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In this issue we publish the Proceedings of the International Conference **Mathematical Challenge of Quantum Transport in Nanosystems. "Pierre Duclos Workshop"** organized by Saint Petersburg National Research University of Information Technologies, Mechanics, and Optics in September 2014. This workshop was the eighth of a series which has the aim to bring together specialists in nanosystem modeling, mathematicians and condensed matter physicists.

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A NEW MODEL FOR QUANTUM DOT LIGHT EMITTING-ABSORBING DEVICES: PROOFS AND SUPPLEMENTS

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Motivated by the Jaynes-Cummings (JC) model, we consider here a quantum dot coupled simultaneously to a reservoir of photons and to two electric leads (free-fermion reservoirs). This new Jaynes-Cummings-Leads (JCL) model permits a fermion current through the dot to create a photon flux, which describes a light-emitting device. The same model is also used to describe the transformation of a photon flux into a current of fermions, i.e. a quantum dot light-absorbing device. The key tool to obtain these results is the abstract Landauer-Büttiker formula.

Keywords: Landauer-Büttiker formula, Jaynes-Cummings model, coupling to leads, light emission, solar cells.

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1. Introduction

In the following the fermion current going through a quantum dot is analyzed as a function of

(1) the electro-chemical potentials on leads and of
(2) the contact with the external photon reservoir.

Although the latter is the canonical JC-interaction, the coupling of the JC model with leads needs certain precautions, if we wish to remain in the one-particle quantum mechanical Hamiltonian approach and scattering theory framework. To this end, we proposed a new Jaynes-Cummings-Leads (JCL-) model [19]. This model makes possible a photon flux into the resonator, created by a fermion current through the dot; i.e. it describes a *light-emitting* device, as well as to transform the external photon flux into a current of fermions, which corresponds to a quantum dot *light-absorbing* device.

The paper is an extended version of [19], which means that the JCL-model, as well as all theorems, corollaries of this article one can already find in [19], however, without any proofs. In the following article, we are going to close this gap and give full proofs of all statements. In doing so, we have added some statements absent in [19].

The paper is organized as follows. The JCL-model is introduced and discussed in Sections 2.1-2.7. For simplicity, we choose for the lead Hamiltonians the one-particle discrete Schrödinger operators, with constant one-site (electric) potentials on each of leads. In Section 2.5, we show that the our model fits into the framework of *trace-class scattering*. In Section 2.7, we verify

the important property that the coupled Hamiltonian has no singular continuous spectrum. Our main tool for analysis of different currents is an abstract Landauer-Büttiker-type formula applied in Sections 3.1 and 3.2 to the case of the JCL-model. This allows us to calculate the outgoing flux of photons induced by electric current via leads. This corresponds to a *light-emitting* device. We also found that pumping the JCL quantum dot with a photon flux from a resonator may induce a current of fermions into the leads. This reversing imitates a quantum *light-absorbing* cell device. These are the main properties of our model and the main application of the Landauer-Büttiker-type formula of Sections 3.1 and 3.2. They are presented in Sections 4 and 5, where we distinguish *contact-induced* and *photon-induced* fermion currents.

To describe the results of Sections 4 and 5, note that in our setup, the sample Hamiltonian is a *two-level* quantum dot *decoupled* from the one-mode photon resonator. Then, the unperturbed Hamiltonian H_0 describes a collection of *four* totally decoupled sub-systems: a sample, a resonator and two leads. The perturbed Hamiltonian H is a fully coupled system, and the feature of our model is that it is *totally* (i.e. including the leads) *embedded* in the external electromagnetic field of the resonator. Hence, each electron can be interpreted as a fermion with *internal* harmonic degrees of freedom, or a Fermi-particle caring its individual *photon cloud*.

Similar to the "Black Box" system-leads (SL-) model $\{H_{SL}, H_0\}$, [1], [4], it turns out that the JCL-model also fits into the framework of the abstract Landauer-Büttiker formula, and in particular, is a trace-class scattering system $\{H_{JCL} = H, H_{SL}\}$. The current in the SL-model is called the *contact-induced* current J^c_{el}. This current was the subject of numerous papers, see e.g. [1,5], or [4]. Note that the current J_{el} is due to the difference of the electro-chemical potentials between two leads, but it may be *zero* even if this difference is not null [12, 13].

The fermion current in the JCL-model, takes into account the effect of the electron-photon interaction under the assumption that the leads are already coupled. This is called the *photon-induced* component J^{ph}_{el} of the total current. To the best of our knowledge, the present paper is the first which rigorously studies this phenomenon. We show that the total free-fermion current J_{el} in the JCL-model decomposes into a sum of the contact- and the photon-induced currents: $J_{el} := J^c_{el} + J^{ph}_{el}$. An extreme case is when the contact-induced current is zero, but the photon-induced component is not, c.f. Section 5.1. In this case, the flux of photons J_{ph} out of the quantum dot (sample) is also non-zero, i.e. the dot serves as a light emitting device, c.f. Section 5.2. In general the $J_{ph} \neq 0$ only when the photon-induced component $J^{ph}_{el} \neq 0$.

By choosing the parameters of the model in an suitable manner, one can get either a photon emitting or a photon absorbing system. Hence, the JCL-model can be used either as a light emission device or as a solar cell. Proofs of explicit formulas for fermion and photon currents $J^{ph}_{l,el}$, J_{ph} are contained in Sections 4 and 5.

Note that the JCL-model is called *mirror symmetric* if (roughly speaking) one can interchange left and right leads and the JCL-model remains unchanged. In Section 5 we discuss a surprising example of a mirror symmetric JCL-model such that the free-fermion current is *zero* but the model is photon emitting. This peculiarity is due to a specific choice of the *photon-electron* interaction, which produces fermions with internal harmonic degrees of freedom.

2. Jaynes-Cummings quantum dot coupled to leads

2.1. Jaynes-Cummings model

The starting point for the construction of our JCL-model is the quantum optics Jaynes-Cummings Hamiltonian H^{JC}. Its simplest version is a *two-level* system (quantum dot) with the energy spacing ε, defined by Hamiltonian h_S on the Hilbert space $\mathfrak{h}_S = \mathbb{C}^2$, see e.g. [16]. It is assumed that this system is "open" and interacts with the one-mode ω photon resonator with Hamiltonian h^{ph}.

Since mathematically h^{ph} coincides with a quantum harmonic oscillator, the Hilbert space of the resonator is the boson Fock space $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C})$ over $\mathbb{C}$ and

$$h^{ph} = \omega\, b^* b\,. \tag{2.1}$$

Here, b^* and b are verifying the Canonical Commutation Relations (CCR) creation and annihilation operators with domains in $\mathfrak{F}_+(\mathbb{C}) \simeq \ell^2(\mathbb{N}_0)$. Operator (2.1) is self-adjoint on its domain:

$$\mathrm{dom}(h^{ph}) = \left\{ (k_0, k_1, k_2, \ldots) \in \ell^2(\mathbb{N}_0) : \sum_{n\in\mathbb{N}_0} n^2 |k_n|^2 < \infty \right\}.$$

Note that the canonical basis $\{\phi_n := (0, 0, \ldots, k_n = 1, 0, \ldots)\}_{n\in\mathbb{N}_0}$ in $\ell^2(\mathbb{N}_0)$ consists of eigenvectors of operator (2.1): $h^{ph}\phi_n = n\omega\,\phi_n$.

To model the *two-level* system with the energy spacing ε, one fixes in $\mathbb{C}^2$ two ortho-normal vectors $\{e_0^S, e_1^S\}$, for example $e_0^S := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $e_1^S := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, which are eigenvectors of Hamiltonian h_S with eigenvalues $\{\lambda_0^S = 0,\ \lambda_1^S = \varepsilon\}$. To this end, we set:

$$h_S := \varepsilon \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\ , \tag{2.2}$$

and we introduce two *ladder* operators:

$$\sigma^+ := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \sigma^- := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{2.3}$$

Then, one obtains $h_S = \varepsilon\ \sigma^+\sigma^-$ as well as $e_1^S = \sigma^+ e_0^S$, $e_0^S = \sigma^- e_1^S$ and $\sigma^- e_0^S = 0$. So, e_0^S is the ground state of Hamiltonian h_S. Note that the *non-interacting* Jaynes-Cummings Hamiltonian H_0^{JC} resides in the space $\mathfrak{H}^{JC} = \mathfrak{h}_S \otimes \mathfrak{h}^{ph} = \mathbb{C}^2 \otimes \mathfrak{F}_+(\mathbb{C})$ and it is defined as the *matrix* operator:

$$H_0^{JC} := h_S \otimes I_{\mathfrak{h}^{ph}} + I_{\mathfrak{h}_S} \otimes h^{ph}\ . \tag{2.4}$$

Here, $I_{\mathfrak{h}^{ph}}$ denotes the identity operator in the Fock space $\mathfrak{h}^{ph}$, whereas $I_{\mathfrak{h}_S}$ stays for the identity matrix in the space $\mathfrak{h}_S$.

With operators (2.3), the interaction V_{Sb} between quantum dot and photons (bosons) in the resonator is defined (in the rotating-wave approximation [16]) by the operator:

$$V_{Sb} := g_{Sb}\ (\sigma^+ \otimes b + \sigma^- \otimes b^*)\ . \tag{2.5}$$

Operators (2.4) and (2.5) define the Jaynes-Cummings model Hamiltonian:

$$H_{JC} := H_0^{JC} + V_{Sb}\ , \tag{2.6}$$

which is a self-adjoint operator on the common domain $\mathrm{dom}(H_0^{JC}) \cap \mathrm{dom}(V_{Sb})$. The standard interpretation of H_{JC} is that (2.6) describes an "open" two-level system interacting with an external one-mode electromagnetic field [16].

Since the one-mode resonator is able to absorb *infinitely* many bosons, this interpretation sounds reasonable, but one can see that the spectrum $\sigma(H^{JC})$ of the Jaynes-Cummings model is *discrete*. To this end, note that the so-called number operator $\mathfrak{N}_{JC} := \sigma^+\sigma^- \otimes I_{\mathfrak{h}^{ph}} + I_{\mathfrak{h}_S} \otimes b^* b$ commutes with H_{JC}. Then, since for any $n \geqslant 0$:

$$\mathfrak{H}_{n>0}^{JC} := \{\zeta_0 e_0^S \otimes \phi_n + \zeta_1 e_1^S \otimes \phi_{n-1}\}_{\zeta_{0,1}\in\mathbb{C}}\ ,\ \mathfrak{H}_{n=0}^{JC} := \{\zeta_0 e_0^S \otimes \phi_0\}_{\zeta_0\in\mathbb{C}}\ ,$$

are eigenspaces of operator $\mathfrak{N}_{JC}$, they reduce H_{JC}, i.e. $H_{JC} : \mathfrak{H}_n^{JC} \to \mathfrak{H}_n^{JC}$. Note that $\mathfrak{H}^{JC} = \bigoplus_{n\geqslant 0} \mathfrak{H}_n^{JC}$, where each $\mathfrak{H}_n^{JC}$ is invariant subspace of operator (2.6). Therefore, it has

the representation:

$$H_{JC} = \bigoplus_{n\in\mathbb{N}_0} H_{JC}^{(n)}\ ,\ \ n>1\ ,\ H_{JC}^{(0)} = 0\,. \tag{2.7}$$

Here operators $H_{JC}^{(n)}$ are the restrictions of H_{JC}, which act in each $\mathfrak{H}_n^{JC}$ as follows:

$$\begin{aligned} &H_{JC}^{(n)}(\zeta_0\, e_0^S\otimes\phi_n + \zeta_1\, e_1^S\otimes\phi_{n-1}) \\ &\quad = [\zeta_0 n\omega + \zeta_1 g_{Sb}\sqrt{n}]\, e_0^S\otimes\phi_n + [\zeta_1(\varepsilon+(n-1)\omega) + \zeta_0 g_{Sb}\sqrt{n}]\, e_1^S\otimes\phi_{n-1}\ . \end{aligned} \tag{2.8}$$

Hence, the spectrum $\sigma(H_{JC}) = \bigcup_{n\geqslant 0}\sigma(H_{JC}^{(n)})$. By virtue of (2.8), the spectrum $\sigma(H_{JC}^{(n)})$ is defined for $n\geqslant 1$ by eigenvalues $E(n)$ of two-by-two matrix $\widehat{H}_{JC}^{(n)}$ acting on the coefficient space $\{\zeta_0,\zeta_1\}$:

$$\widehat{H}_{JC}^{(n)}\begin{pmatrix}\zeta_1\\ \zeta_0\end{pmatrix} = \begin{pmatrix}\varepsilon+(n-1)\,\omega & g_{Sb}\sqrt{n}\\ g_{Sb}\sqrt{n} & n\omega\end{pmatrix}\begin{pmatrix}\zeta_1\\ \zeta_0\end{pmatrix} = E(n)\begin{pmatrix}\zeta_1\\ \zeta_0\end{pmatrix}\ . \tag{2.9}$$

Then, (2.7) and (2.9) imply that the spectrum of the Jaynes-Cummings model Hamiltonian H_{JC} is *pure point*:

$$\sigma(H_{JC}) = \sigma_{p.p.}(H_{JC}) = \{0\}\cup\bigcup_{n\in\mathbb{N}}\left\{n\omega + \frac{1}{2}(\varepsilon-\omega) \pm \sqrt{(\varepsilon-\omega)^2/4 + g_{Sb}^2 n}\right\}.$$

This property evidently persists for any system Hamiltonian h_S with discrete spectrum and linear interaction (2.5) with a finite mode photon resonator [16].

We resume the above observations concerning the Jaynes-Cummings model, which is our starting point, by following remarks:

(a) The standard Hamiltonian (2.6) describes instead of *flux* only oscillations of photons between resonator and quantum dot, i.e. the system h_S is not "open" enough.

(b) Since one our aim is to model a *light-emitting* device, the system h_S needs an *external* source of energy to pump it into the dot, which will be transformed by interaction (2.5) into the outgoing *photon current* by pumping the resonator.

(c) To reach this aim we extend the standard Jaynes-Cummings model to our JCL-model by attaching to the quantum dot h_S (2.2) two *leads*, which are (infinite) reservoirs of *free* fermions. Manipulating with *electro-chemical* potentials of fermions in these reservoirs we can force one of them to inject fermions in the quantum dot, whereas another one to absorb the fermions out the quantum dot with the same rate. This current of fermions throughout the dot will pump the dot and induce a photon current according scenario (b).

(d) The most subtle point is to invent a *leads-dot* interaction V_{lS}, which ensures the above mechanism and which is simple enough that one would still be able to treat this JCL-model using our extension of the Landauer-Büttiker formalism.

2.2. The JCL-model

First, let us make some general remarks and formulate certain indispensable conditions when one follows the modeling (d).

(1) Note that since the Landauer-Büttiker formalism [13] is essentially a scattering theory on a contact between two subsystems, it is developed only on a "one-particle" level. This allows one to study with this formalism only ideal (*non-interacting*) many-body systems. We impose this condition on many-body fermion systems (electrons) in two leads. Thus, only direct interaction between different components of the system: dot-photons V_{Sb} and electron-dot V_{lS} are allowed.

(2) It is well-known that fermion reservoirs are technically simpler to treat than boson ones [13]. Moreover, in the framework of our model, it is also very natural since we study electric current, although produced by "non-interacting electrons". So, below we use fermions/electrons synonymously.
(3) In spite of the precautions formulated above, the first difficulty to consider in an ideal many-body system interacting with quantized electromagnetic field (photons) is induced *indirect* interaction. If electrons can emit and absorb photons, it is possible for one electron to emit a photon that another electron absorbs, thus creating an indirect photon-mediated electron-electron interaction. This interaction makes it impossible to develop the Landauer-Büttiker formula, which requires a non-interacting framework.

Assumption 2.1. To solve this difficulty, we forbid in our model the photon-mediated interaction. To this end, we assume that every electron (in leads and in dot) interacts with its *own* distinct copy of the electromagnetic field. So, considering electrons together with their photon fields as non-interacting "composed particles", allows us to apply the Landauer-Büttiker approach. Formally, it corresponds to the "one-electron" Hilbert space $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$, where $\mathfrak{h}^{ph}$ is the Hilbert space of the individual photon field. The fermion description of composed-particles $\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$ corresponds to the antisymmetric Fock space $\mathfrak{F}_-(\mathfrak{h}^{el} \otimes \mathfrak{h}^{ph})$.

The composed-particle assumption 2.1 allows us to use the Landauer-Büttiker formalism developed for ideal many-body fermion systems. Now, we come closer to the formal description of our JCL-model with two (infinite) leads and a one-mode quantum resonator.

Recall that the Hilbert space of the Jaynes-Cummings Hamiltonian with two energy levels is $\mathfrak{H}^{JC} = \mathbb{C}^2 \otimes \mathfrak{F}_+(\mathbb{C})$. The boson Fock space is constructed from a one-dimensional Hilbert space, since we consider only photons of a single fixed frequency. We model the electrons in the leads as free fermions residing on discrete semi-infinite lattices. Thus:

$$\mathfrak{h}^{el} = \ell^2(\mathbb{N}) \oplus \mathbb{C}^2 \oplus \ell^2(\mathbb{N}) = \mathfrak{h}^{el}_l \oplus \mathfrak{h}_S \oplus \mathfrak{h}^{el}_r, \tag{2.10}$$

is the one-particle Hilbert space for the electrons and for the dot. Here, $\mathfrak{h}^{el}_\alpha$, $\alpha \in \{l, r\}$, are the respective Hilbert spaces of the *left* and *right* lead, while $\mathfrak{h}_S = \mathbb{C}^2$ is the Hilbert space of the quantum dot. We denote by:

$$\{\delta^\alpha_n\}_{n\in\mathbb{N}}, \qquad \{\delta^S_n\}^1_{j=0},$$

the canonical basis consisting of individual lattice sites of $\mathfrak{h}^{el}_\alpha$, $\alpha \in \{l, r\}$, and of $\mathfrak{h}_S$, respectively. With the Hilbert space for photons, $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C}) \simeq \ell^2(\mathbb{N}_0)$, we define the Hilbert space of the *full* system, i.e. quantum dot with leads and with the photon field, as follows:

$$\mathfrak{H} = \mathfrak{h}^{el} \otimes \mathfrak{h}^{ph} = \Big(\ell^2(\mathbb{N}) \oplus \mathbb{C}^2 \oplus \ell^2(\mathbb{N})\Big) \otimes \ell^2(\mathbb{N}_0). \tag{2.11}$$

Remark 2.2. Note that the structure of full space (2.11) takes into account the condition 2.1 and produces composed fermions via the last tensor product. It also manifests that electrons *in the dot* as well as those *in the leads* are composed with photons. This is different than the picture imposed by the the Jaynes-Cummings model, when *only the dot* is composed with photons:

$$\mathfrak{H} = \ell^2(\mathbb{N}) \oplus \mathbb{C}^2 \otimes \ell^2(\mathbb{N}_0) \oplus \ell^2(\mathbb{N}) \quad , \quad \mathfrak{H}^{JC} = \mathbb{C}^2 \otimes \ell^2(\mathbb{N}_0)\,, \tag{2.12}$$

see (2.4), (2.5) and (2.6), where $\mathfrak{H}^{JC} = \mathfrak{h}_S \otimes \mathfrak{h}^{ph}$. The next step is a choice of interactions between subsystems: dot-resonator-leads.

According to (2.10), the decoupled leads-dot Hamiltonian is the matrix operator:

$$h^{el}_0 = \begin{pmatrix} h^{el}_l & 0 & 0 \\ 0 & h_S & 0 \\ 0 & 0 & h^{el}_r \end{pmatrix} \text{ on } u = \begin{pmatrix} u_l \\ u_S \\ u_r \end{pmatrix} \,,\ \{u_\alpha \in \ell^2(\mathbb{N})\}_{\alpha\in\{l,r\}}\,,\ u_S \in \mathbb{C}^2\,,$$

where $h^{el}_{\alpha} = -\Delta^D + v_\alpha$ with a constant potential bias $v_\alpha \in \mathbb{R}$, $\alpha \in \{l, r\}$, and h_S can be any self-adjoint two-by-two matrix with eigenvalues $\{\lambda^S_0, \lambda^S_1 := \lambda^S_0 + \varepsilon\}$, $\varepsilon > 0$, and eigenvectors $\{e^S_0, e^S_1\}$, cf (2.2). Here, Δ^D denotes the discrete Laplacian on $\ell^2(\mathbb{N})$ with homogeneous Dirichlet boundary conditions given by:

$$\begin{aligned}(\Delta^D f)(x) &:= f(x+1) - 2f(x) + f(x-1), \quad x \in \mathbb{N},\\ \mathrm{dom}(\Delta^D) &:= \{f \in \ell^2(\mathbb{N}_0) : f(0) := 0\},\end{aligned}$$

which is obviously a bounded self-adjoint operator. Notice that $\sigma(\Delta^D) = [0, 4]$.

We define the *lead-dot interaction* for coupling $g_{el} \in \mathbb{R}$ by the matrix operator acting in (2.10) as follows:

$$v_{el} = g_{el} \begin{pmatrix} 0 & \langle \cdot, \delta^S_0\rangle \delta^l_1 & 0 \\ \langle \cdot, \delta^l_1\rangle \delta^S_0 & 0 & \langle \cdot, \delta^r_1\rangle \delta^S_1 \\ 0 & \langle \cdot, \delta^S_1\rangle \delta^r_1 & 0 \end{pmatrix} , \tag{2.13}$$

where non-trivial off-diagonal entries are *projection* operators in the Hilbert space (2.10) with the scalar product $u, v \mapsto \langle u, v\rangle$ for $u, v \in \mathfrak{h}^{el}$. Here, $\{\delta^S_0, \delta^S_1\}$ is ortho-normal basis in $\mathfrak{h}^{el}_S$, which in general may be different from $\{e^S_0, e^S_1\}$. Hence, interaction (2.13) describes quantum *tunneling* between leads and the dot via contact sites of the leads, which are supports of δ^l_1 and δ^r_1.

Then we define the Hamiltonian for the system of interacting leads and dot as $h^{el} := h^{el}_0 + v_{el}$. Here, both h^{el}_0 and h^{el} are bounded self-adjoint operators on $\mathfrak{h}^{el}$.

Recall that photon Hamiltonian in the one-mode resonator is defined by operator $h^{ph} = \omega b^* b$ with domain in the Fock space $\mathfrak{F}_+(\mathbb{C}) \simeq \ell^2(\mathbb{N}_0)$, (2.1). We denote the canonical basis in $\ell^2(\mathbb{N}_0)$ by $\{\Upsilon_n\}_{n\in\mathbb{N}_0}$. Then for the spectrum of h^{ph} one obviously gets:

$$\sigma(h^{ph}) = \sigma_{pp}(h^{ph}) = \bigcup_{n\in\mathbb{N}_0} \{n\omega\}. \tag{2.14}$$

We introduce the following decoupled Hamiltonian H_0, which describes the system when the leads are decoupled from the quantum dot and the electron does not interact with the photon field:

$$H_0 := H^{el}_0 + H^{ph}, \tag{2.15}$$

where

$$H^{el}_0 := h^{el}_0 \otimes I_{\mathfrak{h}^{ph}} \quad \text{and} \quad H^{ph} := I_{\mathfrak{h}^{el}} \otimes h^{ph}.$$

The operator H_0 is self-adjoint on $\mathrm{dom}(H_0) = \mathrm{dom}(I_{\mathfrak{h}^{el}} \otimes h^{ph})$. Recall that h^{el}_0 and h^{ph} are bounded self-adjoint operators. Hence, H^{el}_0 and H^{el} are semi-bounded from below, which yields that H_0 is semi-bounded from below.

The interaction of the photons and the electrons in the quantum dot is given by the coupling of the dipole moment of the electrons to the electromagnetic field in the rotating wave approximation. Namely:

$$V_{ph} = g_{ph} \left((\cdot, e^S_0) e^S_1 \otimes b + (\cdot, e^S_1) e^S_0 \otimes b^* \right), \tag{2.16}$$

for some coupling constant $g_{ph} \in \mathbb{R}$. The total Hamiltonian is given by:

$$H := H^{el} + H^{ph} + V_{ph} = H_0 + V_{el} + V_{ph}, \tag{2.17}$$

where $H^{el} := h^{el} \otimes I_{\mathfrak{h}^{ph}}$ and $V_{el} := v_{el} \otimes I_{\mathfrak{h}^{ph}}$.

In the following, we call $\mathcal{S} = \{H, H_0\}$ the Jaynes-Cummings-leads system, in short JCL-model, which we are going to analyze. In particular, we are interested in the electron and photon currents for that system. The analysis will be based on the abstract Landauer-Büttiker formula, cf. [1, 13].

Lemma 2.3. *H is bounded from below self-adjoint such that* $\mathrm{dom}(H) = \mathrm{dom}(H_0)$.

Proof. Let $c \geqslant 2$. Then,

$$\|b\Upsilon_n\|^2 \leqslant \|b^*\Upsilon_n\|^2 = n+1 \leqslant c^{-1}n^2 + c, \quad n \in \mathbb{N}_0.$$

Consider elements $f \in \mathfrak{h}_S \otimes \mathfrak{h}^{ph} \cap \mathrm{dom}(I_{\mathfrak{h}^{el}} \otimes h^{ph})$ with the following:

$$f = \sum_{j,l} \beta_{jl} e_j \otimes \Upsilon_l, \quad j \in \{0,1\}, \quad l \in \mathbb{N}_0,$$

which are dense in $\mathfrak{H}^{JC} := \mathfrak{h}^{el}_S \otimes h^{ph}$. Then, $\|f\|^2 = \sum_{j,l}|\beta_{jl}|^2$ and $\|(I_{\mathfrak{h}^{el}} \otimes b^*b)f\|^2 = \sum_{j,l=1}|\beta_{jl}|^2 l^2$. We obtain the following:

$$\|((\cdot, e_1^S)e_0^S \otimes b)f\|^2 \leqslant \sum_{j,l}|\beta_{jl}|^2 \|b\Upsilon_l\|^2 \leqslant$$

$$\sum_{j,l}|\beta_{jl}|^2(c^{-1}l^2 + c) = c^{-1}\|(I_{\mathfrak{h}^{el}} \otimes b^*b)f\|^2 + c\|f\|^2$$

Similarly,

$$\|((\cdot, e_1^S)e_0^S \otimes b^*)f\|^2 \leqslant c^{-1}\|(I_{\mathfrak{h}^{el}} \otimes b^*b)f\|^2 + c\,\|f\|^2.$$

If $c \geqslant 2$ is large enough, then we obtain that V_{ph} is dominated by H^{ph} with relative bound less than one. Hence, H is self-adjoint and $\mathrm{dom}(H_0) = \mathrm{dom}(H)$. Since H_0^{el} and V_{el} are bounded and H^{ph} is self-adjoint and bounded from below, it follows that $H = H_0^{el} + H^{ph} + V_{el} + V_{ph}$ is bounded from below [17, Thm. V.4.1]. □

2.3. Time reversible symmetric systems

A system described by the Hamiltonian H is called time reversible symmetric if there is a conjugation Γ defined on $\mathfrak{H}$ such that $\Gamma H = H\Gamma$. Recall that Γ is a conjugation if the conditions $\Gamma^2 = I$ and $(\Gamma f, \Gamma g) = \overline{(f,g)}$, $f, g \in \mathfrak{H}$.

Let $\mathfrak{h}^{ph}_n$, $n \in \mathbb{N}_0$, the subspace spanned by the eigenvector Υ_n in $\mathfrak{h}^{ph}$. We set:

$$\mathfrak{H}_{n_\alpha} := \mathfrak{h}^{el}_\alpha \otimes \mathfrak{h}^{ph}_n, \quad n \in \mathbb{N}_0, \quad \alpha \in \{l, r\}. \tag{2.18}$$

Notice that

$$\mathfrak{H} = \bigoplus_{n \in \mathbb{N}_0, \alpha \in \{l,r\}} \mathfrak{H}_{n_\alpha}$$

Definition 2.4. The JCL-model is called time reversible symmetric if there is a conjugation Γ acting on $\mathfrak{H}$ such that H and H_0 are time reversible symmetric and the subspaces $\mathfrak{H}_{n_\alpha}$, $n \in \mathbb{N}_0$, $\alpha \in \{l, r\}$, reduces Γ.

Example 2.5. Let γ^{el}_α and γ^{el}_S be conjugations defined by the following:

$$\gamma^{el}_\alpha f_\alpha := \overline{f_\alpha} := \{\overline{f_\alpha(k)}\}_{k \in \mathbb{N}}, \quad f_\alpha \in \mathfrak{h}^{el}_\alpha, \quad \alpha \in \{l, r\},$$

and

$$\gamma^{el}_S f_S = \gamma^{el}_S \begin{pmatrix} f_S(0) \\ f_S(1) \end{pmatrix} := \begin{pmatrix} \overline{f_S(0)} \\ \overline{f_S(1)} \end{pmatrix}$$

We set $\gamma^{el} := \gamma^{el}_l \oplus \gamma^{el}_S \oplus \gamma^{el}_r$. Further, we set:

$$\gamma^{ph}\psi := \overline{\psi} = \{\overline{\psi(n)}\}_{n \in \mathbb{N}_0}, \quad \psi \in \mathfrak{h}^{ph}.$$

Let $\Gamma := \gamma^{el} \otimes \gamma^{ph}$. One easily checks that Γ is a conjugation on $\mathfrak{H} = \mathfrak{h}^{el} \otimes \mathfrak{h}^{ph}$.

Lemma 2.6. *Let γ^{el}_α, $\alpha \in \{S, l, r\}$, and γ^{ph} be given by Example 2.5.*

(i) *If the conditions $\gamma^{el}_S e^S_0 = e^S_0$ and $\gamma^{el}_S e^S_1 = e^S_1$ are satisfied, then H_0 is time reversible symmetric with respect to Γ and, moreover, the subspaces $\mathfrak{H}_{n_\alpha}$, $n \in \mathbb{N}_0$, $\alpha \in \{l, r\}$, reduces Γ.*

(ii) *If in addition the conditions $\gamma_S^{el}\delta_0^S = \delta_0^S$ and $\gamma_S^{el}\delta_1^S = \delta_1^S$ are satisfied, then JCL-model is time reversible symmetric.*

Proof. (i) Obviously we have

$$\gamma_\alpha^{el} h_\alpha^{el} = h_\alpha^{el}\gamma_\alpha^{el}, \quad \alpha \in \{l, r\}, \quad \text{and} \quad \gamma^{ph} h^{ph} = h^{ph}\gamma^{ph}.$$

If $\gamma_S^{el} e_0^S = e_0^S$ and $\gamma_S^{el} e_1^S = e_1^S$ are satisfied, then $\gamma_S^{el} h_S^{el} = h_S^{el}\gamma_S^{el}$ which yields $\gamma^{el} h_0^{el} = h_0^{el}\gamma^{el}$ and, hence, $\Gamma H_0 = \Gamma H_0$. Since $\gamma^{el}\mathfrak{h}_\alpha^{el} = \mathfrak{h}_\alpha^{el}$ and $\gamma^{ph}\mathfrak{h}^{ph} = \mathfrak{h}^{ph}$ one gets $\Gamma\mathfrak{H}_{n_\alpha} = \mathfrak{H}_{n_\alpha}$ which shows that $\mathfrak{H}_{n_\alpha}$ reduces Γ.

(ii) Notice that $\gamma_\alpha^{el}\delta_1^\alpha = \delta_1^\alpha$, $\alpha \in \{l, r\}$. If in addition the conditions $\gamma_S^{el}\delta_0^S = \delta_0^S$ and $\gamma_S^{el}\delta_1^S = \delta_1^S$ are satisfied, then $\gamma^{el} v_{el} = v_{el}\gamma^{el}$ is valid, which yields $\gamma^{el} h^{el} = h^{el}\gamma^{el}$. Hence, $\Gamma H = H\Gamma$. Together with (i), this proves that the JCL-model is time reversible symmetric. □

Choosing the following:

$$e_0^S := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e_1^S := \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \delta_0^S := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \delta_1^S := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{2.19}$$

one satisfies the condition $\gamma_S^{el} e_0^S = e_0^S$ and $\gamma_S^{el} e_1^S = e_1^S$ as well as $\gamma_S^{el} e_0^S = e_0^S$ and $\gamma_S^{el} e_1^S = e_1^S$.

2.4. Mirror symmetric systems

A unitary operator U acting on $\mathfrak{H}$ is called a mirror symmetry if the following conditions are met:

$$U\mathfrak{H}_{n_\alpha} = \mathfrak{H}_{n_{\alpha'}}, \quad \alpha, \alpha' \in \{l, r\}, \quad \alpha \neq \alpha'$$

are satisfied. In particular, this yields $U\mathfrak{H}^{JC} = \mathfrak{H}^{JC}$, $\mathfrak{H}^{JC} := \mathfrak{h}_S^{el} \otimes \mathfrak{h}^{ph}$.

Definition 2.7. The JCL-model is called mirror symmetric if there is a mirror symmetry commuting with H_0 and H.

One can easily verify that if H_0 is mirror symmetric, then

$$H_{n_{\alpha'}} U = U H_{n_\alpha}, \qquad n \in \mathbb{N}_0, \quad \alpha, \alpha' \in \{l, r\}, \quad \alpha \neq \alpha',$$

where

$$H_{n_\alpha} := h_\alpha^{el} \otimes I_{\mathfrak{h}_n^{ph}} + I_{\mathfrak{h}_\alpha^{el}} \otimes h_n^{ph} = h_\alpha^{el} + n\omega, \quad n \in \mathbb{N}_0, \quad \alpha, \alpha' \in \{l, r\}, \quad \alpha \neq \alpha'.$$

In particular, this yields that $v_\alpha = v_{\alpha'}$. Moreover, one gets $UH_S = H_S U$ where $H_S := h_S^{el} \otimes I_{\mathfrak{h}^{ph}} + I_{\mathfrak{h}^{el}} \otimes h^{ph}$.

Notice that if H and H_0 commute with the same mirror symmetry U, then also the operator $H_c := h^{el} \otimes I_{\mathfrak{h}^{ph}} + I_{\mathfrak{h}^{el}} \otimes h^{ph}$ also commutes with U, i.e, is mirror symmetric.

Example 2.8. Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Let $v_l = v_r$ and let e_0^S and e_1^S as well as δ_0^S and δ_1^S be given by (2.19). We set:

$$u_S^{el} e_0^S := e_0^S \quad \text{and} \quad u_S^{el} e_1^S = -e_1^S, \tag{2.20}$$

as well as

$$u^{ph}\Upsilon_n = e^{-in\pi}\Upsilon_n, \quad n \in \mathbb{N}_0. \tag{2.21}$$

Obviously, $U_S := u_S^{el} \otimes u^{ph}$ defines a unitary operator on $\mathfrak{H}^{JC}$. Straightforward computation shows that:

$$U_S H_S = H_S U_S \quad \text{and} \quad U_S V_{ph} = V_{ph} U_S. \tag{2.22}$$

Furthermore, we set:

$$u_{rl}^{el}\delta_n^l := \delta_n^r, \quad \text{and} \quad u_{lr}^{el}\delta_n^r = \delta_n^l, \quad n \in \mathbb{N}, \tag{2.23}$$

and

$$u^{el} := \begin{pmatrix} 0 & 0 & u^{el}_{lr} \\ 0 & u^{el}_S & 0 \\ u^{el}_{lr} & 0 & 0 \end{pmatrix}.$$

We thus have the following:

$$v_{el}\, u^{el} \begin{pmatrix} f_l \\ f_S \\ f_r \end{pmatrix} = \begin{pmatrix} < f_S, (u^{el}_S)^* \delta^S_0 > \delta^l_1 \\ < f_r, (u^{el}_{lr})^* \delta^l_1 > \delta^S_0 + < f_l, (u^{el}_{rl})^* \delta^r_1 > \delta^S_1 \\ < f_S, (u^{el}_S)^* \delta^S_1 > \delta^r_1 \end{pmatrix} \tag{2.24}$$

Since $\delta^S_0 := \frac{1}{\sqrt{2}}(e^S_0 + e^S_1)$ and $\delta^S_1 := \frac{1}{\sqrt{2}}(e^S_0 - e^S_1)$ we get from (2.20)

$$(u^{el}_S)^* \delta^S_0 = \delta^S_1 \quad \text{and} \quad (u^{el}_S)^* \delta^S_1 = \delta^S_0. \tag{2.25}$$

Obviously, we then have

$$(u^{el}_{lr})^* \delta^l_1 = \delta^r_1 \qquad (u^{el}_{rl})^* \delta^r_1 = \delta^l_1. \tag{2.26}$$

Inserting (2.25) and (2.26) into (2.24), we find

$$v_{el}\, u^{el} \begin{pmatrix} f_l \\ f_S \\ f_r \end{pmatrix} = \begin{pmatrix} < f_S, \delta^S_1 > \delta^l_1 \\ < f_r, \delta^r_1 > \delta^S_0 + < f_l, \delta^l_1 > \delta^S_1 \\ < f_S, \delta^S_0 > \delta^r_1 \end{pmatrix} \tag{2.27}$$

Further, we have:

$$u^{el} v_{el} \begin{pmatrix} f_l \\ f_S \\ f_r \end{pmatrix} = \begin{pmatrix} < f_S, \delta^S_1 > \delta^l_1 \\ < f_l, \delta^l_1 > \delta^S_1 + < f_r, \delta^r_1 > \delta^S_0 \\ < f_s, \delta^S_0 > \delta^r_1 \end{pmatrix}. \tag{2.28}$$

Comparing (2.27) and (2.28), we get $u^{el} v_{el} = v_{el} u^{el}$. Setting $U := u^{el} \otimes u^{ph}$ one immediately proves that $UH_0 = H_0 U$ and $UH = HU$. Since $U\mathfrak{H}_{n_\alpha} = \mathfrak{H}_{n_{\alpha'}}$, it is satisfied that $\mathcal{S}$ is mirror symmetric.

We note that Example 2.8 $\mathcal{S}$ is also time-reversible symmetric.

2.5. Spectral properties of H: first part

In the following, our goal is to apply the Landauer-Büttiker formula to the JCL-model. By $\mathfrak{L}_p(\mathfrak{H})$, $1 \leqslant p \leqslant \infty$, we denote in the following the Schatten-v.Neumann ideals.

Proposition 2.9. *If $\mathcal{S} = \{H, H_0\}$ is the JCL-model, then $(H+i)^{-1} - (H_0+i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. In particular, the absolutely continuous parts H^{ac} and H^{ac}_0 are unitarily equivalent.*

Proof. We have

$$\begin{aligned}(H+i)^{-1} - (H_0+i)^{-1} &= (H_0+i)^{-1} V (H+i)^{-1} = \\ &(H_0+i)^{-1} V (H_0+i)^{-1} - (H_0+i)^{-1} V (H_0+i)^{-1} V (H+i)^{-1},\end{aligned}$$

where $V = H - H_0 = V_{el} + V_{ph}$. Taking into account Lemma 2.3, it suffices to prove that $(H_0+i)^{-1} V (H_0+i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. Using the spectral decomposition of h^{ph} with respect to $\mathfrak{h}^{ph} = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}^{ph}_n$, where $\mathfrak{h}^{ph}_n$ are the subspaces spanned by Υ_n, we obtain the following:

$$(H_0+i)^{-1} = \bigoplus_{n\in\mathbb{N}_0} (h^{el}_0 + n\omega + i)^{-1} \otimes I_{\mathfrak{h}^{ph}_n}. \tag{2.29}$$

We have $(H_0+i)^{-1}V(H_0+i)^{-1} = (H_0+i)^{-1}(V_{el}+V_{ph})(H_0+i)^{-1}$. Since v_{el} is a finite rank operator, we have $\|v_{el}\|_{\mathfrak{L}_1} < \infty$. Furthermore, $\mathfrak{h}^{ph}_n$ is obviously one-dimensional for any $n \in \mathbb{N}_0$. Hence, $\|I_{\mathfrak{h}^{ph}_n}\|_{\mathfrak{L}_1} = 1$. From (2.29) and $V_{el} = v_{el} \otimes I_{\mathfrak{h}^{ph}}$, we obtain the following:

$$\begin{aligned}\|(H_0+i)^{-1}V_{el}(H_0+i)^{-1}\|_{\mathfrak{L}_1} &= \sum_{n\in\mathbb{N}_0} \|(h_0^{el}+n\omega+i)^{-1}v_{el}(h_0^{el}+n\omega+i)^{-1}\|_{\mathfrak{L}_1} \\ &\leqslant \sum_{n\in\mathbb{N}_0} \|(h_0^{el}+n\omega+i)^{-2}\|\ \|v_{el}\|_{\mathfrak{L}_1}\end{aligned}$$

Since h_0^{el} is bounded, we get:

$$\|(h_0^{el}+n\omega+i)^{-1}\| = \sup_{\lambda\in\sigma(h_0^{el})} \Big(\sqrt{(\lambda+n\omega)^2+1}\Big)^{-1} \leqslant c(n+1)^{-1}, \tag{2.30}$$

for some $c > 0$. This immediately implies that $\|(H_0+i)^{-1}V_{el}(H_0+i)^{-1}\|_{\mathfrak{L}_1} < \infty$.

We are going to handle $(H_0+i)^{-1}V_{ph}(H_0+i)^{-1}$. Let p_n^{ph} be the projection from $\mathfrak{h}^{ph}$ onto $\mathfrak{h}^{ph}_n$. We have the following:

$$\begin{aligned}&(H_0+i)^{-1}\,(\cdot,e_0^S)e_1^S\otimes b\,(H_0+i)^{-1} \\ &= \sum_{m,n\in\mathbb{N}_0} (h_0^{el}+m\omega+i)^{-1}(\cdot,e_0^S)e_1^S\,(h_0^{el}+n\omega+i)^{-1}\otimes p_m^{ph}bp_n^{ph} \\ &= \sum_{n\in\mathbb{N}} (h_0^{el}+(n-1)\omega+i)^{-1}\,(\cdot,e_0^S)e_1^S\,(h_0^{el}+n\omega+i)^{-1}\otimes\sqrt{n}\Upsilon_{n-1}\langle\cdot,\Upsilon_n\rangle\end{aligned}$$

From (2.30), we get the following:

$$\Big\|(h_0^{el}+(n-1)\omega+i)^{-1}\,(\cdot,e_0^S)e_1^S\,(h_0^{el}+n\omega+i)^{-1}\Big)\otimes\sqrt{n}\Upsilon_n\langle\cdot,\Upsilon_n\rangle\Big\|_{\mathfrak{L}_1} \leqslant c^2\frac{\sqrt{n}}{n(n+1)},$$

$n\in\mathbb{N}$, which yields:

$$\|(H_0+i)^{-1}\,(\cdot,e_0^S)e_1^S\otimes b\,(H_0+i)^{-1}\|_{\mathfrak{L}_1} \leqslant c^2\sum_{n\in\mathbb{N}}^{\infty}\frac{\sqrt{n}}{n(n+1)} < \infty.$$

Since

$$\|(H_0+i)^{-1}\,(\cdot,e_1^S)e_0^S\otimes b^*\,(H_0+i)^{-1}\|_{\mathfrak{L}_1} = \|(H_0+i)^{-1}\,(\cdot,e_0^S)e_1^S\otimes b\,(H_0+i)^{-1}\|_{\mathfrak{L}_1},$$

one gets $(H_0+i)^{-1}V_{ph}(H_0+i)^{-1}\in\mathfrak{L}_1(\mathfrak{H})$, which completes the proof. □

Thus, the JCL-model $\mathcal{S} = \{H, H_0\}$ is a $\mathfrak{L}_1$-scattering system. Let us recall that $h_\alpha^{el} = -\Delta^D + v_\alpha$, $\alpha\in\{l,r\}$, on $\mathfrak{h}_l^{el} = \mathfrak{h}_r^{el} = \ell^2(\mathbb{N})$.

Lemma 2.10. *Let $\alpha\in\{l,r\}$. We have the following:*

$$\sigma(h_\alpha^{el}) = \sigma_{ac}(h_\alpha^{el}) = [v_\alpha, 4+v_\alpha].$$

The normalized generalized eigenfunctions of h_α^{el} are given by:

$$g_\alpha(x,\lambda) = \pi^{-\frac{1}{2}}(1-(-\lambda+2+v_\alpha)^2/4)^{-\frac{1}{4}}\sin\Big(\arccos((-\lambda+2+v_\alpha)/2)x\Big)$$

for $x\in\mathbb{N}$, $\lambda\in(v_\alpha,4+v_\alpha)$.

Proof. We prove the absolute continuity of the spectrum by showing that:

$$\{g_\alpha(x,\lambda)\,|\,\lambda\in(-2,2)\}$$

is a complete set of generalized eigenfunctions. Note that it suffices to prove the lemma for

$$((\Delta^D+2)f)(x) = f(x+1)+f(x-1), \qquad f(0)=0.$$

The lemma then follows by replacing λ with $-\lambda + 2 + v_\alpha$. Let $\lambda \in (-2, 2)$ and

$$g_{\Delta^D}(x, \lambda) = \pi^{-\frac{1}{2}}(1 - \lambda^2/4)^{-\frac{1}{4}} \sin\Big(\arccos(\lambda/2)x\Big).$$

Note that $g_{\Delta^D}(0, \lambda) = 0$, when the boundary condition is satisfied. We substitute $\mu = \arccos(\lambda/2) \in (0, \pi)$, i.e. $\lambda = 2\cos(\mu)$ and obtain the following:

$$\sin(\mu(x + 1)) + \sin(\mu(x - 1)) = 2\sin(\mu x)\cos(\mu),$$

when $g_{\Delta^D}(x, \lambda)$ satisfies the eigenvalue equation. It is obvious that $g_{\Delta^D}(\cdot, \lambda) \notin \ell^2(\mathbb{N}_0)$ for $\lambda \in (-2, 2)$. To complete the proof of the lemma, it remains to show the ortho-normality and the completeness. For the ortho-normality, we have to show that

$$\sum_{x\in\mathbb{N}} g_{\Delta^D}(x, \lambda)g_{\Delta^D}(x, \nu) = \delta(\lambda - \nu).$$

Let $\psi \in C_0^\infty\Big((-2, 2)\Big)$. We use the substitution $\mu = \arccos(\nu/2)$ and the relation

$$\sin(\arccos(y)) = (1 - y^2)^{-\frac{1}{2}}$$

to obtain the following:

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu \sum_{x\in\mathbb{N}} g_{\Delta^D}(x, \lambda)g_{\Delta^D}(x, \nu)\psi(\nu) \\
&= 2\pi^{-1} \int_0^\pi \mathrm{d}\mu \sum_{x\in\mathbb{N}} \frac{\sin(\mu)\sin\Big(\arccos(\lambda/2)x\Big)\sin(\mu x)}{(\sin(\mu))^{\frac{1}{2}}(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}}\psi(2\cos(\mu)) \\
&= (2\pi)^{-1} \int_0^\pi \mathrm{d}\mu \sum_{x\in\mathbb{N}} \frac{(\sin(\mu))^{\frac{1}{2}}}{(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}}\Big(e^{i(\arccos(\lambda/2)-\mu)x} + \\
&e^{-i(\arccos(\lambda/2)-\mu)x} - e^{i(\arccos(\lambda/2)+\mu)x} - e^{-i(\arccos(\lambda/2)+\mu)x}\Big)\psi(2\cos(\mu)).
\end{aligned}$$

Observe that for the Dirichlet kernel:

$$\sum_{x\in\mathbb{N}_0} (e^{ixy} + e^{-ixy}) - 1 = 2\pi\,\delta(y),$$

when

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu \sum_{x\in\mathbb{N}} g_{\Delta^D}(x, \lambda)g_{\Delta^D}(x, \nu)\psi(\nu) = \\
&\int_0^\pi \mathrm{d}\mu \frac{(\sin(\mu))^{\frac{1}{2}}}{(\sin(\arccos(\lambda/2)))^{\frac{1}{2}}} \left(\delta(\arccos(\lambda/2) - \mu) + \delta(\arccos(\lambda/2) + \mu)\right)\psi(2\cos(\mu)) = \psi(\lambda).
\end{aligned}$$

In the second equality we use that the summand containing $\delta(\arccos(\lambda/2) + \mu)$ is zero since both $\arccos(\lambda/2) > 0$ and $\mu > 0$. Thus, the generalized eigenfunctions are orthonormal. Finally, using once more the substitution $\mu = \arccos(\nu/2)$, we obtain the following:

$$\begin{aligned}
&\int_{-2}^{2} \mathrm{d}\nu\, g_{\Delta^D}(x, \nu)g_{\Delta^D}(y, \nu) = \\
&\int_{-2}^{2} \mathrm{d}\nu \left(1 - (\nu/2)^2\right)^{-\frac{1}{2}} \sin\Big(\arccos(\nu/2)x\Big)\sin\Big(\arccos(\nu/2)y\Big) = \\
&2\pi^{-1} \int_0^\pi \mathrm{d}\mu\, (\sin(\mu))^{-1} \sin(\mu) sin(\mu x)\sin(\mu y) = \delta_{xy},
\end{aligned}$$

for $x, y \in \mathbb{N}$, when the family of generalized eigenfunctions is also complete. □

From these two lemmas, we obtain the following corollary that gives us the spectral properties of H_0.

Proposition 2.11. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Then, $\sigma(H_0) = \sigma_{ac}(H_0) \cup \sigma_{pp}(H_0)$, where*

$$\sigma_{ac}(H_0) = \bigcup_{n\in\mathbb{N}_0} [v_l + n\omega, v_l + 4 + n\omega] \cup [v_r + n\omega, v_r + 4 + n\omega]$$

and

$$\sigma_{pp}(H_0) = \bigcup_{n\in\mathbb{N}_0} \{\lambda_j^S + n\omega : j = 0, 1\}.$$

The eigenvectors are given by $\widetilde{g}(m, n) = e_m^S \otimes \Upsilon_n$, $m = 0, 1$, $n \in \mathbb{N}_0$. The generalized eigenfunctions are given by $\widetilde{g}_\alpha(\cdot, \lambda, n) = g_\alpha(\cdot, \lambda - n\omega) \otimes \Upsilon_n$ for $\lambda \in \sigma_{ac}(H_0)$, $n \in \mathbb{N}_0$, $\alpha \in \{l, r\}$.

Proof. It is well known (see e.g. [15]) that for two self-adjoint operators A and B with $\sigma_{sc}(A) = \sigma_{sc}(B) = \emptyset$, we have $\sigma_{sc}(A \otimes 1 + 1 \otimes B) = \emptyset$,

$$\sigma_{ac}(A \otimes 1 + 1 \otimes B) = \Big(\sigma_{ac}(A) + \sigma(B)\Big) \cup \Big(\sigma(A) + \sigma_{ac}(B)\Big)$$

and

$$\sigma_{pp}(A \otimes 1 + 1 \otimes B) = \sigma_{pp}(A) + \sigma_{pp}(B).$$

Furthermore, if $\psi_A(\lambda_A)$ and $\psi_B(\lambda_B)$ are (generalized) eigenfunctions of A and B, respectively, then $\psi_A(\lambda_A) \otimes \psi_B(\lambda_B)$ is a (generalized) eigenfunction of $A \otimes I + I \otimes B$ for the (generalized) eigenvalue $\lambda_A + \lambda_B$.

The lemma follows now with $A = h_0^{el}$ and $B = h^{ph}$ using Lemmata 2.10 and (2.14) and the fact that h_S has eigenvectors $\{e_0^S, e_1^S\}$ with eigenvalues $\{\lambda_0^S, \lambda_1^S = \lambda_0^S + \varepsilon\}$. □

2.6. Spectral representation

For the convenience of the reader, we define here what we mean under a spectral representation of the absolutely continuous part K_0^{ac} of a self-adjoint operator K_0 on a separable Hilbert space $\mathfrak{K}$. Let $\mathfrak{k}$ be an auxiliary separable Hilbert space. We consider the Hilbert space $L^2(\mathbb{R}, d\lambda, \mathfrak{k})$. By $\mathcal{M}$, we define the multiplication operator induced by the independent variable λ in $L^2(\mathbb{R}, d\lambda, \mathfrak{k})$. Let $\Phi : \mathfrak{K}^{ac}(K_0) \longrightarrow L^2(\mathbb{R}, d\lambda, \mathfrak{k})$ be an isometry acting from $\mathfrak{K}^{ac}(K_0)$ into $L^2(\mathbb{R}, d\lambda, \mathfrak{k})$ such that: $\Phi\mathrm{dom}(K_0^{ac}) \subseteq \mathrm{dom}(\mathcal{M})$ and

$$\mathcal{M}\Phi f = \Phi K_0^{ac} f, \quad f \in \mathrm{dom}(K_0^{ac}).$$

Obviously, the orthogonal projection $P := \Phi\Phi^*$ commutes with $\mathcal{M}$ which yields the existence of a measurable family, $\{P(\lambda)\}_{\lambda\in\mathbb{R}}$, such that:

$$(P\,\widehat{f}\,)(\lambda) = P(\lambda)\,\widehat{f}\,(\lambda), \qquad \widehat{f}\, \in L^2(\mathbb{R}, \lambda, \mathfrak{k}).$$

We set $L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)) := PL^2(\mathbb{R}, \lambda, \mathfrak{k})$, $\mathfrak{k}(\lambda) := P(\lambda)\mathfrak{k}$, and call the triplet

$$\Pi(K_0^{ac}) := \{L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)), \mathcal{M}, \Phi\}$$

a spectral representation of K_0^{ac}. If $\{L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)), \mathcal{M}, \Phi\}$ is a spectral representation of K^{ac}, then K^{ac} is unitarily equivalent $\mathcal{M}_0 := \mathcal{M} \restriction L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda))$. Indeed, one has $\Phi K_0^{ac}\Phi^* = \mathcal{M}_0$. The function $\xi_{K_0}^{ac}(\lambda) := \mathrm{dom}(\mathfrak{k}(\lambda))$, $\lambda \in \mathbb{R}$, is called the spectral multiplicity function of K_0^{ac}. Notice that $0 \leqslant \xi_{K_0}^{ac}(\lambda) \leqslant \infty$ for $\lambda \in \mathbb{R}$.

For $\alpha \in \{l, r\}$, the generalized eigenfunctions of h_α^{el} define generalized Fourier transforms by $\phi_\alpha^{el} : \mathfrak{h}_\alpha^{el} = \mathfrak{h}_\alpha^{el,ac}(h_\alpha^{el}) \to L^2([v_\alpha, v_\alpha + 4])$ and

$$(\phi_\alpha^{el} f_\alpha)(\lambda) = \sum_{x\in\mathbb{N}_0} g_\alpha(x, \lambda) f_\alpha(x), \quad f_\alpha \in \mathfrak{h}_\alpha^{el}. \tag{2.31}$$

We then set:

$$\mathfrak{h}^{el}_\alpha(\lambda) := \begin{cases} \mathbb{C} & \lambda \in [v_\alpha, v_\alpha + 4] \\ 0 & \lambda \in \mathbb{R} \setminus [v_\alpha, v_\alpha + 4]. \end{cases} \tag{2.32}$$

One can easily verify that $\Pi(h^{el}_\alpha) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}^{el}_\alpha(\lambda)), \mathcal{M}, \phi^{el}_\alpha\}$ is a spectral representation of $h^{el}_\alpha = h^{el,ac}_\alpha$, $\alpha = l, r$, where we always assumed implicitly that $(\phi^{el}_\alpha f_\alpha)(\lambda) = 0$ for $\lambda \in \mathbb{R} \setminus [v_\alpha, v_\alpha + 4]$. Setting:

$$\mathfrak{h}^{el}(\lambda) := \begin{matrix} \mathfrak{h}^{el}_l(\lambda) \\ \oplus \\ \mathfrak{h}^{el}_r(\lambda) \end{matrix} \subseteq \mathbb{C}^2, \quad \lambda \in \mathbb{R}, \tag{2.33}$$

and introducing the map:

$$\phi^{el} : \mathfrak{h}^{el,ac}(h^{el}_0) = \begin{matrix} \mathfrak{h}^{el}_l \\ \oplus \\ \mathfrak{h}^{el}_r \end{matrix} \longrightarrow L^2(\mathbb{R}, d\lambda, \mathfrak{h}^{el}(\lambda)), \tag{2.34}$$

defined by:

$$\phi^{el} f := \begin{pmatrix} \phi^{el}_l f_l \\ \phi^{el}_r f_r \end{pmatrix}, \quad \text{where} \quad f := \begin{pmatrix} f_l \\ f_r \end{pmatrix} \tag{2.35}$$

we obtain a spectral representation $\Pi(h^{el,ac}_0) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}^{el}(\lambda)), \mathcal{M}, \phi^{el}\}$ of the absolutely continuous part $h^{el,ac}_0 = h^{el}_l \oplus h^{el}_r$ of h^{el}_0. One easily verifies that $0 \leqslant \xi^{ac}_{h^{el}_0}(\lambda) \leqslant 2$ for $\lambda \in \mathbb{R}$. Introducing:

$$\lambda^{el}_{\min} := \min\{v_l, v_r\} \quad \text{and} \quad \lambda^{el}_{\max} := \max\{v_l + 4, v_r + 4\}, \tag{2.36}$$

one easily verifies that $\xi^{ac}_{h^{el}_0}(\lambda) = 0$ for $\lambda \in \mathbb{R} \setminus [\lambda^{el}_{\min}, \lambda^{el}_{\max}]$.

Notice, if $v_r + 4 \leqslant v_l$, then

$$\mathfrak{h}^{el}(\lambda) = \begin{cases} \mathbb{C}, & \lambda \in [v_r, v_r + 4] \cup [v_l, v_l + 4], \\ \{0\}, & \text{otherwise} \end{cases}$$

which shows that h^{el}_0 has a simple spectrum. In particular, it holds $\xi^{ac}_{h^{el}_0}(\lambda) = 1$ for $\lambda \in [v_r, v_r + 4] \cup [v_l, v_l + 4]$ and otherwise $\xi^{ac}_{h^{el}_0}(\lambda) = 0$.

Let us introduce the Hilbert space $\mathfrak{h} := l^2(\mathbb{N}_0, \mathbb{C}^2) = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}_n$, $\mathfrak{h}_n := \mathbb{C}^2$, $n \in \mathbb{N}_0$. Regarding $\mathfrak{h}^{el}(\lambda - n\omega)$ as a subspace of $\mathfrak{h}_n$, one regards:

$$\mathfrak{h}(\lambda) := \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}_n(\lambda), \quad \mathfrak{h}_n(\lambda) := \mathfrak{h}^{el}(\lambda - n\omega), \quad \lambda \in \mathbb{R}, \tag{2.37}$$

as a measurable family of subspaces in $\mathfrak{h}$. Notice that $0 \leqslant \dim(\mathfrak{h}(\lambda)) < \infty$, $\lambda \in \mathbb{R}$. We consider the Hilbert space $L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda))$.

Furthermore, we introduce the isometric map $\Phi : \mathfrak{H}(H^{ac}_0) \longrightarrow L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda))$ defined by

$$(\Phi f)(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \begin{pmatrix} (\phi^{el}_l f_l(n))(\lambda - n\omega) \\ (\phi^{el}_r f_r(n))(\lambda - n\omega) \end{pmatrix}, \quad \lambda \in \mathbb{R}, \tag{2.38}$$

where

$$\bigoplus_{n\in\mathbb{N}_0} \begin{pmatrix} f_l(n) \\ f_r(n) \end{pmatrix} \in \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}^{el,ac}(h^{el}_0) \otimes \mathfrak{h}^{ph}_n = \bigoplus_{n\in\mathbb{N}} \begin{pmatrix} \mathfrak{h}^{el}_l \otimes h^{ph}_n \\ \oplus \\ \mathfrak{h}^{el}_r \otimes h^{ph}_n \end{pmatrix}$$

where $\mathfrak{h}_{ph} = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}^{ph}_n$ and $\mathfrak{h}^{ph}_n$ is the subspace spanned by the eigenvectors Υ_n of h^{ph}. One easily verifies that Φ is an isometry acting from $\mathfrak{H}^{ac}(H^{ac}_0)$ onto $L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda))$.

Lemma 2.12. *The triplet* $\{L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda)), \mathcal{M}, \Phi\}$ *forms a spectral representation of* H_0^{ac}*, that is,* $\Pi(H_0^{ac}) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda)), \mathcal{M}, \Phi\}$ *where there is a constant* $d \in \mathbb{N}_0$ *such that* $0 \leqslant \xi_{H_0}^{ac}(\lambda) \leqslant 2d_{\max}$ *for* $\lambda \in \mathbb{R}$ *where* $d_{\max} := \frac{\lambda_{\max}^{el} - \lambda_{\min}^{el}}{\omega}$ *and* $\lambda_{\max}^{el}$ *and* $\lambda_{\min}^{el}$ *are given by* (2.36)*.*

Proof. It remains to be shown that Φ transforms H_0^{ac} into the multiplication operator $\mathcal{M}$. We have

$$H_0^{ac} f = \bigoplus_{n\in\mathbb{N}_0} \begin{pmatrix} (h_l^{el} f_l)(n) + n\omega f_l(n) \\ (h_r^{el} f_r)(n) + n\omega f_r(n) \end{pmatrix}$$

which yields the following:

$$\begin{aligned}(\Phi H_0^{ac} f)(\lambda) &= \bigoplus_{n\in\mathbb{N}_0} \begin{pmatrix} (\phi_l^{el}(h_l^{el} f_l)(n))(\lambda - n\omega) + n\omega(\phi_l^{el} f_l(n))(\lambda - n\omega) \\ (\phi_r^{el}(h_r^{el} f_r)(n))(\lambda - n\omega) + n\omega(\phi_r^{el} f_r(n))(\lambda - n\omega) \end{pmatrix} \\ &= \bigoplus_{n\in\mathbb{N}_0} \begin{pmatrix} \lambda(\phi_l^{el} f_l(n))(\lambda - n\omega) \\ \lambda(\phi_r^{el} f_r(n))(\lambda - n\omega) \end{pmatrix} = (\mathcal{M}\Phi f)(\lambda), \quad \lambda \in \mathbb{R}.\end{aligned}$$

which proves the desired property.

One easily checks that $\mathfrak{h}(\lambda)$ might only be only non-trivial if $\lambda - n\omega \in [\lambda_{\min}^{el}, \lambda_{\max}^{el}]$. Hence, we obtain that $\mathfrak{h}(\lambda)$ is non-trivial if the condition:

$$\frac{\lambda - \lambda_{\max}^{el}}{\omega} \leqslant n \leqslant \frac{\lambda - \lambda_{\min}^{el}}{\omega}$$

is satisfied. Hence,

$$0 \leqslant \xi_{H_0}^{ac}(\lambda) \leqslant 2 \text{ card} \left\{ n \in \mathbb{N}_0 : \frac{\lambda - \lambda_{\max}^{el}}{\omega} \leqslant n \leqslant \frac{\lambda - \lambda_{\min}^{el}}{\omega} \right\}, \quad \lambda \in \mathbb{R}.$$

or

$$0 \leqslant \xi_{H_0}^{ac}(\lambda) \leqslant 2\text{card} \left\{ n \in \mathbb{N}_0 : 0 \leqslant n \leqslant \frac{\lambda_{\max}^{el} - \lambda_{\max}^{el}}{\omega} \right\}, \quad \lambda \in \mathbb{R}.$$

Hence $0 \leqslant \xi_{H_0}^{ac}(\lambda) \leqslant d_{\max}$ for $\lambda \in \mathbb{R}$. □

In the following we denote the orthogonal projection from $\mathfrak{h}(\lambda)$ onto $\mathfrak{h}_n(\lambda)$ by $P_n(\lambda)$, $\lambda \in \mathbb{R}$, cf (2.37). Since $\mathfrak{h}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \mathfrak{h}_n(\lambda)$ we have $I_{\mathfrak{h}(\lambda)} = \sum_{n\in\mathbb{N}_0} P_n(\lambda)$, $\lambda \in \mathbb{R}$. Further, we introduce the following subspaces:

$$\mathfrak{h}_{n_\alpha}(\lambda) := \mathfrak{h}_\alpha^{el}(\lambda - n\omega), \quad \lambda \in \mathbb{R}, \quad n \in \mathbb{N}_0.$$

Notice that:

$$\mathfrak{h}_n(\lambda) = \bigoplus_{\alpha\in\{l,r\}} \mathfrak{h}_{n_\alpha}(\lambda), \quad \lambda \in \mathbb{R}, \quad n \in \mathbb{N}_0.$$

By $P_{n_\alpha}(\lambda)$ we denote the orthogonal projection from $\mathfrak{h}(\lambda)$ onto $\mathfrak{h}_{n_\alpha}(\lambda)$, $\lambda \in \mathbb{R}$. Clearly, we have $P_n(\lambda) = \sum_{\alpha\in\{l,r\}} P_{n_\alpha}(\lambda)$, $\lambda \in \mathbb{R}$.

Example 2.13. In general, the direct integral $\Pi(H_0^{ac})$ can be very complicated, in particular, the structure of $\mathfrak{h}(\lambda)$ given by (2.37) is difficult to analyze. However, there are interesting simple cases:
(i) Let $v = v_l = v_r$ and $4 \leqslant \omega$. In this case we have $\mathfrak{h}^{el}(\lambda) = \mathbb{C}^2$ for $[v, v+4]$ and

$$\mathfrak{h}(\lambda) = \begin{cases} \mathbb{C}^2, & \lambda \in [v + n\omega, v + n\omega + 4], \quad n \in \mathbb{N}_0, \\ \{0\}, & \text{otherwise.} \end{cases}$$

(ii) Let $v_r = 0$, $v_l = 4$, $\omega_0 = 4$. Then

$$\mathfrak{h}(\lambda) = \begin{cases} \mathfrak{h}_r^{el}(\lambda) = \mathbb{C}, & \lambda \in [0,4), \\ \mathfrak{h}_{lr}^{el}(\lambda) = \mathbb{C}^2, & \lambda \in [4,8), \\ \mathfrak{h}_{rl}^{el}(\lambda) = \mathbb{C}^2, & \lambda \in [8,12), \\ \cdots \end{cases}$$

where

$$\mathfrak{h}_{\alpha\alpha'}^{el}(\lambda) = \begin{matrix} \mathfrak{h}_{\alpha}^{el}(\lambda) \\ \oplus \\ \mathfrak{h}_{\alpha'}^{el}(\lambda) \end{matrix}, \qquad \alpha, \alpha' \in \{l, r\}, \quad \alpha \neq \alpha'.$$

Hence, $\dim(\mathfrak{h}(\lambda)) = 2$ for $\lambda \geqslant 4$. □

Let Z be a bounded operator acting on $\mathfrak{H}^{ac}(H_0)$ and commuting with H_0^{ac}. Since Z commutes with H_0^{ac} there is a measurable family $\{Z(\lambda)\}_{\lambda\in\mathbb{R}}$ of bounded operators acting on $\mathfrak{h}(\lambda)$ such that Z is unitarily equivalent to the multiplication operator induced by $\{Z(\lambda)\}_{\lambda\in\mathbb{R}}$ in $\Pi(H_0^{ac})$. We then set:

$$Z_{m_\alpha n_\varkappa}(\lambda) := P_{m_\alpha}(\lambda) Z(\lambda) \restriction \mathfrak{h}_{n_\varkappa}(\lambda), \quad \lambda \in \mathbb{R}, \qquad m, n \in \mathbb{N}_0, \quad \alpha, \varkappa \in \{l, r\}.$$

Let $Z_{m_\alpha n_\varkappa} := P_{m_\alpha} Z P_{n_\varkappa}$ where P_{m_α} is the orthogonal projection from $\mathfrak{H}$ onto $\mathfrak{H}_{m_\alpha} \subseteq \mathfrak{H}^{ac}(H_0)$, cf. (2.18). Clearly, the multiplication operator induced $\{Z_{m_\alpha n_\varkappa}(\lambda)\}_{\lambda\in\mathbb{R}}$ in $\Pi(H_0^{ac})$ is unitarily equivalent to $Z_{m_\alpha n_\varkappa}$.

Since, by Lemma 2.12, $\mathfrak{h}(\lambda)$ is a finite dimensional space, the operators $Z(\lambda)$ are finite dimensional ones and we can introduce the following quantity:

$$\sigma_{m_\alpha n_\varkappa}(\lambda) := \mathrm{tr}(Z_{m_\alpha n_\varkappa}(\lambda)^* Z_{m_\alpha n_\varkappa}(\lambda)), \quad \lambda \in \mathbb{R}, \qquad m, n \in \mathbb{N}_0, \quad \alpha, \varkappa \in \{l, r\}.$$

Lemma 2.14. *Let H_0 be the self-adjoint operator defined by* (2.15) *on $\mathfrak{H}$. Furthermore, let Z be a bounded operator on $\mathfrak{H}^{ac}(H_0)$ commuting with H_0^{ac}*
(i) *Let Γ be a conjugation on $\mathfrak{H}$, cf. Section 2.3. If Γ commutes with H_0 and P_{n_α}, $n \in \mathbb{N}_0$, $\alpha \in \{l, r\}$ and $\Gamma Z \Gamma = Z^*$ holds, then $\sigma_{m_\alpha n_\varkappa}(\lambda) = \sigma_{n_\varkappa m_\alpha}(\lambda)$, $\lambda \in \mathbb{R}$.*
(ii) *Let U be a mirror symmetry on $\mathfrak{H}$. If U commutes with H_0 and Z, then $\sigma_{m_\alpha n_\varkappa}(\lambda) = \sigma_{m_{\alpha'} n_{\varkappa'}}(\lambda)$, $\lambda \in \mathbb{R}$, $m, n \in \mathbb{N}_0$, $\alpha, \alpha', \varkappa, \varkappa' \in \{l, r\}$, $\alpha \neq \alpha'$, $\varkappa \neq \varkappa'$.*

Proof. (i) Since Γ commutes with H_0 the conjugation Γ is reduce by $\mathfrak{H}^{ac}(H_0)$. So without loss of generality, we assume that Γ acts on $\mathfrak{H}^{ac}(H_0)$. We set $\Gamma_{n_\alpha} := \Gamma \restriction \mathfrak{H}_{n_\alpha}$. Notice that:

$$\Gamma = \bigoplus_{n\in\mathbb{N}_0, \alpha\in\{l,r\}} \Gamma_{n_\alpha}.$$

There is a measurable family $\{\Gamma(\lambda)\}_{\lambda\in\mathbb{R}}$ of conjugations such that the multiplication operator induced by $\{\Gamma(\lambda)\}_{\lambda\in\mathbb{R}}$ in $\Pi(H_0^{ac})$ is unitarily equivalent to Γ. Moreover, since Γ commutes with P_{n_α}, we see that the multiplication operator induced by the measurable family:

$$\Gamma_{n_\alpha}(\lambda) := \Gamma(\lambda) \restriction \mathfrak{h}_{n_\alpha}(\lambda), \quad \lambda \in \mathbb{R}, \quad m \in \mathbb{N}_0, \quad \alpha \in \{l, r\},$$

is unitarily equivalent to Γ_{n_α}. Using $\Gamma Z \Gamma = Z^*$ we get $\Gamma_{m_\alpha} Z_{m_\alpha n_\varkappa} \Gamma_{n_\varkappa} = Z_{n_\varkappa m_\alpha}^*$. Hence,

$$\Gamma_{m_\alpha}(\lambda) Z_{m_\alpha n_\varkappa}(\lambda) \Gamma_{n_\varkappa}(\lambda) = Z_{n_\varkappa m_\alpha}(\lambda)^*, \quad \lambda \in \mathbb{R}. \tag{2.39}$$

If X is a trace class operator, then $\mathrm{tr}(\Gamma X \Gamma) = \overline{\mathrm{tr}(X)}$. Using that we find

$$\sigma_{m_\alpha n_\varkappa}(\lambda) = \overline{\mathrm{tr}(\Gamma_{n_\varkappa}(\lambda) Z_{m_\alpha n_\varkappa}(\lambda)^* Z_{m_\alpha n_\varkappa}(\lambda) \Gamma_{n_\varkappa}(\lambda))} = \overline{\mathrm{tr}(\Gamma_{n_\varkappa}(\lambda) Z_{m_\alpha n_\varkappa}(\lambda)^* \Gamma_{m_\alpha} \Gamma_{m_\alpha} Z_{m_\alpha n_\varkappa}(\lambda) \Gamma_{n_\varkappa}(\lambda))}$$

From (2.39), we obtain the following:

$$\sigma_{m_\alpha n_\varkappa}(\lambda) = \overline{\mathrm{tr}(Z_{n_\varkappa m_\alpha}(\lambda) Z_{n_\varkappa m_\alpha}(\lambda)^*)} = \sigma_{n_\varkappa m_\alpha}(\lambda), \quad \lambda \in \mathbb{R},$$

which proves (i).

(ii) Again, without loss of generality we can assume that U acts only $\mathfrak{H}^{ac}(H_0)$. Since U commutes with H_0, there is a measurable family $\{U(\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators acting on $\mathfrak{h}(\lambda)$ such that the multiplication operator induced by $\{U(\lambda)\}_{\lambda\in\mathbb{R}}$ is unitarily equivalent to U. Since $U\mathfrak{H}_{n_\alpha} = \mathfrak{H}_{n_{\alpha'}}$ we have $U(\lambda)\mathfrak{h}_{n_\alpha}(\lambda) = \mathfrak{h}_{n_{\alpha'}}(\lambda)$, $\lambda \in \mathbb{R}$. Hence,

$$\sigma_{m_\alpha n_\varkappa}(\lambda) = \mathrm{tr}(U(\lambda) Z_{m_\alpha n_\varkappa}(\lambda)^* Z_{m_\alpha n_\varkappa}(\lambda) U(\lambda)^*) = \mathrm{tr}(U(\lambda) Z_{m_\alpha, n_\varkappa}(\lambda)^* U(\lambda)^* U(\lambda) Z_{m_\alpha, n_\varkappa}(\lambda) U(\lambda)^*).$$

Hence,

$$\sigma_{m_\alpha n_\varkappa}(\lambda) = \mathrm{tr}(P_{n_{\varkappa'}} U(\lambda) Z(\lambda)^* U(\lambda)^* P_{m_{\alpha'}}(\lambda) U(\lambda) Z(\lambda) U(\lambda)^* P_{n_{\varkappa'}}(\lambda)).$$

Since U commutes with Z, we find that:

$$\sigma_{m_\alpha n_\varkappa}(\lambda) = \mathrm{tr}(P_{n_{\varkappa'}} Z(\lambda)^* P_{m_{\alpha'}}(\lambda) Z(\lambda) P_{n_{\varkappa'}}(\lambda)) = \sigma_{m_{\alpha'} n_{\varkappa'}}(\lambda), \quad \lambda \in \mathbb{R},$$

which proves (ii). □

2.7. Spectral properties of H: second part

Since we have full information for the spectral properties of H_0, we can use this to show that H has no singular continuous spectrum. Crucial for that is the following lemma: with the help of [6, Cor. IV.15.19], which establishes existence and completeness of wave operators and absence of singular continuous spectrum through a time-falloff method. We cite it as a Lemma for convenience, with slight simplifications that suffice for our purposes.

Lemma 2.15 ([6, Corollary IV.15.19])**.** *Let $\{H_0, H\}$ be a scattering system and let Λ be a closed countable set. Let F_+ and F_- be two self-adjoint operators such that $F_+ + F_- = P^{ac}_{H_0}$ and*

$$s - \lim_{t\to\infty} e^{\mp itH_0} F_\pm e^{\pm itH_0} = 0.$$

If $(H-i)^{-1} - (H_0 - i)^{-1} \in \mathfrak{L}_\infty(\mathfrak{H})$, $(1 - P^{ac}_{H_0})\gamma(H_0) \in \mathfrak{L}_\infty(\mathfrak{H})$, and

$$\Big| \int_0^{\pm\infty} \mathrm{d}t \Big\| \Big((H_0 - i)^{-1} - (H - i)^{-1} \Big) e^{-itH_0} \gamma(H_0) F_\pm \Big\| \Big| < \infty$$

for all $\gamma \in C_0^\infty(\mathbb{R} \setminus \Lambda)$, then $W_\pm(H, H_0)$ exist and are complete and $\sigma_{sc}(H) = \sigma_{sc}(H_0) = \emptyset$. Furthermore, each eigenvalue of H and H_0 in $\mathbb{R} \setminus \Lambda$ is of finite multiplicity and these eigenvalues accumulate the most at points of Λ or at $\pm\infty$.

We already know that the wave operators exist and are complete since the resolvent difference is trace class. Hence, we need Lemma 2.15 only to prove the following proposition.

Proposition 2.16. *The Hamiltonian H defined by* (2.17) *has no singular continuous spectrum, that is, $\sigma_{sc}(H) = \emptyset$.*

Proof. At first we have to construct the operators $F_\pm$. To this end, let $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the usual Fourier transform, i.e

$$(\mathcal{F}f)(\mu) := \widehat{f}\,(\mu) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\mu x} f(x) dx, \quad f \in L^2(\mathbb{R}, dx), \quad \mu \in \mathbb{R}.$$

Further, let $\Pi_\pm$ be the orthogonal projection onto $L^2(\mathbb{R}_\pm)$ in $L^2(\mathbb{R})$. We set:

$$F_\pm = \Phi^* \mathcal{F} \Pi_\pm \mathcal{F}^* \Phi,$$

where Φ is given by (2.38). We immediately obtain $F_- + F_+ = P_{ac}(H_0)$. We still have to show that:

$$s - \lim_{t\to\infty} \|e^{\mp itH_0}\Phi^*\mathcal{F}\Pi_\pm\mathcal{F}^*\Phi e^{\pm itH_0} f\| = 0$$

for $f \in \mathfrak{H}^{ac}(H_0)$. We prove the relation only for F_+ since the proof for F_- is essentially identical. We have the following:

$$\Big(\Pi_+\mathcal{F}^*\Phi e^{itH_0} f\Big)(x) = (2\pi)^{-\frac{1}{2}}\chi_{\mathbb{R}_+}(x)\int_{\mathbb{R}} \mathrm{d}\mu\, e^{i(x+t)\mu}\widehat{f}(\mu) = \chi_{\mathbb{R}_+}(x)\psi(x+t)$$

with $\psi = \mathcal{F}\widehat{f}$. Now,

$$\|e^{-itH_0}\Phi^*\mathcal{F}\Pi_+\mathcal{F}^*\Phi e^{itH_0} f\|^2 =$$
$$\|\Pi_+\mathcal{F}^*\Phi e^{itH_0} f\|^2 = \int_{\mathbb{R}_+} \mathrm{d}x\Big|\psi(x+t)\Big|^2 = \int_t^\infty \mathrm{d}x\Big|\psi(x)\Big|^2 \overset{t\to\infty}{\longrightarrow} 0.$$

Concerning the compactness condition, we already know that $(H-i)^{-1} - (H_0-i)^{-1} \in \mathfrak{L}_1(\mathfrak{H}) \subset \mathfrak{L}_\infty(\mathfrak{H})$ from Proposition 2.9. Let

$$\Lambda := \bigcup_{n\in\mathbb{N}_0} \{v_l + n\omega, v_r + n\omega, v_l + 4 + n\omega, v_r + 4 + n\omega\},$$

which is closed and countable. We know from Corollary 2.11 that H_0 has no singular continuous spectrum and the eigenvalues are of finite multiplicity. It follows then that $(1 - P_{ac}(H_0))\gamma(H_0)$ is compact for every $\gamma \in C_0^\infty(\mathbb{R}\setminus\Lambda)$. The remaining assumption of Lemma 2.15 is as follows:

$$\left|\int_0^{\pm\infty} \mathrm{d}t\, \Big\|\Big((H-i)^{-1} - (H_0-i)^{-1}\Big)\gamma(H_0)e^{-itH_0}F_\pm\Big\|\right| < \infty.$$

If we can prove this, then we immediately obtain that H has no singular continuous spectrum. Now $(H-i)^{-1} - (H_0-i)^{-1} = (H-i)^{-1}(V_{el}+V_{ph})(H_0-i)^{-1}$. But $(H-i)^{-1}$ is bounded,

$$\mathrm{ran}(F_\pm) \subset \mathfrak{H}^{ac}(H_0) = (\mathfrak{h}_l^{el} \oplus \mathfrak{h}_r^{el}) \otimes \mathfrak{h}^{ph},$$

and $V_{ph}P^{ac}(H_0) = 0$. Also, $V_{el} = v_{el} \otimes I_{\mathfrak{h}^{ph}}$ and

$$\ker(v_{el})^\perp \subset \mathbb{C}\delta_1^l \oplus \mathfrak{h}_S \oplus \mathbb{C}\delta_1^r.$$

Hence, it suffices to prove:

$$\left|\int_0^{\pm\infty} \mathrm{d}t\, \Big\|P_1^\alpha(H_0-i)^{-1}\gamma(H_0)e^{-itH_0}F_\pm\Big\|\right| < \infty,$$

$\alpha \in \{l, r\}$, where $P_1^\alpha = p_1^\alpha \otimes I_{\mathfrak{h}^{ph}}$ and p_1^α is the orthogonal projection onto $\mathfrak{h}_\alpha^{el}$. In the following we treat only the case F_+. The calculations for F_- are completely analogous. We use that Φ maps H_0^{ac} into the multiplication operator $\mathcal{M}$ induced by λ. Hence, we get the following:

$$\Big\|P_1^\alpha\widetilde{\gamma}(H_0)e^{-itH_0}\Phi^*\mathcal{F}f\Big\| = \Big\|P_1^\alpha\Phi^*\Phi\widetilde{\gamma}(H_0)e^{-itH_0}\Phi^*\mathcal{F}f\Big\| =$$
$$= (2\pi)^{-\frac{1}{2}}\Big(\sum_{n\in\mathbb{N}_0}\Big|\int_{\delta_{\alpha,n}} \mathrm{d}\lambda\; g_\alpha(1,\lambda-n\omega)\widetilde{\gamma}(\lambda)\int_{\mathbb{R}_+}\mathrm{d}x\, e^{-i\lambda(x+t)}f(x)\Big|^2\Big)^{\frac{1}{2}},$$

where $\mathrm{supp}\,(f) \subseteq \mathbb{R}_+$, $\widetilde{\gamma}(\lambda) := (\lambda-i)^{-1}\gamma(\lambda)$, $\lambda \in \mathbb{R}$, and $\delta_{\alpha,n} := [v_\alpha + n\omega_0, v_\alpha + n\omega + 4]$. Notice that $\widetilde{\gamma}(\lambda) \in C_0^\infty(\mathbb{R}\setminus\Lambda)$. We find:

$$\int_{\delta_{j,n}} \mathrm{d}\lambda\; g_\alpha(1,\lambda-n\omega)\widetilde{\gamma}(\lambda)\int_{\mathbb{R}_+}\mathrm{d}x\, e^{-i\lambda(x+t)}f(x) =$$
$$\int_{v_\alpha}^{v_\alpha+4} \mathrm{d}\lambda\; g_\alpha(1,\lambda)\widetilde{\gamma}(\lambda+n\omega)\int_{\mathbb{R}_+}\mathrm{d}x\, e^{-i(\lambda+n\omega)(x+t)}f(x)$$

which yields:

$$\left\|P_1^\alpha \Phi^* \Phi \widetilde{\gamma}(H_0) e^{-itH_0} \Phi^* \mathcal{F} f\right\| =$$
$$(2\pi)^{-\frac{1}{2}} \Big(\sum_{n\in\mathbb{N}_0} \Big| \int_{v_\alpha}^{v_\alpha+4} \mathrm{d}\lambda \; g_\alpha(1,\lambda) \widetilde{\gamma}(\lambda+n\omega_0) \int_{\mathbb{R}_+} \mathrm{d}x \, e^{-i(\lambda+n\omega_0)(x+t)} f(x) \Big|^2 \Big)^{\frac{1}{2}}.$$

Since the support of $\gamma(\lambda)$ is compact, we see that the sum $\sum_{n\in\mathbb{N}_0}$ is finite. Changing the integrals, we get:

$$\int_{\delta_{\alpha,n}} \mathrm{d}\lambda \; g_\alpha(1,\lambda-n\omega) \widetilde{\gamma}(\lambda) \int_{\mathbb{R}_+} \mathrm{d}x \, e^{-i\lambda(x+t)} f(x) =$$
$$\int_{\mathbb{R}_+} \mathrm{d}x \, f(x) e^{-in\omega_0(x+t)} \int_{v_\alpha}^{v_\alpha+4} \mathrm{d}\lambda \; g_\alpha(1,\lambda) \widetilde{\gamma}(\lambda+n\omega) e^{-i\lambda(x+t)}$$

Integrating by parts m-times, we obtain:

$$\int_{\delta_{\alpha,n}} \mathrm{d}\lambda \; g_\alpha(1,\lambda-n\omega) \widetilde{\gamma}(\lambda) \int_{\mathbb{R}_+} \mathrm{d}x \, e^{-i\lambda(x+t)} f(x) =$$
$$(-i)^m \int_{\mathbb{R}_+} \mathrm{d}x \, f(x) \frac{e^{-in\omega(x+t)}}{(x+t)^m} \int_{v_\alpha}^{v_\alpha+4} \mathrm{d}\lambda \; e^{-i\lambda(x+t)} \frac{d^m}{d\lambda^m} \left(g_\alpha(1,\lambda) \widetilde{\gamma}(\lambda+n\omega) \right)$$

Hence,

$$\Big| \int_{\delta_{\alpha,n}} \mathrm{d}\lambda \; g_\alpha(1,\lambda-n\omega) \widetilde{\gamma}(\lambda) \int_{\mathbb{R}_+} \mathrm{d}x \, e^{-i\lambda(x+t)} f(x) \Big|^2 \leqslant C_n^2 \left(\int_{\mathbb{R}_+} \mathrm{d}x \, |f(x)| \frac{1}{(x+t)^m} \right)^2$$

which yields:

$$\Big| \int_{\delta_{\alpha,n}} \mathrm{d}\lambda \; g_\alpha(1,\lambda-n\omega) \widetilde{\gamma}(\lambda) \int_{\mathbb{R}_+} \mathrm{d}x \, e^{-i\lambda(x+t)} f(x) \Big|^2 \leqslant C_n^2 \frac{1}{t^{(2m-1)}} \|f\|^2$$

for $m \in \mathbb{N}$ where:

$$C_n := \int_{v_\alpha}^{v_\alpha+4} \mathrm{d}\lambda \left| \frac{d^m}{d\lambda^m} \left(g_\alpha(1,\lambda) \widetilde{\gamma}(\lambda+n\omega) \right| \right).$$

Notice that $C_n = 0$ for sufficiently large $n \in \mathbb{N}$. Therefore,

$$\left\|P_1^\alpha \widetilde{\gamma}(H_0) e^{-itH_0} \Phi^* \mathcal{F} f\right\| \leqslant \left(\sum_{n\in\mathbb{N}_0} C_n^2 \right)^{1/2} \frac{1}{t^{m-1/2}} \|f\|, \quad f \in L^2(\mathbb{R}_+, dx),$$

which shows that $\left\|P_1^\alpha \widetilde{\gamma}(H_0) e^{-itH_0} F_+\right\| \in L^1(\mathbb{R}_+, dt)$ for $m \geqslant 2$. □

3. Landauer-Büttiker formula and applications

3.1. Landauer-Büttiker formula

The abstract Landauer-Büttiker formula can be used to calculate currents through devices. Usually one considers a pair $\mathcal{S} = \{K, K_0\}$ be of self-adjoint operators where the unperturbed Hamiltonian K_0 describes a totally decoupled system, that means, the inner system is closed and the leads are decoupled from it, while the perturbed Hamiltonian K describes the system where the leads are coupled to the inner system. An important component is system $\mathcal{S} = \{K, K_0\}$, which represents a complete scattering or even a trace class scattering system.

In [1], an abstract Landauer-Büttiker formula was derived in the framework of a trace class scattering theory for semi-bounded self-adjoint operators which allows one to reproduce the results of [18] and [7] rigorously. In [13], the results of [1] were generalized to non-semi-bounded operators. Following [1], we consider a trace class scattering system $\mathcal{S} = \{K, K_0\}$. We

recall that $\mathcal{S} = \{K, K_0\}$ is called a trace class scattering system if the resolvent difference of K and K_0 belongs to the trace class. If $\mathcal{S} = \{K, K_0\}$ is a trace class scattering system, then the wave operators $W_\pm(K, K_0)$ exist and are complete. The scattering operator is defined by $S(K, K_0) := W_+(K, K_0)^* W_-(K, K_0)$. The main components, besides the trace class scattering system $\mathcal{S} = \{K, K_0\}$, are the density and the charge operators ρ and Q, respectively.

The density operator ρ is a non-negative bounded self-adjoint operator commuting with K_0. The charge Q is a bounded self-adjoint operator commuting also with K_0. If K has no singular continuous spectrum, then the current related to the density operator ρ and the charge Q is defined as follows:

$$J^{\mathcal{S}}_{\rho,Q} = -i \operatorname{tr} \left(W_-(K, K_0) \rho W_-(K, K_0)^* [K, Q] \right), \tag{3.1}$$

where $[K, Q]$ is the commutator of K and Q. In fact, the commutator $[K, Q]$ might be not defined. In this case, the regularized definition:

$$J^{\mathcal{S}}_{\rho,Q} = -i \operatorname{tr} \left(W_-(K, K_0)(I + K_0^2) \rho W_-(K, K_0)^* \frac{1}{K - i} [K, Q] \frac{1}{K + i} \right), \tag{3.2}$$

is used, where it is assumed that $(I + K_0^2)\rho$ is a bounded operator. Since the condition $(H - i)^{-1}[H, Q](H + i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ is satisfied, definition (3.2) makes sense. By $\mathfrak{L}_1(\mathfrak{H})$ is the ideal of trace class operators is denoted.

Let K_0 be self-adjoint operator on the separable Hilbert space $\mathfrak{K}$. We call ρ be a density operator for K_0 if ρ is a bounded non-negative self-adjoint operator commuting with K_0. Since ρ commutes with K_0, one sees that ρ leaves invariant the subspace $\mathfrak{K}^{ac}(K_0)$. We then set

$$\rho_{ac} := \rho \restriction \mathfrak{K}^{ac}(K_0).$$

call ρ_{ac} the ac-density part of ρ.

A bounded self-adjoint operator, Q, commuting with K_0, is called a charge. If Q is the charge, then:

$$Q_{ac} := Q \restriction \mathfrak{K}^{ac}(K_0),$$

is called its ac-charge component.

Let $\Pi(K_0^{ac}) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)), \mathcal{M}, \Phi\}$ be a spectral representation of K_0^{ac}. If ρ is a density operator, then there is a measurable family $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ of bounded self-adjoint operators such that the multiplication operator:

$$(\mathcal{M}_{\rho_{ac}} \widehat{f})(\lambda) := \rho_{ac}(\lambda)\, \widehat{f}\,(\lambda), \quad \widehat{f} \in \operatorname{dom}(M_{\rho_{ac}}) := L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)),$$

is unitarily equivalent to the ac-part ρ_{ac}, that is, $\mathcal{M}_{\rho_{ac}} = \Phi \rho_{ac} \Phi^*$. In particular, this yields that: ess-sup $_{\lambda\in\mathbb{R}} \|\rho_{ac}(\lambda)\|_{\mathcal{B}(\mathfrak{k}(\lambda)} = \|\rho_{ac}\|_{\mathcal{B}(\mathfrak{K}^{ac}(K_0))}$. In the following, we call $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ the density matrix of ρ_{ac}.

Similarly, one obtains that if Q is a charge, then there is a measurable family $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ of bounded self-adjoint operators, such that the multiplication operator:

$$\begin{aligned} (\mathcal{M}_{Q_{ac}} \widehat{f})(\lambda) &:= Q_{ac}(\lambda)\, \widehat{f}\,(\lambda), \\ \widehat{f} \in \operatorname{dom}(Q_{ac}) &:= \{f \in L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda)) : Q_{ac}(\lambda)\, \widehat{f}\,(\lambda) \in L^2(\mathbb{R}, d\lambda, \mathfrak{k}(\lambda))\}, \end{aligned}$$

is unitarily equivalent to Q_{ac}, i.e. $\mathcal{M}_{Q_{ac}} = \Phi Q_{ac} \Phi^*$. In particular, one has:

$$\text{ess-sup}_{\lambda\in\mathbb{R}} \|Q_{ac}(\lambda)\|_{\mathcal{B}(\mathfrak{k}(\lambda))} = \|Q_{ac}\|_{\mathcal{B}(\mathfrak{K}^{ac}(K_0))}. \tag{3.3}$$

If Q is a charge, then the family $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ is called the charge matrix of the ac-component of Q.

Let $\mathcal{S} = \{K, K_0\}$ be a trace scattering system. By $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$, we denote the scattering matrix, which corresponds to the scattering operator $S(K, K_0)$ with respect to the spectral representation $\Pi(K_0^{ac})$. The operator $T := S(K, K_0) - P^{ac}(K_0)$ is called the transmission operator.

By $\{T(\lambda)\}_{\lambda\in\mathbb{R}}$, we denote the transmission matrix which is related to the transmission operator. Scattering and transmission matrices are related by $S(\lambda) = T_{\mathfrak{k}(\lambda)} + T(\lambda)$ for a.e. $\lambda \in \mathbb{R}$. Notice that $T(\lambda)$ belongs for to the trace class a.e. $\lambda \in \mathbb{R}$.

Theorem 3.1 ([13, Corollary 2.14]). *Let $\mathcal{S} := \{K, K_0\}$ be a trace class scattering system and let $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ be the scattering matrix of $\mathcal{S}$ with respect to the spectral representation $\Pi(K_0^{ac})$. Furthermore, let ρ and Q be density and charge operators and let $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ be the density and charge matrices of the ac-components ρ_{ac} and charge Q_{ac} with respect to $\Pi(K_0^{ac})$, respectively. If $(I + K_0^2)\rho$ is bounded, then the current $J^{\mathcal{S}}_{\rho,Q}$ defined by* (3.2) *admits the representation:*

$$J^{\mathcal{S}}_{\rho,Q} = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}\Big(\rho_{ac}(\lambda)(Q_{ac}(\lambda) - S^*(\lambda)Q_{ac}(\lambda)S(\lambda))\Big)\mathrm{d}\lambda, \tag{3.4}$$

where the integrand on the right side and the current $J^{\mathcal{S}}_{\rho,Q}$ satisfy the estimate:

$$\begin{aligned}|\mathrm{tr}\,(\rho_{ac}(\lambda)(Q_{ac}(\lambda) - S^*(\lambda)Q_{ac}(\lambda)S(\lambda)))| \leqslant \\ 4\|\rho(\lambda)\|_{\mathfrak{L}(\mathfrak{k}(\lambda))}\|T(\lambda)\|_{\mathfrak{L}_1(\mathfrak{k}(\lambda))}\|Q(\lambda)\|_{\mathfrak{L}(\mathfrak{k}(\lambda))},\end{aligned} \tag{3.5}$$

for a.e. $\lambda \in \mathbb{R}$ and

$$|J^{\mathcal{S}}_{\rho,Q}| \leqslant C_0\|(H + i)^{-1} - (H_0 + i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}, \tag{3.6}$$

where $C_0 := \frac{2}{\pi}\|(1 + H_0^2)\rho\|_{\mathfrak{L}(\mathfrak{K})}$.

In applications, not every charge Q is a bounded operator. We say the self-adjoint operator Q commuting with K_0 is a p-tempered charge if $Q(H_0 - i)^{-p}$ is a bounded operator for $p \in \mathbb{N}_0$. As above, we can introduce $Q_{ac} := Q \restriction \mathrm{dom}(Q) \cap \mathfrak{K}^{ac}(K_0)$. It follows that $QE_{K_0}(\Delta)$ is a bounded operator for any bounded Borel set Δ. This yields that the corresponding charge matrix, $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$, is a measurable family of bounded self-adjoint operators such that:

$$\text{ess-sup}_{\,\lambda\in\mathbb{R}}(1 + \lambda^2)^{p/2}\|Q_{ac}(\lambda)\|_{\mathfrak{L}(\mathfrak{k}(\lambda))} < \infty.$$

To generalize the current $J^{\mathcal{S}}_{\rho,Q}$ to tempered charges Q, one uses the fact that $Q(\Delta) := QE_{K_0}(\Delta)$ is a charge for any bounded Borel set Δ. Hence, the current $J^{\mathcal{S}}_{\rho,Q(\Delta)}$ is well-defined by (3.2) for any bounded Borel set Δ. Using Theorem 3.1 one gets that for p-tempered charges, the limit

$$J^{\mathcal{S}}_{\rho,Q} := \lim_{\Delta\to\mathbb{R}} J^{\mathcal{S}}_{\rho,Q(\Delta)} \tag{3.7}$$

exists, provided $(H_0 - i)^{p+2}\rho$ is a bounded operator. This gives rise to the following corollary:

Corollary 3.2. *Let the assumptions of the Theorem 3.1 be satisfied. If for some $p \in \mathbb{N}_0$ the operator $(H_0 - i)^{p+2}\rho$ is bounded and Q is a p-tempered charge for K_0, then the current defined by* (3.7) *admits the representation* (3.4)*, where the right hand side of* (3.4) *satisfies the estimate* (3.5)*. Moreover, the current $J^{\mathcal{S}}_{\rho,Q}$ can be estimated in the following manner:*

$$|J^{\mathcal{S}}_{\rho,Q}| \leqslant C_p\|(H + i)^{-1} - (H_0 + i)^{-1}\|_{\mathfrak{L}_1(\mathfrak{K})}, \tag{3.8}$$

where $C_p := \frac{2}{\pi}\|(1 + H_0^2)^{p+2/2}\rho\|_{\mathfrak{L}(\mathfrak{K})}\|Q(I + H_0^2)^{-p/2}\|_{\mathfrak{L}(\mathfrak{K})}$.

At first glance, the formula (3.4) is not very similar to the original Landauer-Büttiker formula of [7, 18]. To make the formula more convenient, we recall that a standard application example for the Landauer-Büttiker formula is the so-called black-box model, cf. [1]. In this case, the Hilbert space $\mathfrak{K}$ is given by:

$$\mathfrak{K} = \mathfrak{K}_S \oplus \bigoplus_{j=1}^{N} \mathfrak{K}_j, \quad 2 \leqslant N < \infty. \tag{3.9}$$

and K_0 by:

$$K_0 = K_S \oplus \bigoplus_{j=1}^{N} K_j, \quad 2 \leqslant N < \infty. \tag{3.10}$$

The Hilbert space $\mathfrak{K}_S$ is called the sample or dot and K_S is the sample or dot Hamiltonian. The Hilbert spaces $\mathfrak{K}_j$ are called reservoirs or leads and K_j are the reservoir or lead Hamiltonians. For simplicity, we assume that the reservoir Hamiltonians K_j are absolutely continuous and the sample Hamiltonian K_S has a point spectrum. A typical choice for the density operator is:

$$\rho = f_S(K_S) \oplus \bigoplus_{j=1}^{N} f_j(K_j), \tag{3.11}$$

where $f_S(\cdot)$ and $f_j(\cdot)$ are non-negative bounded Borel functions, and for the charge:

$$Q = g_S(H_s) \oplus \bigoplus_{j=1}^{N} g_j(H_j), \tag{3.12}$$

where $g_S(\cdot)$ and $g_j(\cdot)$ a bounded Borel functions. Making this choice the Landauer-Büttiker formula (3.4) takes the form:

$$J^{\mathcal{S}}_{\rho,Q} = \frac{1}{2\pi} \sum_{j,k=1}^{N} \int_{\mathbb{R}} (f_j(\lambda) - f_k(\lambda)) g_j(\lambda) \sigma_{jk}(\lambda) d\lambda, \tag{3.13}$$

where

$$\sigma_{jk}(\lambda) := \mathrm{tr}(T_{jk}(\lambda)^* T_{jk}(\lambda)), \quad j,k = 1, \ldots, N, \quad \lambda \in \mathbb{R}, \tag{3.14}$$

are called the *total transmission probability* from reservoir k to reservoir j, cf. [1]. We call it the *cross-section* of the scattering process going from channel k to channel j at energy $\lambda \in \mathbb{R}$. $\{T_{jk}(\lambda)\}_{\lambda \in \mathbb{R}}$ is called the transmission matrix from channel k to channel j at energy $\lambda \in \mathbb{R}$ with respect to the spectral representation $\Pi(K_0^{ac})$. We note that $\{T_{jk}(\lambda)\}_{\lambda \in \mathbb{R}}$ corresponds to the transmission operator:

$$T_{jk} := P_j T(K, K_0) P_k, \quad T(K, K_0) := S(K, K_0) - P^{ac}(K_0), \tag{3.15}$$

acting from the reservoir k to reservoir j where $T(K, K_0)$ is called the transmission operator. Let $\{T(\lambda)\}_{\lambda \in \mathbb{R}}$ be the transmission matrix. Following [1], the current $J^{\mathcal{S}}_{\rho,Q}$ given by (3.13) is directed from the reservoirs into the sample.

The quantity $\|T(\lambda)\|_{\mathfrak{L}_2} = \mathrm{tr}(T(\lambda)^* T(\lambda))$ is well-defined and is called the cross-section of the scattering system $\mathcal{S}$ at energy $\lambda \in \mathbb{R}$. Notice that:

$$\sigma(\lambda) = \|T(\lambda)\|_{\mathfrak{L}_2} = \mathrm{tr}(T(\lambda)^* T(\lambda)) = \sum_{j,k=1}^{N} \sigma_{jk}(\lambda). \quad \lambda \in \mathbb{R},$$

We point out that the channel cross-sections $\sigma_{jk}(\lambda)$ admit the property:

$$\sum_{j=1}^{N} \sigma_{jk}(\lambda) = \sum_{j=1}^{N} \sigma_{kj}(\lambda), \quad \lambda \in \mathbb{R}, \tag{3.16}$$

which is a consequence of the unitarity of the scattering matrix. Moreover, if there is a conjugation J, such that $KJ = JK$ and $K_0 J = J K_0$ holds, that is, if the scattering system $\mathcal{S}$ is time reversible symmetric, then we have even more, namely, it holds that:

$$\sigma_{jk}(\lambda) = \sigma_{kj}(\lambda), \quad \lambda \in \mathbb{R}. \tag{3.17}$$

Usually, the Landauer-Büttiker formula (3.13) is used to calculated the electron current entering the reservoir j from the sample. In this case one has to choose $Q := Q_j^{el} := -\mathfrak{e} P_j$ where

P_j is the orthogonal projection form $\mathfrak{K}$ onto $\mathfrak{K}_j$ and $\mathfrak{e} > 0$ is the magnitude of the elementary charge. This is equivalent to choosing $g_j(\lambda) = -\mathfrak{e}$ and $g_k(\lambda) = 0$ for $k \neq j$, $\lambda \in \mathbb{R}$. In doing so, we get the Landauer-Büttiker formula simplifying to:

$$J^{\mathcal{S}}_{\rho,Q^{el}_j} = -\frac{\mathfrak{e}}{2\pi} \sum_{k=1}^{N} \int_{\mathbb{R}} (f_j(\lambda) - f_k(\lambda)) \sigma_{jk}(\lambda) d\lambda. \tag{3.18}$$

To restore the original Landauer-Büttiker formula, one sets:

$$f_j(\lambda) = f(\lambda - \mu_j), \quad \lambda \in \mathbb{R}, \tag{3.19}$$

where μ_j is the chemical potential of the reservoir $\mathfrak{K}_j$ and $f(\cdot)$ is a bounded non-negative Borel function called the distribution function. This gives rise to the following formula:

$$J^{\mathcal{S}}_{\rho,Q^{el}_j} = -\frac{\mathfrak{e}}{2\pi} \sum_{k=1}^{N} \int_{\mathbb{R}} (f(\lambda - \mu_j) - f(\lambda - \mu_k)) \sigma_{jk}(\lambda) d\lambda. \tag{3.20}$$

In particular, if we choose one:

$$f(\lambda) := f_{FD}(\lambda) := \frac{1}{1 + e^{\beta\lambda}}, \quad \beta > 0, \quad \lambda \in \mathbb{R}, \tag{3.21}$$

where $f_{FD}(\cdot)$ is the Fermi-Dirac distribution function, and inserting (3.21) into (3.20) we obtain:

$$J^{\mathcal{S}}_{\rho,Q^{el}_j} = -\frac{\mathfrak{e}}{2\pi} \sum_{k=1}^{N} \int_{\mathbb{R}} (f_{FD}(\lambda - \mu_j) - f_{FD}(\lambda - \mu_k)) \sigma_{jk}(\lambda) d\lambda. \tag{3.22}$$

If we have only two reservoirs, then they are usually denoted by l (left) and r (right). Let $j = l$ and $k = r$. Then,

$$J^{\mathcal{S}}_{\rho,Q^{el}_l} = -\frac{\mathfrak{e}}{2\pi} \int_{\mathbb{R}} (f_{FD}(\lambda - \mu_l) - f_{FD}(\lambda - \mu_r)) \sigma_{lr}(\lambda) d\lambda. \tag{3.23}$$

One easily checks that $J^{\mathcal{S}}_{\rho,Q_l} \leqslant 0$ if $\mu_l \geqslant \mu_r$. That means, the current is leaving the left reservoir and is entering the right one which is in accordance with physical expectations.

Example 3.3. Notice that $s_c := \{h^{el}, h^{el}_0\}$ is a $\mathfrak{L}_1$ scattering system. The Hamiltonian h^{el} takes into account the effect of coupling of reservoirs or leads $\mathfrak{h}_l := l^2(\mathbb{N})$ and $\mathfrak{h}_r := l^2(\mathbb{N})$ to the sample $\mathfrak{h}_S = \mathbb{C}^2$ which is also called the quantum dot. The Hamiltonians for the leads are given by: $h^{el}_\alpha = -\Delta^D + v_\alpha$, $\alpha = l, r$. The sample or quantum dot Hamiltonian is given by h^{el}_S. The wave operators are given by:

$$w_\pm(h^{el}, h^{el}_0) := s\text{-}\lim_{t\to\infty} e^{ith^{el}} e^{-ith^{el}_0} P^{ac}(h^{el}_0). \tag{3.24}$$

The scattering operator is given by $s_c := w_+(h^{el}, h^{el}_0)^* w_-(h^{el}, h^{el}_0)$. Let $\Pi(h^{el,ac}_0)$ be the spectral representation of $h^{el,ac}_0$ introduced in Section 2.6. If ρ^{el} and q^{el} are density and charge operators for h^{el}_0, then the Landauer-Büttiker formula takes the following form:

$$J^{s_c}_{\rho^{el},q^{el}} = \frac{1}{2\pi} \int_{\mathbb{R}} \operatorname{tr}\left(\rho^{el}_{ac}(\lambda)\left(q^{el}_{ac} - s_c(\lambda)^* q^{el}_{ac}(\lambda) s_c(\lambda)\right)\right), \tag{3.25}$$

where $\{s_c(\lambda)\}_{\lambda\in\mathbb{R}}$, $\{q^{el}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{\rho^{el}(\lambda)\}_{\lambda\in\mathbb{R}}$ are the scattering, charge and density matrices with respect to $\Pi(h^{el,ac}_0)$, respectively. The condition that $((h^{el}_0)^2 + I_{\mathfrak{h}^{el}})\rho^{el}$ is a bounded operator is superfluous because h^{el}_0 is a bounded operator. For the same reason we have that every p-tempered charge q^{el} is in fact a charge, that means, q^{el} is a bounded self-adjoint operator.

The scattering system s_c is a black-box model with reservoirs $\mathfrak{h}^{el}_l$ and $\mathfrak{h}^{el}_r$. Choosing

$$\rho^{el} = f_l(h^{el}) \oplus f_S(h^{el}_S) \oplus f_r(h^{el}_r),$$

where $f_\alpha(\cdot)$, $\alpha = l, r$, are bounded Borel functions, and

$$q^{el} = g_l(h_l^{el}) \oplus g_S(h_S^{el}) \oplus g_r(h_r^{el}),$$

where $g_\alpha(\cdot)$, $\alpha \in \{l, r\}$, are locally bounded Borel functions, then from (3.13) it follows that:

$$J^{s_c}_{\rho^{el},q^{el}} = \frac{1}{2\pi} \sum_{\substack{\alpha,\varkappa\in\{l,r\}\\ \alpha\neq\varkappa}} \int_{\mathbb{R}} (f_\alpha(\lambda) - f_\varkappa(\lambda)) g_\alpha(\lambda)\sigma_c(\lambda) d\lambda,$$

where $\{\sigma_c(\lambda)\}_{\lambda\in\mathbb{R}}$ is the channel cross-section from left to right and vice versa. Indeed, let $\{t_c(\lambda)\}_{\lambda\in\mathbb{R}}$ be the transition matrix which corresponds to the transition operator $t_c := s_c - I_{\mathfrak{h}^{el}}$. Clearly, one has $t_c(\lambda) = I_{\mathfrak{h}(\lambda)} - s_c(\lambda)$, $\lambda \in \mathbb{R}$. Let $\{p^{el}_\alpha(\lambda)\}_{\lambda\in\mathbb{R}}$ be the matrix which corresponds to the orthogonal projection p^{el}_α from $\mathfrak{h}^{el}$ onto $\mathfrak{h}^{el}_\alpha$. Further, let $t^c_{rl}(\lambda) := p^{el}_r(\lambda) t_c(\lambda) p^{el}_l$ and $t^c_{lr} := p^{el}_l(\lambda) t_c(\lambda) p^{el}_r$. Notice that both quantities are in fact scalar functions. Accordingly, the channel cross-sections $\sigma^c_{lr}(\lambda)$ and $\sigma^c_{rl}(\lambda)$ at energy $\lambda \in \mathbb{R}$ are given by $\sigma_c(\lambda) := \sigma^c_{lr}(\lambda) = |t^c_{lr}(\lambda)|^2 = |t^c_{rl}(\lambda)|^2 = \sigma^c_{rl}(\lambda)$, $\lambda \in \mathbb{R}$.

In particular, if $g_l(\lambda) = 1$ and $g_r = 0$, then:

$$J^{s_c}_{\rho^{el},q^{el}_l} = \frac{1}{2\pi} \int_{\mathbb{R}} (f_l(\lambda) - f_r(\lambda)) \sigma_c(\lambda) d\lambda, \tag{3.26}$$

and $q^{el}_l := p^{el}_l$. Following [1], $J^{s_c}_{\rho^{el},q^{el}_l}$ denotes the current entering the quantum dot from the left lead.

3.2. Application to the JCL-model

Let $\mathcal{S} = \{H, H_0\}$ now be the JCL-model. Furthermore, let ρ and Q be the density operator and a charge for H_0, respectively. Under these assumptions, the current $J^{\mathcal{S}}_{\rho,Q}$ is defined by:

$$J^{\mathcal{S}}_{\rho,Q} := -i\mathrm{tr}\left(W_-(H, H_0)(I + H_0^2)\rho W_-(H, H_0)^* \frac{1}{H - i}[H, Q]\frac{1}{H + i}\right), \tag{3.27}$$

and admits representation (3.4). If Q is a p-tempered charge and $(H_0 - i)^{p+2}\rho$ is a bounded operator, then the current $J^{\mathcal{S}}_{\rho,Q}$ is defined in accordance with (3.7) and the Landauer-Büttiker formula (3.4) is also valid.

We introduce the intermediate scattering system $\mathcal{S}_c := \{H, H_c\}$, where:

$$H_c := h^{el} \otimes I_{\mathfrak{h}^{ph}} + I_{\mathfrak{h}^{el}} \otimes h^{ph} = H_0 + V_{el}.$$

The Hamiltonian H_c describes the coupling of the leads to the quantum dot, but under the assumption that the photon interaction is not switched on.

Accordingly, $\mathcal{S}_{ph} := \{H, H_c\}$ and $\mathcal{S}_c := \{H_c, H_0\}$ are $\mathfrak{L}_1$-scattering systems. The corresponding scattering operators are denoted by S_{ph} and S_c, respectively. Let $\Pi(H^{ac}_c) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}_c(\lambda)), \mathcal{M}, \Phi_c\}$ of H^{ac}_c be a spectral representation of H_c. The scattering matrix of the scattering system $\{H, H_c\}$ with respect to $\Pi(H^{ac}_c)$ is denoted by $\{S_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$. The scattering matrix of the scattering system $\{H_c, H_0\}$ with respect to $\Pi(H^{ac}_0) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}_0(\lambda)), \mathcal{M}, \Phi_0\}$ is denoted by $\{S_c(\lambda)\}_{\lambda\in\mathbb{R}}$.

Since $\mathcal{S}_c$ is a $\mathfrak{L}_1$-scattering system, the wave operators $W_\pm(H_c, H_0)$ exist and are complete and since $\Phi_c W_\pm(H_c, H_0)\Phi_0^*$ commutes with $\mathcal{M}$, there are measurable families $\{W_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$ of isometries acting from $\mathfrak{h}_0(\lambda)$ onto $\mathfrak{h}_c(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ such that:

$$(\Phi_c W_\pm(H_c, H_0)\Phi_0^* \widehat{f}\,)(\lambda) = W_\pm(\lambda)\, \widehat{f}\,(\lambda), \quad \lambda \in \mathbb{R}, \quad \widehat{f} \in L^2(\mathbb{R}, d\lambda, \mathfrak{h}_0(\lambda)).$$

The families $\{W_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$ are called wave matrices.

Straightforward computation shows that $\widehat{S}_{ph} := W_+(H_c, H_0)^* S_{ph} W_+(H_c, H_0)$ commutes with H_0. Hence, with respect to the spectral representation $\Pi(H^{ac}_0)$, the operator $\widehat{S}_{ph}$ is unitarily

equivalent to a multiplication induced by a measurable family $\{\widehat{S}_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators in $\mathfrak{h}_0(\lambda)$. Straightforward computation shows that:

$$\widehat{S}_{ph}(\lambda) = W_+(\lambda)^* S_{ph}(\lambda) W_+(\lambda), \tag{3.28}$$

for a.e. $\lambda \in \mathbb{R}$. Roughly speaking, $\{\widehat{S}_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ is the scattering matrix of S_{ph} with respect to the spectral representation $\Pi(H_0^{ac})$.

Furthermore, let

$$\rho^c := W_-(H_c, H_0)\rho W_-(H_c, H_0)^* \tag{3.29}$$

and

$$Q^c := W_+(H_c, H_0) Q W_+(H_c, H_0)^*. \tag{3.30}$$

The operators ρ^c and Q^c are the density and tempered charge operators for the scattering system $\mathcal{S}_{ph}$. Indeed, one easily verifies that ρ^c and Q^c are commute with H_c. Moreover, ρ^c is non-negative. Furthermore, if Q is a charge, then Q^c is also a charge. This gives rise to the introduction of currents $J^c_{\rho,Q} := J^{\mathcal{S}_c}_{\rho,Q}$,

$$J^c_{\rho,Q} := -i\mathrm{tr}\left(W_-(H_c, H_0)\rho W_-(H_c, H_0)^* \frac{1}{H_c - i}[H_c, Q]\frac{1}{H_c + i}\right), \tag{3.31}$$

and $J^{ph}_{\rho,Q} := J^{\mathcal{S}_{ph}}_{\rho^c,Q^c}$,

$$J^{ph}_{\rho,Q} := -i\mathrm{tr}\left(W_-(H, H_c)\rho^c W_-(H, H_c)^* \frac{1}{H - i}[H, Q^c]\frac{1}{H + i}\right), \tag{3.32}$$

which are well defined. If Q is p-tempered charge and $(H_0 - i)^{p+2}\rho$ is a bounded operator, then one easily checks that Q^c is a p-tempered charge and $(H_c - i)^{p+2}\rho^c$ is a bounded operator. Hence the definition of the currents $J^{\mathcal{S}_c}_{\rho^c,Q^c}$ can be extended to this case and the Landauer-Büttiker formula (3.4) holds.

Finally, we note that the corresponding matrices $\{\rho^c_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{Q^c_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ are related to the matrices $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ by

$$\rho^c_{ac}(\lambda) = W_-(\lambda)\rho_{ac}(\lambda)W_-(\lambda)^* \quad \text{and} \quad Q^c_{ac}(\lambda) = W_+(\lambda)Q_{ac}(\lambda)W_+(\lambda)^* \tag{3.33}$$

for a.e. $\lambda \in \mathbb{R}$.

Proposition 3.4 (Current decomposition)**.** *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Furthermore, let ρ and Q be the density operator and a p-tempered charge, $p \in \mathbb{N}_0$, for H_0, respectively. If $(H_0 - i)^{p+2}\rho$ is a bounded operator, then the decomposition,*

$$J^{\mathcal{S}}_{\rho,Q} = J^c_{\rho,Q} + J^{ph}_{\rho,Q}, \tag{3.34}$$

holds where $J^c_{\rho,Q}$ and $J^{ph}_{\rho,Q}$ are given by (3.31) *and* (3.32)*.*

In particular, let $\{S_c(\lambda)\}_{\lambda\in\mathbb{R}}$, $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ be scattering, density and charge matrices of S_c, ρ and Q with respect to $\Pi(H_0^{ac})$ and let $\{S_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$, $\{\rho^c_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\{Q^c_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ be the scattering, density and charge matrices of the scattering operator S_{ph}, density operator ρ^c, cf. (3.29)*, and charge operator Q^c, cf.* (3.30)*, with respect to the spectral representation $\Pi(H_c^{ac}\}$. Then, the following representations:*

$$J^c_{\rho,Q} := \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}(\rho_{ac}(\lambda)(Q_{ac}(\lambda) - S_c(\lambda)^* Q_{ac}(\lambda) S_c(\lambda))d\lambda, \tag{3.35}$$

$$J^{ph}_{\rho,Q} := \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}(\rho^c_{ac}(\lambda)(Q^c_{ac}(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda)))d\lambda, \tag{3.36}$$

take place.

Proof. Since $\mathcal{S}_c$ and $\mathcal{S}_{ph}$ are $\mathfrak{L}_1$-scattering systems from Theorem 3.1 the representations (3.35) and (3.36) are easily follow. Taking into account (3.33), we get the following:

$$\begin{aligned}&\mathrm{tr}(\rho^c_{ac}(\lambda)(Q^c_{ac}(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda))) = \\ &\quad \mathrm{tr}(W_-(\lambda)\rho_{ac} W_-(\lambda)^*(W_+(\lambda)Q_{ac}(\lambda)W_+(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda))).\end{aligned}$$

Using $S_c(\lambda) = W_+(\lambda)^* W_-(\lambda)$ we find that:

$$\begin{aligned}&\mathrm{tr}(\rho^c_{ac}(\lambda)(Q^c_{ac}(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda))) = \mathrm{tr}\,(\rho_{ac}(\lambda)\times \\ &(S_c(\lambda)^* Q_{ac}(\lambda) S_c(\lambda) - W_-(\lambda)^* S_{ph}(\lambda)^* W_+(\lambda) Q_{ac}(\lambda) W_+(\lambda)^* S_{ph}(\lambda) W_-(\lambda)))\,.\end{aligned} \tag{3.37}$$

Since $\{H_c, H_0\}$ and $\{H, H_c\}$ are $\mathfrak{L}_1$-scattering systems, the existence of the wave operators $W_\pm(H, H_c)$ and $W_\pm(H_c, H_0)$ follows. Using the chain rule, we find $W_\pm(H, H_0) = W_\pm(H, H_c)W_\pm(H_c, H_0)$ which yields:

$$\begin{aligned}S &= W_+(H, H_0)^* W_+(H, H_0) \\ &= W_+(H_c, H_0)^* W_+(H, H_c) W_-(H, H_c) W_-(H_c, H_0) = W_+(H_c, H_0)^* S_{ph} W_-(H_c, H_0).\end{aligned}$$

Hence, the scattering matrix $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ of $\{H, H_0\}$ admits the representation

$$S(\lambda) = W_+(\lambda)^* S_{ph}(\lambda) W_-(\lambda), \quad \lambda \in \mathbb{R}. \tag{3.38}$$

Inserting (3.38) into (3.37), we get the following:

$$J^{ph}_{\rho,Q} = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}(\rho_{ac}(\lambda)(S_c(\lambda)^* Q_{ac}(\lambda) S_c(\lambda) - S(\lambda)^* Q_{ac}(\lambda) S(\lambda)))d\lambda \tag{3.39}$$

Using (3.39), we obtain the following:

$$J^c_{\rho,Q} + J^{ph}_{\rho,Q} = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}(\rho_{ac}(\lambda)(Q_{ac}(\lambda) - S(\lambda)^* Q_{ac}(\lambda) S(\lambda)))d\lambda.$$

Finally, taking into account (3.4), we obtain (3.34). □

Remark 3.5.
(i) The current $J^c_{\rho,Q}$ is due to the coupling of the leads to the quantum dot and it is therefore called the *contact induced current*.
(ii) The current $J^{ph}_{\rho,Q}$ is due to the interaction of photons with electrons and it is called the *photon induced current*. Notice the this current is calculated under the assumption that the leads are already in contact with the dot.

Corollary 3.6. *Let the assumptions of Proposition 3.4 be satisfied. With respect to the spectral representation $\Pi(H^{ac}_0)$ of H^{ac}_0 the photon induced current $J^{ph}_{\rho,Q}$ can be represented by:*

$$J^{ph}_{\rho,Q} := \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}(\,\widehat{\rho}_{ac}(\lambda)\,(Q_{ac}(\lambda) - \,\widehat{S}_{ph}(\lambda)^*\,Q_{ac}(\lambda)\,\widehat{S}_{ph}\,(\lambda)))d\lambda, \tag{3.40}$$

where the measurable families $\{\,\widehat{S}_{ph}(\lambda)\,\}_{\lambda\in\mathbb{R}}$ and $\{\,\widehat{\rho}_{ac}(\lambda)\,\}_{\lambda\in\mathbb{R}}$ are given by (3.28) *and*

$$\widehat{\rho}_{ac}(\lambda) := S_c(\lambda)\rho_{ac}(\lambda)S_c(\lambda)^* \quad \lambda \in \mathbb{R}, \tag{3.41}$$

respectively.

Proof. Using (3.33) and $S_c(\lambda) = W_+(\lambda)^* W_-(\lambda)$, we find:

$$\begin{aligned}&\mathrm{tr}(\rho^c_{ac}(\lambda)(Q^c_{ac}(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda))) = \\ &\quad \mathrm{tr}\,(S_c(\lambda)\rho_{ac}(\lambda)S_c(\lambda)^*\,(Q_{ac}(\lambda) - W_+(\lambda)^* S_{ph}(\lambda)^* W_+(\lambda) Q_{ac}(\lambda) W_+(\lambda)^* S_{ph}(\lambda) W_+(\lambda)))\,.\end{aligned}$$

Taking into account the representations (3.28) and (3.41), we get the following:

$$\begin{aligned}&\mathrm{tr}(\rho^c_{ac}(\lambda)(Q^c_{ac}(\lambda) - S_{ph}(\lambda)^* Q^c_{ac}(\lambda) S_{ph}(\lambda))) = \\ &\quad \mathrm{tr}(S_c(\lambda)\rho_{ac}(\lambda)S_c(\lambda)^*(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^*\, Q_{ac}(\lambda)\, \widehat{S}_{ph}(\lambda))),\end{aligned}$$

which immediately yields (3.40). □

Remark 3.7. In the following, we call $\{\,\widehat{\rho}_{ac}(\lambda)\,\}_{\lambda\in\mathbb{R}}$, cf. (3.41), the photon modified electron density matrix. Notice that $\{\,\widehat{\rho}_{ac}(\lambda)\,\}_{\lambda\in\mathbb{R}}$ might be non-diagonal, even if the electron density matrix $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ is diagonal.

4. Analysis of currents

In the following, we analyze currents $J^c_{\rho,Q}$ and $J^{ph}_{\rho,Q}$ under the assumption that ρ and Q have the tensor product structure:

$$\rho = \rho^{el}\otimes\rho^{ph} \quad \text{and} \quad Q = q^{el}\otimes q^{ph}, \tag{4.1}$$

where ρ^{el} and ρ^{ph} as well as q^{el} and q^{ph} are density operators and (tempered) charges for h^{el}_0 and h^{ph}, respectively. Since ρ^{ph} commutes with h^{ph}, which is discrete, the operator ρ^{ph}has the form:

$$\rho^{ph} = \sum_{n\in\mathbb{N}_0} \rho^{ph}(n)(\cdot,\Upsilon_n)\Upsilon_n, \tag{4.2}$$

where $\rho^{ph}(n)$ are non-negative numbers. Similarly, q^{ph} can be represented as:

$$q^{ph} = \sum_{n\in\mathbb{N}_0} q^{ph}(n)(\cdot,\Upsilon_n)\Upsilon_n, \tag{4.3}$$

where $q^{ph}(n)$ are real numbers.

Lemma 4.1. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Assume that $\rho \neq 0$ and Q have the structure* (4.1) *where ρ^{el} is a density operator and q^{el} is a charge for h^{el}_0.*

(i) *The operator $(H_0 - i)^{p+2}\rho$, $p\in\mathbb{N}_0$, is bounded if and only if the condition:*

$$\sup_{n\in\mathbb{N}_0} \rho^{ph}(n) n^{p+2} < \infty, \tag{4.4}$$

is satisfied.

(ii) *The charge Q is p-tempered if and only if:*

$$\sup_{n\in\mathbb{N}} |q^{ph}(n)| n^{-p} < \infty, \tag{4.5}$$

is valid

Proof. (i) The operator $(H_0 - i)^{p+2}\rho$ admits the representation:

$$(H_0 - i)^{p+2}\rho = \bigoplus_{p\in\mathbb{N}_0} \rho^{ph}(n)(h^{el}_0 + n\omega - i)^{p+2}\rho^{el}.$$

We have:

$$\begin{aligned}\|(H_0 - i)^{p+2}\rho\|_{\mathfrak{L}(\mathfrak{H})} &= \sup_{p\in\mathbb{N}_0} \rho^{ph}(n)\|(h^{el}_0 + n\omega - i)^{p+2}\rho^{el}\|_{\mathfrak{L}(\mathfrak{h}^{el})} \\ &= \sup_{p\in\mathbb{N}_0} \rho^{ph}(n) n^{p+2} n^{-(p+2)} \left\|(h^{el}_0 + n\omega - i)^{p+2}\rho^{el}\right\|_{\mathfrak{L}(\mathfrak{h}^{el})}.\end{aligned} \tag{4.6}$$

Since $\lim_{n\to\infty} n^{-(p+2)} \left\|(h^{el}_0 + n\omega - i)^{p+2}\rho^{el}\right\|_{\mathfrak{L}(\mathfrak{h}^{el})} = \omega^{p+2}\|\rho^{el}\|_{\mathfrak{L}(\mathfrak{h}^{el})}$, we obtain for sufficiently large $n\in\mathbb{N}_0$ that:

$$\frac{\omega^{p+2}}{2}\|\rho^{el}\|_{\mathfrak{L}(\mathfrak{h}^{el})} \leqslant n^{-(p+2)}\|(h^{el}_0 + n\omega - i)^{p+2}\rho^{el}\|_{\mathfrak{L}(\mathfrak{h}^{el})}.$$

Using that and (4.6), we immediately obtain (4.4). Conversely, from (4.6) and (4.4), we obtain that $(H_0 - i)^{p+2}\rho$ is a bounded operator.

(ii) As above, we have:

$$Q(H_0 - i)^{-p} = \bigoplus_{n\in\mathbb{N}_0} q^{ph}(n)q^{el}.$$

Hence:

$$\|Q(H_0 - i)^{-p}\|_{\mathfrak{L}(\mathfrak{H})} = \sup_{n\in\mathbb{N}_0} |q^{ph}(n)| \|q^{el}(h_0^{el} + n\omega - i)^{-p}\|_{\mathfrak{L}(\mathfrak{h}^{el})}.$$

Since $\lim_{n\to\infty} n^p \|(h_0^{el} + n\omega - i)^{-p}\|_{\mathfrak{L}(\mathfrak{h}^{el})} = \omega^{-p}\|q^{el}\|_{\mathfrak{L}(\mathfrak{h}^{el})}$, we similarly obtain, as above, that (4.5) holds. The converse is obvious. □

4.1. Contact induced current

Let us recall that $\mathcal{S}_c = \{H_c, H_0\}$ is a $\mathfrak{L}_1$-scattering system. Straightforward computation shows that:

$$W_\pm(H_c, H_0) = w_\pm(h^{el}, h_0^{el}) \otimes I_{\mathfrak{h}^{ph}},$$

where $w_\pm(h^{el}, h_0^{el})$ is given by (3.24). Hence:

$$S_c = s_c \otimes I_{\mathfrak{h}^{ph}}, \quad \text{where} \quad s_c := w_+(h_c^{el}, h_0^{el})^* w_-(h_c^{el}, h_0^{el}).$$

Proposition 4.2. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Assume that ρ and Q are given by* (4.1) *where ρ^{el} and q^{el} are density and charge operators for h_0^{el} and ρ^{ph} and q^{ph} for h^{ph}, respectively. If for some $p \in \mathbb{N}_0$ the conditions* (4.4) *and* (4.5) *are satisfied, then the current $J^c_{\rho,Q}$ is well defined and admits the representation:*

$$J^c_{\rho,Q} = \gamma J^{s_c}_{\rho^{el},q^{el}}, \qquad \gamma := \sum_{n\in\mathbb{N}_0} q^{ph}(n)\rho^{ph}(n), \tag{4.7}$$

where $J^{s_c}_{\rho^{el},q^{el}}$ is defined by (3.2). *In particular, if $\mathrm{tr}(\rho^{ph}) = 1$ and $q^{ph} = I_{\mathfrak{h}^{ph}}$, then $J^c_{\rho,Q} = J^{s_c}_{\rho^{el},q^{el}}$.*

Proof. First, we note that by lemma 4.1 the operator $(H_0 - i)^{p+2}\rho$ is bounded and Q is p-tempered. Hence, the current $J^{\mathcal{S}_c}_{\rho,Q}$ is correctly defined and the Landauer-Büttiker formula (3.4) is valid.

With respect to the spectral representation $\Pi(H_0^{ac})$ of Lemma 2.12, the charge matrix $\{Q_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ of $Q_{ac} = q_{ac}^{el} \otimes q^{ph}$ admits the representation:

$$Q_{ac}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} q_{ac}^{el}(\lambda - n\omega)q^{ph}(n), \quad \lambda \in \mathbb{R}. \tag{4.8}$$

Since $S_c = s_c \otimes I_{\mathfrak{h}^{ph}}$, the scattering matrix $\{S_c(\lambda)\}_{\lambda\in\mathbb{R}}$ admits the representation:

$$S_c(\lambda) = \bigoplus_{n\in\mathbb{N}_0} s_c(\lambda - n\omega), \quad \lambda \in \mathbb{R}.$$

Hence:

$$\begin{aligned} &Q_{ac}(\lambda) - S_c(\lambda)^* Q_{ac}(\lambda) S_c(\lambda) = \\ &\quad \bigoplus_{n\in\mathbb{N}_0} q^{ph}(n) \left(q_{ac}^{el}(\lambda - n\omega) - s_c(\lambda - n\omega)^* q_{ac}^{el}(\lambda - \omega n) s_c(\lambda - n\omega) \right). \end{aligned} \tag{4.9}$$

Moreover, the density matrix $\{\rho_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ admits the representation:

$$\rho_{ac}(\lambda) = \bigoplus_{n\in\mathbb{N}_0} \rho^{ph}(n)\rho_{ac}^{el}(\lambda - n\omega) \tag{4.10}$$

Inserting (4.10) into (4.9) we find the following:

$$\rho^{ac}(\lambda)\left(Q_{ac}(\lambda)-S_c(\lambda)^*Q_{ac}(\lambda)S_c(\lambda)\right)= \bigoplus_{n\in\mathbb{N}_0} q^{ph}(n)\rho^{ph}(n)\rho^{el}_{ac}(\lambda-n\omega)\left(q^{el}_{ac}(\lambda-\omega n)-s_c(\lambda-n\omega)^*q^{el}_{ac}(\lambda-\omega n)s_c(\lambda-n\omega)\right)$$

Since $\gamma=\sum_{n\in\mathbb{N}_0} q^{ph}(n)\rho^{ph}(n)$ is absolutely convergent by (4.4) and (4.5), we obtain that:

$$\mathrm{tr}\left(\rho^{ac}(\lambda)\left(Q_{ac}(\lambda)-S_c(\lambda)^*Q_{ac}(\lambda)S_c(\lambda)\right)\right)= \sum_{n\in\mathbb{N}_0} q^{ph}(n)\rho^{ph}(n)\mathrm{tr}\left(\rho^{el}_{ac}(\lambda-n\omega)\left(q^{el}_{ac}(\lambda-\omega n)-s_c(\lambda-n\omega)^*q^{el}_{ac}(\lambda-\omega n)s_c(\lambda-n\omega)\right)\right) \tag{4.11}$$

Clearly, we have:

$$\left|\mathrm{tr}\left(\rho^{el}_{ac}(\lambda-n\omega)\left(q^{el}_{ac}(\lambda-\omega n)-s_c(\lambda-n\omega)^*q^{el}_{ac}(\lambda-\omega n)s_c(\lambda-n\omega)\right)\right)\right|\leqslant 4\|\rho^{el}_{ac}(\lambda-n\omega)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))}\|q^{el}_{ac}(\lambda-n\omega)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))},\quad \lambda\in\mathbb{R}.$$

We insert (4.11) into the Landauer-Büttiker formula (3.35). Using (4.4) and (4.5) as well as

$$\int_{\mathbb{R}}\|\rho^{el}_{ac}(\lambda)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))}\|q^{el}_{ac}(\lambda)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))}d\lambda<\infty,$$

we see that we can interchange the integral and the sum. By doing so, we get:

$$J^c_{\rho,Q}=\sum_{n\in\mathbb{N}_0} q^{ph}(n)\rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\rho^{el}_{ac}(\lambda-n\omega)\times \left(q^{el}_{ac}(\lambda-\omega n)-s_c(\lambda-n\omega)^*q^{el}_{ac}(\lambda-\omega n)s_c(\lambda-n\omega)\right)\right)d\lambda.$$

Using (3.25) we prove (4.7).

If $\mathrm{tr}(\rho^{ph})=1$, then $\sum_{\mathbb{N}_0}\rho^{ph}(n)=1$. Furthermore, if $\rho^{ph}=I_{\mathfrak{h}^{ph}}$, then $q^{ph}(n)=1$. Hence, $\gamma=1$. □

4.2. Photon induced current

To calculate the current $J^{ph}_{\rho,Q}$, we use representation (3.40). We then set:

$$\widehat{S}^{ph}_{mn}(\lambda):=P_m(\lambda)\,\widehat{S}_{ph}(\lambda)\upharpoonright\mathfrak{h}_n(\lambda),\quad \lambda\in\mathbb{R},$$

where $\{\widehat{S}_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ is defined by (3.28) and $P_m(\lambda)$ is the orthogonal projection from $\mathfrak{h}(\lambda)$, cf. (2.37), onto $\mathfrak{h}_m(\lambda):=\mathfrak{h}^{el}(\lambda-m\omega)$, $\lambda\in\mathbb{R}$.

Proposition 4.3. *Let $\mathcal{S}=\{H,H_0\}$ be the JCL-model. Assume that ρ and Q are given by* (4.1) *where ρ^{el} and q^{el} are density and charge operators for h^{el}_0 and ρ^{ph} and q^{ph} for h^{ph}, respectively. If for some $p\in\mathbb{N}_0$ the conditions* (4.4) *and* (4.5) *are satisfied, then the current $J^{ph}_{\rho,Q}$ is well-defined and it admits the following representation:*

$$J^{ph}_{\rho,Q}=\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)\sum_{n\in\mathbb{N}_0}q^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}d\lambda\,\mathrm{tr}\left(\widehat{\rho}^{el}_{ac}(\lambda-m\omega)\times \left(q^{el}_{ac}(\lambda-n\omega)\delta_{mn}-\widehat{S}^{ph}_{nm}(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)\right)\right), \tag{4.12}$$

where $\{\widehat{\rho}^{el}_{ac}(\lambda)\}_{\lambda\in\mathbb{R}}$ is the photon modified electron density defined, cf. (3.41)*, which takes the following form:*

$$\widehat{\rho}^{el}_{ac}(\lambda)=s_c(\lambda)\rho^{el}(\lambda)s_c(\lambda)^*,\quad \lambda\in\mathbb{R}. \tag{4.13}$$

Proof. By Lemma 4.1 we get that that the charge Q is p-tempered and $(H_0 - i)^p \rho$ is a bounded operator. By Corollary 3.2, the current $J^{ph}_{\rho,Q} := J^{S_{ph}}_{\rho^c,Q^c}$ is well-defined.

Since $\left(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right)$ is a trace class operator for $\lambda \in \mathbb{R}$, we get from (3.40) and (4.10) that:

$$\mathrm{tr}\left(\widehat{\rho}_{ac}(\lambda) \left(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right)\right) = \sum_{m\in\mathbb{N}_0} \rho^{ph}(m) \mathrm{tr}\left(\widehat{\rho}^{el}(\lambda - m\omega) P_m(\lambda) \left(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right) P_m(\lambda)\right)$$

Furthermore, we have:

$$\begin{aligned} P_m(\lambda) \left(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right) P_m(\lambda) \\ = q^{ph}(m) \left(q^{el}(\lambda - m\omega) - P_m(\lambda) \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right) P_m(\lambda) \\ = q^{ph}(m) q^{el}(\lambda - m\omega) - \sum_{n\in\mathbb{N}_0} q^{ph}(n) \widehat{S}^{ph}_{nm}(\lambda)^* q^{el}(\lambda - n\omega) \widehat{S}^{ph}_{nm}(\lambda), \end{aligned}$$

for $\lambda \in \mathbb{R}$ where $\widehat{S}^{ph}_{nm}(\lambda)^* := P_n(\lambda) \widehat{S}_{ph}(\lambda) P_m(\lambda)$, $\lambda \in \mathbb{R}$. Notice that $\sum_{n\in\mathbb{N}_0}$ is a sum with a finite number of summands. Hence:

$$\mathrm{tr}\left(\widehat{\rho}_{ac}(\lambda) \left(Q_{ac}(\lambda) - \widehat{S}_{ph}(\lambda)^* Q_{ac}(\lambda) \widehat{S}_{ph}(\lambda)\right)\right) = \sum_{m\in\mathbb{N}_0} \rho^{ph}(m) \sum_{n\in\mathbb{N}_0} q^{ph}(n) \times \mathrm{tr}\left(\widehat{\rho}^{el}(\lambda - m\omega) \left(q^{el}(\lambda - m\omega)\delta_{mn} - \widehat{S}^{ph}_{nm}(\lambda)^* q^{el}(\lambda - n\omega) \widehat{S}^{ph}_{nm}(\lambda)\right)\right)$$

We are going to show that

$$\sum_{m\in\mathbb{N}_0} \rho^{ph}(m) \sum_{n\in\mathbb{N}_0} |q^{ph}(n)| \int_{\mathbb{R}} \left|\mathrm{tr}\left(\widehat{\rho}^{el}(\lambda - m\omega) \times \left(q^{el}(\lambda - m\omega)\delta_{mn} - \widehat{S}^{ph}_{nm}(\lambda)^* q^{el}(\lambda - n\omega) \widehat{S}^{ph}_{nm}(\lambda)\right)\right)\right| d\lambda < \infty.$$

Clearly, one has the following estimate:

$$\left|\mathrm{tr}\left(\widehat{\rho}^{el}(\lambda - m\omega) \left(q^{el}(\lambda - m\omega)\delta_{mn} - \widehat{S}^{ph}_{nm}(\lambda)^* q^{el}(\lambda - n\omega) \widehat{S}^{ph}_{nm}(\lambda)\right)\right)\right| \leqslant 2 \| \widehat{\rho}^{el}(\lambda - m\omega) \|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} \left(\|q^{el}(\lambda - m\omega)\|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))}\delta_{nm} + \|q^{el}(\lambda - n\omega)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))}\right).$$

Furthermore, we get:

$$\int_{\lambda\in\mathbb{R}} \| \widehat{\rho}^{el}(\lambda - m\omega) \|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} \|q^{el}(\lambda - m\omega)\|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))}\delta_{nm} \leqslant \int_{\lambda\in\mathbb{R}} \| \widehat{\rho}^{el}(\lambda) \|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} \|q^{el}(\lambda)\|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} d\lambda$$

and

$$\int_{\mathbb{R}} \| \widehat{\rho}^{el}(\lambda - m\omega) \|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} \|q^{el}(\lambda - n\omega)\|_{\mathfrak{L}(\mathfrak{h}_n(\lambda))} d\lambda \leqslant \|q^{el}_{ac}\|_{\mathfrak{L}(\mathfrak{h}^{el})} \int_{\lambda\in\mathbb{R}} \| \widehat{\rho}^{el}(\lambda - (m-n)\omega) \|_{\mathfrak{L}(\mathfrak{h}_{m-n}(\lambda))} d\lambda$$

If the conditions (4.4) and (4.5) are satisfied, then

$$\sum_{m\in\mathbb{N}_0} \rho^{ph}(m) |q^{ph}(m)| \int_{\mathbb{R}} \| \widehat{\rho}^{el}(\lambda) \|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} \|q^{el}(\lambda)\|_{\mathfrak{L}(\mathfrak{h}_m(\lambda))} d\lambda < \infty.$$

Furthermore, we obtain:

$$\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)\sum_{n\in\mathbb{N}_0}|q^{ph}(n)|\int_{\lambda\in\mathbb{R}}\|\,\widehat{\rho}^{el}(\lambda-(m-n)\omega)\,\|_{\mathfrak{L}(\mathfrak{h}_{m-n}(\lambda))}d\lambda\leqslant$$
$$(v_{\max}-v_{\min}+4)\|\rho^{el}_{ac}\|_{\mathfrak{L}(\mathfrak{h}^{el})}\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)\sum_{|m-n|\leqslant d_{\max}}|q^{ph}(n)|<\infty,$$

where $d_{\max}$ is introduced by Lemma 2.12. To prove the following:

$$\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)\sum_{|m-n|\leqslant d_{\max}}|q^{ph}(n)|<\infty,$$

we again use (4.4) and (4.5). The last step allows us to interchange the integral and the sums, which immediately proves (4.12). □

Corollary 4.4. *Let $\mathcal{S}=\{H,H_0\}$ be the JCL-model. We assume that ρ and Q are given by* (4.1)*, where ρ^{el} and q^{el} are density and charge operators for h^{el}_0 and ρ^{ph} and q^{ph} for h^{ph}, respectively. If ρ^{el} is an equilibrium state, i.e. $\rho^{el}=f^{el}(h^{el}_0)$, then:*

$$J^{ph}_{\rho,Q}=\sum_{m,n\in\mathbb{N}_0}q^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}\Big(\rho^{ph}(n)f^{el}(\lambda-n\omega)-\rho^{ph}(m)f^{el}(\lambda-m\omega)\Big)\times$$
$$\mathrm{tr}\Big(\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big)\,d\lambda. \tag{4.14}$$

Proof. From (4.12), we obtain the following:

$$J^{ph}_{\rho,Q}=\sum_{n\in\mathbb{N}_0}q^{ph}(n)\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}d\lambda\;f^{el}(\lambda-m\omega)\times$$
$$\mathrm{tr}\Big(q^{el}_{ac}(\lambda-n\omega)\delta_{mn}-\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big).$$

Hence,

$$J^{ph}_{\rho,Q}=\sum_{n\in\mathbb{N}_0}q^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}d\lambda\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)f^{el}(\lambda-m\omega)\times$$
$$\mathrm{tr}\Big(q^{el}_{ac}(\lambda-n\omega)\delta_{mn}-\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big).$$

This gives the following:

$$J^{ph}_{\rho,Q}=\sum_{n\in\mathbb{N}_0}q^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}d\lambda\,\Big(\rho^{ph}(n)f^{el}(\lambda-n\omega)\mathrm{tr}\Big(q^{el}_{ac}(\lambda-n\omega)\Big)- \tag{4.15}$$
$$\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)f^{el}(\lambda-m\omega)\mathrm{tr}\Big(\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big)\Big).$$

Since

$$\sum_{m\in\mathbb{N}_0}\rho^{ph}(m)f^{el}(\lambda-m\omega)\mathrm{tr}\Big(\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big)=$$
$$\sum_{m\in\mathbb{N}_0}\Big(\rho^{ph}(m)f^{el}(\lambda-m\omega)-\rho^{ph}(n)f^{el}(\lambda-n\omega)\Big)\,\mathrm{tr}\Big(\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big)+$$
$$\rho^{ph}(n)f^{el}(\lambda-n\omega)\sum_{m\in\mathbb{N}_0}\mathrm{tr}\Big(\,\widehat{S}^{ph}_{nm}\,(\lambda)^*q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}\,(\lambda)\Big),$$

then inserting this into (4.15) we obtain (4.14). □

5. Electron and photon currents

5.1. Electron current

To calculate the electron current induced by contacts and photon contact, we make the following choice throughout this section. We set

$$Q^{el}_\alpha := q^{el}_\alpha \otimes q^{ph}, \quad q^{el}_\alpha := -\mathfrak{e}p^{el}_\alpha \quad \text{and} \quad q^{ph} := I_{\mathfrak{h}^{ph}}, \quad \alpha \in \{l, r\}, \tag{5.1}$$

where p^{el}_α denotes the orthogonal projection from $\mathfrak{h}^{el}$ onto $\mathfrak{h}^{el}_\alpha$. By $\mathfrak{e} > 0$, we denote the magnitude of the elementary charge. Since p^{el}_α commutes with h^{el}_α, one can easily verify that Q^{el}_α commutes with H_0, which shows that Q^{el}_α is a charge. Following [1], the flux related to Q^{el}_α gives us the electron current $J^{\mathcal{S}}_{\rho,Q^{el}_\alpha}$ entering the lead α from the sample. Notice $Q^{el}_\alpha = -\mathfrak{e}P_\alpha$ where P_α is the orthogonal projection from $\mathfrak{H}$ onto $\mathfrak{H}_\alpha := \mathfrak{h}^{el}_\alpha \otimes \mathfrak{h}^{ph}$. Since $q^{ph} = I_{\mathfrak{h}^{ph}}$, condition (4.5) is immediately satisfied for any $p \geqslant 0$.

Let $f(\cdot) : \mathbb{R} \longrightarrow \mathbb{R}$ be a non-negative bounded measurable function. We set:

$$\rho^{el} = \rho^{el}_l \oplus \rho^{el}_S \oplus \rho^{el}_r, \quad \rho^{el}_\alpha := f(h^{el}_\alpha - \mu_\alpha), \quad \alpha \in \{l, r\}, \tag{5.2}$$

and $\rho = \rho^{el} \otimes \rho^{ph}$. By μ_α the chemical potential of the lead α is denoted. In applications, one sets $f(\lambda) := f_{FD}(\lambda)$, $\lambda \in \mathbb{R}$, where $f_{FD}(\lambda)$ is the so-called Fermi-Dirac distribution given by (3.21). If $\beta = \infty$, then $f_{FD}(\lambda) := \chi_{\mathbb{R}_-}(\lambda)$, $\lambda \in \mathbb{R}$. Notice that $[\rho^{el}, p^{el}] = 0$. For ρ^{ph}, we choose the Gibbs state:

$$\rho^{ph} := \frac{1}{Z} e^{-\beta h^{ph}}, \quad Z = \mathrm{tr}(e^{-\beta h^{ph}}) = \frac{1}{1 - e^{-\beta\omega}}. \tag{5.3}$$

Hence, $\rho^{ph} = (1 - e^{-\beta\omega})e^{-\beta h^{ph}}$. If $\beta = \infty$, then $\rho^{ph} := (\cdot, \Upsilon_0)\Upsilon_0$. Clearly, $\mathrm{tr}(\rho^{ph}) = 1$. We note that $\rho^{ph}(n) = (1 - e^{-\beta\omega})e^{-n\beta\omega}$, $n \in \mathbb{N}_0$, satisfies the condition (4.4) for any $p \geqslant 0$. Accordingly, $\rho_0 = \rho^{el} \otimes \rho^{ph}$ is the density operator for H_0.

Definition 5.1. Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. If $Q := Q^{el}_\alpha$, where Q^{el}_α is given by (5.1), and $\rho := \rho_0 := \rho^{el} \otimes \rho^{ph}$, where ρ^{el} and ρ^{ph} are given by (5.2) and (5.3), then $J^{el}_{\rho_0,Q^{el}_\alpha} := J^{\mathcal{S}}_{\rho_0,Q^{el}_\alpha}$ is called the electron current entering the lead α. The currents $J^{c}_{\rho_0,Q^{el}_\alpha}$ and $J^{ph}_{\rho_0,Q^{el}_\alpha}$ are called the contact-induced and photon-induced electron currents.

5.1.1. Contact induced electron current. The following proposition immediately follows from Proposition 4.2.

Proposition 5.2. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Then the contact induced electron current $J^{c}_{\rho_0,Q^{el}_\alpha}$, $\alpha \in \{l, r\}$, is given by $J^{c}_{\rho_0,Q^{el}_\alpha} = J^{s_c}_{\rho^{el},q^{el}_\alpha}$. In particular, one has:*

$$J^{c}_{\rho_0,Q^{el}_\alpha} = -\frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}} (f(\lambda - \mu_\alpha) - f(\lambda - \mu_\varkappa)\sigma_c(\lambda)d\lambda, \quad \alpha, \varkappa \in \{l, r\}, \quad \alpha \neq \varkappa, \tag{5.4}$$

where $\{\sigma_c(\lambda)\}_{\lambda\in\mathbb{R}}$ is the channel cross-section from left to the right of the scattering system $s_c = \{h^{el}, h^{el}_0\}$, cf. Example 3.3.

Proof. Since $\mathrm{tr}(\rho^{ph}) = 1$ it follows from Proposition 4.2 that $J^{c}_{\rho_0,Q^{el}_\alpha} = J^{s_c}_{\rho^{el},q^{el}_\alpha}$. From (3.26), cf. Example 3.3, we find (5.4). □

If $\mu_l > \mu_r$ and $f(\cdot)$ is decreasing, then $J^{c}_{\rho_0,Q^{el}_l} < 0$. Hence, the electron contact current is going from the left lead to the right which is in accordance with the physical expectations. In particular, this is valid for the Fermi-Dirac distribution.

Proposition 5.3. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Further, let ρ^{el} and ρ^{ph} be given by* (5.2) *and* (5.3)*, respectively. If the charge Q^{el}_α is given by* (5.1)*, then the following holds:*

(E) If $\mu_l = \mu_r$, then $J^c_{\rho_0,Q^{el}_\alpha} = 0$, $\alpha \in \{l, r\}$.
(S) If $v_l \geqslant v_r + 4$, then $J^c_{\rho_0,Q^{el}_\alpha} = 0$, $\alpha \in \{l, r\}$, even if $\mu_l \neq \mu_l$.
(C) If $e^S_0 = \delta^S_0$ and $e^S_1 = \delta^S_1$, then $J^c_{\rho_0,Q^{el}_\alpha} = 0$, $\alpha \in \{l, r\}$, even if $\mu_l \neq \mu_l$.

Proof. (E) If $\mu_l = \mu_r$, then $f(\lambda - \mu_l) = f(\lambda - \mu_r)$. Applying formula (5.4) we obtain $J^c_{\rho_0,Q^{el}_\alpha} = 0$.

(S) If $v_l \geqslant v_r + 4$, then $h^{el,ac}_0$ has simple spectrum. Hence the scattering matrix $\{s_c(\lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $s_c = \{h^{el}, h^{el}_0\}$ is a scalar function which immediately yields $\sigma_c(\lambda) = 0$, $\lambda \in \mathbb{R}$, which yields $J^c_{\rho_0,Q^{el}_\alpha} = 0$.

(C) In this case, the Hamiltonian h^{el} decomposes into the direct sum of two non-interacting Hamiltonians. Hence, the scattering matrix of $\{s_c(\lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $s_c = \{h^{el}, h^{el}_0\}$ is diagonal, which immediately yields $J^c_{\rho_0,Q^{el}_\alpha} = 0$. □

5.1.2. Photon induced electron current. It is hopeless to analyze the properties of (4.12) if we make no assumptions concerning ρ^{el} and the scattering operator s_c. The simplest assumptions is that ρ^{el} and s_c commute. In this case, we get $\widehat{\rho}^{el}(\lambda) = \rho^{el}(\lambda)$, $\lambda \in \mathbb{R}$.

Lemma 5.4. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Furthermore, let ρ^{el} be given by* (5.2)*. If one of the cases (E), (S) or (C) of Proposition 5.3 is realized, then the ρ^{el} and s_c commute.*

Proof. If (E) holds, then $\rho^{el} = f(h^{el}_0)$ which yields $[\rho^{el}, s_c] = 0$. If (S) is valid, then the scattering matrix $\{s_c(\lambda)\}_{\lambda\in\mathbb{R}}$ is a scalar function which shows $[\rho^{el}, s_c] = 0$. Finally, if (C) is realized, then the scattering matrix $\{s_c(\lambda)\}_{\lambda\in\mathbb{R}}$ diagonal. Since the ρ^{el} is given by (5.2) we get $[\rho^{el}, s_c] = 0$. □

We will now calculate the current $J^{ph}_{\rho_0,Q^{el}_\alpha}$, see (4.12). Clearly, we have $P_\alpha(\lambda) = \sum_{n\in\mathbb{N}_0} p^{el}_\alpha(\lambda - n\omega)$ and $I_{\mathfrak{h}(\lambda)} = P_l(\lambda) + P_r(\lambda)$, $\lambda \in \mathbb{R}$. We then set:

$$P_{n_\alpha}(\lambda) := P_\alpha(\lambda)P_n(\lambda) = P_n(\lambda)P_\alpha(\lambda) = p^{el}_\alpha(\lambda - n\omega),\ \alpha \in \{l, r\},$$

$n \in \mathbb{N}_0$, $\lambda \in \mathbb{R}$. In the following we use the notation $\widehat{T}_{ph}(\lambda) = \widehat{S}_{ph}(\lambda) - I_{\mathfrak{h}(\lambda)}$, $\lambda \in \mathbb{R}$, where $\{\widehat{T}_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ is called the transition matrix and $\{\widehat{S}_{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ is given by (3.28). We set:

$$\widehat{T}^{ph}_{k_\alpha m_\varkappa}(\lambda) := P_{k_\alpha}(\lambda)\,\widehat{T}_{ph}(\lambda)P_{m_\varkappa}(\lambda), \quad \lambda \in \mathbb{R}, \quad \alpha, \varkappa \in \{l, r\}, \quad k, m \in \mathbb{N}_0,$$

and:

$$\widehat{\sigma}^{ph}_{k_\alpha m_\varkappa}(\lambda) = \mathrm{tr}(\,\widehat{T}^{ph}_{k_\alpha m_\varkappa}(\lambda)^*\ \widehat{T}^{ph}_{k_\alpha m_\varkappa}(\lambda)\,), \quad \lambda \in \mathbb{R}, \tag{5.5}$$

which is the cross-section between the channels k_α and $m_\varkappa$.

Proposition 5.5. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model.*
(i) *If ρ^{el} commutes with the scattering operator s_c and q^{el}, then:*

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{\substack{m,n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}} \frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}} \Big(\rho^{ph}(n)f(\lambda - \mu_\alpha - n\omega) - \rho^{ph}(m)f(\lambda - \mu_\varkappa - m\omega)\Big)\ \widehat{\sigma}^{ph}_{n_\alpha m_\varkappa}(\lambda)\,d\lambda. \tag{5.6}$$

(ii) *If in addition $\mathcal{S} = \{H, H_0\}$ is time reversible symmetric, then*

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{m,n\in\mathbb{N}_0} \frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}} \Big(\rho^{ph}(n)f(\lambda - \mu_\alpha - n\omega) - \rho^{ph}(m)f(\lambda - \mu_{\alpha'} - m\omega)\Big)\ \widehat{\sigma}^{ph}_{n_\alpha m_{\alpha'}}(\lambda)\,d\lambda, \tag{5.7}$$

$\alpha, \alpha' \in \{l, r\}$, $\alpha \neq \alpha'$.

Proof. (i) Let us assume that:

$$q^{el} = \sum_{\varkappa\in\{l,r\}} g_\varkappa(h^{el}_\varkappa),$$

Notice that

$$q^{el}_{ac}(\lambda) = \sum_{\varkappa\in\{l,r\}} g_\varkappa(\lambda)p^{el}_\varkappa(\lambda), \quad \lambda\in\mathbb{R}. \tag{5.8}$$

Inserting (5.8) into (4.12) and using $q^{ph} = I_{\mathfrak{h}^{ph}}$, we obtain the following:

$$J^{ph}_{\rho_0,Q} = \sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(m) \sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}} \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\alpha(\lambda-m\omega)g_\varkappa(\lambda-n\omega)\times$$
$$\mathrm{tr}\left(p^{el}_\alpha(\lambda-m\omega)\left(p^{el}_\varkappa(\lambda-n\omega)\delta_{mn} - \widehat{S}^{ph}_{nm}(\lambda)^* p^{el}_\varkappa(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)\right)\right),$$

where, for simplicity, we have set:

$$\phi_\alpha(\lambda) := f(\lambda-\mu_\alpha), \quad \lambda\in\mathbb{R}, \quad n\in\mathbb{N}_0, \quad \alpha\in\{l,r\}. \tag{5.9}$$

Accordingly, we get:

$$J^{ph}_{\rho_0,Q} = \sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}} \rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\varkappa(\lambda-n\omega)g_\varkappa(\lambda-n\omega)\mathrm{tr}\left(p^{el}_\varkappa(\lambda-n\omega)\right) -$$
$$\sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}}\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\alpha(\lambda-m\omega)g_\varkappa(\lambda-n\omega)\times \tag{5.10}$$
$$\mathrm{tr}\left(p^{el}_\alpha(\lambda-m\omega)\,\widehat{S}^{ph}_{nm}(\lambda)^* p^{el}_\varkappa(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)p^{el}_\alpha(\lambda-m\omega)\right).$$

Since the scattering matrix $\{\,\widehat{S}^{ph}(\lambda)\}_{\lambda\in\mathbb{R}}$ is unitary, we have:

$$p^{el}_\varkappa(\lambda-n\omega) = \sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} p^{el}_\varkappa(\lambda-n\omega)\,\widehat{S}^{ph}_{mn}(\lambda)^* p^{el}_\alpha(\lambda-m\omega)\,\widehat{S}^{ph}_{mn}(\lambda)p^{el}_\varkappa(\lambda-n\omega), \tag{5.11}$$

for $n\in\mathbb{N}_0$ and $\varkappa\in\{l,r\}$. Inserting (5.11) into (5.10), we find that:

$$J^{ph}_{\rho_0,Q} = \sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}}\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\varkappa(\lambda-n\omega)g_\varkappa(\lambda-n\omega)\times$$
$$\mathrm{tr}\left(p^{el}_\varkappa(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)^* p^{el}_\alpha(\lambda-m\omega)\,\widehat{S}^{ph}_{mn}(\lambda)p^{el}_\varkappa(\lambda-n\omega)\right) -$$
$$\sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}}\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\alpha(\lambda-m\omega)g_\varkappa(\lambda-n\omega)\times$$
$$\mathrm{tr}\left(p^{el}_\alpha(\lambda-m\omega)\,\widehat{S}^{ph}_{nm}(\lambda)^* p^{el}_\varkappa(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)p^{el}_\alpha(\lambda-m\omega)\right).$$

Using the notation (5.5), we find the following:

$$J^{ph}_{\rho_0,Q} = \sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}}\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\varkappa(\lambda-n\omega)g_\varkappa(\lambda-n\omega)\,\widehat{\sigma}^{ph}_{m_\alpha n_\varkappa}(\lambda) -$$
$$\sum_{\substack{n\in\mathbb{N}_0\\ \varkappa\in\{l,r\}}}\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\ \phi_\alpha(\lambda-m\omega)g_\varkappa(\lambda-n\omega)\,\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)\,.$$

By (3.16), we find that:

$$\sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \widehat{\sigma}^{ph}_{m_\alpha n_\varkappa}(\lambda) \;=\; \sum_{\substack{m\in\mathbb{N}_0\\ \alpha\in\{l,r\}}} \widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda) \quad \lambda\in\mathbb{R}.$$

Using that, we obtain the following:

$$J^{ph}_{\rho_0,Q} = \sum_{\substack{m,n\in\mathbb{N}_0\\ \alpha,\varkappa\in\{l,r\}}} \frac{1}{2\pi}\int_{\mathbb{R}} \times \tag{5.12}$$

$$\Big(\rho^{ph}(n)\phi_\varkappa(\lambda-n\omega)-\rho^{ph}(m)\phi_\alpha(\lambda-m\omega)\Big)\, g_\varkappa(\lambda-n\omega)\,\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)\,d\lambda.$$

Setting $g_\alpha(\lambda)=-\mathfrak{e}$ and $g_\varkappa(\lambda)\equiv 0$, $\varkappa\neq\alpha$, we obtain (5.6).

(ii) Straightforward computation shows that:

$$\sum_{n,m\in\mathbb{N}_0}\int_{\mathbb{R}}\Big(\rho^{ph}(n)f(\lambda-\mu_a-n\omega)-\rho^{ph}(m)f(\lambda-\mu_a-m\omega)\Big)\,\widehat{\sigma}^{ph}_{n_\alpha m_\alpha}(\lambda)\,d\lambda =$$

$$\sum_{n,m\in\mathbb{N}_0}\int_{\mathbb{R}}\Big(\rho^{ph}(m)f(\lambda-\mu_a-m\omega)-\rho^{ph}(n)f(\lambda-\mu_a-n\omega)\Big)\,\widehat{\sigma}^{ph}_{m_\alpha n_\alpha}(\lambda)\,d\lambda.$$

Since $\sigma^{ph}_{m_\alpha n_\alpha}(\lambda)=\sigma^{ph}_{n_\alpha m_\alpha}(\lambda)$, $\lambda\in\mathbb{R}$, we obtain the following:

$$\sum_{n,m\in\mathbb{N}_0}\int_{\mathbb{R}}\Big(\rho^{ph}(n)f(\lambda-\mu_a-n\omega)-\rho^{ph}(m)f(\lambda-\mu_a-m\omega)\Big)\,\widehat{\sigma}^{ph}_{n_\alpha m_\alpha}(\lambda)\,d\lambda =$$

$$-\sum_{n,m\in\mathbb{N}_0}\int_{\mathbb{R}}\Big(\rho^{ph}(n)f(\lambda-\mu_a-n\omega)-\rho^{ph}(m)f(\lambda-\mu_a-m\omega)\Big)\,\widehat{\sigma}^{ph}_{n_\alpha m_\alpha}(\lambda)\,d\lambda$$

which yields:

$$\sum_{n,m\in\mathbb{N}_0}\int_{\mathbb{R}}\Big(\rho^{ph}(n)f(\lambda-\mu_a-n\omega)-\rho^{ph}(m)f(\lambda-\mu_a-m\omega)\Big)\,\widehat{\sigma}^{ph}_{n_\alpha m_\alpha}(\lambda)\,d\lambda=0.$$

Using that, we immediately obtain the representation (5.7) from (5.6). □

Corollary 5.6. *Let $\mathcal{S}=\{H,H_0\}$ be the JCL-model.*
(i) *If the cases cases (E), (S) or (C) of Proposition 5.3 are realized, then the representation* (5.6) *holds.*
(ii) *If the case (E) of Proposition 5.3 is realized and the system $\mathcal{S}=\{H,H_0\}$ is time reversible symmetric, then*

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{m,n\in\mathbb{N}_0}\frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}}(\rho^{ph}(n)f(\lambda-\mu-n\omega)-\rho^{ph}(m)f(\lambda-\mu-m\omega))\,\widehat{\sigma}^{ph}_{n_\alpha m_{\alpha'}}(\lambda)d\lambda \tag{5.13}$$

$n\in\mathbb{N}_0$, $\alpha\in\{l,r\}$ where $\mu:=\mu_l=\mu_r$ and $\alpha\neq\alpha'$.
(iii) *If the case (E) of Proposition 5.3 is realized and the system $\mathcal{S}=\{H,H_0\}$ is time reversible and mirror symmetric, then $J^{ph}_{\rho_0,Q^{el}_\alpha}=0$.*

Proof. (i) The statement follows from Proposition 5.5(i) and Lemma 5.4.

(ii) Setting $\mu_\alpha=\mu_{\alpha'}$ formula (5.13) follows (5.7).

(iii) If $\mathcal{S}=\{H,H_0\}$ is time reversible and mirror symmetric, we obtain from Lemma 2.14 (ii) that $\widehat{\sigma}^{ph}_{n_\alpha m_{\alpha'}}(\lambda)=\widehat{\sigma}^{ph}_{n_{\alpha'} m_\alpha}(\lambda)$, $\lambda\in\mathbb{R}$, $n,m\in\mathbb{N}_0$, $\alpha,\alpha'\in\{l,r\}$, $\alpha\neq\alpha'$. Using that, we obtain from (5.13) the following:

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{m,n\in\mathbb{N}_0}\frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}}(\rho^{ph}(n)f(\lambda-\mu-n\omega)-\rho^{ph}(m)f(\lambda-\mu-m\omega))\,\widehat{\sigma}^{ph}_{n_{\alpha'} m_\alpha}(\lambda)d\lambda.$$

Interchanging m and n, we obtain:

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{m,n\in\mathbb{N}_0} \frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}} (\rho^{ph}(m)f(\lambda-\mu-m\omega) - \rho^{ph}(n)f(\lambda-\mu-n\omega))\,\widehat{\sigma}^{ph}_{m_{\alpha'}n_\alpha}(\lambda)d\lambda.$$

Using that $\mathcal{S}$ is time reversible symmetric we get from Lemma 2.14 (i) that:

$$J^{ph}_{\rho_0,Q^{el}_\alpha} = -\sum_{m,n\in\mathbb{N}_0} \frac{\mathfrak{e}}{2\pi}\int_{\mathbb{R}} (\rho^{ph}(m)f(\lambda-\mu-m\omega) - \rho^{ph}(n)f(\lambda-\mu-n\omega))\,\widehat{\sigma}^{ph}_{n_\alpha m_{\alpha'}}(\lambda)d\lambda.$$

which shows that $J^{ph}_{\rho_0,Q^{el}_\alpha} = -J^{ph}_{\rho_0,Q^{el}_\alpha}$. Hence $J^{ph}_{\rho_0,Q^{el}_\alpha} = 0$. □

We note that by Proposition 5.3, the contact induced current is zero, i.e. $J^{c}_{\rho_0,Q^{el}_\alpha} = 0$. Hence, if the $\mathcal{S}$ is time reversible and mirror symmetric, then the total current is zero, i.e. $J^{\mathcal{S}}_{\rho_0,Q^{el}_\alpha} = 0$.

Remark 5.7. Let the case (E) of Proposition 5.3 be realized, that is, $\mu_l = \mu_r$. Moreover, we assume for simplicity that $0 =: v_r \leqslant v := v_l$.

(i) If $\beta = \infty$, then $\rho^{ph}(n) = \delta_{0n}$, $n \in \mathbb{N}_0$. From (5.6), we immediately obtain that $J^{ph}_{\rho^{el},Q^{el}_\alpha} = 0$. That means, if the temperature is zero, then the photon-induced electron current is zero.

(ii) The photon-induced electron current might be zero even if $\beta < \infty$. Indeed, let $\mathcal{S} = \{H, H_0\}$ be time reversible symmetric and let the case (E) be realized. If $\omega \geqslant v+4$ and $\mathfrak{h}^{el}(\lambda) := \mathfrak{h}^{el}_n(\lambda) = \mathfrak{h}^{el}(\lambda - n\omega)$, $n \in \mathbb{N}_0$. Hence, one always has $n = m$ in formula (5.13), which immediately yields $J^{ph}_{\rho_0,Q^{el}_\alpha} = 0$.

(iii) The photon-induced electron current might be different than zero. Indeed, let $\mathcal{S} = \{H, H_0\}$ be time reversible symmetric and let $v = 2$ and $\omega = 4$, then one sees that to calculate the $J^{ph}_{\rho_0,Q^{el}_l}$, one has to consider $m = n+1$ in formula (5.13). Therefore, we find that:

$$J^{ph}_{\rho_0,Q^{el}_l} = -\sum_{n\in\mathbb{N}_0} \frac{\mathfrak{e}}{2\pi}\times$$

$$\int_{\mathbb{R}} d\lambda \left(\rho^{ph}(n)f(\lambda-\mu-n\omega) - \rho^{ph}(n+1)f(\lambda-\mu-(n+1)\omega)\right)\widehat{\sigma}^{ph}_{n_l\,(n+1)_r}(\lambda).$$

If ρ^{ph} is given by (5.3) and $f(\lambda) = f_{FD}(\lambda)$, cf. (3.21), then one easily verifies that

$$\frac{\partial}{\partial x}\rho^{ph}(x)f_{FD}(\lambda-\mu-x\omega) < 0, \quad x,\mu,\lambda \in \mathbb{R}.$$

Hence, $\rho^{ph}(n)f_{FD}(\lambda-\mu-n\omega)$ is decreasing in $n \in \mathbb{N}_0$ for $\lambda,\mu \in \mathbb{R}$ which yields $\left(\rho^{ph}(n)f(\lambda-\mu-n\omega) - \rho^{ph}(n+1)f(\lambda-\mu-(n+1)\omega)\right) \geqslant 0$. Therefore, $J^{ph}_{\rho_0,Q^{el}_l} \leqslant 0$ which means that the photon-induced current leaves the left-hand side and enters the right-hand side. In fact, $J^{ph}_{\rho_0,Q^{el}_l} = 0$ implies that $\widehat{\sigma}^{ph}_{n_l\,(n+1)_r}(\lambda) = 0$ for $n \in \mathbb{N}_0$ and $\lambda \in \mathbb{R}$, which means that there is no scattering from the left-hand side to the right one and vice versa which can be excluded generically.

5.2. Photon current

The photon current is related to the charge by equation:

$$Q := Q^{ph} = -I_{\mathfrak{h}^{el}} \otimes \mathfrak{n},$$

where $\mathfrak{n} = \mathrm{d}\Gamma(1) = b^*b$ is the photon number operator on $\mathfrak{h}^{ph} = \mathfrak{F}_+(\mathbb{C})$, which is self-adjoint and commutes with h^{ph}. It follows that Q^{ph} is also self-adjoint and commutes with H_0. It is not bounded, but since $\mathrm{dom}(\mathfrak{n}) = \mathrm{dom}(h^{ph})$, it is immediately obvious that $Q^{ph}(H_0+\theta)^{-1}$ is bounded,

when $\mathfrak{N}$ is a tempered charge. Its charge matrix with respect to the spectral representation $\Pi(H_0^{ac})$ of Lemma 2.12 is given by:

$$Q_{ac}^{ph}(\lambda) = -\bigoplus_{n\in\mathbb{N}_0} nP_n(\lambda).$$

We recall that $P_n(\lambda)$ is the orthogonal projection from $\mathfrak{h}(\lambda)$ onto $\mathfrak{h}_n(\lambda) = \mathfrak{h}^{el}(\lambda - n\omega)$, $\lambda \in \mathbb{R}$. We will now calculate the photon current or, as it is also known, the photon production rate.

5.2.1. Contact induced photon current. The following proposition is, in fact, in accordance with the physical intuition.

Proposition 5.8. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model. Then $J^c_{\rho_0,Q^{ph}} = 0$.*

Proof. We note that $q^{el}_{ac}(\lambda) = I_{\mathfrak{h}^{el}(\lambda)}$, $\lambda \in \mathbb{R}$. Inserting this into (3.25), we obtain $J^{s_c}_{\rho^{el},q^{el}} = 0$. Applying Proposition 4.2 we prove $J^c_{\rho_0,Q^{ph}} = 0$. □

The result reflects the fact that the lead contact does not contribute to the photon current, which is plausible from the physical point of view.

5.2.2. Photon current. From Proposition 5.8, we see that only the photon-induced photon current $J^{ph}_{\rho_0,Q^{ph}}$ contributes to the photon current $J^{\mathcal{S}}_{\rho_0,Q^{ph}}$. Since $J^{\mathcal{S}}_{\rho_0,Q^{ph}} = J^{ph}_{\rho_0,Q^{ph}}$, we call $J^{ph}_{\rho_0,Q^{ph}}$ simply the *photon current*.

Using the notation $\widehat{T}^{ph}_{nm}(\lambda) := P_n(\lambda)\,\widehat{T}_{ph}(\lambda) \restriction \mathfrak{h}^{el}(\lambda - m\omega)$, $\lambda \in \mathbb{R}$, $m, n \in \mathbb{N}_0$. We set:

$$\widetilde{T}^{ph}_{nm}(\lambda) = \widehat{T}^{ph}_{nm}(\lambda) s_c(\lambda - m\omega), \quad \lambda \in \mathbb{R}, \quad m, n \in \mathbb{N}_0, \tag{5.14}$$

and

$$\widetilde{T}^{ph}_{n_\varkappa m_\alpha}(\lambda) := P_{n_\varkappa}(\lambda)\widetilde{T}^{ph}_{nm}(\lambda) \restriction \mathfrak{h}^{el}_\alpha(\lambda - m\omega), \quad \lambda \in \mathbb{R}, \tag{5.15}$$

$m, n \in \mathbb{N}_0$, $\alpha, \varkappa \in \{l, r\}$, as well as $\widetilde{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda) := \mathrm{tr}(\widetilde{T}^{ph}_{n_\varkappa m_\alpha}(\lambda)^* \widetilde{T}^{ph}_{n_\varkappa m_\alpha}(\lambda))$, $\lambda \in \mathbb{R}$.

Proposition 5.9. *Let $\mathcal{S} = \{H, H_0\}$ be the JCL-model.*
(i) *Then:*

$$J^{ph}_{\rho_0,Q^{ph}} = \sum_{\substack{m,n\in\mathbb{N}_0 \\ \alpha,\varkappa\in\{l,r\}}} (n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} f(\lambda - \mu_\alpha - m\omega)\widetilde{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)d\lambda. \tag{5.16}$$

(ii) *If ρ^{el} commutes with s_c, then:*

$$J^{ph}_{\rho_0,Q^{ph}} = \sum_{\substack{m,n\in\mathbb{N}_0 \\ \alpha,\varkappa\in\{l,r\}}} (n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} f(\lambda - \mu_\alpha - m\omega)\,\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)d\lambda. \tag{5.17}$$

(iii) *If ρ^{el} commutes with s_c and $\mathcal{S} = \{H, H_0\}$ is time reversible symmetric, then:*

$$J^{ph}_{\rho_0,Q^{ph}} = \sum_{\substack{m,n\in\mathbb{N}_0, n>m \\ \varkappa,\alpha\in\{l,r\}}} \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda \times \tag{5.18}$$

$$(n-m)\left(\rho^{ph}(m)f(\lambda - \mu_\alpha - m\omega) - \rho^{ph}(n)f(\lambda - \mu_\varkappa - n\omega)\right)\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda),$$

where $\alpha' \in \{l, r\}$ and $\alpha' \neq \alpha$.

Proof. (i) From (4.12) we get

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{m,n\in\mathbb{N}_0} n\rho^{ph}(m)\times$$
$$\frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\,\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\left(P_n(\lambda)\delta_{mn} - \widehat{S}^{ph}_{nm}(\lambda)^* q^{el}_{ac}(\lambda-n\omega)\,\widehat{S}^{ph}_{nm}(\lambda)\right)\right).$$

Hence:

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{m\in\mathbb{N}_0} m\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\left(P_m(\lambda) - \widehat{S}^{ph}_{mm}(\lambda)^* P_m(\lambda)\,\widehat{S}^{ph}_{mm}(\lambda)\right)\right)d\lambda +$$
$$\sum_{\substack{m,n\in\mathbb{N}_0\\ m\neq n}} n\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\widehat{S}^{ph}_{nm}(\lambda)^* P_n(\lambda)\,\widehat{S}^{ph}_{nm}(\lambda)\right)d\lambda.$$

Using the relation $P_m(\lambda) = I_{\mathfrak{h}(\lambda)} - \sum_{n\in\mathbb{N}_0, m\neq n} P_n(\lambda)$, $\lambda\in\mathbb{R}$, we obtain the following:

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{\substack{m,n\in\mathbb{N}_0\\ m\neq n}} m\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\left(\widehat{S}^{ph}_{nm}(\lambda)^* P_n(\lambda)\,\widehat{S}^{ph}_{nm}(\lambda)\right)\right)d\lambda +$$
$$\sum_{\substack{m,n\in\mathbb{N}_0\\ m\neq n}} n\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\widehat{S}^{ph}_{nm}(\lambda)^* P_n(\lambda)\,\widehat{S}^{ph}_{nm}(\lambda)\right)d\lambda.$$

Since $\widehat{T}_{ph}(\lambda) = \widehat{S}_{ph}(\lambda) - I_{\mathfrak{h}(\lambda)}$, $\lambda\in\mathbb{R}$, we find

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{m,n\in\mathbb{N}_0}(m-n)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\widehat{\rho}^{\,el}_{ac}(\lambda-m\omega)\,\widehat{T}^{ph}_{nm}(\lambda)^*\,\widehat{T}^{ph}_{nm}(\lambda)\right)d\lambda.$$

Using (4.13) and definition (5.14) one readily sees that:

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{m,n\in\mathbb{N}_0}(m-n)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\rho^{el}_{ac}(\lambda-m\omega)\widetilde{T}^{ph}_{nm}(\lambda)^*\widetilde{T}^{ph}_{nm}(\lambda)\right)d\lambda\,.$$

Since $\rho^{el}_{ac} = \rho^{el}_l \oplus \rho^{el}_r$ where ρ^{el}_α is given by (5.2), we find the following:

$$J^{ph}_{\rho_0,Q^{ph}} = -\sum_{\substack{m,n\in\mathbb{N}_0\\ \alpha,\varkappa\in\{l,r\}}}(m-n)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} f(\lambda-\mu_\alpha-m\omega)\mathrm{tr}\left(\widetilde{T}^{ph}_{n\varkappa m_\alpha}(\lambda)^*\widetilde{T}^{ph}_{n\varkappa m_\alpha}(\lambda)\right)d\lambda,$$

where we have used (5.15). Using $\widetilde{\sigma}^{ph}_{n\varkappa m_\alpha}(\lambda) = \mathrm{tr}(\widetilde{T}^{ph}_{n\varkappa m_\alpha}(\lambda)^*\widetilde{T}^{ph}_{n\varkappa m_\alpha}(\lambda))$, we prove (5.16).

(ii) If ρ^{el}_{ac} commutes with s_c, then $\widehat{\rho}^{\,el}_{ac}(\lambda) = \rho^{el}_{ac}(\lambda)$, $\lambda\in\mathbb{R}$, which yields that one can replace $\widetilde{\sigma}^{ph}_{n\varkappa m_\alpha}(\lambda)$ by $\widehat{\sigma}^{ph}_{n\varkappa m_\alpha}(\lambda)$, $\lambda\in\mathbb{R}$. Therefore, (5.17) holds.

(iii) Clearly, we have:

$$J^{ph}_{\rho_0,Q^{ph}} = \tag{5.19}$$
$$\sum_{\substack{m,n\in\mathbb{N}_0, n>m\\ \alpha,\varkappa\in\{l,r\}}}(n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} f(\lambda-\mu_\alpha-m\omega)\,\widehat{\sigma}^{ph}_{n\varkappa m_\alpha}(\lambda)d\lambda +$$
$$\sum_{\substack{m,n\in\mathbb{N}_0, n<m\\ \alpha,\varkappa\in\{l,r\}}}(n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}} f(\lambda-\mu_\alpha-m\omega)\,\widehat{\sigma}^{ph}_{n\varkappa m_\alpha}(\lambda)d\lambda\,.$$

Moreover, a straightforward computation shows the following:

$$\sum_{\substack{m,n\in\mathbb{N}_0,n<m\\ \alpha,\varkappa\in\{l,r\}}}(n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}f(\lambda-\mu_\alpha-m\omega)\,\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)d\lambda=$$

$$\sum_{\substack{m,n\in\mathbb{N}_0,n>m\\ \alpha,\varkappa\in\{l,r\}}}(m-n)\rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}f(\lambda-\mu_\varkappa-n\omega)\,\widehat{\sigma}^{ph}_{m_\alpha n_\varkappa}(\lambda)d\lambda.$$

Since $\mathcal{S}=\{H,H_0\}$ is time reversible symmetric, we find the following:

$$\sum_{\substack{m,n\in\mathbb{N}_0,n<m\\ \alpha,\varkappa\in\{l,r\}}}(n-m)\rho^{ph}(m)\frac{1}{2\pi}\int_{\mathbb{R}}f(\lambda-\mu_\alpha-m\omega)\,\widehat{\sigma}^{ph}_{m_\alpha n_\varkappa}(\lambda)d\lambda= \tag{5.20}$$

$$\sum_{\substack{m,n\in\mathbb{N}_0,n>m\\ \alpha,\varkappa\in\{l,r\}}}(m-n)\rho^{ph}(n)\frac{1}{2\pi}\int_{\mathbb{R}}f(\lambda-\mu_\varkappa-n\omega)\,\widehat{\sigma}^{ph}_{n_\varkappa m_\alpha}(\lambda)d\lambda.$$

Inserting (5.20) into (5.19), we obtain (5.18). □

Corollary 5.10. *Let $\mathcal{S}=\{H,H_0\}$ be the JCL-model and let $f=f_{FD}$. If case (E) of Proposition 5.3 is realized and $\mathcal{S}=\{H,H_0\}$ is time reversible symmetric, then $J^{ph}_{\rho_0,Q^{ph}}\geqslant 0$.*

Proof. We set $\mu:=\mu_l=\mu_r$. One has:

$$\rho^{ph}(m)f(\lambda-\mu-m\omega)-\rho^{ph}(n)f(\lambda-\mu-n\omega)=$$
$$e^{-m\beta\omega}(1-e^{-(n-m)\beta\omega})f_{FD}(\lambda-\mu-m\omega)f_{FD}(\lambda-\mu-n\omega)\geqslant 0,$$

for $n>m$. From (5.18), we see that $J^{ph}_{\rho_0,Q^{ph}}\geqslant 0$. □

Remark 5.11. We will now comment the results. If $J^{ph}_{\rho_0,Q^{ph}}\geqslant 0$, then system $\mathcal{S}$ is called light emitting. Similarly, if $J^{ph}_{\rho_0,Q^{ph}}\leqslant 0$, then we call it light absorbing. Of course if $\mathcal{S}$ is light emitting and absorbing, then $J^{ph}_{\rho_0,Q^{ph}}=0$.

(i) If $\beta=\infty$, then $\rho^{ph}(m)=\delta_{0m}$, $m\in\mathbb{N}_0$. Inserting this into (5.16), we get:

$$J^{ph}_{\rho_0,Q^{ph}}=\sum_{\substack{n\in\mathbb{N}_0\\ \alpha,\varkappa\in\{l,r\}}}n\frac{1}{2\pi}\int_{\mathbb{R}}f(\lambda-\mu_\alpha)\widetilde{\sigma}^{ph}_{n_\varkappa 0_\alpha}(\lambda)d\lambda\geqslant 0$$

Hence, the system $\mathcal{S}$ is light emitting.

(ii) Let us show $\mathcal{S}$ might be light emitting even if $\beta<\infty$. We consider the case (E) of Proposition 5.3. If $\mathcal{S}$ is time reversible symmetric, then it follows from Corollary 5.10 that the system is light emitting.

If the system $\mathcal{S}$ is time reversible and mirror symmetric, then $J^{ph}_{\rho_0,Q^{el}_\alpha}=0$, $\alpha\in\{l,r\}$, by Corollary 5.6(iii) . Since $J^{c}_{\rho_0,Q^{el}}=0$ by Proposition 5.3, we get that $J^{\mathcal{S}}_{\rho_0,Q^{el}_\alpha}=0$ but the photon current is larger than zero. So our JCL-model is light emitting by a zero total electron current $J^{\mathcal{S}}_{\rho_0,Q^{el}_\alpha}$.

Let $v_r=0$, $v_l=2$ and $\omega=4$. Hence $\mathcal{S}$ is not mirror symmetric. Then, we get from Remark 5.7(iii) that $J^{ph}_{\rho_0,Q^{el}_l}=-J^{ph}_{\rho_0,Q^{el}_r}\leqslant 0$. Hence, there is an electron current from the left to the right lead. Notice that by Proposition 5.3 $J^{c}_{\rho_0,Q^{el}_l}=0$. Hence, $J^{\mathcal{S}}_{\rho_0,Q^{el}_l}\leqslant 0$.

(iii) To realize a light absorbing situation, we consider the case (S) of Proposition 5.3 and assume that $\mathcal{S}$ is time reversible symmetric. Notice that by Lemma 5.4, s_c commutes with ρ^{el}. We make the following choices:

$$v_r = 0, \quad v_l \geqslant 4, \quad \omega = v_l, \quad \mu_l = 0, \quad \mu_r = \omega = v_l.$$

It follows out that with respect to the representation (5.18) one has only to $m = n - 1$, $\varkappa = r$ and $\alpha = l$. Hence,

$$J^{ph}_{\rho_0,Q^{ph}} = \sum_{n\in\mathbb{N}} \frac{1}{2\pi} \times \int_{\mathbb{R}} d\lambda \left(\rho^{ph}(n-1) f(\lambda - (n-1)\omega) - \rho^{ph}(n) f(\lambda - (n+1)\omega)\right) \widehat{\sigma}^{ph}_{n_l(n-1)_r}(\lambda)$$

Since, $f(\lambda) = f_{FD}(\lambda)$, we find:

$$\begin{aligned} &\rho^{ph}(n-1) f(\lambda - (n-1)\omega) - \rho^{ph}(n) f(\lambda - (n+1)\omega) = \\ &\quad \rho^{ph}(n-1) f(\lambda - (n-1)\omega) f(\lambda - (n+1)\omega) \times \\ &\quad \left(1 + e^{\beta(\lambda - (n+1)\omega)} - e^{-\beta\omega}(1 + e^{\beta(\lambda - \omega(n-1))})\right), \end{aligned}$$

or

$$\begin{aligned} &\rho^{ph}(n-1) f(\lambda - (n-1)\omega) - \rho^{ph}(n) f(\lambda - (n+1)\omega) = \\ &\quad \rho^{ph}(n-1) f(\lambda - (n-1)\omega) f(\lambda - (n+1)\omega)(1 - e^{-\beta\omega})(1 - e^{\beta(\lambda - \omega n)}). \end{aligned}$$

Since $\lambda - n\omega \geqslant 0$ we find $\rho^{ph}(n-1) f(\lambda - (n-1)\omega) - \rho^{ph}(n) f(\lambda - (n+1)\omega) \leqslant 0$ which yields $J^{ph}_{\rho_0,Q^{ph}} \leqslant 0$.

To calculate $J^{ph}_{\rho_0,Q^{el}_l}$, we use formula (5.7). Setting $\alpha = l$, we obtain $\alpha' = r$, which yields

$$J^{ph}_{\rho_0,Q^{el}_l} = -\sum_{m,n\in\mathbb{N}_0} \frac{\mathfrak{e}}{2\pi} \times \int_{\mathbb{R}} d\lambda \left(\rho^{ph}(n) f(\lambda - \mu_r - n\omega) - \rho^{ph}(m) f(\lambda - \mu_l - m\omega)\right) \widehat{\sigma}^{ph}_{n_l m_r}(\lambda)\,.$$

One verifies that $\widehat{\sigma}^{ph}_{0_l 0_r}(\lambda) = 0$ and $\widehat{\sigma}^{ph}_{n_l m_r}(\lambda) = 0$ for $m \neq n+1$, $n \in \mathbb{N}$. Hence,

$$J^{ph}_{\rho_0,Q^{el}_l} = -\sum_{n\in\mathbb{N}} \frac{\mathfrak{e}}{2\pi} \times \int_{\mathbb{R}} d\lambda \left(\rho^{ph}(n) f(\lambda - \mu_r - n\omega) - \rho^{ph}(n-1) f(\lambda - \mu_l - (n+1)\omega)\right) \widehat{\sigma}^{ph}_{n_l(n+1)_r}(\lambda)\,,$$

Since $\mu_r = \omega$ and $\mu_l = 0$, we find:

$$J^{ph}_{\rho_0,Q^{el}_l} = -\sum_{n\in\mathbb{N}} \frac{\mathfrak{e}}{2\pi} \times \int_{\mathbb{R}} f(\lambda - (n+1)\omega) \rho^{ph}(n-1)(1 - e^{-\beta\omega})\, \widehat{\sigma}^{ph}_{n_l(n+1)_r}(\lambda)\, d\lambda \leqslant 0.$$

Hence, there is electron current flowing from the left to right induced by photons. We recall that $J^{c}_{\rho_0,Q^{el}_l} = 0$.

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ON THE ROBIN EIGENVALUES OF THE LAPLACIAN IN THE EXTERIOR OF A CONVEX POLYGON

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Let $\Omega \subset \mathbb{R}^2$ be the exterior of a convex polygon whose side lengths are $\ell_1, \dots, \ell_M$. For a real constant α, let H^Ω_α denote the Laplacian in Ω, $u \mapsto -\Delta u$, with the Robin boundary conditions $\partial u/\partial \nu = \alpha u$ at $\partial\Omega$, where ν is the outer unit normal. We show that, for any fixed $m \in \mathbb{N}$, the mth eigenvalue $E^\Omega_m(\alpha)$ of H^Ω_α behaves as $E^\Omega_m(\alpha) = -\alpha^2 + \mu^D_m + \mathcal{O}(\alpha^{-1/2})$ as $\alpha \to +\infty$, where μ^D_m stands for the mth eigenvalue of the operator $D_1 \oplus \dots \oplus D_M$ and D_n denotes the one-dimensional Laplacian $f \mapsto -f''$ on $(0, \ell_n)$ with the Dirichlet boundary conditions.

Keywords: eigenvalue asymptotics, Laplacian, Robin boundary condition, Dirichlet boundary condition.

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1. Introduction

1.1. Laplacian with Robin boundary conditions

Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$, be a connected domain with a compact Lipschitz boundary $\partial\Omega$. For $\alpha > 0$, let H^Ω_α denote the Laplacian $u \mapsto -\Delta u$ in Ω with the Robin boundary conditions $\partial u/\partial \nu = \alpha u$ at $\partial\Omega$, where ν stands for the outer unit normal. More precisely, H^Ω_α is the self-adjoint operator in $L^2(\Omega)$ generated by the sesquilinear form:

$$h^\Omega_\alpha(u,u) = \iint\limits_\Omega |\nabla u|^2 \, \mathrm{d}x - \alpha \int\limits_{\partial\Omega} |u|^2 \, \mathrm{d}\sigma, \quad \mathcal{D}(h^\Omega_\alpha) = W^{1,2}(\Omega).$$

Here and below, σ denotes the $(d-1)$-dimensional Hausdorff measure.

One checks in the standard way that the operator H^Ω_α is semibounded from below. If Ω is bounded (i.e. Ω is an interior domain), then it has a compact resolvent, and we denote by $E^\Omega_m(\beta)$, $m \in \mathbb{N}$, its eigenvalues taken according to their multiplicities and enumerated in the non-decreasing order. If Ω is unbounded (i.e. Ω is an exterior domain), then the essential spectrum of H^Ω_α coincides with $[0, +\infty)$, and the discrete spectrum consists of finitely many eigenvalues which will be denoted again by $E^\Omega_m(\alpha)$, $m \in \{1, \dots, K_\alpha\}$, and enumerated in the non-decreasing order taking into account the multiplicities.

We are interested in the behavior of the eigenvalues $E^\Omega_m(\alpha)$ for large α. It seems that the problem was introduced by Lacey, Ockedon, Sabina [11] when studying a reaction-diffusion system. Giorgi and Smits [6] studied a link to the theory of enhanced surface superconductivity. Recently, Freitas and Krejčiřík [10] and then Pankrashkin and Popoff [15] studied the eigenvalue asymptotics in the context of the spectral optimization.

Let us list some available results. Under various assumptions one showed the asymptotics of the form:

$$E_m^\Omega(\alpha) = -C_\Omega \alpha^2 + o(\alpha^2) \text{ as } \alpha \text{ tends to } +\infty, \tag{1}$$

where $C_\Omega \geq 1$ is a constant depending on the geometric properties of Ω. Lacey, Ockedon, Sabina [11] showed (1) with $m = 1$ for C^4 compact domains, for which $C_\Omega = 1$, and for triangles, for which $C_\Omega = 2/(1 - \cos\theta)$, where θ is the smallest corner. Lu and Zhu [13] showed (1) with $m = 1$ and $C_\Omega = 1$ for compact C^1 smooth domains, and Daners and Kennedy [2] extended the result to any fixed $m \in \mathbb{N}$. Levitin and Parnovski [12] showed (1) with $m = 1$ for domains with piecewise smooth compact Lipschitz boundaries. They proved, in particular, that if Ω is a curvilinear polygon whose smallest corner is θ, then for $\theta < \pi$ there holds $C_\Omega = 2/(1 - \cos\theta)$, otherwise $C_\Omega = 1$. Pankrashkin [14] considered two-dimensional domains with a piecewise C^4 smooth compact boundary and without convex corners, and it was shown that $E_1^\Omega(\alpha) = -\alpha^2 - \gamma\alpha + \mathcal{O}(\alpha^{2/3})$, where γ is the maximum of the signed curvature at the boundary. Exner, Minakov, Parnovski [4] showed that for compact C^4 smooth domains the same asymptotics $E_m^\Omega(\alpha) = -\alpha^2 - \gamma\alpha + \mathcal{O}(\alpha^{2/3})$ holds for any fixed $m \in \mathbb{N}$. Similar results were obtained by Exner and Minakov [3] for a class of two-dimensional domains with non-compact boundaries and by Pankrashkin and Popoff [15] for C^3 compact domains in arbitrary dimensions. Cakoni, Chaulet, Haddar [1] studied the asymptotic behavior of higher eigenvalues.

1.2. Problem setting and the main result

The computation of further terms in the eigenvalue asymptotics needs more precise geometric assumptions. To our knowledge, such results are available for the two-dimensional case only. Helffer and Pankrashkin [9] studied the tunneling effect for the eigenvalues of a specific domain with two equal corners, and Helffer and Kachmar [8] considered the domains whose boundary curvature has a unique non-degenerate maximum. The machinery of both papers is based on the asymptotic properties of the eigenfunctions: it was shown that the eigenfunctions corresponding to the lowest eigenvalues concentrate near the smallest convex corner at the boundary or, if no convex corners are present, near the point of the maximum curvature, and this is used to obtain the corresponding eigenvalue asymptotics.

The aim of the present note is to consider a new class of two-dimensional domains Ω. Namely, our assumption is as follows:

The domain $\mathbb{R}^2 \setminus \overline{\Omega}$ is a convex polygon (with straight edges).

Such domains are not covered by the above cited works: all the corners are non-convex, and the curvature is constant on the smooth part of the boundary, and it is not clear how the eigenfunctions are concentrated along the boundary. We hope that our result will be of use for the understanding of the role of non-convex corners.

In order to formulate the main result, we first need some notation. We denote the vertices of the polygon $\mathbb{R}^2 \setminus \overline{\Omega}$ by $A_1, \ldots, A_M \in \mathbb{R}^2$, $M \geq 3$, and assume that they are enumerated is such a way that the boundary $\partial\Omega$ is the union of the M line segments $L_n := [A_n, A_{n+1}]$, $n \in \{1, \ldots, M\}$, where we denote $A_{M+1} := A_1$, $A_0 := A_M$. It is also assumed that there are no artificial vertices, i.e. that $A_n \notin [A_{n-1}, A_{n+1}]$ for any $n \in \{1, \ldots, M\}$.

Furthermore, we denote by ℓ_n the length of the side L_n, and by D_n the Dirichlet Laplacian $f \mapsto -f''$ on $(0, \ell_n)$ viewed as a self-adjoint operator in $L^2(0, \ell_n)$. The main result of the present note is as follows:

Theorem 1. *For any fixed $m \in \mathbb{N}$ there holds:*

$$E_m^\Omega(\alpha) = -\alpha^2 + \mu_m^D + \mathcal{O}\Big(\frac{1}{\sqrt{\alpha}}\Big) \text{ as } \alpha \text{ tends to } +\infty,$$

where μ_m^D is the mth eigenvalue of the operator $D_1 \oplus \cdots \oplus D_M$.

The proof is based on the machinery proposed by Exner and Post [5] to study the convergence on graph-like manifolds. In reality, our construction appears to be quite similar to that of Post [16], which was used to study decoupled waveguides.

We remark that due to the presence of non-convex corners the domain of the operator H_α^Ω contains singular functions and is not included in $W^{2,2}(\Omega)$, see e.g. Grisvard [7]. This does not produce any difficulties, as our approach is purely variational and is entirely based on analysis of the sesqulinear form.

2. Preliminaries

2.1. Auxiliary operators

For $\alpha > 0$, we denote by T_α the following self-adjoint operator in $L^2(\mathbb{R}_+)$:

$$T_\alpha v = -v'', \quad \mathcal{D}(T_\alpha) = \big\{v \in W^{2,2}(\mathbb{R}_+) : \, v'(0) + \alpha v(0) = 0\big\}.$$

It is well known that:

$$\operatorname{spec} T_\alpha = \{-\alpha^2\} \cup [0, +\infty), \quad \ker(T + \alpha^2) = \mathbb{C}\varphi_\alpha, \quad \varphi_\alpha(s) := \frac{e^{-\alpha s}}{\sqrt{2\alpha}}. \tag{2}$$

The sesqulinear form t_α for the operator T_α looks as follows:

$$t_\alpha(v, v) = \int\limits_0^\infty \big|v'(s)\big|^2 \mathrm{d}s - \alpha\big|v(0)\big|^2, \quad \mathcal{D}(t_\alpha) = W^{1,2}(\mathbb{R}_+).$$

Lemma 2. *For any $v \in W^{1,2}(\mathbb{R}_+)$, there holds:*

$$\int\limits_0^\infty \big|v(s)\big|^2 \mathrm{d}s - \bigg|\int\limits_0^\infty \varphi_\alpha(s) v(s) \mathrm{d}s\bigg|^2 \le \frac{1}{\alpha^2}\bigg(\int\limits_0^\infty \big|v'(s)\big|^2 \mathrm{d}s - \alpha\big|v(0)\big|^2 + \alpha^2 \int\limits_0^\infty \big|v(s)\big|^2 \mathrm{d}s\bigg).$$

Proof. We denote by P the orthogonal projector on $\ker(T_\alpha + \alpha^2)$ in $L^2(\mathbb{R}_+)$, then by the spectral theorem, we have:

$$t_\alpha(v, v) + \alpha^2 \|Pv\|^2 = t_\alpha(v - Pv, v - Pv) \ge 0,$$

for any $v \in \mathcal{D}(t_\alpha)$. As φ_α is normalized, there holds

$$\bigg|\int\limits_0^\infty \varphi_\alpha(x) v(x) \mathrm{d}x\bigg| = \|Pv\|,$$

and we arrive at the conclusion. □

Another important estimate is as follows, see Lemmas 2.6 and 2.8 in [12]:

Lemma 3. *Let $\Lambda \subset \mathbb{R}^2$ be an infinite sector of opening $\theta \in (0, 2\pi)$, then for any $\varepsilon > 0$ and any function $v \in W^{1,2}(\Lambda)$ there holds:*

$$\int\limits_{\partial\Lambda} |v|^2 \mathrm{d}s \le \varepsilon \iint\limits_\Lambda |\nabla v|^2 \mathrm{d}x + \frac{C_\theta}{\varepsilon} \iint\limits_\Lambda |v|^2 \mathrm{d}x \quad \textit{with} \quad C_\theta = \begin{cases} \dfrac{2}{1 - \cos\theta}, & \theta \in (0, \pi), \\ 1, & \theta \in [\pi, 2\pi). \end{cases} \tag{3}$$

2.2. Decomposition of Ω

Let us proceed with a decomposition of the domain Ω which will be used through the proof. Let $n \in \{1, \dots, M\}$. We denote by S_n^1 and S_n^2 the half-lines originating respectively at A_n and A_{n+1}, orthogonal to L_n and contained in Ω. By Π_n, we denote the half-strip bounded by the half-lines S_n^1 and S_n^2 and the line segment L_n, and by Λ_n we denote the infinite sector bounded by the lines S_{n-1}^2 and S_n^1 and contained in Ω. The constructions are illustrated in Fig. 1. We note that the $2M$ sets Λ_n and Π_n, $n \in \{1, \dots, M\}$, are non-intersecting and that $\overline{\Omega} = \bigcup_{n=1}^M \overline{\Lambda}_n \cup \bigcup_{n=1}^M \overline{\Pi}_n$.

We deduce from Lemma 3:

Lemma 4. *There exists a constant $C > 0$ such that for any $\varepsilon > 0$, any $n \in \{1, \dots, M\}$ and any $v \in W^{1,2}(\Lambda_n)$ there holds*

$$\int\limits_{\partial\Lambda_n} |v|^2 \mathrm{d}\sigma \le C\varepsilon\Big(\iint\limits_{\Lambda_n} |\nabla v|^2 \mathrm{d}x + \frac{1}{\varepsilon^2} \iint\limits_{\Lambda_n} |v|^2 \mathrm{d}x \Big).$$

Furthermore, for each $n \in \{1, \dots, M\}$ we denote by Θ_n the uniquely defined isometry $\mathbb{R}^2 \to \mathbb{R}^2$ such that:

$$A_n = \Theta_n(0,0) \quad \text{and} \quad \Pi_n = \Theta_n\big((0,\ell_n) \times \mathbb{R}_+\big) :$$

We remark that due to the spectral properties of the above operator T_α, see (2), we have, for any $u \in W^{1,2}(\Pi_n)$,

$$\begin{aligned}
&\int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| \frac{\partial}{\partial s} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t - \alpha \int\limits_0^{\ell_n} \Big| u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}t + \alpha^2 \int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t \\
&\qquad = \int\limits_0^{\ell_n} \Big(\int\limits_0^{\infty} \Big| \frac{\partial}{\partial s} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s - \alpha \Big| u\big(\Theta_n(t,0)\big) \Big|^2 + \alpha \int\limits_0^{\infty} \Big| u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s \Big) \mathrm{d}t \ge 0,
\end{aligned}$$

which implies, in particular, the following:

$$\begin{aligned}
0 \le &\int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| \frac{\partial}{\partial t} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t \\
&\le \int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| \frac{\partial}{\partial t} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t + \int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| \frac{\partial}{\partial s} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t \\
&\quad - \alpha \int\limits_0^{\ell_n} \Big| u\big(\Theta_n(t,0)\big) \Big|^2 \mathrm{d}t + \alpha^2 \int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big| u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t \\
&\quad = \iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \alpha \int\limits_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint\limits_{\Pi_n} |u|^2 \mathrm{d}x. \quad (4)
\end{aligned}$$

2.3. Eigenvalues and identification maps

We will use an eigenvalue estimate which is based on the max-min principle and is just a suitable reformulation of Lemma 2.1 in [5] or of Lemma 2.2 in [16]:

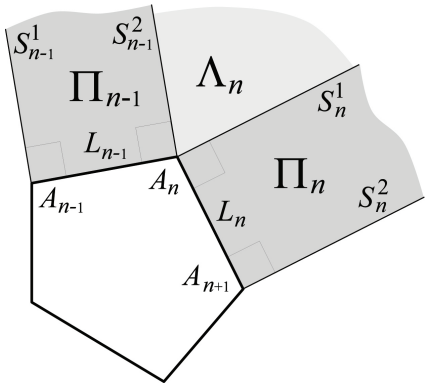

FIG. 1. Decomposition of the domain

Proposition 5. *Let B and B' be non-negative self-adjoint operators acting respectively in Hilbert space $\mathcal{H}$ and $\mathcal{H}'$ and generated by sesqulinear form b and b'. Choose $m \in \mathbb{N}$ and assume that the operator B has at least m eigenvalues $\lambda_1 \leq \dots \leq \lambda_m < \inf \operatorname{spec}_{\mathrm{ess}} B$ and that the operator B' has a compact resolvent. If there exists a linear map $J : \mathcal{D}(b) \to \mathcal{D}(b')$ (identification map) and two constants $\delta_1, \delta_2 > 0$ such that $\delta_1 \leq (1+\lambda_m)^{-1}$, and that for any $u \in \mathcal{D}(b)$ there holds:*

$$\|u\|^2 - \|Ju\|^2 \leq \delta_1 \Big(b(u,u) + \|u\|^2 \Big),$$
$$b'(Ju,Ju) - b(u,u) \leq \delta_2 \Big(b(u,u) + \|u\|^2 \Big),$$

then

$$\lambda'_m \leq \lambda_m + \frac{(\lambda_m \delta_1 + \delta_2)(1+\lambda_m)}{1-(1+\lambda_m)\delta_1},$$

where λ'_m is the mth eigenvalue of the operator B'.

3. Proof of Theorem 1

3.1. Dirichlet-Neumann bracketing

Consider the following sesqulinear form:

$$h^{\Omega,D}_\alpha(u,u) = \sum_{n=1}^M \iint\limits_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \sum_{n=1}^M \Big(\iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \alpha \int\limits_{L_n} |u|^2 \mathrm{d}\sigma \Big),$$
$$\mathcal{D}(h^{\Omega,D}_\alpha) = \bigoplus_{n=1}^M W^{1,2}_0(\Lambda_n) \oplus \bigoplus_{n=1}^M \widetilde{W}^{1,2}_0(\Pi_n),$$
$$\widetilde{W}^{1,2}_0(\Pi_n) := \big\{ f \in W^{1,2}(\Pi_n) : f = 0 \text{ at } S^1_n \cup S^2_n \big\},$$

and denote by $H^{\Omega,D}_\alpha$ the associated self-adjoint operator in $L^2(\Omega)$. Clearly, the form $h^{\Omega,D}_\alpha$ is a restriction of the initial form h^Ω_α, and due to the max-min principle we have:

$$E^\Omega_m(\alpha) \leq E^{\Omega,D}_m(\alpha),$$

where $E_m^{\Omega,D}(\alpha)$ is the mth eigenvalue of $H_\alpha^{\Omega,D}$ (as soon at it exists). On the other hand, we have the decomposition:

$$H_\alpha^{\Omega,D} = \bigoplus_{n=1}^{M} \big(- \Delta_n^D \big) \oplus \bigoplus_{n=1}^{M} G_{n,\alpha}^D,$$

where $(-\Delta_n^D)$ is the Dirichlet Laplacian in $L^2(\Lambda_n)$ and $G_{n,\alpha}^D$ is the self-adjoint operator in $L^2(\Pi_n)$ generated by the sesquilinear form:

$$g_{n,\alpha}^D(u,u) = \iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \alpha \int\limits_{L_n} |u|^2 \mathrm{d}\sigma, \quad \mathcal{D}(g_{n,\alpha}^D) = \widetilde{W}_0^{1,2}(\Pi_n).$$

Consider the following unitary maps:

$$U_n : L^2(\Pi_n) \to L^2\big((0,\ell_n)\times\mathbb{R}_+\big), \quad U_n f := f \circ \Theta_n, \quad n \in \{1,\dots,M\},$$

then it is straightforward to check that $U_n G_{n,\alpha}^D U_n^* = D_n \otimes 1 + T_\alpha \otimes 1$. As the operators $(-\Delta_n^D)$ are non-negative, it follows that $\operatorname{spec}_{\mathrm{ess}} H_\alpha^{\Omega,D} = [0,+\infty)$ and that $E_m^{\Omega,D}(\alpha) = -\alpha^2 + \mu_m^D$, which gives the majoration:

$$E_m^\Omega(\alpha) \le -\alpha^2 + \mu_m^D, \tag{5}$$

for all m with $\mu_m^D < \alpha^2$. In particular, the inequality (5) holds for any fixed m as α tends to $+\infty$.

Similarly, we introduce the following sesquilinear form:

$$h_\alpha^{\Omega,N}(u,u) = \sum_{n=1}^{M} \iint\limits_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \sum_{n=1}^{M} \bigg(\iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \alpha \int\limits_{L_n} |u|^2 \mathrm{d}\sigma \bigg),$$

$$\mathcal{D}(h_\alpha^{\Omega,N}) = \bigoplus_{n=1}^{M} W^{1,2}(\Lambda_n) \oplus \bigoplus_{n=1}^{M} W^{1,2}(\Pi_n),$$

and denote by $H_\alpha^{\Omega,N}$ the associated self-adjoint operator in $L^2(\Omega)$. Clearly, the initial form h_α^Ω is a restriction of the form $h_\alpha^{N,\Omega}$, and due to the max-min principle we have:

$$E_m^{\Omega,N}(\alpha) \le E_m^\Omega(\alpha),$$

where $E_m^{\Omega,N}(\alpha)$ is the mth eigenvalue of $H_\alpha^{\Omega,N}$, and the inequality holds for those m for which $E_m^\Omega(\alpha)$ exists. On the other hand, we have the decomposition:

$$H_\alpha^{\Omega,N} = \bigoplus_{n=1}^{M} \big(- \Delta_n^N \big) \oplus \bigoplus_{n=1}^{M} G_{n,\alpha}^N,$$

where $(-\Delta_n^N)$ denotes the Neumann Laplacian in $L^2(\Lambda_n)$ and $G_{n,\alpha}^N$ is the self-adjoint operator in $L^2(\Pi_n)$ generated by the sesquilinear form

$$g_{n,\alpha}^N(u,u) = \iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \alpha \int\limits_{L_n} |u|^2 \mathrm{d}\sigma, \quad \mathcal{D}(g_{n,\alpha}^N) = W^{1,2}(\Pi_n).$$

There holds $U_n G_{n,\alpha}^N U_n^* = N_n \otimes 1 + T_\alpha \otimes 1$, where N_n is the operator $f \mapsto -f''$ on $(0,\ell_n)$ with the Neumann boundary condition viewed as a self-adjoint operator in the Hilbert space $L^2(0,\ell_n)$, $n \in \{1,\dots,M\}$. The operators $(-\Delta_n^N)$ are non-negative, and we have $\operatorname{spec}_{\mathrm{ess}} H_\alpha^{\Omega,N} = [0,+\infty)$ and $E_m^{\Omega,N}(\alpha) = -\alpha^2 + \mu_m^N$, where μ_m^N is the mth eigenvalue of the operator $N_1 \oplus \cdots \oplus N_M$. Thus, we obtain the minorations:

$$H_\alpha^\Omega \ge -\alpha^2 \text{ and } E_m^\Omega(\alpha) \ge -\alpha^2 + \mu_m^N, \tag{6}$$

which holds for any fixed m as α tends to $+\infty$. By combining the inequalities (5) and (6) we also obtain the rough estimate:

$$E_m^\Omega(\alpha) = -\alpha^2 + \mathcal{O}(1) \quad \text{for any fixed } m \text{ and for } \alpha \text{ tending to } +\infty. \tag{7}$$

3.2. Construction of an identification map

In order to conclude the proof of Theorem 1, we will apply Proposition 5 to the operators:

$$B = H_\alpha^\Omega + \alpha^2, \quad B' = D_1 \oplus \cdots \oplus D_n,$$

which will allow us to obtain another inequality between the quantities:

$$\lambda_m = E_m^\Omega(\alpha) + \alpha^2, \quad \lambda'_m = \mu_m^D.$$

Note that for any fixed $m \in \mathbb{N}$, one has $\lambda_m = \mathcal{O}(1)$ for large α, see (7). Therefore, it is sufficient to construct an identification map $J = J_\alpha$ as in Proposition 5 with $\delta_1 + \delta_2 = \mathcal{O}(\alpha^{-1/2})$. Recall that the respective forms b and b' in our case are given by:

$$b(u,u) = h_\alpha^\Omega(u,u) + \alpha^2\|u\|^2, \quad \mathcal{D}(b) = \mathcal{D}(h_\alpha^\Omega) = W^{1,2}(\Omega),$$

$$b'(f,f) = \sum_{n=1}^{M} \int_0^{\ell_n} \big|f_n'(t)\big|^2 \mathrm{d}t, \quad \mathcal{D}(b') = \big\{f = (f_1,\dots,f_M) : f_n \in W_0^{1,2}(0,\ell_n)\big\}.$$

Here and below, by $\|u\|$ we mean the usual norm in $L^2(\Omega)$. The positivity of b' is obvious, and the positivity of b follows from (6).

Consider the maps:

$$P_{n,\alpha} : W^{1,2}(\Pi_n) \to L^2(0,\ell_n), \quad (P_{n,\alpha}u)(t) = \int_0^\infty \varphi_\alpha(s) u\big(\Theta_n(t,s)\big)\mathrm{d}s, \quad n \in \{1,\dots,M\}.$$

If $u \in W^{1,2}(\Omega)$, then $u \in W^{1,2}(\Pi_n)$ for any $n \in \{1,\dots,M\}$, and one can estimate, using the Cauchy-Schwarz inequality:

$$\begin{aligned}\big|(P_{n,\alpha}u)(0)\big|^2 + \big|(P_{n,\alpha}u)(\ell_n)\big|^2 &\le \int_0^\infty \big|u\big(\Theta_n(0,s)\big)\big|^2\mathrm{d}s + \int_0^\infty \big|u\big(\Theta_n(\ell_n,s)\big)\big|^2\mathrm{d}s \\ &= \int_{S_n^1} |u|^2\mathrm{d}\sigma + \int_{S_n^2} |u|^2\mathrm{d}\sigma.\end{aligned}$$

As $S_{n-1}^2 \cup S_n^1 = \partial\Lambda_n$, we can use Lemma 4 with $\varepsilon = \alpha^{-1}$, which gives:

$$\begin{aligned}\sum_{n=1}^M \Big(\big|(P_{n,\alpha}u)(0)\big|^2 + \big|(P_{n,\alpha}u)(\ell_n)\big|^2\Big) &\le \sum_{n=1}^M \Big(\int_{S_n^1} |u|^2\mathrm{d}\sigma + \int_{S_n^2} |u|^2\mathrm{d}\sigma\Big) \\ &= \sum_{n=1}^M \int_{\partial\Lambda_n} |u|^2\mathrm{d}\sigma \le \frac{C}{\alpha}\sum_{n=1}^M \Big(\iint_{\Lambda_n} |\nabla u|^2\mathrm{d}x + \alpha^2 \iint_{\Lambda_n} |u|^2\mathrm{d}x\Big). \end{aligned} \tag{8}$$

For each $n \in \{1,\dots,M\}$, we introduce a map:

$$\pi_n : (0,\ell_n) \to \{0,\ell_n\}, \quad \pi_n(t) = 0 \text{ for } t < \frac{\ell_n}{2}, \quad \pi_n(t) = \ell_n \text{ otherwise},$$

and choose a function: $\rho_n \in C^\infty\big([0,\ell_n]\big)$ with $\rho_n(0)=\rho_n(\ell_n)=1$ and $\rho_n\Big(\dfrac{\ell_n}{2}\Big)=0$.

Finally, we define:

$$J_\alpha : W^{1,2}(\Omega) \to \bigoplus_{n=1}^{M} L^2(0,\ell_n), \quad (J_\alpha u)_n(t) = (P_{n,\alpha}u)(t) - (P_{n,\alpha}u)\big(\pi_n(t)\big)\rho_n(t).$$

We remark that $(J_\alpha u)_n \in W_0^{1,2}(0,\ell_n)$ for any $u \in W^{1,2}(\Omega)$ and $n \in \{1,\dots,M\}$, i.e. J_α maps $\mathcal{D}(b)$ into $\mathcal{D}(b')$ and will be used as an identification map.

3.3. Estimates for the identification map

Take any $\delta > 0$. Using the following inequality:

$$(a_1+a_2)^2 \geq (1-\delta)a_1^2 - \frac{1}{\delta}\,a_2^2, \quad a_1, a_2 \geq 0,$$

we estimate:

$$\|u\|^2 - \|J_\alpha u\|^2 = \sum_{n=1}^{M} \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x + \sum_{n=1}^{M} \Big(\iint\limits_{\Pi_n} |u|^2 \mathrm{d}x - \int\limits_0^{\ell_n} \Big| \big(P_{n,\alpha}u\big)(t) - \big(P_{n,\alpha}u\big)\big(\pi(t)\big)\rho(t) \Big|^2 \mathrm{d}t \Big)$$

$$\leq \sum_{n=1}^{M} \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x + \sum_{n=1}^{M} \Big(\iint\limits_{\Pi_n} |u|^2 \mathrm{d}x - (1-\delta) \int\limits_0^{\ell_n} \big|\big(P_{n,\alpha}u\big)(t)\big|^2 \mathrm{d}t + \frac{1}{\delta} \int\limits_0^{\ell_n} \big|\big(P_{n,\alpha}u\big)\big(\pi(t)\big)\rho(t)\big|^2 \mathrm{d}t \Big)$$

$$= \sum_{n=1}^{M} \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x + \sum_{n=1}^{M} \Big(\iint\limits_{\Pi_n} |u|^2 \mathrm{d}x - \int\limits_0^{\ell_n} \big|\big(P_{n,\alpha}u\big)(t)\big|^2 \mathrm{d}t \Big)$$

$$+\delta \sum_{n=1}^{M} \int\limits_0^{\ell_n} \big|\big(P_{n,\alpha}u\big)(t)\big|^2 \mathrm{d}t + \frac{1}{\delta} \sum_{n=1}^{M} \int\limits_0^{\ell_n} \Big|\big(P_{n,\alpha}u\big)\big(\pi(t)\big)\rho_n(t)\Big|^2 \mathrm{d}t$$

$$=: I_1 + I_2 + I_3 + I_4.$$

We have the trivial inequality:

$$I_1 \leq \frac{1}{\alpha^2} \sum_{n=1}^{M} \Big(\iint\limits_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \alpha^2 \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x \Big).$$

To estimate the term I_2, we use Lemma 2 and then (4):

$$I_2 = \sum_{n=1}^{M} \int\limits_0^{\ell_n} \Big(\int\limits_0^{\infty} \big|u\big(\Theta_n(t,s)\big)\big|^2 \mathrm{d}s - \Big| \int\limits_0^{\infty} \varphi_\alpha(s) u\big(\Theta_n(t,s)\big) \mathrm{d}s \Big|^2 \Big) \mathrm{d}t$$

$$\leq \frac{1}{\alpha^2} \sum_{n=1}^{M} \int\limits_0^{\ell_n} \Big(\int\limits_0^{\infty} \Big|\frac{\partial}{\partial s} u\big(\Theta_n(t,s)\big)\Big|^2 \mathrm{d}s - \alpha \big|u\big(\Theta_n(t,0)\big)\big|^2 + \alpha^2 \int\limits_0^{\infty} \big|u\big(\Theta_n(t,s)\big)\big|^2 \mathrm{d}s \Big) \mathrm{d}t$$

$$\leq \frac{1}{\alpha^2} \sum_{n=1}^{M} \Big(\iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int\limits_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint\limits_{\Pi_n} |u|^2 \mathrm{d}x \Big),$$

which gives:

$$I_1 + I_2 \le \frac{1}{\alpha^2}\Big(h_\alpha^\Omega(u,u) + \alpha^2\|u\|^2\Big).$$

Furthermore, with the help of the Cauchy-Schwarz inequality, we have:

$$I_3 \le \delta \sum_{n=1}^{M} \int\limits_0^{\ell_n} \int\limits_0^{\infty} \Big|u\big(\Theta_n(t,s)\big)\Big|^2 \mathrm{d}s\,\mathrm{d}t = \delta \sum_{n=1}^{M} \iint\limits_{\Pi_n} |u|^2 \mathrm{d}x \le \delta\|u\|^2,$$

To estimate the last term, I_4, we introduce the following constant:

$$R := \max\Big\{ \int\limits_0^{\ell_n} \big|\rho_n(t)\big|^2 \mathrm{d}t : \ n \in \{1,\dots,M\}\Big\},$$

then, using first the estimate (8), and then the inequality (4),

$$\begin{aligned}
I_4 &\le \frac{R}{\delta} \sum_{n=1}^{M} \sup_{t\in(0,\ell_n)} \Big|\big(P_{n,\alpha}u\big)\big(\pi_n(t)\big)\Big|^2 \\
&\le \frac{R}{\delta} \sum_{n=1}^{M} \Big(\big|(P_{n,\alpha}u)(0)\big|^2 + \big|(P_{n,\alpha}u)(\ell_n)\big|^2\Big) \\
&\le \frac{RC}{\delta\alpha} \sum_{n=1}^{M} \Big(\iint\limits_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \alpha^2 \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x\Big) \\
&\le \frac{RC}{\delta\alpha} \Big[\sum_{n=1}^{M} \Big(\iint\limits_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \alpha^2 \iint\limits_{\Lambda_n} |u|^2 \mathrm{d}x\Big) \\
&\qquad + \sum_{n=1}^{M} \Big(\iint\limits_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int\limits_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint\limits_{\Pi_n} |u|^2 \mathrm{d}x\Big)\Big] \\
&= \frac{RC}{\delta\alpha}\Big(h_\alpha^\Omega(u,u) + \alpha^2\|u\|\Big).
\end{aligned}$$

Choosing $\delta = \alpha^{-1/2}$ and summing up the four terms, we see that:

$$\|u\|^2 - \|J_\alpha u\|^2 \le \frac{c_1}{\sqrt{\alpha}}\Big(h_\alpha^\Omega(u,u) + \alpha^2\|u\|^2 + \|u\|^2\Big) \equiv \frac{c_1}{\sqrt{\alpha}}\Big(b(u,u) + \|u\|^2\Big),$$

with a suitable constant $c_1 > 0$.

Now, we need to compare $b'(J_\alpha u, J_\alpha u)$ and $b(u,u)$. Take $\delta \in (0,1)$ and use the inequality:

$$(a_1 + a_2)^2 \le (1+\delta)a_1^2 + \frac{2}{\delta}\,a_2^2, \quad a_1, a_2 \ge 0,$$

Then:

$$
\begin{aligned}
b'(J_\alpha u, J_\alpha u) - b(u,u) &= \sum_{n=1}^{M} \int_0^{\ell_n} \Big| (P_{n,\alpha}u)' - \rho_n' \big[(P_{n,\alpha}u)\circ\pi_n\big] \Big|^2 \mathrm{d}t - \Big(h_\alpha^\Omega(u,u) + \alpha^2 \|u\|^2 \Big) \\
&\le (1+\delta) \sum_{n=1}^{M} \int_0^{\ell_n} \Big| (P_{n,\alpha}u)' \Big|^2 \mathrm{d}t + \frac{2}{\delta} \sum_{n=1}^{M} \int_0^{\ell_n} \Big| \rho_n' \big[(P_{n,\alpha}u)\circ\pi_n\big] \Big|^2 \mathrm{d}t \\
&\quad - \sum_{n=1}^{M} \Big(\iint_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \alpha^2 \iint_{\Lambda_n} |u|^2 \mathrm{d}x \Big) \\
&\quad - \sum_{n=1}^{M} \Big(\iint_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint_{\Pi_n} |u|^2 \mathrm{d}x \Big) \qquad (9) \\
&\le (1+\delta) \sum_{n=1}^{M} \int_0^{\ell_n} \Big| (P_{n,\alpha}u)' \Big|^2 \mathrm{d}t + \frac{2}{\delta} \sum_{n=1}^{M} \int_0^{\ell_n} \Big| \rho_n' \big[(P_{n,\alpha}u)\circ\pi_n\big] \Big|^2 \mathrm{d}t \\
&\quad - \sum_{n=1}^{M} \Big(\iint_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint_{\Pi_n} |u|^2 \mathrm{d}x \Big).
\end{aligned}
$$

Using first the Cauchy-Schwarz inequality and then inequality (4), we have:

$$
\int_0^{\ell_n} \big|(P_{n,\alpha}u)'\big|^2 \mathrm{d}t \le \int_0^{\ell_n} \int_0^{\infty} \Big| \frac{\partial}{\partial t} u\big(\Theta_n(t,s)\big) \Big|^2 \mathrm{d}s\,\mathrm{d}t \le \iint_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint_{\Pi_n} |u|^2 \mathrm{d}x.
$$

Substituting the last inequality into (9), we arrive at:

$$
\begin{aligned}
b'(J_\alpha u, J_\alpha u) - b(u,u) \le \delta \sum_{n=1}^{M} \Big(\iint_{\Pi_n} |\nabla u|^2 \mathrm{d}x - \int_{L_n} |u|^2 \mathrm{d}\sigma + \alpha^2 \iint_{\Pi_n} |u|^2 \mathrm{d}x \Big) \\
+ \frac{2}{\delta} \sum_{n=1}^{M} \int_0^{\ell_n} \Big| \rho_n' \big[(P_{n,\alpha}u)\circ\pi_n\big] \Big|^2 \mathrm{d}t.
\end{aligned} \qquad (10)
$$

Furthermore, using the constant:

$$
R' := \max\Big\{ \int_0^{\ell_n} \big|\rho_n'(t)\big|^2 \mathrm{d}t : \, n \in \{1,\dots,M\} \Big\},
$$

and the inequality (8), we have:

$$
\begin{aligned}
&\sum_{n=1}^{M} \int_0^{\ell_n} \Big| \rho_n' \big[(P_{n,\alpha}u)\circ\pi_n\big] \Big|^2 \mathrm{d}t \le R' \sum_{n=1}^{M} \sup_{t\in(0,\ell_n)} \big|(P_{n,\alpha}u)\big(\pi_n(t)\big)\big|^2 \\
&\le R' \sum_{n=1}^{M} \Big(\big|(P_{n,\alpha}u)(0)\big|^2 + \big|(P_{n,\alpha}u)(\ell_n)\big|^2 \Big) \le \frac{R'C}{\alpha} \sum_{n=1}^{M} \Big(\iint_{\Lambda_n} |\nabla u|^2 \mathrm{d}x + \alpha^2 \iint_{\Lambda_n} |u|^2 \mathrm{d}x \Big).
\end{aligned}
$$

The substitution of this inequality into (10) and the choice $\delta = \alpha^{-1/2}$ then leads to:

$$b'(Ju, Ju) - b(u, u) \leq \frac{c_2}{\sqrt{\alpha}}\Big(h^\Omega_\alpha(u, u) + \alpha^2\|u\|^2\Big) \leq \frac{c_2}{\sqrt{\alpha}}\Big(b(u, u) + \|u\|^2\Big),$$

with a suitable constant $c_2 > 0$. By Proposition 5, for any fixed $m \in \mathbb{N}$ and for large α, we have the estimate $\mu^D_m \leq E^\Omega_m(\alpha) + \alpha^2 + \mathcal{O}(\alpha^{-1/2})$. The combination with (5) gives the result.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 57–62

THERMALLY INDUCED TRANSITIONS AND MINIMUM ENERGY PATHS FOR MAGNETIC SYSTEMS

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Thermally induced magnetic transitions are rare events as compared with vibrations of individual magnetic moments. Timescales for these processes differ by 10 orders of magnitude or more. Therefore, the standard Monte-Carlo simulation is not suitable for the theoretical description of such phenomena. However, a statistical approach based on transition state theory is applicable for calculations of the transition rates. It presupposes finding the minimum energy path (MEP) between stable magnetic states on the multidimensional energy surface of the system. A modification of the Nudged Elastic Band (NEB) method for finding the energy barriers between states is suggested. A barrier on the energy surface corresponds to the difference between maximum energy along the MEP (highest saddle point) and the initial state minimum. The NEB procedure is implemented for spin rotations in Cartesian representation with geometric constraint on the magnitude of the magnetic moment. In this case, the effective magnetic forces are restricted to the tangent plane of the magnetic momentum vector.

Keywords: Potential energy surface, minimum energy path, nudged elastic band method, numerical optimization, quick min-mode.

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1. Introduction

In recent years, there has been large interest in the study of magnetization reversal processes under the action of thermal fluctuations and external perturbations. The stability of magnetic states is of great importance for research and development of miniaturized magnetic storage devices [1]. For estimation of the rates of activated transitions it is essential to know the response of the system to random perturbations. Direct Monte-Carlo simulation of temperature induced magnetization reversal is effectively impossible due to the time-scale difference between high-frequency vibrations of individual moments and low-frequency magnetic transitions between magnetic states of the whole system. However, a statistical approach known as 'transition state theory' [2, 3] can be used in this case. This approach describes transitions through description of behavior of a system in the least observable 'transition state'. Stable states of the system correspond to the minima on the multidimensional energy surface of the system considered as a function of all parameters determining the magnetic configuration. For magnetic systems, these parameters have to determine all spin vectors. These could be Cartesian coordinates of the magnetic moments. However, due to the large difference in the time scale of longitudinal and transverse relaxation of the magnetic moment, the length can be taken to be fixed and thereby decrease the number of independent variables. Transition rates depend on the height of energy barriers, which correspond to saddle points on minimum energy paths (MEP), as well as on the shape of the energy surface at the minimum and saddle points [2]. A popular and efficient approach used for calculation of MEP for atomic rearrangements is the nudged elastic band (NEB) method [3]. A transition path is represented there by a chain of images (replicas) of the system between two local minima on the potential energy surface; each image

corresponds to specific configuration of the system with known potential energy. The images are connected with artificial springs to keep them well separated and prevent them from falling into the minima. The images give a discrete representation of the path on the energy surface. An iterative algorithm moves the images under the action of a force that contains the transverse component of the real force and parallel component of the spring force. Detailed description of this procedure, taking into account the constraint on the modulus of magnetic moments, is given below.

2. Method

2.1. Minimization technique

The system is defined by the Hamiltonian which gives the energy of the system for any configuration of the spin vectors. It can be either an analytical function of spin vectors, or numerical procedure, such as DFT calculations [4]. A constraint on the length of the spin vectors confining them to the surface of a sphere or a self-consistent determination of the modulus of magnetic moments require specific measures to be incorporated into the implementation of the NEB method. Common constrained-optimization techniques, such as Lagrange multipliers method, are not suitable in this case due to the computational cost which tends to be high for non-analytical Hamiltonians [3,5]. In addition, in most cases pure analytical methods for finding extrema are unsuitable due to the computational difficulty for evaluating the second derivatives of the Hamiltonian. Thereby, the implementation method itself should preferably incorporate these constraints. One way to do this is to use a coordinate system that is bounded to surface of the sphere, such as spherical or stereographical coordinates [5]. This approach is quite successful; however, it suffers from topological artifacts of a sphere, such as coordinate periodicity and problems with pole regions. As an alternative to using sphere-specific coordinates and unconstrained transformations, we propose to use Cartesian coordinates and sphere-specific constrained transformations, e.g. rotations. Using this approach in the optimization procedure allows one to overcome most of the topological artifacts of a sphere and prevent violation of native constraints.

We use a minimization technique known as ‘quick-min’ or ‘velocity projection optimization’ [4, 5], which is essentially a gradient descent method, optimized with accumulation of velocity in direction of minimization movement. An iteration step can be formulated in four stages as follows:

$$\vec{a}_i = -\frac{1}{m}\nabla E\left(\vec{S}_i\right),$$

$$\vec{v}_i = \vec{v}_{i-1} + \frac{\vec{a}_i + \vec{a}_{i-1}}{2}\Delta t,$$

$$\vec{v}_i = \left\|\vec{v}_i\right\| \langle \vec{a}_{i0}|\vec{v}_{i0}\rangle \, \chi\left(\langle \vec{a}_{i0}|\vec{v}_{i0}\rangle\right) \vec{a}_{i0} = \frac{\langle \vec{a}_i|\vec{v}_i\rangle \, \chi\left(\langle \vec{a}_{i0}|\vec{v}_{i0}\rangle\right)}{\left\|\vec{a}_i\right\|^2}\vec{a}_i,$$

$$\vec{S}_{i+1} = \vec{S}_i + \vec{v}_i\Delta t + \frac{\vec{a}_i}{2}\Delta t^2,$$

where m and Δt are optimization parameters and χ is Heaviside function. The method is inspired by the velocity Verlet integration of motion equation. The native constraint requires the force to be restricted to the tangent plane of the current spin vector. If so, movement on tangent plane can be calculated. An infinitesimal movement in the tangent plane is equal to movement on the surface of the sphere; thereby we can transform that shift into rotation in

movement plane. We can construct rotation matrix in axis-angle representation from $\vec{n}$ – normal to movement plane and θ – rotation angle:

$$R(\vec{n},\theta) = \begin{pmatrix} n_x^2 + \cos\theta\,(1-n_x^2) & n_x n_y\,(1-\cos\theta) - n_z\sin\theta & n_x n_z\,(1-\cos\theta) + n_y\sin\theta \\ n_x n_y\,(1-\cos\theta) + n_z\sin\theta & n_y^2 + \cos\theta\,(1-n_y^2) & n_y n_z\,(1-\cos\theta) - n_x\sin\theta \\ n_x n_z\,(1-\cos\theta) - n_y\sin\theta & n_y n_z\,(1-\cos\theta) + n_x\sin\theta & n_z^2 + \cos\theta\,(1-n_z^2) \end{pmatrix}. \quad (1)$$

The minimization step is performed by using matrix (1) in following form:

$$\vec{S}_{i+1} = R(\vec{n}_i,\theta_i)\cdot\vec{S}_i.$$

In principle, instead of rotation matrices, another type of object can be used – unit quaternions, also known as versors. From $\vec{n}$, θ, quaternion describing the same rotation is defined as follows:

$$q(s,\vec{v}) = \left(\cos\frac{\theta}{2}, \vec{n}\sin\frac{\theta}{2}\right). \quad (2)$$

If quaternion is defined as in (2), then minimization step can be written in following form:

$$\vec{S}_{i+1} = q_i\cdot\vec{S}_i\cdot q_i^{-1},$$

where $\vec{S}_i$ is converted to quaternion by adding unit scalar part to it.

Accurately implemented, both rotation matrix approach and quaternion approach have similar computational cost. Quaternions have major computational benefit: the composition of the rotations can be calculated by simple multiplication of corresponding quaternions, which is much faster than multiplication of rotation matrices, but the difference was not significant in the present applications. However, it seems worth looking into yet another spin representation for this task: each spin vector as unit vector of a surface of a sphere can be constructed by rotation from a selected start vector. Therefore, it is possible to use rotations as coordinates. It may be of large interest to implement the procedure described above solely using quaternion terms.

2.2. Calculation of minimum energy path

The NEB method is implemented as minimization of all intermediate images of the path, using the specially modified force. In addition to the true force, each image is affected by forces of artificial springs that connect it to its neighbors. This force for each spring is determined from length of arc segment between two spin vectors in different images. To prevent the 'corner-cutting' effect [3], nudging direction is introduced using 'upwind tangent" approach [6]. In this approach, nudging direction is chosen as direction to highest energy neighbor. After that, forces are projected dependent on that direction:

$$\vec{F}_\Sigma = \vec{F}_{T\perp} + \vec{F}_{E||}.$$

With this modified force, the iterative minimization procedure moves the images to the MEP. The saddle point, which corresponds to maximum energy on MEP, can be estimated from two neighboring images with highest energy. In addition, 'climbing-image' (CI) modification [7] can be used: The highest energy image marked as 'climbing', is free from spring forces and parallel component of the true force is inverted to move that image higher along MEP to the saddle point.

3. Test cases

Two simple systems were chosen as test cases. Both represent a single atom with two degrees of freedom to make it easier to visualize. In that case potential energy surface can be shown as a two-dimensional surface in three-dimensional space. In these particular cases, spherical coordinates were used for plotting: ϕ – azimuth angle and θ – elevation angle. The potential energy surfaces, plotted as function of these angles, are shown in Fig. 1 and Fig. 2. In both cases there are two minima corresponding to $\phi = \theta = 0$ and $\phi = \pi$, $\theta = 0$. The initial path corresponds to the chain shown with empty circles and is chosen to be the same in both cases. Images of a system in that state were intentionally distributed non-equidistantly through predetermined randomized procedure to show that NEB procedure is not constricted to a limited set of initial path configurations. The final MEP, obtained using the algorithm described above, corresponds to the chain shown with solid circles. The saddle point is denoted by a cross mark.

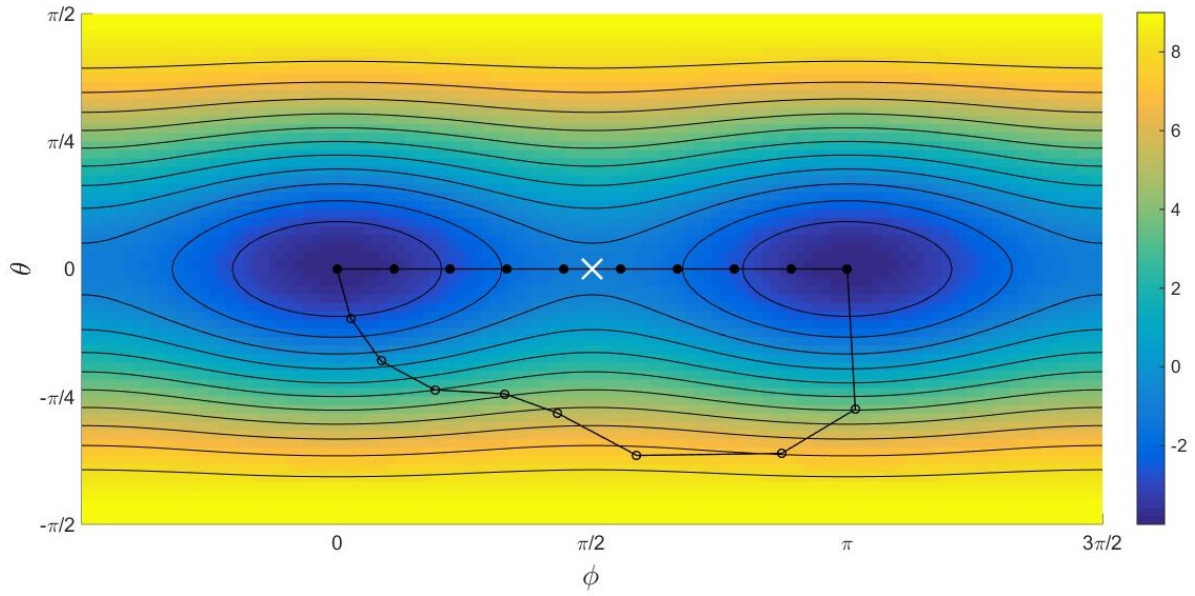

FIG. 1. Potential energy surface for single spin with spin Hamiltonian (3). Calculation of MEP without Climbing Image. Saddle point is directly between minima. Maximums are in pole regions ($\theta = \pm\pi/2$)

The first system is a single spin with Hamiltonian containing only internal anisotropy part:

$$H = \vec{S}^T \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -9 \end{pmatrix} \vec{S}. \tag{3}$$

For this system, the MEP is expected to be a straight line between the local minima. In Fig. 1, this case is displayed, with even number of intermediary images and without CI. The saddle point is estimated to be between the two images with highest energy on opposite slopes. Due to symmetry, the point in the center is the saddle point. Also, if an odd number of intermediate images were used, then the middle image would be expected to get to saddle point even without using CI. Note that in Fig. 1, the distances between adjacent images in the final configuration of the path are equal.

The second system is single spin with Gaussian Hamiltonian:

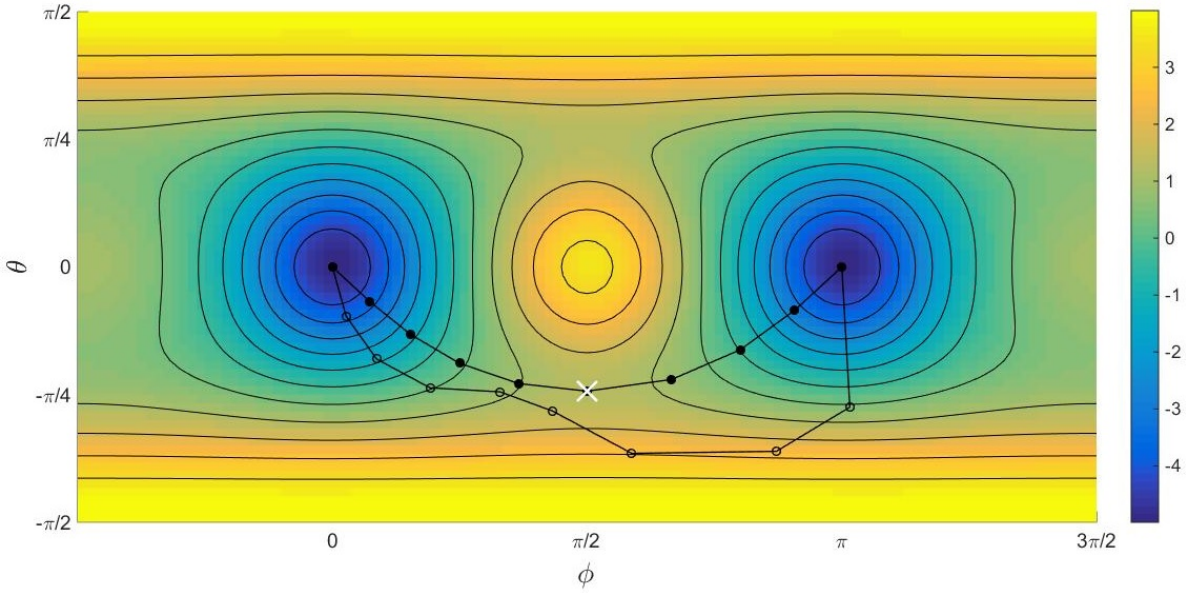

FIG. 2. Potential energy surface for single spin with Gaussian Hamiltonian (4). Calculation of MEP with Climbing Image. Saddle point is exactly in climbed image. There are maximums in pole regions ($\theta = \pm\pi/2$), and there is maximum directly between minima ($\varphi = \pi/2$, $\theta = 0$), which results in curved form of MEP

$$
\begin{gathered}
H = \sum_i w_i \exp\left(-\frac{\alpha_i}{0.35}\right), \\
w = \left\{ \begin{array}{cccccc} -5, & -5, & 1, & 3.5, & 4, & 4 \end{array} \right\}, \\
P = \left\{ \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\},
\end{gathered}
\tag{4}
$$

where α_i is the angle between $\vec{P}_i$ and spin vector.

For this system, the MEP is non-trivial; it is a curved line since now there is a maximum in the energy at the center. In Fig. 2, the results of a calculation which was carried out with CI turned on. The saddle point is estimated to be exactly at the climbing image. The usage of CI results in splitting the band in two parts, separated by saddle point, with a different distance between adjacent images on the two sides. Due to symmetry, if either number of images were odd or CI were turned off, then the images would have even distribution of distances between them. Note that in Fig. 1, there are two possible MEPs, and in Fig. 2, there are four. This illustrates that the NEB method finds the local MEP closest to the initial path, not necessarily the global MEP. The final configuration depends in that way on the initial path.

These cases show that the NEB implementation described above is in accordance with theoretical description [3] and behaves in the expected way. There are no problems specific to pole regions or periodicity of coordinates, which is good for application to magnetic systems. In the future, this implementation should be compared with other implementations in terms of speed of convergence. Also, it may be interesting to try a pure quaternion implementation.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 63–78

ON SOME APPLICATIONS OF THE BOUNDARY CONTROL METHOD TO SPECTRAL ESTIMATION AND INVERSE PROBLEMS

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We consider applications of the Boundary Control (BC) method to generalized spectral estimation problems and to inverse source problems. We derive the equations of the BC method for these problems and show that the solvability of these equations crucially depends on the controllability properties of the corresponding dynamical system and properties of the corresponding families of exponentials.

Keywords: spectral estimation problem, boundary control method, identification problem, inverse problem, Schrödinger equation, hyperbolic system.

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1. Introduction

The classical spectral estimation problem consists of recovering the coefficients a_n, λ_k, $k = 1, \dots, N,\ N \in \mathbb{N}$, of a signal

$$s(t) = \sum_{n=1}^{N} a_k e^{\lambda_k t}, \quad t \geqslant 0$$

from the given observations $s(j)$, $j = 0, \dots, 2N-1$, where the coefficients a_k, λ_k may be arbitrary complex numbers. The literature describing various methods for solving the spectral estimation problem is very extensive: see for example the list of references in [1, 2]. In these papers a new approach to this problem was proposed: a signal $s(t)$ was treated as a kernel of a certain convolution operator corresponding to an input-output map for some linear discrete-time dynamical system. While the system realized from the input-output map is not unique, the coefficients a_n and λ_n can be determined uniquely using the non-selfadjoint version of the boundary control method [3].

In [4, 8], this approach has been generalized to the infinite-dimensional case: more precisely, the problem of the recovering the coefficients $a_k, \lambda_k \in \mathbb{C}$, $k \in \mathbf{N}$, of the given signal:

$$S(t) = \sum_{k=1}^{\infty} a_k(t) e^{\lambda_k t}, \quad t \in (0, 2T), \tag{1.1}$$

from the given data $S \in L_2(0, 2T)$ was considered. In [4], the case $a_k \in \mathbb{C}$ has been treated, in [8] the case when for each k, $a_k(t) = \sum_{i=0}^{L_k - 1} a_k^i t^i$ are polynomials of the order $L_k - 1$ with complex valued coefficients a_k^i was studied.

Recently, it was observed [9, 15] that the results of [4, 8] are closely related to the dynamical inverse source problem: let H be a Hilbert space, A be an operator in H with the domain $D(A)$, Y be another Hilbert space, $O : H \supset D(O) \mapsto Y$ be an observation operator (see [18]). Given the dynamical system in H:

$$\begin{cases} u_t - Au = 0, \quad t > 0, \\ u(0) = a, \end{cases} \tag{1.2}$$

we denote by u^a its solution, and by $y(t) := (Ou^a)(t)$ the observation (output of this system). The operator that realizes the correspondence $a \mapsto (Ou^a)(t)$ is called the *observation* operator $\mathbb{O}^T : H \mapsto L_2(0, T; Y)$. We fix some $T > 0$ and assume that $y(t) \in L_2(0, T; Y)$. One can pose the following questions: what information on the operator A could be recovered from the observation $y(t)$? We mention works on the multidimensional inverse problems for the Schrödinger, heat and wave equations by one measurement, concerning this subject. Some of the results (for the Schrödinger equation) are given in [9, 10, 16]. To answer this question in the abstract setting, in [15] the authors derived the version of the BC-method equations under the condition that A is self-adjoint and $Y = \mathbb{R}$. In the present paper, we address the same question without the assumption about selfajointness of A . The possibility of recovering the spectral data from the dynamical one is well-known for the dynamical system with a boundary control [11, 12]. We extend these ideas to the case of the dual (observation) system.

The solvability of the BC-method equations for the spectral estimation problem critically depends on the properties of corresponding exponential family. The solvability of the BC-method equations for system (1.2) depends on the controllability properties of the dual system. We point out the close relation between these two problems: they both leads to essentially the same equations (see section 4 for applications), and conditions for the solvability of these equations are the same (on the connections between the controllability of a dynamical systems and properties of exponential families see [5]).

In the second section, we outline the solution for the spectral estimation problem in infinite dimensional spaces (see [8] for details). In the third section, we derive the equations of the BC-method for problem (1.2), extending the results of [15] to the case of non self-adjoint operator. Also, we answer the question on the extension of the observation $y(t) = (\mathbb{O}a)(t)$. The last section is devoted to the applications to inverse problem by one measurement of the Schrödinger equation on the interval and to the problem of extending the inverse data for the first order hyperbolic system on the interval, see also [4, 7–9].

2. The spectral estimation problem in infinite dimensional spaces

The problem is set up in the following way: given the signal (1.1), $S \in L_2(0, 2T)$, for $T > 0$, to recover the coefficients $a_k(t)$, λ_k, $k \in \mathbb{N}$. Below, we outline the procedure of recovering unknown parameters, for the details see [8].

We consider the dynamical systems in a complex Hilbert space H:

$$\dot{x}(t) = Ax(t) + bf(t), \quad t \in (0, T), \quad x(0) = 0. \tag{2.1}$$

$$\dot{y}(t) = A^*y(t) + dg(t), \quad t \in (0, T), \quad y(0) = 0, \tag{2.2}$$

here $b, d \in H$, $f, g \in L_2(0, T)$, and we assume that the spectrum of the operator A, $\{\lambda_k\}_{k=1}^{\infty}$ is not simple. We denote the algebraic multiplicity of λ_k by L_k, $k \in \mathbb{N}$, and also assume that the set of all root vectors $\{\phi_k^i\}$, $i = 1, \dots, L_k$, $k \in \mathbb{N}$, forms a Riesz basis in H. Here, the vectors from the chain $\{\phi_k^i\}_{i=1}^{L_k}$, $k \in \mathbb{N}$, satisfy the equations:

$$(A - \lambda_k)\,\phi_k^1 = 0, \quad (A - \lambda_k)\,\phi_k^i = \phi_k^{i-1}, \ 2 \leqslant i \leqslant L_k.$$

The spectrum of A^* is $\{\overline{\lambda}_k\}_{k=1}^{\infty}$ and the root vectors $\{\psi_k^i\}$, $i = 1, \ldots, L_k$, $k \in \mathbb{N}$, also form a Riesz basis in H and satisfy the equations:

$$\left(A^* - \overline{\lambda}_k\right) \psi_k^{L_k} = 0, \quad \left(A^* - \overline{\lambda}_k\right) \psi_k^i = \psi_k^{i+1}, \ 1 \leqslant i \leqslant L_k - 1.$$

Moreover, the root vectors of A and A^* are normalized, in accordance with the following:

$$\left\langle \phi_k^i, \psi_l^j \right\rangle = 0, \text{ if } k \neq l \text{ or } i \neq j;$$
$$\left\langle \phi_k^i, \psi_k^i \right\rangle = 1, \ \ i = 1, \ldots, L_k, \ k \in \mathbb{N}.$$

We consider f and g as the inputs of the systems (2.1) and (2.2) and define the outputs z and w by the formulas:

$$z(t) = \langle x(t), d \rangle , \quad w(t) = \langle y(t), b \rangle .$$

We assume that $b = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} b_k^i \phi_k^i$, $d = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} d_k^i \psi_k^i$. While searching for the solution to (2.1) in the form $x(t) = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} c_k^i(t) \phi_k^i$, we arrive at the following representation for the output:

$$z(t) = \langle x(t), d \rangle = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} c_k^i(t) d_k^i = \int_0^t r(t-\tau) f(\tau) \, d\tau,$$

where the *response function* $r(t)$ is defined as:

$$r(t) = \sum_{k=1}^{\infty} e^{\lambda_k t} \left[a_k^1 + a_k^2 t + a_k^3 \frac{t^2}{2} + \ldots + a_k^{L_k - 1} \frac{t^{L_k - 2}}{(L_k - 2)!} + a_k^{L_k} \frac{t^{L_k - 1}}{(L_k - 1)!} \right], \tag{2.3}$$

with a_k^j being defined as:

$$a_k^j = \sum_{i=j}^{L_k} b_k^i d_k^{i-j+1}, \quad j = 1, \ldots, L_k, \ k \in \mathbb{N}. \tag{2.4}$$

It is important to note that $r(t)$ has the form of the series in (1.1).

Analogously, looking for the solution of (2.2) in the form:

$$y(t) = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} h_k^i(t) \psi_k^i,$$

we arrive at:

$$w(t) = \langle y(t), b \rangle = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} h_k^i(t) b_k^i = \int_0^t \overline{r(t-\tau)} g(\tau) \, d\tau.$$

We introduce the *connecting operator* $C^T : L_2(0,T) \mapsto L_2(0,T)$, defined through its bilinear form by the formula:

$$\left\langle C^T f, g \right\rangle = \langle x(T), y(T) \rangle .$$

In [8], the representation for C^T was obtained:

Lemma 1. *The connecting operator C^T has a representation*

$$(C^T f)(t) = \int_0^T r(2T - t - \tau) f(\tau) \, d\tau.$$

We assume that the systems (2.1), (2.2) are spectrally controllable in time T. This means that for any $i \in \{1, \dots, L_k\}$, and any $k \in \mathbb{N}$, there exist $f_k^i,\, g_k^i \in H_0^1(0,T)$, such that $x^{f_k^i}(T) = \phi_k^i,\ y^{g_k^i}(T) = \psi_k^i$. Using ideas of the BC method [13], we are able to extract the spectral data, $\left\{\lambda_k, a_k^j\right\},\ j = 1, \dots, L_k,\ k \in \mathbb{N}$, from the dynamical one, $r(t),\ t \in (0, 2T)$, (see [4, 8] for more details):

Proposition 1. *The set $\lambda_k,\ f_k^i,\ i = 1, \dots, L_k,\ k \in \mathbb{N}$, are eigenvalues and root vectors of the following generalized eigenvalue problem in $L_2(0,T)$:*

$$\int_0^T \left(r'(2T - t - \tau) - \lambda r(2T - t - \tau)\right) f(\tau)\, d\tau = 0. \tag{2.5}$$

The set $\overline{\lambda}_k,\ g_k^i,\ k = 1, \dots \infty,\ i = 1, \dots, L_k$ are eigenvalues and root vectors of the generalized eigenvalue problem in $L_2(0,T)$:

$$\int_0^T \left(\overline{r'(2T - t - \tau)} - \lambda \overline{r(2T - t - \tau)}\right) g(\tau)\, d\tau = 0. \tag{2.6}$$

Now, we describe the algorithm of recovering $a_k^1, \dots a_k^{L_k},\ k \in \mathbb{N}$ (see the representation (2.3)). We normalize the solutions to (2.5), (2.6) by the rule:

$$\left\langle C^T \widetilde{f}_k^i, \widetilde{g}_k^i \right\rangle = 1, \tag{2.7}$$

and define:

$$\widetilde{b}_k^i = \left\langle y^{\widetilde{g}_k^i}(T), b \right\rangle = \int_0^T \overline{r}(T - \tau) \widetilde{g}_k^i(\tau)\, d\tau, \tag{2.8}$$

$$\widetilde{d}_k^i = \left\langle x^{\widetilde{f}_k^i}(T), d \right\rangle = \int_0^T r(T - \tau) \widetilde{f}_k^i(\tau)\, d\tau. \tag{2.9}$$

Then (see (2.4))

$$a_k^1 = \sum_{i=1}^{L_k} \widetilde{b}_k^i \widetilde{d}_k^i. \tag{2.10}$$

We denote by ∂ and I the differentiation operator and the identity operator in $L_2(0,T)$. We normalize the solutions to (2.5), (2.6) (for $i > l$) by the following rule:

$$\left\langle \left[C^T (\partial - \lambda_k I)\right]^l \widehat{f}_k^i, \widehat{g}_k^{i-l} \right\rangle = 1, \tag{2.11}$$

we define $\widehat{b}_k^i,\ \widehat{d}_k^i$ by (2.8), (2.9) and evaluate:

$$a_k^l = \sum_{i=l}^{L_k} \widehat{b}_k^i \widehat{d}_k^{i-l+1}, \quad l = 2, \dots, L_k. \tag{2.12}$$

We conclude this section with the algorithm for solving the spectral estimation problem: suppose that we are given with the function $r \in L_2(0, 2T)$ of the form (2.3) and the family $\bigcup_{k=1}^{\infty} \{e^{\lambda_k t}, \dots, t^{L_k - 1} e^{\lambda_k t}\}$ is minimal in $L_2(0,T)$. Then, to recover λ_k, L_k and coefficients of polynomials, one should utilize the following:

Algorithm

a) solve generalized eigenvalue problems (2.5), (2.6) to find λ_k, L_k and non-normalized controls.
b) Normalize $\widetilde{f}_k^i$, $\widetilde{g}_k^i$ by (2.7), define $\widetilde{b}_k^i$, $\widetilde{d}_k^i$ by (2.8), (2.9) to recover a_k^1 by (2.10).
c) Normalize $\widehat{f}_k^i$, $\widehat{g}_k^{i-l}$ by (2.11), define $\widehat{b}_k^i$, $\widehat{d}_k^i$ by (2.8), (2.9) to recover a_k^l by (2.12), $l = 2, \dots, L_k - 1$.

3. Equations of the BC method

Let us denote by A^* the operator adjoint to A and $B := O^*$, $B : Y \mapsto H$. Along with system (1.2), we consider the following dynamical control system:

$$\begin{cases} v_t + A^* v = Bf, \quad t < T, \\ v(T) = 0, \end{cases} \tag{3.1}$$

and denote its solution by v^f. The reason we consider the system (3.1) reverse in time is that it is adjoint to (1.2) (see [5, 15]).

For every $0 \leqslant s < T$, we introduce the *control* operator by $W^s f := v^f(s)$. It is easy to verify that $-W^0$ is adjoint to $\mathbb{O}^T$. Indeed, taking $f \in L_2(0, T; Y)$, $a \in H$ we show [15] that:

$$\int_0^T (f, \mathbb{O}a)_Y = -\left(W^0 f, a\right)_H, \tag{3.2}$$

here $\mathbb{O}a = (Ou^a)(t)$. Due to the arbitrariness of f and a, the last equality is equivalent to $\left(\mathbb{O}^T\right)^* = -W^0$.

We assume that the operator A satisfies the following assumptions:

Assumption 1. a) *The spectrum of the operator A, $\{\lambda_k\}_{k=1}^{\infty}$ consists of the eigenvalues λ_k with algebraic multiplicity L_k, $k \in \mathbb{N}$, and the set of all root vectors $\{\phi_k^i\}$, $i = 1, \dots, L_k$, $k \in \mathbb{N}$, form a Riesz basis in H. Here, the vectors from the chain $\{\phi_k^i\}_{i=1}^{L_k}$, $k \in \mathbb{N}$, satisfy the equations*

$$(A - \lambda_k)\,\phi_k^1 = 0, \quad (A - \lambda_k)\,\phi_k^i = \phi_k^{i-1},\ 2 \leqslant i \leqslant L_k.$$

The root vectors of A^*, $\{\psi_k^i\}$, $i = 1, \dots, L_k$, $k \in \mathbb{N}$, form a Riesz basis in H and satisfy:

$$\left(A^* - \overline{\lambda}_k\right)\psi_k^{L_k} = 0, \quad \left(A^* - \overline{\lambda}_k\right)\psi_k^i = \psi_k^{i+1},\ 1 \leqslant i \leqslant L_k - 1.$$

b) *The system (3.1) is spectrally controllable in time T: i.e. there exists the controls $f_k^i \in H_0^1(0, T; Y)$ such that $W^0 f_k^i = \psi_k^i$, for $i = 1, \dots, L_k$, $k \in \mathbb{N}$.*

We say that the vector a is *generic* if its Fourier representation in the basis $\{\phi_k^i\}_{k=1}^{\infty}$, $a = \sum_{k=1}^{\infty} \sum_{i=1}^{L_k} a_k^i \phi_k^i$, is such that $a_k^i \neq 0$ for all k, i. We assume that the controls from the Assumption 1 are extended by zero outside the interval $(0, T)$. Now, we are ready to formulate.

Theorem 1. *If A satisfies Assumption 1, $Y = \mathbb{R}$, and source a is generic, then the spectrum of A and controls f_k^i are the spectrum and the root vectors of the following generalized spectral problem:*

$$\int_0^{2T} \Big((\dot{O}a)(t) - \lambda_k (Oa)(t), f_k(t - T + \tau) \Big)_Y \, dt = 0, \quad 0 < \tau < T. \tag{3.3}$$

Here, by dot, we denote the differentiation with respect to t.

Proof. We denote by $\{\widetilde{f}_k^i\}$ the set of controls which satisfy $W^0\widetilde{f}_k^i = \psi_k^i$. By $\{f_k^i\}$ we denote the set of shifted controls: $f_k^i(t) = \widetilde{f}_k^i(t-T)$. Thus, the control f_k^i acts on the time interval $(T, 2T)$. Let us fix some $i \in 1, \dots, L_k$, $k \in \mathbb{N}$, $\tau \in (0, T)$ and consider $W^0\left(\dot{f}_k^i(\cdot+\tau)\right)$:

$$W^0\left(\dot{f}_k^i(\cdot+\tau)\right) = v^{\dot{f}_k^i(\cdot+\tau)}(0) = v_t^{f_k^i(\cdot+\tau)}(0) = \left(Bf_k^i(\cdot+\tau)\right)(0) - A^* v^{f_k^i(\cdot+\tau)}(0). \tag{3.4}$$

Since $f_k^i \in H_0^1(T, 2T, Y)$, $\left(Bf_k^i(\cdot+\tau)\right)(0) = 0$. The second term on the right side of (3.4) could be evaluated using the following reasons. The function $v^{f_k^i}$ solves:

$$\begin{gathered} v_t^{f_k^i(\cdot+\tau)} + A^* v^{f_k^i(\cdot+\tau)} = 0, \quad 0 \leqslant t \leqslant T-\tau, \\ v^{f_k^i(\cdot+\tau)}(T-\tau) = \psi_k^i. \end{gathered}$$

We are looking for a solution in the form $v^{f_k^i(\cdot+\tau)}(t) = \sum_{j=1}^{L_k} c_k^j(t)\psi_k^j$, then c_k^j satisfies boundary conditions $c_k^j(0) = \delta_{ij}$ and equation:

$$\begin{aligned} &\frac{d}{dt}c_k^1 + \overline{\lambda}_k c_k^1 = 0, \\ &\frac{d}{dt}c_k^j + \overline{\lambda}_k c_k^j + c_k^{j-1} = 0, \quad j = 2, \dots, L_k. \end{aligned}$$

Solving this system, we obtain the following expansion:

$$v^{f_k^i(\cdot+\tau)}(t) = \sum_{j=i}^{L_k} \frac{(T-\tau-t)^{j-i}}{(j-i)!} e^{\overline{\lambda}_k(T-\tau-t)}\psi_k^j. \tag{3.5}$$

Evaluating $A^* v^{f_k^i(\cdot+\tau)}(0)$, making use of (3.5) and properties of the root vectors, we arrive at:

$$\begin{aligned} &A^* v^{f_k^{L_k}(\cdot+\tau)}(0) = \overline{\lambda}_k v^{f_k^{L_k}(\cdot+\tau)}(0), \\ &A^* v^{f_k^i(\cdot+\tau)}(0) = \overline{\lambda}_k v^{f_k^i(\cdot+\tau)}(0) + v^{f_k^{i+1}(\cdot+\tau)}(0), \ i < L_k. \end{aligned}$$

Then, continuing (3.4), we obtain:

$$W^0\left(\dot{f}_k^{L_k}(\cdot+\tau)\right) = -A^* v^{f_k^{L_k}(\cdot+\tau)}(0) = -\overline{\lambda}_k W^0 f_k^{L_k}, \tag{3.6}$$

$$W^0\left(\dot{f}_k^i(\cdot+\tau)\right) = -\overline{\lambda}_k W^0 f_k^i - \overline{\lambda}_k W^0 f_k^{i+1}, \ i < L_k. \tag{3.7}$$

Integrating by parts and taking into account that $f_k^i(0) = f_k^i(T) = 0$ for $i = 1, \dots, L_k$, we get:

$$\begin{aligned} &\int_0^{2T} \left((Oa)(t), \dot{f}_k^i(t+\tau)\right)_Y dt = -\int_0^{2T} \left((\dot{O}a)(t), f_k^i(t+\tau)\right)_Y dt \\ &+ \left((\dot{O}a)(t+\tau), f_k^i(t)\right)_Y\Big|_{t=0}^{t=2T} = -\int_0^{2T} \left((\dot{O}a)(t), f_k^i(t+\tau)\right)_Y dt \end{aligned} \tag{3.8}$$

Conversely, using the duality between W^0 and $\mathbb{O}^T$ and (3.6), (3.7), we have for $i = L_k$:

$$\int_0^{2T} \Big((Oa)(t), \dot{f}_k^{L_k}(t+\tau)\Big)_Y \, dt = -\Big(a, W^0 \dot{f}_k^{L_k}(\cdot+\tau)\Big)_H = \Big(a, \overline{\lambda}_k W^0 f_k^{L_k}(\cdot+\tau)\Big)_H =$$

$$\Big(\lambda_k a, W^0 f_k^{L_k}(\cdot+\tau)\Big)_H = -\int_0^{2T} \Big(\lambda_k (Oa)(t), f_k^{L_k}(t+\tau)\Big)_Y \, dt \quad (3.9)$$

and for $i < L_k$:

$$\int_0^{2T} \Big((Oa)(t), \dot{f}_k^{i}(t+\tau)\Big)_Y \, dt = \big(a, \overline{\lambda}_k W^0 f_k^i(\cdot+\tau) + W^0 f_k^{i+1}(\cdot+\tau)\big)_H =$$

$$-\lambda_k \int_0^{2T} \big((Oa)(t), f_k^i(t+\tau)\big)_Y \, dt - \int_0^{2T} \big((Oa)(t), f_k^{i+1}(t+\tau)\big)_Y \, dt \quad (3.10)$$

In what follows, we assume that elements with index $i = L_k + 1$ or $i = 0$ are zero. Combining (3.8) and (3.9), (3.10), we see that the pair λ_k, f_k satisfies on $0 < \tau < T$, $i = 1, \dots, L_k$:

$$\int_0^{2T} \Big((\dot{Oa})(t) - \lambda_k (Oa)(t), f_k^i(t+\tau)\Big)_Y \, dt = \int_0^{2T} \big((Oa)(t), f_k^{i+1}(t+\tau)\big)_Y \, dt. \quad (3.11)$$

Now we prove the converse; solving the generalized eigenvalue problem:

$$\int_0^{2T} \Big((\dot{Oa})(t) - \lambda (Oa)(t), f(t+\tau)\Big)_Y \, dt = 0 \quad (3.12)$$

yields $\{\lambda_k\}_{k=1}^{\infty}$ eigenvalues of A and controls $\{f_k^i\}$, $i = 1, \dots, L_k$, $k \in \mathbb{N}$.

Let the functions $\{f_1, \dots, f_L\}$ satisfying (3.11) constitute the chain for (3.12) for some λ. Then, as it follows from the proof that for $\tau \in (0, T)$:

$$\Big(a, W^0 \dot{f}_i(t+\tau)\Big)_H + \lambda \big(a, W^0 f_i(t+\tau)\big)_H = -\big(a, W^0 f_{i+1}(t+\tau)\big)_H,$$

which is equivalent to

$$-\big(a, A^* v^{f_i(t+\tau)}(0)\big)_H + \lambda \big(a, v^{f_i(t+\tau)}(0)\big)_H = -\big(a, v^{f_{i+1}(t+\tau)}(0)\big)_H, \ \tau \in (0, T). \quad (3.13)$$

First, we consider case $i = L$. We rewrite the last equality (using the notation $f = f_L$) as:

$$\big(a, A^* v^{f(t+\tau)}(0) - \overline{\lambda} v^{f(t+\tau)}(0)\big)_H = 0, \quad \tau \in (0, T). \quad (3.14)$$

We assume that $v^{f(t+\tau)}(T-\tau) = \sum_{\substack{k\in\mathbb{N} \\ i=1,\dots,L_k}} c_k^i \psi_k^i$. Then, developing v^f in the Fourier series as we did in (3.5), we arrive at:

$$v^{f(t+\tau)}(0) = \sum_{\substack{k\in\mathbb{N} \\ i=1,\dots,L_k}} c_k^i \sum_{j=1}^{L_k} \frac{(T-\tau)^{j-i}}{(j-i)!} e^{\overline{\lambda}_k (T-\tau)} \psi_k^j. \quad (3.15)$$

Applying operator A^* and using the property $A^*\psi_k^j = \overline{\lambda}_k\psi_k^j + \psi_k^{j+1}$, we obtain:

$$A^*v^{f(t+\tau)}(0) = \sum_{\substack{k\in\mathbb{N}\\ i=1,\dots,L_k}} c_k^i \sum_{j=1}^{L_k} \frac{(T-\tau)^{j-i}}{(j-i)!} e^{\overline{\lambda}_k(T-\tau)} \left(\overline{\lambda}_k\psi_k^j + \psi_k^{j+1}\right). \tag{3.16}$$

Introducing the notation:

$$g(\tau) := A^*v^{f(t+\tau)}(0) - \overline{\lambda}v^{f(t+\tau)}(0) = \sum_{\substack{k\in\mathbb{N}\\ i=1,\dots,L_k}} g_k^i(\tau)\psi_k^i, \tag{3.17}$$

relation (3.14) yields:

$$0 = (a,g)_H = \sum_{\substack{k\in\mathbb{N}\\ i=1,\dots,L_k}} a_k^i g_k^i(\tau), \quad \tau\in(0,T). \tag{3.18}$$

The functions $g_k^i(\tau)$ are combination of products of $e^{\overline{\lambda}_k(T-\tau)}$ and polynomials $\frac{(T-\tau)^\alpha}{\alpha!}$. Then, we can rewrite (3.18) as follows:

$$0 = \sum_{\substack{k\in\mathbb{N}\\ i=1,\dots,L_k}} b_k^i \frac{(T-\tau)^{i-1}}{(i-1)!} e^{\overline{\lambda}_k(T-\tau)}, \quad \tau\in(0,T). \tag{3.19}$$

If $Y=\mathbb{R}$, the controllability of the dynamical system (3.1) imply [5] the minimality of the family $\bigcup_{k=1}^\infty\{e^{\overline{\lambda}_k t}, te^{\overline{\lambda}_k t}\dots, t^{L_k-1}e^{\overline{\lambda}_k t}\}$ in $L_2(0,T)$ in $L_2(0,T)$, so we have $b_k^i=0$ for all k,i. However, as follows from (3.15), (3.16):

$$b_k^{L_k} = c_k^1\overline{\lambda}_k a_k^1 - \overline{\lambda}c_k^1 a_k^1 = 0.$$

Then, since a is generic, either $\lambda=\lambda_k$ or $c_k^1=0$.

Let $\lambda\neq\lambda_k$, so $c_k^1=0$. Then, for $b_k^{L_k-1}$, we have:

$$b_k^{L_k-1} = c_k^2\overline{\lambda}_k a_k^2 - \overline{\lambda}c_k^2 a_k^2 = 0,$$

from which the equality $c_k^2=0$ follows. Repeating this procedure for $b_k^{L_k-i}$, $i\geqslant 2$, we obtain:

$$\text{If } \lambda\neq\lambda_k, \text{ then } c_k^i=0,\ i=1,\dots,L_k. \tag{3.20}$$

We consider the second option; let $\lambda=\lambda_k$. Then, from (3.15) and (3.16):

$$b_k^{L_k-1} = c_k^1 = 0, \quad b_k^{L_k-2} = c_k^2 a_k^3 = 0, \dots, b_k^1 = c_k^{L_k-1}a_k^{L_k} = 0.$$

So, we arrive at the following:

$$\text{If } \lambda=\lambda_k, \text{ then } c_k^i=0,\ i=1,\dots,L_k-1, \text{ and } c_k^{L_k} \text{ could be arbitrary.} \tag{3.21}$$

Finally (3.20), (3.21) imply that $\lambda=\lambda_{k'}$ and $f=c_{k'}f_{k'}^{L_{k'}}$, $c_{k'}\neq 0$, for some k'.

Thus, on the first step we already obtained that $\lambda=\lambda_{k'}$ for some k' and $f_L = c_{k'}f_{k'}^{L_{k'}}$. The second vector f in the Jordan chain satisfies

$$\int_0^{2T} \left((\dot{Oa})(t) - \lambda_{k'}(Oa)(t), f(t+\tau)\right)_Y dt = \int_0^{2T} \left((Oa)(t), c_{k'}f_{k'}^{L_{k'}}(t+\tau)\right)_Y dt.$$

We rewrite (3.13) in our case:

$$-\left(a, A^*v^{f(t+\tau)}(0)\right)_H + \lambda_{k'}\left(a, v^{f(t+\tau)}(0)\right)_H = -\left(a, c_{k'}v^{f_{k'}^{L_{k'}}(t+\tau)}(0)\right)_H, \ \tau\in(0,T). \tag{3.22}$$

In this case, g, introduced in (3.17), has the form:

$$g(\tau) = \sum_{\substack{k\in\mathbb{N}\\ i=1,\dots,L_k}} c_k^i \sum_{j=1}^{L_k} \frac{(T-\tau)^{j-i}}{(j-i)!} e^{\overline{\lambda}_k(T-\tau)} \left(\left(\overline{\lambda}_k - \overline{\lambda}_{k'}\right)\psi_k^j + \psi_k^{j+1}\right),$$

and rewrite (3.22) as:

$$(a,g)_H = \left(a, v^{f_{k'}^{L_{k'}}(\cdot+\tau)}\right)_H = c_{k'} a_{k'}^{L_{k'}} e^{\overline{\lambda}_{k'}(T-\tau)} \tag{3.23}$$

Using the same notations in (3.18) and (3.19), we transcribe the equalities for coefficients b_k^i for (3.23) to get:

$$b_{k'}^1 = c_{k'} a_{k'}^{L_{k'}}, \quad b_k^i = 0, \quad k \neq k',$$

In the case $k \neq k'$, we repeat the arguments used above and find that:

$$c_k^i = 0, \quad i = 1, \dots, L_k.$$

When $k = k'$, we have:

$$b_{k'}^{L_{k'}} = 0, \quad b_{k'}^{L_{k'}-1} = c_{k'}^1 a_{k'}^{L_{k'}} = 0, \quad b_{k'}^{L_{k'}-2} = c_{k'}^2 a_{k'}^{L_{k'}} = 0,$$
$$b_{k'}^2 = c_{k'}^{L_{k'}-2} a_{k'}^{L_{k'}} = 0, \quad b_{k'}^1 = c_{k'}^{L_{k'}-1} a_{k'}^{L_{k'}} = c_{k'} a_{k'}^{L_{k'}}.$$

So, we find:

$$c_{k'}^i = 0, \quad i < L_{k'} - 1, \quad c_{k'}^{L_{k'}-1} = c_{k'}, \quad c_{k'}^{L_{k'}} \text{ is arbitrary.}$$

So, finally we arrive at for some c_{L-1}:

$$f = f_{L-1} = c_{k'} f_{k'}^{L_{k'}-1} + c_{L-1} f_{k'}^{L_{k'}}$$

Arguing in the same fashion, we obtain that:

$$f_i = c_{k'} f_{k'}^{L_{k'}-i} + c_i f_{k'}^{L_{k'}}, \quad 1 \leqslant i < L_{k'} - 1.$$

So, we have shown that the elements of the Jordan chain for (3.3) which correspond to eigenvalue $\lambda_{k'}$ are the linear combination of corresponding controls and eigenvector (i.e. the control that generate the eigenvector of A^*). □

Remark 1. *The solution to (3.3) yields $\{\lambda_k\}_{k=1}^{\infty}$ eigenvalues of A and (non-normalized) root vectors $\{\widehat{f_k^i}\}$, $\widehat{f_k^i} = c_k f_k^i + c_k^i f_k^{L_k}$ $k \in \mathbb{N}$, $i = 1, \dots, L_k$, $c_k^{L_k} = 0$.*

For the dynamical system (1.2), under the conditions on A, Y, formulated in Theorem 1, there is the possibility to extend the observation $y(t) = (Ou^a)(t)$ defined for $t \in (0, 2T)$ to $t \in \mathbb{R}_+$. To this end, we show that for an observation having the form:

$$\mathbb{O}a = \sum_{k\in\mathbb{N}} e^{\lambda_k t} \sum_{j=1}^{L_k} \frac{b_k^j t^{L_k - j}}{(L_k - j)!}, \tag{3.24}$$

we can recover the coefficients b_k^j.

Take $i \in \{1, \dots, L_k\}$ and search for the solution to (1.2) with $a = \phi_k^i$ in the form $u = \sum_{l=1}^{L_k} c_l(t)\phi_k^l$, we arrive at the system (here $c_{L_k+1} = 0$):

$$\frac{d}{dt}c_l(t) - \lambda_k c_l(t) = c_{l+1}(t), \quad l = 1, \dots, L_k,$$
$$c_l(0) = \delta_{li}.$$

whose solution is:

$$c_l(t) = \frac{t^{i-l}}{(i-l)!} e^{\lambda_k t}, \quad l \leqslant i,$$
$$c_l(t) = 0, \quad l > i.$$

Thus,

$$u^{\phi_k^i} = \sum_{l=1}^{i} \frac{t^{i-l}}{(i-l)!} e^{\lambda_k t} \phi_k^l. \tag{3.25}$$

For the initial state $a = \sum_{k\in\mathbb{N}} \sum_{i=1}^{L_k} a_k^i \phi_k^i$, we obtain:

$$u^a = \sum_{k\in\mathbb{N}} e^{\lambda_k t} \sum_{j=1}^{L_k} \frac{t^{L_k-j}}{(L_k-j)!} \sum_{l=1}^{j} a_k^{L_k-j+l} \phi_k^l.$$

So, for observation $(\mathbb{O}a)(t) = (Ou^a)(t)$, we derive the representation (3.24) with coefficients b_k^j, defined by:

$$b_k^j := \sum_{l=1}^{j} a_k^{L_k-j+l} O\phi_k^l, \quad k \in \mathbb{N},\ j = 1, \dots, L_k. \tag{3.26}$$

Making use of Theorem 1 (see also Remark 1), we have:

$$W^0 \widehat{f_k^i} = c_k \psi_k^i + c_k^i \psi_k^{L_k}, \quad k \in \mathbb{N},\ i = 1, \dots, L_k,\ c_k^{L_k} = 0. \tag{3.27}$$

Counting (3.2), we write:

$$\left(W^0 \widehat{f_k^i}, a\right)_H = -\int_0^T Ou^a \widehat{f_k^i}\, dt.$$

We plug $a = \phi_k^i$ into the last equality and use (3.27) to get:

$$c_k = \left(c_k \psi_k^i + c_k^i \psi_k^{L_k}, \phi_k^i\right)_H = -\int_0^T Ou^{\phi_k^i} \widehat{f_k^i}\, dt. \tag{3.28}$$

We evaluate the right side of (3.28) for all i. For $i = 1$ we get (see (3.25)):

$$c_k = -O\phi_k^1 \int_0^T e^{\lambda_k t} \widehat{f_k^1}\, dt.$$

Or equivalently:

$$\frac{c_k}{O\phi_k^1} = -\int_0^T e^{\lambda_k t} \widehat{f_k^1}\, dt. \tag{3.29}$$

Evaluating (3.28) for $i = 2$, counting (3.25), we obtain:

$$c_k = -O\phi_k^2 \int_0^T e^{\lambda_k t} \widehat{f_k^2}\, dt - O\phi_k^1 \int_0^T t e^{\lambda_k t} \widehat{f_k^2}\, dt.$$

We divide this equality by c_k and plug (3.29) in to find:

$$\frac{c_k}{O\phi_k^2} = -\frac{\int\limits_0^T e^{\lambda_k t}\widehat{f}_k^1\,dt\int\limits_0^T e^{\lambda_k t}\widehat{f}_k^2\,dt}{\int\limits_0^T e^{\lambda_k t}\widehat{f}_k^1\,dt - \int\limits_0^T te^{\lambda_k t}\widehat{f}_k^2\,dt} \tag{3.30}$$

Suppose we already found $\frac{c_k}{O\phi_k^l}$ for $l = 1, \dots, i-1$. To find this quantity for $l = i$, we evaluate (3.28), plugging the expression for $u^{\phi_k^i}$ (3.25):

$$c_k = -\sum_{l=1}^{i} O\phi_k^l \int\limits_0^T \frac{t^{i-l}}{(i-l)!}e^{\lambda_k t}\widehat{f}_k^i\,dt.$$

We divide last equality by c_k to find:

$$\frac{c_k}{O\phi_k^i} = -\frac{\int\limits_0^T e^{\lambda_k t}\widehat{f}_k^i\,dt}{1+\sum\limits_{l=1}^{i-1}\int\limits_0^T \frac{t^{i-l}}{(i-l)!}e^{\lambda_k t}\widehat{f}_k^i\,dt\left(\frac{c_k}{O\phi_k^l}\right)^{-1}}. \tag{3.31}$$

Observe that in the right side of (3.31) in view of (3.30), we know all terms.

To evaluate a_k^i, we use, see (3.27):

$$a_k^i = \left(a,\psi_k^i\right)_H = \left(a, W^0\widehat{f}_k^i - c_k^i\psi_k^{L_k}\right)_H\frac{1}{c_k} = -\int\limits_0^T Ou^a\widehat{f}_k^i\,dt\frac{1}{c_k} - a_k^{L_k}\frac{c_k^i}{c_k} \tag{3.32}$$

We multiply (3.27) by $\phi_k^{L_k}$ and obtain for $i < L_k$:

$$\begin{aligned} c_k^i = \left(W^0 f_k^i, \phi_k^{L_k}\right)_H &= -\int\limits_0^T f_k^i(t)\left(Ou^{\phi_k^{L_k}}\right)(t)\,dt \\ &= -\sum_{l=1}^{L_k} O\phi_k^l\int\limits_0^T\frac{t^{L_k-l}}{(L_k-l)!}e^{\lambda_k t}f_k^i(t)\,dt. \end{aligned}$$

Dividing the last equality by c_k, we obtain:

$$\frac{c_k^i}{c_k} = -\sum_{l=1}^{L_k}\left(\frac{c_k}{O\phi_k^l}\right)^{-1}\int\limits_0^T\frac{t^{L_k-l}}{(L_k-l)!}e^{\lambda_k t}f_k^i(t)\,dt, \quad i < L_k. \tag{3.33}$$

Notice that in view of (3.31), we know all terms in the right hand side in (3.33). Now, we multiply (3.32) by c_k:

$$a_k^i c_k = -\int\limits_0^T Ou^a\widehat{f}_k^i\,dt - a_k^{L_k}c_k\frac{c_k^i}{c_k}.$$

Since $c_k^{L_k} = 0$, we have for $i = L_k$:

$$a_k^{L_k}c_k = -\int\limits_0^T \widehat{f}_k^{L_k}(t)\left(Ou^a\right)(t)\,dt,$$

and finally:

$$a_k^i c_k = -\int_0^T \widehat{f}_k^i(t)\,(Ou^a)\,(t)\,dt + \int_0^T \widehat{f}_k^{L_k}(t)\,(Ou^a)\,(t)\,dt\frac{c_k^i}{c_k}. \tag{3.34}$$

In view of (3.33), we know all terms on the right side of (3.34).

Now, we rewrite formula for b_k^j (3.26):

$$b_k^j := \sum_{l=1}^{j} \left\{a_k^{L_k-j+l} c_k\right\} \left(\frac{O\phi_k^l}{c_k}\right) \quad k \in \mathbb{N},\ j = 1, \dots, L_k, \tag{3.35}$$

and observe that the first term in each summand is given by (3.34), while the second term by (3.31). So, we know right hand side in (3.35).

After we recovered all b_k^j by (3.35), we can extend the observation $(\mathbb{O}a)(t)$ by formula (3.24) for $t > 2T$.

4. Application to inverse problems

Here, we provide two applications of the above-developed theory to inverse problems. Other applications of the BC approach to the spectral estimation problem can be found in [1, 2, 4, 7–9, 15].

4.1. Reconstructing the potential for the 1D Schrödinger equation from boundary measurements

Let the real potential $q \in L^1(0,1)$ and $a \in H_0^1(0,1)$ be fixed, we consider the boundary value problem:

$$\begin{cases} iu_t(x,t) - u_{xx}(x,t) + q(x)u(x,t) = 0 & t > 0, \quad 0 < x < 1 \\ u(0,t) = u(1,t) = 0 & t > 0, \\ u(x,0) = a(x) & 0 < x < 1. \end{cases} \tag{4.1}$$

Assuming that the initial datum a is generic (but unknown), the inverse problem we are interested in is to determine the potential q from the trace of the derivative of the solution u to (4.1) on the boundary:

$$\{r_0(t), r_1(t)\} := \{u_x(0,t), u_x(1,t)\}, \quad t \in (0, 2T),$$

It is well known that the self-adjoint operator A defined on $L^2(0,1)$ by:

$$A\phi = -\phi'' + q\phi, \quad D(A) := H^2(0,1) \cap H_0^1(0,1), \tag{4.2}$$

admits a family of eigenfunctions $\{\phi_k\}_{k=1}^{\infty}$ forming a orthonormal basis in $L^2(0,1)$, and associated sequence of eigenvalues $\lambda_k \to +\infty$. Using the Fourier method, we can represent the solution of (4.1) in the form:

$$u(x,t) = \sum_{k=1}^{\infty} a_k e^{i\lambda_k t}\phi_k(x), \quad a_k = (a, \phi_k)_{L^2(0,1)} \tag{4.3}$$

The inverse data admits the representation:

$$\{r_0(t), r_1(t)\} = \left\{\sum_{k=1}^{\infty} a_k e^{i\lambda_k t}\phi_k'(0), \sum_{k=1}^{\infty} a_k e^{i\lambda_k t}\phi_k'(1)\right\}. \tag{4.4}$$

One can prove that $r_0, r_1 \in L^2(0,T)$. Using the method from the first section, we recover the eigenvalues λ_k of A and the products $\phi_k'(0)a_k$ and $\phi_k'(1)a_k$. So (as a is generic) we recovered the spectral data consisting of:

$$D := \left\{ \lambda_k, \frac{\phi_k'(1)}{\phi_k'(0)} \right\}_{k=1}^{\infty}. \tag{4.5}$$

Now from D we construct the spectral function associated with A.

Given $\lambda \in \mathbb{C}$, we denote by $y(\cdot,\lambda)$ the solution to:

$$\begin{cases} -y''(x,\lambda) + q(x)y(x,\lambda) = \lambda y(x,\lambda), & 0 < x < 1, \\ y(0,\lambda) = 0, \quad y'(0,\lambda) = 1. \end{cases}$$

Then, the eigenvalues of the Dirichlet problem of A are exactly the zeros of the function $y(1,\lambda)$, while a family of normalized corresponding eigenfunctions is given by $\phi_k(x) = \dfrac{y(x,\lambda_k)}{\|y(\cdot,\lambda_k)\|}$. Thus, we can rewrite the second components in D in the following way:

$$\frac{\phi_k'(1)}{\phi_k'(0)} = \frac{y'(1,\lambda_k)}{y'(0,\lambda_k)} = y'(1,\lambda_k) =: A_k. \tag{4.6}$$

Let us denote by dot the derivative with respect to λ and λ_n be an eigenvalue of A. We borrowed the following fact from [17, p. 30]:

$$\|y(\cdot,\lambda_k)\|_{L^2}^2 = y'(1,\lambda_k)\dot{y}(1,\lambda_k),$$

$$y(1,\lambda) = \prod_{n\geqslant 1} \frac{\lambda_n - \lambda}{n^2\pi^2}$$

$$\dot{y}(1,\lambda_k) = -\frac{1}{k^2\pi^2} \prod_{n\geqslant 1, n\neq k} \frac{\lambda_n - \lambda_k}{n^2\pi^2} =: B_k.$$

Notice that the set of pairs $\{\lambda_k, \|y(\cdot,\lambda_k)\|_{L^2}^2\}_{k=1}^{\infty} =: \widetilde{D}$ is "classical" spectral data. Using the above relations, we come to $\widetilde{D} = \{\lambda_k, A_kB_k\}_{k=1}^{\infty}$. Let $\alpha_k^2 := \|y(\cdot,\lambda_k)\|_{L^2}^2 = A_kB_k$, we introduce the spectral function associated with A:

$$\rho(\lambda) = \begin{cases} -\sum\limits_{\lambda\leqslant\lambda_k\leqslant 0} \frac{1}{\alpha_k^2} & \lambda \leqslant 0, \\ \sum\limits_{0<\lambda_k\leqslant\lambda} \frac{1}{\alpha_k^2} & \lambda > 0, \end{cases}$$

which is a monotonously increasing function having jumps at the points of the Dirichlet spectra. The regularized spectral function is introduced by:

$$\sigma(\lambda) = \begin{cases} \rho(\lambda) - \rho_0(\lambda) & \lambda \geqslant 0, \\ \rho(\lambda) & \lambda < 0, \end{cases} \qquad \rho_0(\lambda) = \sum_{0<\lambda_k^0\leqslant\lambda} \frac{1}{(\alpha_k^0)^2} \quad \lambda > 0,$$

where ρ_0 is the spectral function associated with the operator A with $q \equiv 0$. The potential can thus be recovered from $\sigma(\lambda)$ by Gelfand-Levitan, Krein or the BC method (see [6, 14]). Once the potential has been found, we can recover the eigenfunctions ϕ_k, the traces $\phi_k'(0)$ and Fourier coefficients a_k, $k = 1, \ldots \infty$. Thus, the initial state can be recovered via its Fourier series.

4.2. Extension of the inverse data

We fix $p_{ij} \in C^1([0,1];\mathbb{C})$, $d_1, d_2 \in L_2(0,1;\mathbb{C})$ and consider on interval $(0,1)$ the initial boundary value problem:

$$\begin{cases} \frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} - \frac{\partial}{\partial x}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} - \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = 0, \quad t > 0, \\ u(0,t) = u(1,t) = 0, \quad t > 0, \\ \begin{pmatrix} u(x,0) \\ v(x,0) \end{pmatrix} = \begin{pmatrix} d_1(x) \\ d_2(x) \end{pmatrix}, \quad 0 \leqslant x \leqslant 1. \end{cases} \tag{4.7}$$

We fix some $T > 0$ and define $R(t) := \{v(0,t), v(1,t)\}$, $0 \leqslant t \leqslant T$. Here, we focus on the problem of the continuation of the inverse data: we assume that $R(t)$ is known on the interval $(0,T)$, $T > 2$, and recover it on the whole real axis. The problem of recovering unknown coefficients p_{ij} and initial state $c_{1,2}$ has been considered in [19,20], where the authors established the uniqueness result, having the response $R(t)$ on the interval $(-T,T)$ for large enough T.

We introduce the notations $B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $P = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix}$, $D = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}$ and the operators A, A^* acting by the rule:

$$A = B\frac{d}{dx} + P, \quad \text{on } (0,1),$$
$$A^*\psi = -B\frac{d}{dx} + P^T, \quad \text{on } (0,1),$$

with the domains:

$$D(A) = D(A^*) = \left\{ \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \in H^1(0,1;\mathbb{C}^2) \,|\, \varphi_1(0) = \varphi_1(1) = 0 \right\}.$$

The spectrum of the operator A has the following structure (see [19, 20]): $\sigma(A) = \Sigma_1 \cup \Sigma_2$, where $\Sigma_1 \cap \Sigma_2 = \emptyset$ and there exists $N_1 \in \mathbb{N}$ such that

1) Σ_1 consists of $2N_1 - 1$ eigenvalues including algebraical multiplicities
2) Σ_2 consists of infinite number of eigenvalues of multiplicity one
3) Root vectors of A form a Riesz basis in $L_2(0,1;\mathbb{C}^2)$.

Let m denote the algebraical multiplicity of eigenvalue λ, and we introduce the notations:

$$\Sigma_1 = \left\{\lambda^i \in \sigma(A),\, m_i \geqslant 2,\, 1 \leqslant i \leqslant N\right\},$$
$$\Sigma_2 = \left\{\lambda_n \in \sigma(A),\, \lambda_n \text{ is simple },\, n \in \mathbb{Z}\right\}.$$

Let $e_1 := \binom{0}{1}$. The root vectors are introduced in the following way:

$$\left(A - \lambda^i\right)\phi_1^i = 0, \quad \left(A - \lambda^i\right)\phi_j^i = \phi_{j-1}^i, \quad 2 \leqslant j \leqslant m_i,$$
$$\phi_j^i(0) = e_1,\ \phi_j^i \in D(A),\ 1 \leqslant j \leqslant m_i.$$

For the adjoint operator, the following equalities are valid:

$$\left(A^* - \overline{\lambda}^i\right)\psi_{m_i}^i = 0, \quad \left(A^* - \overline{\lambda}^i\right)\psi_j^i = \psi_{j+1}^i, \quad 1 \leqslant j \leqslant m_i - 1,$$
$$\psi_j^i(0) = e_1,\ \psi_j^i \in D(A^*),\ 1 \leqslant j \leqslant m_i.$$

For the simple eigenvalues, we have:

$$(A-\lambda_n)\,\phi_n=0,\quad \left(A^*-\overline{\lambda}_n\right)\psi_n=0,\quad \text{for } n\in\mathbb{Z},$$
$$\phi_n(0)=\psi_n(0)=e_1,\ \phi_n\in D(A),\ \psi_n\in D(A^*).$$

Moreover, the following biorthogonality conditions hold:

$$\left(\phi_j^i,\psi_n\right)=0,\quad \left(\phi_n,\psi_j^i\right)=0,\quad (\phi_k,\psi_n)=0,$$
$$\left(\phi_j^i,\psi_l^k\right)=0,\quad \text{if } i\neq k \text{ or } j\neq l,$$
$$\rho_j^i=\left(\phi_j^i,\psi_j^i\right),\quad i=1,\dots,N,\quad j=1,\dots,m_i,$$
$$\rho_n=\left(\phi_n,\psi_n\right),\quad n\in\mathbb{Z}.$$

We represent the initial state as the series:

$$D=\sum_{i=1}^{N}\sum_{j=1}^{m_i}d_j^i\phi_j^i(x)+\sum_{n\in\mathbb{Z}}d_n\phi_n(x), \tag{4.8}$$

and search for the solution to (4.7) in the form:

$$\begin{pmatrix}u\\ v\end{pmatrix}(x,t)=\sum_{i=1}^{N}\sum_{j=1}^{m_i}c_j^i(t)\phi_j^i(x)+\sum_{n\in\mathbb{Z}}c_n(t)\phi_n(x).$$

Using the method of moments, we can derive the system of ODe's for c_j^i, $i\in\{1,\dots,N\}$, $j\in\{1,\dots,m_i\}$, c_n, $n\in\mathbb{Z}$, solving which we obtain:

$$c_j^i(t)=e^{\lambda^i t}\left[d_j^i+d_{j+1}^i t+d_{j+2}^i\frac{t^2}{2}+\ldots+d_{m_i}^i\frac{t^{m_i-j}}{(m_i-j)!}\right],\quad c_n(t)=d_n e^{\lambda_n t}.$$

Notice that the response $\{v(0,t),v(1,t)\}$ has a form depicted in (1.1):

$$v(0,t)=\sum_{i=1}^{N}e^{\lambda^i t}a_i^0(t)+\sum_{n\in\mathbb{Z}}e^{\lambda_n t}d_n\left(\phi_n(0)\right)_2, \tag{4.9}$$

$$v(1,t)=\sum_{i=1}^{N}e^{\lambda^i t}a_i^1(t)+\sum_{n\in\mathbb{Z}}e^{\lambda_n t}d_n\left(\phi_n(1)\right)_2, \tag{4.10}$$

where the coefficients of $a_i^0(t)=\sum_{k=0}^{m_i-1}\alpha_k^i t^k$ are given by

$$\alpha_0^i=\sum_{l=1}^{m_i}d_l^i\left(\phi_l^i(0)\right)_2,\quad \alpha_1^i=\sum_{l=2}^{m_i}d_l^i\left(\phi_{l-1}^i(0)\right)_2,\quad \alpha_2^i=\frac{1}{2}\sum_{l=3}^{m_i}d_l^i\left(\phi_{l-2}^i(0)\right)_2,$$
$$\ldots,\alpha_k^i=\frac{1}{k!}\sum_{l=k+1}^{m_i}d_l^i\left(\phi_{l-k}^i(0)\right)_2,\ldots\quad \alpha_{m_i-1}^i=\frac{1}{(m_i-1)!}d_{m_i}^i\left(\phi_1^i(0)\right)_2.$$

The coefficients $a_i^1(t)$, $i=1,\dots,N$ are defined by the similar formulas.

We assume that the initial state D is generic. Introducing the notation $U:=\binom{u}{v}$, we consider the dynamical system with the boundary control $f\in L_2(\mathbb{R}_+)$:

$$\begin{cases}U_t-AU=0,\quad 0\leqslant x\leqslant 1,\ t>0,\\ u(0,t)=f(t),u(1,t)=0,\quad t>0,\\ U(x,0)=0.\end{cases}$$

It is not difficult to show that this system is exactly controllable in time $T\geq 2$. This implies (see [5]) that the family $\bigcup_{i=1}^{N}\{e^{\lambda^i t},\dots,t^{m_i-1}e^{\lambda^i t}\}\cup\{e^{\lambda_n t}\}_{n\in\mathbb{Z}}$ forms a Riesz basis in a closure

of its linear span in $L_2((0,T);\mathbb{C})$. So we can apply the method from the second sections to recover λ^i, m_i, coefficients of polynomials $a_i^{0,1}(t)$ $i = 1, \dots, N$, λ_n, $n \in \mathbb{Z}$. The latter allows one to extend the inverse data $R(t)$ to all values of $t \in \mathbb{R}$ by formulas (4.9), (4.10). This is important for the solution of the identification problem, see [20].

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ON THE DERIVATION OF THE SCHRÖDINGER EQUATION WITH POINT-LIKE NONLINEARITY

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In this report we discuss the problem of approximating nonlinear delta-interactions in dimensions one and three with regular, local or non-local nonlinearities. Concerning the one dimensional case, we discuss a recent result proved in [10], on the derivation of nonlinear delta-interactions as limit of scaled, local nonlinearities. For the three dimensional case, we consider an equation with scaled, non-local nonlinearity. We conjecture that such an equation approximates the nonlinear delta-interaction, and give an heuristic argument to support our conjecture.

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1. Introduction

Point interactions in quantum mechanics describe the dynamics of particles in interaction with potentials supported on a (finite or infinite) set of points. In dimension one, they are quite easily understood as a limit of short range potentials and they have been a subject of study since the very early years of quantum mechanics, a most well-known application is the Kronig-Penney model [17], which describes the dynamics of electrons in crystals. In higher dimensions, the first attempts to use point interaction came from nuclear physics, to describe the short range interactions between nucleons. It was found that to define a potential supported in one point in dimension larger than one is a subtler and less intuitive matter. Indeed, a rigorous mathematical definition of point potentials in dimension three was achieved only in the 1960's with the work of Berezin and Faddeev [7].

At a formal level the Hamiltonian describing a particle in a potential supported by points can be written as: $H_\alpha = -\Delta + \sum_j \alpha_j \delta_{y_j}$, where $\alpha = \{\alpha_j\}$ is a set of assigned real constants, $Y = \{y_j\}$ is a fixed set of points in $\mathbb{R}^d$, and δ_{y_j} is the Dirac delta-distribution centered in y_j. For this reason, H_α is also referred to as delta-interaction. For a thorough discussion on the Hamiltonian H_α see [6], the monograph also includes an historical overview of the topic and an appendix with an update on the progresses in the area.

The subject of this report is the Schrödinger equation associated with a nonlinear version of the Hamiltonian H_α in which the constants α_j depend on the state of the system. Such an equation describes the propagation of a wave function in a medium whose response is nonlinear only in some isolated points. The question that we want to address is whether the solution of the equation with point-like nonlinearities is approximated by the solution of an equation with smooth nonlinear terms.

We shall focus attention only on the one and three dimensional cases. They will be discussed separately, with the related applications and literature, in Sec. 2 and 3 respectively.

In dimension one, a solution to the approximating problem was given in [10]. Here we shall briefly discuss the result and give a sketch of the proof, we refer to [10] for the details.

In dimension three , the problem is still open. Here we shall exhibit an equation that we conjecture to approximate the nonlinear delta-interaction, and give an heuristic argument to support our conjecture.

To the best of our knowledge very little is known about the two dimensional case. Also the correct definition of the limit problem, and the study of the well-posedness, is not yet done. In dimension four or higher, instead, the problem cannot be set up because is not possible to define the Hamiltonian H_α, see [6].

In what follows we shall construct the approximating equation by introducing a small scaling parameter that will be denoted by ε. We shall denote by c a generic positive constant whose value may change from line to line. The constant c may depend on the parameters entering the equations and on the initial data, but in no case c will depend on the scaling parameter.

2. Nonlinear delta-interactions in dimension one

In this section we shall present a review on the Schrödinger equation with delta-like nonlinearities concentrated in a fixed set of points in dimension one. We shall recall the definition of the equation and the basic results about its well-posedness, this part is a survey of the works [4, 5] and [16]. Then we shall state the main result of [10] on the derivation of the equation as the limit of Schrödinger equations with spatially non-homogeneous scaled nonlinearity, and discuss the basic ideas behind the proof. We shall also mention a different approximation method based on non-local smoothed nonlinearities, this method was used in [16] as an intermediate step in the proof of the well-posedness of the limit equation.

To begin, it is worth recalling the definition of the operator H_α in dimension one.

The domain of the self-adjoint operator H_α is

$$D(H_\alpha) = \{\psi \in H^2(\mathbb{R}\backslash Y) \cap H^1(\mathbb{R}) \,:\, \psi'(y_j^+) - \psi'(y_j^-) = \alpha_j \psi(y_j)\}. \tag{1}$$

The operator H_α acts on the elements in its domain as the Laplacian, everywhere, except that in the points y_j, i.e.,

$$H_\alpha \psi = -\psi'' \qquad \forall x \neq y_j,\, j = 1, ..., N \tag{2}$$

for any $\psi \in D(H_\alpha)$.

The form domain of H_α does not depend on the parameters α_j and coincides with $H^1(\mathbb{R})$.

To give a precise definition of the nonlinear dynamics in which we are interested, we start with a discussion on the non-autonomous Hamiltonian $H_{\alpha(t)}$, for which we let the parameters α_j depend on the time variable t. Such Hamiltonians are interesting on their own both from the physical and mathematical point of view, see, e.g., [15, 19] and references therein.

When $\alpha_j(t)$ are assigned real valued functions of time, the domain $D(H_{\alpha(t)})$ changes in time as well. In particular, if $\psi(t) \in D(H_{\alpha(t)})$, then $\psi(t)$ must satisfy the time dependent jump conditions $\psi'(t, y_j^+) - \psi'(t, y_j^-) = \alpha_j(t)\psi(t, y_j)$. Conversely, the form domain of $H_{\alpha(t)}$ does not depend on t and coincides with $H^1(\mathbb{R})$.

Consider the Cauchy problem

$$\begin{cases} i\dfrac{d}{dt}\psi(t) = H_{\alpha(t)}\psi(t) \\ \psi|_{t=0} = \psi_0 \end{cases} \tag{3}$$

The weak solutions of (3) are the solutions of the associated integral equation

$$\psi(t,x) = (U(t) * \psi_0)(x) - i\sum_{j=1}^{N}\int_0^t ds\, U(t-s, x-y_j)\alpha_j(s)\psi(s,y_j), \tag{4}$$

where $U(t)$ is the unitary evolution group associated to the free Laplacian in dimension one, its explicit expression is given by

$$U(t,x) = \frac{e^{i\frac{x^2}{4t}}}{(4\pi i t)^{1/2}}.$$

The solutions of (4) belong to the domain of $H_{\alpha(t)}$ only under suitable assumptions on the initial datum and on the regularity of the functions $\alpha_j(t)$. For a discussion on this problem we refer to the works [15, 19].

From (4), it is clear that the solution $\psi(t,x)$ is fully determined from the quantities $\psi(t,y_j)$, $j = 1, ..., N$. Then, by evaluating the equation (4) in y_k, $k = 1, ..., N$, the problem of finding $\psi(t,x)$ can be reduced to solve a system of N coupled Volterra equations for the functions $\psi(t,y_k)$. This fact will also be used in the analysis of the nonlinear problem.

To define the nonlinear delta-interactions we use the weak formulation (4) and mimic the nonlinear flow on it by letting $\alpha_j(t) \to \alpha_j(|\psi(t,y_j)|^2)$. In this way we give a weak formulation of the problem given by the equation $i\partial_t\psi = -\partial^2_{xx}\psi + \sum_{j=1}^{N}\alpha_j(|\psi(t,y_j)|^2)\,\delta_{y_j}\,\psi$ with initial datum ψ_0. We remark that the choice of the nonlinearity $\alpha_j(|\psi(t,y_j)|^2)$ guarantees that the equation is invariant under phase multiplication and that the nonlinearity is local; strong solutions should satisfy the jump condition $\psi'(t,y_j^+) - \psi'(t,y_j^-) = \alpha_j(|\psi(t,y_j)|^2)\psi(t,y_j)$.

We shall follow [4, 5] and consider only power-type nonlinearities, i.e., $\alpha_j(z) = \gamma_j z^{\mu_j}$ for some real constants γ_j, and $\mu_j > 0$, but more general nonlinearities could be considered, see, e.g., [16]. Our model nonlinear delta-interaction is then defined by the integral equation

$$\psi(t,x) = (U(t) * \psi_0)(x) - i\sum_{j=1}^{N}\gamma_j\int_0^t ds\, U(t-s, x-y_j)|\psi(s,y_j)|^{2\mu_j}\psi(s,y_j). \tag{5}$$

This is a weak formulation of the problem

$$\begin{cases} i\dfrac{\partial}{\partial t}\psi(t,x) = -\dfrac{\partial^2}{\partial x^2}\psi(t,x) + \displaystyle\sum_{j=1}^{N}\gamma_j\,\delta_{y_j}\,|\psi(t,y_j)|^{2\mu_j}\psi(t,x) \\ \psi(0,x) = \psi_0(x). \end{cases}$$

Nonlinear point interactions of this form have been used in solid state physics, see, e.g., [8, 18] (and references therein), and, more recently, to model nonlinear periodic systems, such as Bose-Einstein condensates trapped into optical lattices, see [14].

As for the time dependent delta-interactions, we do not address here the problem of showing under what conditions on γ_j, μ_j and ψ_0, the solution of (5) satisfies the jump condition $\psi'(t,y_j^+) - \psi'(t,y_j^-) = \gamma_j|\psi(t,y_j)|^{2\mu_j}\psi(t,y_j)$. Instead we take initial data in the form domain, $H^1(\mathbb{R})$, and discuss the well-posedness and the approximation problem in $H^1(\mathbb{R})$.

We start by recalling that global well-posedness of (5) for initial data in $H^1(\mathbb{R})$ and under the condition that

$$\mu_j < 1 \quad \text{if} \qquad \gamma_j < 0 \tag{6}$$

was proved in [5] (see also [16] for different kind of nonlinearities).

The proof of global well-posedness as given in [5] follows a standard scheme: first prove local well-posedness; then show that there exist some conserved quantities; finally, extend the well-posedness to an arbitrarily large time T by exploiting the conserved quantities together with results on the existence of global solutions for the Volterra equations. We shall not comment on the first step of the proof, the analysis of the local well-posedness. For the purposes of this report it is enough to discuss the conservation laws and how they affect the proof of the global well-posedness, the discussion will make clear where the condition (6) plays a role.

For any initial state in $H^1(\mathbb{R})$, there exist two quantities which are conserved by the nonlinear flow (5): the L^2-norm (also referred to as *mass*), and the energy

$$E[\psi] = \|\psi'\|^2 + \sum_{j=1}^{N} \frac{\gamma_j}{\mu_j + 1} |\psi(y_j)|^{2\mu_j+2}.$$

Then, if $\psi(t)$ is the solution of (5) with $\psi_0 \in H^1(\mathbb{R})$, one has that $\|\psi(t)\|^2 = \|\psi_0\|^2$ and $E[\psi(t)] = E[\psi_0]$.

One main issue in the proof of the global well-posedness is to prove that the H^1-norm of the solution does not blow-up in finite time, i.e., that there does not exist T such that $\limsup_{t\to T} \|\psi(t)\|_{H^1} < \infty$.

From the conservation of mass, proving that blow-up does not occur is reduced to prove that the *kinetic energy* $\|\psi'(t)\|^2$ does not blow-up in finite time.

If $\gamma_j \geqslant 0$ for all j, the conservation of the energy immediately implies that $\|\psi'(t)\| \leqslant c$ (as well as $|\psi(t, y_j)| \leqslant c$). Then no restriction on the power of the nonlinearity is needed.

If for some j, $\gamma_j < 0$, then the conservation of the energy alone is not enough to guarantee that $\|\psi'(t)\|$ stays bounded. One needs to be sure that in the energy the growth of $\|\psi'(t)\|$ cannot be compensated by the negative term $\sum_{j:\gamma_j<0} \frac{\gamma_j}{\mu_j+1} |\psi(t, y_j)|^2$. This is achieved by using the well known Gagliardo-Nirenberg inequality

$$\|\psi\|_\infty \leqslant c \|\psi'\|^{\frac{1}{2}} \|\psi\|^{\frac{1}{2}}. \tag{7}$$

Inequality (7), together with the energy and mass conservation, imply

$$\begin{aligned} E[\psi_0] = E[\psi(t)] &= \|\psi'(t)\|^2 + \sum_{j:\gamma_j \geqslant 0} \frac{\gamma_j}{\mu_j + 1} |\psi(t, y_j)|^{2\mu_j+2} - \sum_{j:\gamma_j<0} \frac{|\gamma_j|}{\mu_j + 1} |\psi(t, y_j)|^{2\mu_j+2} \\ &\geqslant \|\psi'(t)\|^2 - c \sum_{j:\gamma_j<0} \|\psi'(t)\|^{\mu_j+1}. \end{aligned} \tag{8}$$

The bound (8) makes clear where the condition (6) comes from: if $\mu_j < 1$ for all the j's such that $\gamma_j < 0$, then the inequality (8) implies that $\|\psi'(t)\| \leqslant c$; otherwise the negative term at the r.h.s. dominates for $\|\psi'(t)\|$ large, and the inequality (8) does not imply that $\|\psi'(t)\|$ is bounded.

We note that in [5], it is shown that for $N = 1$ the condition (6) is indeed sharp. In the sense that for $\mu \equiv \mu_1 \geqslant 1$, it is possible to find an initial datum $\psi_0 \in H^1(\mathbb{R})$ such that there exists $t_c < \infty$ for which $\limsup_{t\to t_c} \|\psi(t)\|_{H^1(\mathbb{R})} = \infty$, i.e., the solution blows-up in finite time.

2.1. Point-like limit of scaled spatially non-homogeneous nonlinearities in dimension one

Here we discuss the approximating equation used in [10] and give a sketch of the proof of the convergence of the solutions.

For any $\varepsilon > 0$, consider the nonlinear flow

$$\psi^\varepsilon(t,x) = (U(t) * \psi_0)(x) - i\sum_{j=1}^{N}\int_0^t ds\big(U(t-s) * V_j^\varepsilon(\cdot - y_j)|\psi^\varepsilon(s)|^{2\mu_j}\psi^\varepsilon(s)\big)(x) \tag{9}$$

where

$$V_j^\varepsilon(x) = \frac{1}{\varepsilon}V_j\left(\frac{x}{\varepsilon}\right) \qquad \text{with} \quad V_j \in L^1(\mathbb{R}, (1+|x|)dx) \cap L^\infty(\mathbb{R}) \tag{10}$$

and $\mu_j > 0$.

We remark that Eq. (9) is a weak formulation of the Cauchy problem

$$\begin{cases} i\dfrac{\partial}{\partial t}\psi^\varepsilon(t,x) = -\dfrac{\partial^2}{\partial x^2}\psi^\varepsilon(t,x) + \displaystyle\sum_{j=1}^{N} V_j^\varepsilon(x-y_j)|\psi^\varepsilon(t,x)|^{2\mu_j}\psi^\varepsilon(t,x) \\ \psi^\varepsilon(0,x) = \psi_0(x) \end{cases} \tag{11}$$

This describes a situation in which there is a spacial inhomogeneity of the response of the medium to the wave function propagation. The regions in which the response is nonlinear are supported on intervals of length of order ε around the points y_j.

Before discussing the convergence of the solutions of Eq. (9) to the solutions of Eq. (5) we shall comment on the well-posedness of (9). Under the assumption (10), Corollary 6.1.2 of [11] applies, so that, for any $\varepsilon > 0$, one has global existence of strong H^1-solutions for every initial datum $\psi_0 \in H^1(\mathbb{R})$ for any $\mu_j > 0$ if $V_j \geqslant 0$ (defocusing case) and for $0 < \mu_j < 2$ if V_j is negative in some open interval (for $\mu_j = 2$, the critical case, one has global existence for small data, see Remark 6.1.3 of [11]).

As for the limit problem (5), to prove global well-posedness in H^1 one uses the fact that there exist two conserved quantities: the L^2-norm (mass) and the energy

$$E^\varepsilon[\psi] = \|\psi'\|^2 + \sum_{j=1}^{N}\frac{1}{\mu_j+1}\int_{\mathbb{R}} V_j^\varepsilon(y-y_j)|\psi(y)|^{2\mu+2}dy.$$

Precisely one has that, for any $\psi_0 \in H^1(\mathbb{R})$, the solution $\psi^\varepsilon(t)$ of (9) is such that:

$$\|\psi^\varepsilon(t)\|^2 = \|\psi_0\|^2 \qquad \text{and} \qquad E[\psi^\varepsilon(t)] = E[\psi_0].$$

From the mass conservation, to prove that the H^1-norm of $\psi^\varepsilon(t)$ does not blow-up in finite time, one needs to show that the quantity $\|\psi^{\varepsilon\prime}(t)\|$ stays bounded for any t. This is achieved by using the following argument, write V_j as the sum of its positive and negative part, $V_j = V_{j,+} - V_{j,-}$, with $V_{j,+} \geqslant 0$ and $V_{j,-} > 0$. Then, by the Gagliardo-Nirenberg inequality (7),

$$\begin{aligned} \frac{1}{\mu_j+1}\int_{\mathbb{R}} V_j^\varepsilon(y-y_j)|\psi^\varepsilon(y)|^{2\mu_j+2}dy &= \frac{1}{\mu_j+1}\int_{\mathbb{R}}\frac{1}{\varepsilon}V_j\Big(\frac{y-y_j}{\varepsilon}\Big)|\psi^\varepsilon(y)|^{2\mu_j+2}dy \\ &\geqslant -\frac{1}{\mu_j+1}\int_{\mathbb{R}}\frac{1}{\varepsilon}V_{j,-}\Big(\frac{y-y_j}{\varepsilon}\Big)|\psi^\varepsilon(y)|^{2\mu_j+2}dy \\ &\geqslant -\frac{c}{\varepsilon}\|\psi^\varepsilon\|_\infty^{2\mu_j}\int_{\mathbb{R}}|\psi^\varepsilon(y)|^2dy \geqslant -\frac{c}{\varepsilon}\|\psi^{\varepsilon\prime}\|^{\mu_j}\|\psi^\varepsilon\|^2 \end{aligned}$$

We denote by $\mathcal{K} \subseteq \{1, ..., N\}$ the set of indices j such that V_j is negative in some open interval. Then by mass and energy conservation, and the inequality above, one has that,

$$E^\varepsilon[\psi_0] = E^\varepsilon[\psi^\varepsilon(t)] \geqslant \|\psi^{\varepsilon\prime}(t)\|^2 - \frac{c}{\varepsilon}\sum_{j\in\mathcal{K}} \|\psi^{\varepsilon\prime}(t)\|^{\mu_j}. \tag{12}$$

As a consequence, one has $\|\psi^{\varepsilon\prime}(t)\| \leqslant C_\varepsilon$ if $\mu_j < 2$ for all $j \in \mathcal{K}$. We remark that the argument used above gives a bound on $\|\psi^{\varepsilon\prime}(t)\|$ which is not uniform in ε. The constant C_ε depends on ε because ε appears at the denominator of c in Eq. (12). This is enough to obtain global well-posedness for any $\varepsilon > 0$ but it is not enough to prove the convergence result. For that we shall need a bound on $\|\psi^{\varepsilon\prime}(t)\|$ which is uniform in ε, we shall be able to obtain it at the cost of a more restrictive constraint on μ_j.

Now we are ready to state the main result of [10].

Theorem 2.1. *For all $j = 1, ..., N$, take V_j^ε as in (10) and $0 < \mu_j < 1$ if V_j is negative in some open interval. For any $\psi_0 \in H^1(\mathbb{R})$, let ψ be the solution of Eq. (5) with $\gamma_j = \int_{\mathbb{R}} V_j dx$ and ψ^ε be the solution of Eq. (9). Then, for any $T > 0$,*

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,T]} \|\psi(t) - \psi^\varepsilon(t)\|_{H^1(\mathbb{R})} = 0.$$

Outline of the proof of Th. 2.1. We shall discuss only the main ideas behind the proof of Th. (2.1), for the details we refer to [10]. We divide the proof in four steps.

Step 1. The first step is to obtain a bound for $\|\psi^{\varepsilon\prime}(t)\|$ which is uniform in ε. This can be achieved at the cost of a more restrictive constraint on the power of the nonlinear term, precisely we shall need to assume that $\mu_j < 1$, for all $j \in \mathcal{K}$. Writing, as in the proof of the well-posedness of Eq. (9), V_j as the sum of its positive and negative parts, and by assumption (10) and Gagliardo-Nirenberg inequality, we have that

$$\begin{aligned}\frac{1}{\mu_j+1}\int_{\mathbb{R}} V_j^\varepsilon(y-y_j)|\psi^\varepsilon(y)|^{2\mu_j+2}dy &= \frac{1}{\mu_j+1}\int_{\mathbb{R}} \frac{1}{\varepsilon} V_j\Big(\frac{y-y_j}{\varepsilon}\Big)|\psi^\varepsilon(y)|^{2\mu_j+2}dy \\ &\geqslant -\frac{1}{\mu_j+1}\int_{\mathbb{R}} V_{j,-}(y)|\psi^\varepsilon(y_j+\varepsilon y)|^{2\mu_j+2}dy \\ &\geqslant -c\|\psi^{\varepsilon\prime}\|^{\mu_j+1}\end{aligned}$$

The latter bound together with the conservation of the energy, gives

$$E^\varepsilon[\psi_0] = E^\varepsilon[\psi^\varepsilon(t)] \geqslant \|\psi^{\varepsilon\prime}(t)\|^2 - c\sum_{j\in\mathcal{K}} \|\psi^{\varepsilon\prime}(t)\|^{\mu_j+1}.$$

Since

$$\sup_{\varepsilon\in[0,1]} E^\varepsilon[\psi_0] \leqslant \|\psi_0'\|^2 + \|\psi_0\|_\infty^{2\mu+2} \sum_{j=1}^N \frac{1}{\mu_j+1}\int_{\mathbb{R}} dx\ V_{j,+}(x) \equiv K$$

we finally get the inequality:

$$\|\psi^{\varepsilon\prime}(t)\|^2 - c\sum_{j\in\mathcal{K}} \|\psi^{\varepsilon\prime}(t)\|^{\mu_j+1} \leqslant K$$

which implies $\|\psi^{\varepsilon\prime}(t)\| \leqslant c$ if $\mu_j < 1$ for all $j \in \mathcal{K}$ and $t > 0$, by the Gagliardo-Nirenberg inequality, this also implies the bound $\|\psi^\varepsilon(t)\|_\infty \leqslant c$.

Step 2. The solution of the limit problem (5) is completely determined by the values $\psi(t, y_j)$, $j = 1, ..., N$. Then to find $\psi(t, x)$ we must solve first the system of coupled nonlinear

Volterra equations in the variables $\psi(t, y_k)$.

$$\psi(t, y_k) = (U(t) * \psi_0)(y_k) - i \sum_{j=1}^{N} \gamma_j \int_0^t ds\, U(t-s, y_k - y_j) |\psi(s, y_j)|^{2\mu_j} \psi(s, y_j), \tag{13}$$

$k = 1, ..., N$.

For this reason in the second step of the proof we address the problem of showing the convergence of $\psi^\varepsilon(t, y_k)$ to $\psi(t, y_k)$, for all $k = 1, ..., N$. To this end, we compute $\psi^\varepsilon(t, y_k)$ by using Eq. (9), we get

$$\psi^\varepsilon(t, y_k) = (U(t) * \psi_0)(y_k) - i \sum_{j=1}^{N} \int_0^t ds \big(U(t-s) * V_j^\varepsilon(\cdot - y_j) |\psi^\varepsilon(s)|^{2\mu_j} \psi^\varepsilon(s) \big)(y_k).$$

We rewrite the latter equation in a more explicit form as

$$\begin{aligned} \psi^\varepsilon(t, y_k) &= (U(t) * \psi_0)(y_k) \\ &\quad - i \sum_{j=1}^{N} \int_0^t ds \int_{\mathbb{R}} U(t-s,\, y_k - y_j - \varepsilon y)\, V_j(y)\, |\psi^\varepsilon(s, y_j + \varepsilon y)|^{2\mu_j} \psi^\varepsilon(s, y_j + \varepsilon y) dy. \end{aligned} \tag{14}$$

Letting $\varepsilon \to 0$ at the r.h.s. of the latter equation one would expect that

$$\psi^\varepsilon(t, y_k) \simeq (U(t) * \psi_0)(y_k) - i \sum_{j=1}^{N} \int_{\mathbb{R}} V_j(y) dy \int_0^t ds\ \ U(t-s,\, y_k - y_j)\ |\psi^\varepsilon(s, y_j)|^{2\mu_j} \psi^\varepsilon(s, y_j).$$

By comparison with Eq. (13) one notices that $\psi^\varepsilon(t, y_k)$ approximatively satisfies the same equation as $\psi(t, y_k)$ if $\gamma_j = \int_{\mathbb{R}} V_j(y) dy$. To make precise this idea we subtract Eq. (13) from (14). By adding and subtracting suitable terms at the r.h.s. (using the fact that $\gamma_j = \int_{\mathbb{R}} V_j(y) dy$), we end up with the identity

$$\begin{aligned} &\psi^\varepsilon(t, y_k) - \psi(t, y_k) = \\ &- i \sum_{j=1}^{N} \gamma_j \int_0^t ds\ U(t-s, y_k - y_j)\ \big(|\psi^\varepsilon(s, y_j)|^{2\mu_j} \psi^\varepsilon(s, y_j) - |\psi(s, y_j)|^{2\mu_j} \psi(s, y_j) \big) + \mathcal{R}^\varepsilon(t) \end{aligned}$$

where $\mathcal{R}^\varepsilon(t)$ is a remainder that satisfies the bound $\sup_{t\in[0,T]} |\mathcal{R}^\varepsilon(t)| \leqslant c\varepsilon^\delta$ for any $0 < \delta < 1/2$ and $T > 0$, we refer to [10] for the details. Here we use the a priori bounds $\|\psi(t)\|_\infty \leqslant c$ and $\|\psi^\varepsilon(t)\|_\infty \leqslant c$.

From the bound for the remainder $\mathcal{R}^\varepsilon(t)$, the explicit expression of $U(t, x)$, the fact that $||a|^{2\mu} a - |b|^{2\mu} b| \leqslant (|a|^{2\mu} + |b|^{2\mu})|a - b|$ for any $a, b \in \mathbb{C}$, and the a priori bounds $\|\psi(t)\|_\infty \leqslant c$ and $\|\psi^\varepsilon(t)\|_\infty \leqslant c$, we get the inequality:

$$|\psi^\varepsilon(t, y_k) - \psi(t, y_k)| \leqslant c \sum_{j=1}^{N} \int_0^t ds \frac{1}{\sqrt{t-s}} |\psi^\varepsilon(s, y_j) - \psi(s, y_j)| + c\varepsilon^\delta.$$

By a standard argument in the theory of Abel integral operators, we conclude that

$$\sup_{t\in[0,T]} |\psi^\varepsilon(t, y_j) - \psi(t, y_j)| \leqslant c\varepsilon^\delta \tag{15}$$

for any $0 < \delta < 1/2$ and $T > 0$.

Step 3. Now we can proceed to the proof of the convergence in L^2-norm, precisely we shall show that

$$\sup_{t\in[0,T]} \|\psi^\varepsilon(t)-\psi(t)\| \leqslant c\varepsilon^\delta \tag{16}$$

for any $0<\delta<1/2$ and $T>0$.

We rewrite the nonlinear Eq. (9) explicitly, as

$$\begin{aligned}\psi^\varepsilon(t,x) &= (U(t)*\psi_0)(x)\\ &\quad - i\sum_{j=1}^N \int_0^t ds \int_{\mathbb{R}} U(t-s,x-y_j-\varepsilon y)\, V_j(y)\, |\psi^\varepsilon(s,y_j+\varepsilon y)|^{2\mu_j}\psi^\varepsilon(s,y_j+\varepsilon y)dy. \end{aligned}\tag{17}$$

As in Step 2, letting $\varepsilon\to 0$ at the r.h.s. we see that, if $\gamma_j=\int_{\mathbb{R}} V_j dx$, $\psi^\varepsilon(t,x)$ approximately satisfies the same equation as $\psi(t,x)$. To make precise this argument we subtract (17) from (5) and get the identity

$$\begin{aligned}&\psi^\varepsilon(t,x)-\psi(t,x)=\\ &-i\sum_{j=1}^N \gamma_k \int_0^t ds\, U(t-s,x-y_j)\left(|\psi^\varepsilon(s,y_j)|^{2\mu_j}\psi^\varepsilon(s,y_j)-|\psi(s,y_j)|^{2\mu_j}\psi(s,y_j)\right)+\mathcal{T}^\varepsilon(t,x).\end{aligned}$$

where $\mathcal{T}^\varepsilon(t,x)$ is a remainder that satisfies the bound $\sup_{t\in[0,T]}\|\mathcal{T}^\varepsilon(t)\|\leqslant c\varepsilon^\delta$ for any $0<\delta<1/2$ and $T>0$ (see [10] for the details). Taking the L^2-norm of $\psi^\varepsilon(t,x)-\psi(t,x)$ we obtain

$$\begin{aligned}&\sup_{t\in[0,T]}\|\psi^\varepsilon(t)-\psi(t)\|\\ &\leqslant\sum_{j=1}^N|\gamma_j|\sup_{t\in[0,T]}\left\|\int_0^t ds\, U(t-s,\cdot-y_j)\,\left(|\psi^\varepsilon(s,y_j)|^{2\mu_j}\psi^\varepsilon(s,y_j)-|\psi(s,y_j)|^{2\mu_j}\psi(s,y_j)\right)\right\|+c\varepsilon^\delta\\ &\leqslant c\sum_{j=1}^N\sup_{s\in[0,T]}\left||\psi^\varepsilon(s,y_j)|^{2\mu_j}\psi^\varepsilon(s,y_j)-|\psi(s,y_j)|^{2\mu_j}\psi(s,y_j)\right|+c\varepsilon^\delta\\ &\leqslant c\sum_{j=1}^N\sup_{s\in[0,T]}|\psi^\varepsilon(s,y_j)-\psi(s,y_j)|+c\varepsilon^\delta\leqslant c\varepsilon^\delta.\end{aligned}$$

In the second inequality we used the bound

$$\sup_{t\in[0,T]}\left\|\int_0^t U(t-s,\cdot)f(s)\,ds\right\|\leqslant c\sup_{s\in[0,T]}|f(s)|.$$

In the third inequality we used $||a|^{2\mu}a-|b|^{2\mu}b|\leqslant(|a|^{2\mu}+|b|^{2\mu})|a-b|$ and the a priori bounds $\|\psi(t)\|_\infty\leqslant c$, $\|\psi^\varepsilon(t)\|_\infty\leqslant c$. And finally we used the bound (15). This concludes the proof of (16).

Step 4. We are left to prove the convergence in H^1. Since the bound $\|\psi^{\varepsilon\prime}(t)\|\leqslant c$ holds true, there exists a subsequence, that we denote in the same way, such that $\psi^\varepsilon(t)$ converges weakly to $\phi(t)$ in $H^1(\mathbb{R})$. Recalling that $\psi^\varepsilon(t)\to\psi(t)$ in $L^2(\mathbb{R})$ we conclude that $\phi(t)=\psi(t)$ a.e.. Moreover, since:

$$\|\psi^\varepsilon(t)-\psi(t)\|^2_{H^1}=\|\psi^\varepsilon(t)\|^2_{H^1}+\|\psi(t)\|^2_{H^1}-2\,\mathrm{Re}\,(\psi^\varepsilon(t),\psi(t))_{H^1},$$

it is sufficient to prove that

$$\lim_{\varepsilon\to0}\|\psi^\varepsilon(t)\|^2_{H^1}=\|\psi(t)\|^2_{H^1}\ .$$

As in Step 3 we proved the convergence in L^2, we are left to show that

$$\lim_{\varepsilon\to 0}\sup_{t\in[0,T]}\left|\|\psi^{\varepsilon\prime}(t)\|^2-\|\psi'(t)\|^2\right|=0. \tag{18}$$

From the conservation of the energy we obtain

$$\|\psi^{\varepsilon\prime}(t)\|^2=E^\varepsilon[\psi_0]-\sum_{j=1}^N\frac{1}{\mu_j+1}\int dxV_j^\varepsilon(x-y_j)|\psi^\varepsilon(t,x)|^{2\mu_j+2}$$

$$\|\psi'(t)\|^2=E[\psi_0]-\sum_{j=1}^N\gamma_j\frac{1}{\mu_j+1}|\psi(t,y_j)|^{2\mu_j+2}.$$

Since $\lim_{\varepsilon\to 0}E^\varepsilon[\psi_0]=E[\psi_0]$, we have

$$\begin{aligned}&\lim_{\varepsilon\to 0}\sup_{t\in[0,T]}\left|\|\psi^{\varepsilon\prime}(t)\|^2-\|\psi'(t)\|^2\right|\\ =&\lim_{\varepsilon\to 0}\sup_{t\in[0,T]}\left|\sum_{j=1}^N\frac{1}{\mu_j+1}\left(\int_{\mathbb{R}}V_j(x)|\psi^\varepsilon(t,y_j+\varepsilon x)|^{2\mu_j+2}dx-\gamma_j|\psi(t,y_j)|^{2\mu_j+2}\right)\right|.\end{aligned} \tag{19}$$

By Step 2 we have $\lim_{\varepsilon\to 0}\sup_{t\in[0,T]}||\psi^\varepsilon(t,y_j)|^{2\mu_j+2}-|\psi(t,y_j)|^{2\mu_j+2}|=0$. Moreover, since $\gamma_j=\int_{\mathbb{R}}V_jdx$, it follows that

$$\begin{aligned}&\left|\int_{\mathbb{R}}V_j(x)|\psi^\varepsilon(t,y_j+\varepsilon x)|^{2\mu_j+2}dx-\gamma_j|\psi^\varepsilon(t,y_j)|^{2\mu_j+2}\right|\\ &\qquad=\left|\int_{\mathbb{R}}V_j(x)\left(|\psi^\varepsilon(t,y_j+\varepsilon x)|^{2\mu_j+2}-|\psi^\varepsilon(t,y_j)|^{2\mu_j+2}\right)dx\right|\\ &\qquad\leqslant c\sqrt{\varepsilon}\left\||\psi^\varepsilon(t)|^{2\mu_k+2}\right\|_{H^1}\int_{\mathbb{R}}|V_j(x)|\sqrt{|x|}dx\leqslant c\sqrt{\varepsilon}.\end{aligned}$$

The latter bound, together with the equality (19), give (18), and this concludes the proof of Th. 2.1. □

2.2. Remarks on the one dimensional problem

We conclude the discussion on the one dimensional case with several remarks.

We note that the approximating problem (11) imitates the approximation result on the linear delta-interactions. Indeed it is well known, see [6], that the Hamiltonian $H^\varepsilon=-\Delta+\sum_j V_j^\varepsilon(\cdot-y_j)$, with V_j^ε defined as in Eq. (10), converges in the norm resolvent sense to H_α, defined by (1) - (2), with $\alpha_j=\int_{\mathbb{R}}V_jdx$. Recall that this also implies the convergence of associated unitary groups.

For the convergence of the linear problem one only needs to assume $V_j\in L^1(\mathbb{R})$. Also, the well-posedness result for Eq. (9) requires only $V_j\in L^1(\mathbb{R})\cap L^\infty(\mathbb{R})$ (see [11]). This suggests that the assumption $V_j\in L^1(\mathbb{R},(1+|x|)dx)\cap L^\infty(\mathbb{R})$ in Th. (2.1) is not optimal.

Concerning the assumptions on V_j, we also note that the limit problem (5) is well posed for any $\mu_j>0$ if $\gamma_j>0$. Since $\gamma_j=\int_{\mathbb{R}}V_jdx$, one would expect the convergence result to hold true for any $\mu_j>0$ if $\int_{\mathbb{R}}V_jdx>0$. Nevertheless, the argument used to derive the uniform bound, $\|\psi^{\varepsilon\prime}(t)\|\leqslant c$ (step 1 in the proof of Th. 2.1), requires an upper bound on μ_j whenever V_j is negative in some open interval. The same problem appears in the proof of the well-posedness of Eq. (9). This is a consequence of the fact that the argument neglects the positive part of V_j.

In [16], the authors describe a different type of approximating problem which uses a non-local nonlinearity. They consider the equation

$$i\frac{\partial}{\partial t}\psi^\varepsilon(t,x) = -\frac{\partial^2}{\partial x^2}\psi^\varepsilon(t,x) + \rho^\varepsilon(x)\alpha(|\langle\rho^\varepsilon,\psi^\varepsilon(t)\rangle|^2)\langle\rho^\varepsilon,\psi^\varepsilon(t)\rangle, \tag{20}$$

where ρ^ε is a function approximating the Dirac delta-distribution (i.e., $\rho^\varepsilon(x) = \rho(x/\varepsilon)/\varepsilon$ with $\rho \in C_0^\infty[-1,1]$, $\rho \geqslant 0$, and $\int_{\mathbb{R}} \rho dx = 1$) and $\alpha(z)$ is a nonlinear function.

Under suitable assumptions of the nonlinearity, they prove that, for any initial data in $H^1(\mathbb{R})$, the solution of Eq. (20), converges to the solution of the equation $i\partial_t\psi = -\partial^2_{xx}\psi + \alpha(|\psi(t,0)|^2)\,\delta_0\,\psi$.

3. Nonlinear delta-interactions in dimension three

This section is devoted to the analysis of the approximation problem for the Schrödinger equation with nonlinear delta-interactions in dimension three. We will discuss a conjecture on an approximating problem with non-local nonlinearity. For the sake of simplicity we shall restrict the analysis to the case $N = 1$. For a discussion on the generalization of the limit model to $N > 1$ we refer to [1–3].

We shall start by recalling several results from [1] on the well-posedness of the limit model. Since we are setting $N = 1$, we use the notation $\alpha_1 \equiv \alpha$, and set $\mathbf{y}_1 \equiv \mathbf{0}$, i.e., we put the center of interaction in the origin. We set

$$G_0(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|}.$$

In dimension three the operator formally written as $H_\alpha = -\Delta + \alpha\delta_0$ is defined by

$$\begin{aligned} D(H_\alpha) = \Big\{ \psi \in L^2(\mathbb{R}^3) \,:\, & \psi = \phi + qG_0,\ \phi \in H^2_{loc}(\mathbb{R}^3), \\ & \nabla\phi \in L^2(\mathbb{R}^3),\ \Delta\phi \in L^2(\mathbb{R}^3),\ q \in \mathbb{C}, \\ & \lim_{\mathbf{x}\to\mathbf{0}} (\psi(\mathbf{x}) - qG_0(\mathbf{x})) = \alpha q \Big\} \end{aligned} \tag{21}$$

and

$$H_\alpha\psi = -\Delta\psi \qquad \forall \mathbf{x} \neq 0. \tag{22}$$

The quantity q is referred to as *charge* of the wave function ψ. We remark that by the definition of $D(H_\alpha)$, in general one has $\phi \notin H^2(\mathbb{R}^3)$. This is due to the decomposition $\psi = \phi + qG_0$ and to the fact that $G_0 \notin L^2(\mathbb{R}^3)$. Whenever $q = 0$, one has that $\psi = \phi$, and $\psi \in H^2(\mathbb{R})$ with $\psi(\mathbf{0}) = 0$.

The form domain of the operator H_α is

$$V = \left\{ \psi \in L^2(\mathbb{R}^3) \,:\, \psi = \phi + qG_0,\ \phi \in H^1_{loc}(\mathbb{R}^3),\ \nabla\phi \in L^2(\mathbb{R}^3),\ q \in \mathbb{C} \right\}$$

As for the one dimensional case the form domain does not depend on α. Yet, we note one main difference with the one dimensional case: V does not coincide with $H^1(\mathbb{R})$, the form domain of the *free* Laplacian $(-\Delta, H^2(\mathbb{R}^3))$. Then H_α is not a small perturbation, in the sense of quadratic forms, of $-\Delta$.

As for the one dimensional case, to give a precise definition of the nonlinear dynamics we are interested in, we start with a discussion on the non-autonomous Hamiltonian $H_{\alpha(t)}$, where $\alpha(t)$ is an assigned function. Such Hamiltonians have been studied, for example, in relation with the ionization problem (see, e.g., [12, 13] and references therein).

Consider the Cauchy problem (3) in dimension three. From [20], one obtains its solution in terms of the time dependent charge $q(t)$. The charge satisfies the Volterra equation:

$$\frac{q(t)}{4\sqrt{\pi i}} + \int_0^t ds \frac{\alpha(s)q(s)}{\sqrt{t-s}} = \int_0^t ds \frac{(U(s) * \psi_0)(\mathbf{0})}{\sqrt{t-s}}, \tag{23}$$

where $U(t)$ is the unitary group generated by the free Laplacian in dimension three. Its explicit expression is given by

$$U(t, \mathbf{x}) = \frac{e^{i\frac{|\mathbf{x}|^2}{4t}}}{(4\pi i t)^{3/2}},$$

while the solution $\psi(t)$ is completely defined by $q(t)$ through the equation

$$\psi(t, \mathbf{x}) = (U(t) * \psi_0)(\mathbf{x}) + i \int_0^t ds U(t-s, \mathbf{x}) q(s). \tag{24}$$

The solutions defined by equations (23) - (24) belong to $D(H_{\alpha(t)})$ only under certain assumptions on the regularity of the function $\alpha(t)$ and on the initial state ψ_0, see, e.g., [21] and references therein for results in this direction.

To define a nonlinear delta-interaction in dimension three we let $\alpha(t) \to \alpha(|q(t)|^2)$ in equation (23). Following [1], we restrict ourselves to power type nonlinearities, and, as for the one dimensional case, we choose $\alpha(z) = \gamma z^\mu$, with $\gamma \in \mathbb{R}$ and $\mu > 0$.

With this choice the linear Volterra equation (23) is replaced by the nonlinear one

$$\frac{q(t)}{4\sqrt{\pi i}} + \gamma \int_0^t ds \frac{|q(s)|^{2\mu} q(s)}{\sqrt{t-s}} = \int_0^t ds \frac{(U(s) * \psi_0)(\mathbf{0})}{\sqrt{t-s}}. \tag{25}$$

Equation (24) - (25), define our model for a nonlinear delta-interaction in dimension three. We recall that, global well-posedness for the problem (24) - (25) in $\psi_0 \in V$ and under the condition that $\mu < 1$ if $\gamma < 0$ was proved in [1]. In the same paper, the authors also prove that the nonlinear flow admits two conserved quantities: the L^2-norm (mass) and the energy

$$E[\psi] = \|\nabla \phi\|^2 + \frac{\gamma |q|^{2\mu+2}}{\mu + 1},$$

where $\psi = \phi + qG_0 \in V$. So that, for any $\psi_0 \in V$, if $\psi(t)$ is the solution of the problem (24) - (25), one has $\|\psi(t)\|^2 = \|\psi_0\|^2$ and $E[\psi(t)] = E[\psi_0]$.

We remark that by the definition of the form domain of H_α, $\psi \in V$ does not imply $\psi \in H^1(R^3)$, and the well-posedness in V must be understood in the sense that $\|\nabla \phi(t)\|$ and $|q(t)|$ stay bounded.

We also remark that in [1], the authors consider the more general case of finitely many nonlinear delta-interactions, $N \geqslant 1$. The conditions on the initial state which guarantee $\psi(t) \in D(H_{\alpha(|q(t)|^2)})$ are also discussed in [1]. We refer to [2] for the analysis of the blow-up problem and to [3] for the study of the stability/instability properties of the stationary solutions of (24) - (25).

3.1. Point-like limit of scaled non-local nonlinearities in dimension three

In this section we discuss a conjecture about the approximation problem for (24) - (25)through scaled non-local nonlinear flows. We remark that in dimension three the problem of finding an approximation of the nonlinear flow (24) - (25) is subtler than the corresponding problem in dimension one. This is not surprising, as also the problem of finding a regular approximation of the (linear) operator H_α in dimension three requires non-trivial renormalization procedures (see, [6]).

Let ρ be such that $\rho \in C_0^\infty(\mathbb{R}^3)$, $\rho \geqslant 0$, and $\int_{\mathbb{R}^3} \rho \mathrm{d}\mathbf{x} = 1$, then set $\rho^\varepsilon(\mathbf{x}) = \rho(\mathbf{x}/\varepsilon)/\varepsilon^3$, so that ρ^ε converges to the Dirac delta-distribution in dimension three.

We denote by $\tilde{\rho}(\mathbf{k})$ and $\tilde{\rho}^\varepsilon(\mathbf{k})$ the Fourier transform of ρ and ρ^ε respectively, by scaling one has that $\tilde{\rho}^\varepsilon(\mathbf{k}) = \tilde{\rho}(\varepsilon\mathbf{k})$. Moreover, from $\int_{\mathbb{R}^3} \rho \mathrm{d}\mathbf{x} = 1$, it follows that $\tilde{\rho}(\mathbf{0}) = 1$.

We set $M = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}\, (\tilde{\rho}(\mathbf{k}))^2/|\mathbf{k}|^2$ and consider the nonlinear flow (in weak form)

$$\psi^\varepsilon(t,\mathbf{x}) = (U(t) * \psi_0^\varepsilon)(\mathbf{x}) - i\frac{\varepsilon}{M}\int_0^t ds (U(t-s) * \rho^\varepsilon)(\mathbf{x}) \left(-1 + \gamma \frac{\varepsilon^{2\mu+1}|\langle \rho^\varepsilon, \psi^\varepsilon(s)\rangle|^{2\mu}}{M^{2\mu+1}}\right) \langle \rho^\varepsilon, \psi^\varepsilon(s)\rangle. \quad (26)$$

Note that we let the initial datum ψ_0^ε to depend on ε as well. This is due to the fact that we want to compare the solutions of Eq. (26) with the solution of (24) - (25). To do that, one should consider the two nonlinear flows with the same initial datum. In dimension three this is, in general, not possible, because problem (24) - (25) is naturally defined for initial data in V, while problem (26) is naturally defined for initial data in $H^1(\mathbb{R}^3)$. For this reason we let the initial datum in (26) to depend on ε, and assume that ψ_0^ε converges to ψ_0 in a suitable norm as $\varepsilon \to 0$.

To begin, it is also convenient to set $\gamma > 0$ (defocusing nonlinearity), this choice simplifies some issues with the well-posedness, giving at once some useful bounds on relevant quantities, and avoids further constraints on the power of the nonlinearity μ.

We remark that problem (26), is a weak formulation of

$$\begin{cases} i\frac{\partial}{\partial t}\psi^\varepsilon(t,\mathbf{x}) = -\Delta\psi^\varepsilon(t,\mathbf{x}) + \frac{\varepsilon}{M}\left(-1 + \gamma \frac{\varepsilon^{2\mu+1}|\langle \rho^\varepsilon, \psi^\varepsilon(t)\rangle|^{2\mu}}{M^{2\mu+1}}\right) \langle \rho^\varepsilon, \psi^\varepsilon(t)\rangle \rho^\varepsilon(\mathbf{x}) \\ \psi^\varepsilon(0,\mathbf{x}) = \psi_0^\varepsilon(\mathbf{x}) \end{cases}$$

We also note that, also in this case, the nonlinear approximation problem is inspired by the linear one. Indeed, it is easy prove that the (non-local) operator $H^\varepsilon = -\Delta + \frac{\varepsilon}{M}\left(-1 + \alpha\frac{\varepsilon}{M}\right)\langle \rho^\varepsilon, \cdot\rangle \rho^\varepsilon$ converges in norm resolvent sense to the operator H_α defined by (21) - (22).

We conjecture that, for any $\psi_0 \in V$ and $\psi_0^\varepsilon \in H^1(\mathbb{R}^3)$ that converges to ψ_0 in a suitable sense, the solution of Eq. (26) converges to the solution of (24) - (25).

We do not have yet a rigorous proof of this statement, but we are able to give an heuristic argument to support the conjecture.

The basic idea is that the quantity $q^\varepsilon(t) = \frac{\varepsilon}{M}\langle \rho^\varepsilon, \psi^\varepsilon(t)\rangle$, should converge to the charge $q(t)$. Eq. (26), written in terms of $q^\varepsilon(t)$, gives

$$\psi^\varepsilon(t,\mathbf{x}) = (U(t) * \psi_0^\varepsilon)(\mathbf{x}) - i\int_0^t ds (U(t-s) * \rho^\varepsilon)(\mathbf{x}) \left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s). \quad (27)$$

We recall that $\rho^\varepsilon \to \delta_0$, then $(U(t-s) * \rho^\varepsilon)(\mathbf{x}) \to U(t-s,\mathbf{x})$. Assuming, moreover, that $U(t) * \psi_0^\varepsilon \to U(t) * \psi_0$, one expects that

$$\psi^\varepsilon(t,\mathbf{x}) \simeq (U(t) * \psi_0)(\mathbf{x}) + i\int_0^t ds U(t-s,\mathbf{x}) q^\varepsilon(s).$$

By comparison with Eq. (24), this suggests that, if $q^\varepsilon(t)$ converges to $q(t)$, then also $\psi^\varepsilon(t)$ converges to $\psi(t)$.

To support the idea that $q^\varepsilon(t)$ should converge to $q(t)$ we proceed as follows. We take the scalar product of Eq. (27) with ρ^ε, using the definition of $q^\varepsilon(t)$ we get the identity

$$\frac{M}{\varepsilon}q^\varepsilon(t) = \langle \rho^\varepsilon, U(t) * \psi_0^\varepsilon\rangle - i\int_0^t ds \langle \rho^\varepsilon, U(t-s) * \rho^\varepsilon\rangle \left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s). \tag{28}$$

Let $K^\varepsilon(t) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}\,(\tilde\rho^\varepsilon(\mathbf{k}))^2 e^{-i|\mathbf{k}|^2 t}/|\mathbf{k}|^2$. By the definition of $U(t)$ one has that

$$\langle \rho^\varepsilon, U(t) * \rho^\varepsilon\rangle = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}\,(\tilde\rho^\varepsilon(\mathbf{k}))^2 e^{-i|\mathbf{k}|^2 t} = \frac{i}{(2\pi)^3}\frac{d}{dt}\int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}\,\frac{(\tilde\rho^\varepsilon(\mathbf{k}))^2 e^{-i|\mathbf{k}|^2 t}}{|\mathbf{k}|^2} = i\frac{d}{dt}K^\varepsilon(t).$$

Using the latter identity, written as $\langle \rho^\varepsilon, U(t-s) * \rho^\varepsilon\rangle = -i\frac{d}{ds}K^\varepsilon(t-s)$, in (28), and by integration by parts in s, we get

$$\begin{aligned}\frac{M}{\varepsilon}q^\varepsilon(t) = \langle \rho^\varepsilon, U(t) * \psi_0^\varepsilon\rangle &+ \int_0^t ds K^\varepsilon(t-s)\frac{d}{ds}\left[\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s)\right] \\ &- K^\varepsilon(0)\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(t)|^{2\mu}\right) q^\varepsilon(t) + K^\varepsilon(t)\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(0)|^{2\mu}\right) q^\varepsilon(0).\end{aligned}$$

Using the identity $K^\varepsilon(0) = M/\varepsilon$ we see that $\frac{M}{\varepsilon}q^\varepsilon(t)$ cancels, so that, rearranging the terms, we are left with

$$\begin{aligned}\gamma|q^\varepsilon(t)|^{2\mu}q^\varepsilon(t) = \langle \rho^\varepsilon, U(t) * \psi_0^\varepsilon\rangle &+ \int_0^t ds K^\varepsilon(t-s)\frac{d}{ds}\left[\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s)\right] \\ &+ K^\varepsilon(t)\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(0)|^{2\mu}\right) q^\varepsilon(0).\end{aligned}$$

To recover an equation of the form (25), we multiply for $\frac{1}{\sqrt{\tau-t}}$ and integrate in t for $t \in [0,\tau]$. We obtain

$$\begin{aligned}\gamma\int_0^\tau dt \frac{|q^\varepsilon(t)|^{2\mu}q^\varepsilon(t)}{\sqrt{\tau-t}} &= \int_0^\tau dt \frac{\langle \rho^\varepsilon, U(t) * \psi_0^\varepsilon\rangle}{\sqrt{\tau-t}} \\ &+ \int_0^\tau dt \frac{1}{\sqrt{\tau-t}}\int_0^t ds K^\varepsilon(t-s)\frac{d}{ds}\left[\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s)\right] \\ &+ \left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(0)|^{2\mu}\right) q^\varepsilon(0)\int_0^\tau dt \frac{K^\varepsilon(t)}{\sqrt{\tau-t}}.\end{aligned} \tag{29}$$

The heuristic argument showing that $q^\varepsilon(t)$ should converge to $q(t)$ is based on the fact that

$$K^\varepsilon(t) \to \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \mathrm{d}\mathbf{k}\,\frac{e^{-i|\mathbf{k}|^2 t}}{|\mathbf{k}|^2} = \frac{1}{4\pi\sqrt{\pi i}\sqrt{t}}, \tag{30}$$

as $\varepsilon \to 0$. This suggests that Eq. (29) should be approximated by

$$\begin{aligned}\gamma\int_0^\tau dt \frac{|q^\varepsilon(t)|^{2\mu}q^\varepsilon(t)}{\sqrt{\tau-t}} &\simeq \int_0^\tau dt \frac{\langle \rho^\varepsilon, U(t) * \psi_0^\varepsilon\rangle}{\sqrt{\tau-t}} \\ &+ \frac{1}{4\pi\sqrt{\pi i}}\int_0^\tau dt \frac{1}{\sqrt{\tau-t}}\int_0^t ds \frac{1}{\sqrt{t-s}}\frac{d}{ds}\left[\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right) q^\varepsilon(s)\right] \\ &+ \frac{1}{4\pi\sqrt{\pi i}}\left(-1 + \gamma\frac{\varepsilon}{M}|q^\varepsilon(0)|^{2\mu}\right) q^\varepsilon(0)\int_0^\tau dt \frac{1}{\sqrt{\tau-t}}\frac{1}{\sqrt{t}}.\end{aligned}$$

In the second line of the equation above we exchange the integrals in t and s and use the fact that $\int_0^\tau dt \frac{1}{\sqrt{\tau-t}}\frac{1}{\sqrt{t-s}}\mathbf{1}_{\{t>s\}} = \pi$, while in the third line we use $\int_0^\tau dt \frac{1}{\sqrt{\tau-t}}\frac{1}{\sqrt{t}} = \pi$, to get

$$\gamma\int_0^\tau dt\frac{|q^\varepsilon(t)|^{2\mu}q^\varepsilon(t)}{\sqrt{\tau-t}} \simeq \int_0^\tau dt\frac{1}{\sqrt{\tau-t}}\langle\rho^\varepsilon, U(t)*\psi_0^\varepsilon\rangle + \frac{1}{4\sqrt{\pi i}}\int_0^\tau ds\frac{d}{ds}\left[\left(-1+\gamma\frac{\varepsilon}{M}|q^\varepsilon(s)|^{2\mu}\right)q^\varepsilon(s)\right] + \frac{1}{4\sqrt{\pi i}}\left(-1+\gamma\frac{\varepsilon}{M}|q^\varepsilon(0)|^{2\mu}\right)q^\varepsilon(0).$$

Performing the integral in s, and neglecting further terms of order ε, we finally end up with

$$\gamma\int_0^\tau dt\frac{|q^\varepsilon(t)|^{2\mu}q^\varepsilon(t)}{\sqrt{\tau-t}} \simeq \int_0^\tau dt\frac{\langle\rho^\varepsilon, U(t)*\psi_0^\varepsilon\rangle}{\sqrt{\tau-t}} - \frac{q^\varepsilon(\tau)}{4\sqrt{\pi i}}.$$

Comparing the latter formula with Eq. (25), one sees that $q^\varepsilon(t)$ satisfies approximatively the same equation as $q(t)$.

To make rigorous the heuristic argument described above is the goal of a forthcoming work. One would expect that the right approach is to add and subtract to K^ε, in Eq. (29), its limit, given in formula (30), then prove that the remainder (the term containing the difference between K^ε and its limit) is small. One main issue with this approach is the presence of the derivative of $q^\varepsilon(s)$ in Eq. (29), which implies that the remainder depends on $\dot{q}^\varepsilon$. The dependence of the reminder on $\dot{q}^\varepsilon$ is unexpected, because the limit equation does not involve the derivative of q, and difficult to treat, because it requires a bound on $\dot{q}^\varepsilon$. An approach that avoids taking the derivative of q^ε would be preferable.

4. Conclusions

We addressed the problem of finding regular approximations of nonlinear delta-interactions.

We showed that, in dimension one, it is possible to find both local (see [10]) and non-local (see [16]) nonlinearities that converge to the limit problem. The convergence can be rigorously proved for initial data in $H^1(\mathbb{R})$.

For what concerns the three dimensional problem, we suggested an approximation through non-local nonlinearities. The convergence to the limit problem seems to be plausible but it is not yet proved rigorously.

Several problems remain completely open and would deserve some attention. We mention two of them which are strictly related. They concern the approximation of delta-interactions in dimension one and three, through local nonlinearities in the presence of a linear term with a zero energy resonance.

The approximation of H_α in dimension three through Hamiltonians with scaled potentials is not as intuitive as in dimension one. We already noted that in dimension one the operator $-\Delta + V(\cdot/\varepsilon)/\varepsilon$ converges to H_α, with $\alpha = \int_{\mathbb{R}} V dx$. One might then think that also in dimension three, adding a delta-convergent function to the Laplacian would give an operator that converges to H_α. This does not happen to be the case.

To define a sequence of Schrödinger operators that converge to H_α one has to choose a potential V such that the operator $H = -\Delta + V$ has a zero energy resonance. That means that there exists a function ϕ such that $\phi \in L^2_{loc}(\mathbb{R}^3)$, $\nabla\phi \in L^2(\mathbb{R})$ and $H\phi = 0$ in

the distributional sense. Assuming additionally, that V decays fast enough, one has that (see [6])

$$H^\varepsilon = -\Delta + \frac{1+\lambda\varepsilon}{\varepsilon^2} V\left(\frac{\cdot}{\varepsilon}\right), \tag{31}$$

where $\lambda \in \mathbb{R}$ converges (in norm resolvent sense) to H_α, with coupling constant $\alpha = -m\lambda$, where m is a positive constant that depends on V.

One may wonder whether letting $\lambda \to \lambda(\psi)$ would allow to obtain a local approximation of the nonlinear delta-interaction in dimension three.

A similar problem can be formulated in dimension one. Assume that V decays fast enough and that it is such that $H = -\Delta + V$ has a zero energy resonance, i.e., there exists $\phi \in L^\infty(\mathbb{R})$, $\phi \notin L^2(\mathbb{R})$, such that $-\phi'' + V\phi = 0$. Assume also that the resonance ϕ is an even function. Then the operator H^ε in (31), in dimension one, converges in norm resolvent sense to H_α, defined in (1) - (2), with $\alpha = -\widetilde{m}\lambda$, where $\widetilde{m}$ is a positive constant which depends on V (see [9]). In this sense the problems of approximating H_α in dimension one and three are similar. We remark that, in dimension one, also the convergence of the operator $-\Delta + V(\cdot/\varepsilon)/\varepsilon$ relies on the presence of a zero energy resonance of the operator $(-\Delta, H^2(\mathbb{R}))$. In this case the resonance is just the constant function.

Also in the one dimensional case, one might expect that letting $\lambda \to \lambda(\psi)$ in (31) will allow one to construct an approximation of a nonlinear delta-interaction.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 95–99

ON THE POSSIBILITY OF USING OPTICAL Y-SPLITTER IN QUANTUM RANDOM NUMBER GENERATION SYSTEMS BASED ON FLUCTUATIONS OF VACUUM

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Quantum random number generation allows the obtaining of true random numbers that can be used for applications (e.g.,a cryptography) requiring a high degree of randomness. In this paper, we give a mathematical description of a quantum random number generation system using homodyne detection. As a result of the theoretical research, we obtained the description of the relationship between beam splitter input radiation and differential current on detectors after beam splitting. We derived equations allowing one to estimate the scheme parameters imperfection impact on measurement results. We also obtained mathematical expressions, demonstrating the equivalence of quantum description of Y-splitter and beam splitter with two inputs, which allows the use Y-splitter for the implementation of quantum random number generation systems based on vacuum quantum fluctuations.

Keywords: quantum random number generation, beam splitter, Y-splitter, vacuum fluctuations.

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1. Introduction

Random numbers are widely used in classical and quantum cryptography. Perfect randomness is very important for quantum cryptography protocols (see, e.g., [1]), but it is rather difficult to obtain ideally random numbers in real devices. In principle, there are two means to achieve this. The first, one uses special computer algorithms, however, this way leads only to pseudo-random numbers. The second way is to use physical systems with inherent random behavior. It is preferable to have fundamental character of this randomness. The quantum random number generator (QRNG) is one such type of device. Accordingly, QRNG can be divided into several groups, depending upon the physical phenomenon serving as the background for the device: beam separation [2–4], entangled photon states [5, 6], processes of photon emission and detection [7, 8], quantum noise of lasers [9, 10], vacuum fluctuations of the electromagnetic field [11].

2. Quantum random number generation based on the principles of homodyne detection

This type of QRNG is based on the randomness of the quantum noise where the balanced detector subtracts signals received from beam splitter outputs (fig.1).

A coherent state from the laser comes to the first splitter input and in a vacuum state – to another input. The beam splitter prepares the mixture of these signals, then the signals from the beam splitter outputs arrive at the balanced detector. The subtracted signal is

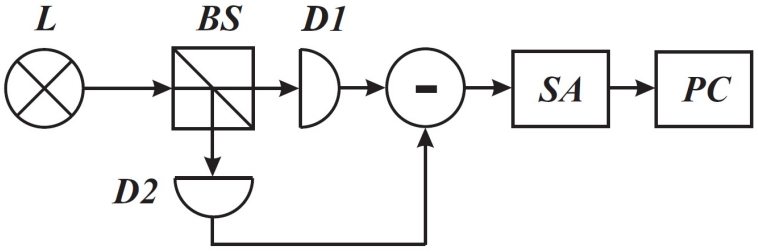

FIG. 1. QRNG scheme, based on vacuum fluctuations: L - laser, BS - beam splitter, D1, D2 - detectors, SA - spectrum analyzer, PC - computer

quantum noise, which can be processed by the PC. Random numbers are thus obtained as a result of the received differential signal processing.

3. Beam splitter

The main element of such schemes is the beam splitter. We consider how it transforms a signal. If incoming signals are a_1 and a_2, then the signals at outputs, b_1 and b_2, can be described by formula (1), where θ - is the angle of the beam splitter.

$$\begin{cases} b_1 = a_1 \cos\theta - a_2 \sin\theta, \\ b_2 = a_1 \sin\theta + a_2 \cos\theta. \end{cases} \tag{1}$$

The radiation is characterized by the Poisson distribution with parameter α (describing mean photon number), which is described as follows (in the operator form)

$$|\alpha\rangle = e^{\alpha a_1^+ - \alpha^* a_1}|0\rangle, \tag{2}$$

where a_1^+ and a_1 are photon creation and annihilation operators at the first input of the beam splitter, $|\alpha\rangle$ is the coherent state, $|0\rangle$ is the vacuum state.

If a coherent state is sent to the first splitter input, and a vacuum state - to another, then the beam splitter input signal is expressed as a tensor product:

$$|\alpha\rangle|0\rangle = e^{\alpha a_1^+ - \alpha^* a_1}|0\rangle_1|0\rangle_2. \tag{3}$$

Let the radiation be characterized by the Poisson distribution with parameter $|\alpha\rangle$. If it passes through the beam splitter with an angle θ (fig.2.*a*), then one of the beam splitter outputs is characterized by the Poisson distribution with parameter $|a\cos\theta\rangle$, and the second is characterized by the Poisson distribution with parameter $|a\sin\theta\rangle$.

In case of symmetric beam splitter we obtain the following expressions for the signals at the both outputs:

$$b_1^+ = b_2^+ = \frac{1}{\sqrt{2}} a_1^+. \tag{4}$$

The differential current can be determined as follows:

$$\Delta i = i_2 - i_1 = \gamma_2 b_2^+ b_2 - \gamma_1 b_1^+ b_1, \tag{5}$$

where i_1 and i_2 are the photocurrents at the first and the second detectors, γ_1 and γ_2 are the quantum efficiencies of the detectors. Correspondingly, the general expression for the differential current is as follows:

$$\langle \Delta i \rangle = \alpha^2(\gamma_2 \sin^2\theta - \gamma_1 \cos^2\theta). \tag{6}$$

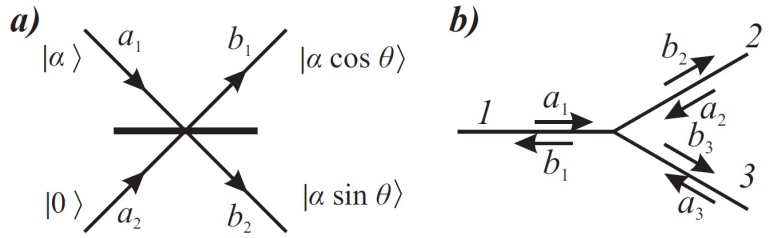

FIG. 2. *a*)Scheme of a beam splitter with angle θ, where to the first splitter input a coherent state is send, and to other input - a vacuum state.*b*)Optical Y-splitter. a_1, a_2, a_3 - input signals of the 1st, 2nd and 3rd ports, respectively, b_1, b_2, b_3 - output signals from the splitter

One can see that in the case of using of a symmetric beam splitter and detectors with identical quantum efficiencies, the mean value of the differential current is zero, and the amplitude of the differential current deviation is proportional to the intensity of the incident radiation:

$$\Delta i = \alpha\gamma. \tag{7}$$

In the case of using an asymmetric beam splitter and detectors with different quantum efficiencies, the amplitude of the differential current deviation is characterized by the following expression:

$$\Delta i = \alpha\sqrt{\gamma_2^2 \sin^2\theta + \gamma_1^2 \cos^2\theta}. \tag{8}$$

4. Y-splitter

In quantum random number generators based on the quantum fluctuations of vacuum, a beam splitter with two inputs and two outputs is normally used. We will consider the possibility of applying a fiber optical Y-splitter for these constructions. For this purpose, it is necessary to compare the quantum descriptions of the beam splitter (Fig. 2.*a*) and Y-splitter (Fig. 2.*b*). We consider the Y-splitter as a system with three inputs and three outputs, because input and output signals can pass through the same channel.

The relationship between the signals at inputs and outputs of the Y-splitter can be described by the following expression:

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} -\sqrt{1-2\lambda^2} & \beta & \beta \\ \lambda & -\gamma & \sqrt{1-\beta^2-\gamma^2} \\ \lambda & \sqrt{1-\beta^2-\gamma^2} & -\gamma \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}. \tag{9}$$

where λ is the real proportionality factor, relating the output signals at the second and the third ports and the input signal applied to the first port; β is the real proportionality factor, relating the output signal at the first port and the input signal applied to the second or the third port; γ is the real proportionality factor, relating the input and the output signals of the second or the third port. Other coefficients are selected in accordance with requirements of the unitary property of the matrix. The following expressions are also caused by the unitarity conditions:

$$\begin{cases} -\sqrt{1-2\lambda^2}\beta - \lambda\gamma + \lambda\sqrt{1-\beta^2-\gamma^2} = 0, \\ -\sqrt{1-2\lambda^2}\beta + \lambda\sqrt{1-\beta^2-\gamma^2} - \lambda\gamma = 0, \\ \beta^2 - 2\gamma\sqrt{1-\beta^2-\gamma^2} = 0. \end{cases} \tag{10}$$

Parameters λ and β can be expressed in terms of γ from this system:

$$\alpha = \beta = \sqrt{2\gamma(1-\gamma)}. \tag{11}$$

Then original matrix takes the form:

$$\begin{pmatrix} 1-2\gamma & \sqrt{2\gamma(1-\gamma)} & \sqrt{2\gamma(1-\gamma)} \\ \sqrt{2\gamma(1-\gamma)} & -\gamma & 1-\gamma \\ \sqrt{2\gamma(1-\gamma)} & 1-\gamma & -\gamma \end{pmatrix}. \tag{12}$$

We consider the special case when the signal from input port 1 is distributed only between ports 2 and 3. In this case, $\sqrt{1-2\lambda^2} = 0$, and $\lambda = \dfrac{1}{\sqrt{2}}$ and by using expressions obtained above, we can obtain the following values: $\beta = \dfrac{1}{\sqrt{2}}$ and $\gamma = \dfrac{1}{2}$.

If the signal a_1 comes to the 1st port of the Y-splitter, then the signals from outputs 2 and 3 can be obtained by using the matrix described above:

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}}a_1 \\ \frac{1}{\sqrt{2}}a_1 \end{pmatrix}. \tag{13}$$

Thus,

$$b_2^+ = b_3^+ = \frac{1}{\sqrt{2}}a_1^+. \tag{14}$$

This result coincides with the signals obtained at the output ports of the symmetric beam splitter (4), when the coherent state a_1 comes to the first splitter input, and a vacuum state - to the other. Thus, as description for the beam splitter and the Y-splitter are the same, to evaluate work of QRNG systems based on the vacuum fluctuations using the Y-splitter we can use results for the beam splitter, obtained earlier. For example, we can estimate the probability of the detecting of N different photons in the substractor [12] (Fig. 3):

$$P_N = exp(-|\alpha|^2) I_{|N|}(|\alpha|^2), \tag{15}$$

where α is the Poisson parameter of the initial radiation, corresponding to the mean number of photons, $I_{|N|}(|\alpha|^2)$ is the modified Bessel function of order $|N|$.

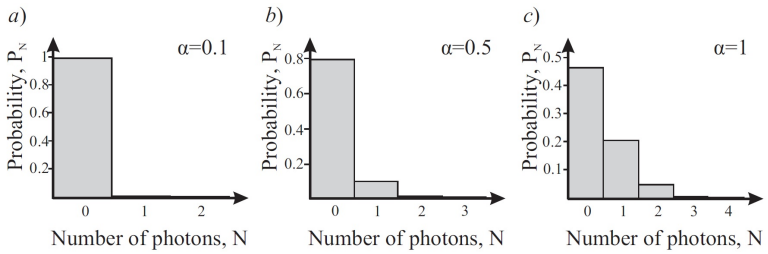

FIG. 3. Probability of detecting of N difference photons at substractor for input radiation with mean number of photons a) α =0.1, b) α=0.5, c) α =1

5. Conclusion

Expressions describing the relationship between the beam splitter input radiation and the differential current were obtained for quantum random number generation scheme using homodyne detection. For this scheme, expressions for estimations of the scheme's parameters imperfection impacts on the measurement results, were also derived. We obtained mathematical expressions demonstrating the formal equivalence for the quantum description of the beam splitter with two inputs and the quantum description of the Y-splitter. This allows us to use the Y-splitter for the implementation of a quantum random number generation system based on the quantum fluctuations of vacuum, and to use the previously obtained formulas for the beam splitter with two inputs and two outputs for the calculation of that system's characteristics.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 100–112

A LINEARIZED MODEL OF QUANTUM TRANSPORT IN THE ASYMPTOTIC REGIME OF QUANTUM WELLS

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The effects of the local accumulation of charges in resonant tunnelling heterostructures have been described using 1D Shrödinger-Poisson Hamiltonians in the asymptotic regime of quantum wells. Taking into account the features of the underling physical system, the corresponding linearized model is naturally related to the adiabatic evolution of shape resonances on a time scale which is exponentially large w.r.t. the asymptotic parameter h. A possible strategy to investigate this problem consists of using a complex dilation to identify the resonances with the eigenvalues of a deformed operator. Then, the adiabatic evolution problem for a sheet-density of charges can be reformulated using the deformed dynamical system which, under suitable initial conditions, is expected to evolve following the instantaneous resonant states.

After recalling the main technical difficulties related to this approach, we introduce a modified model where h-dependent artificial interface conditions, occurring at the boundary of the interaction region, allow one to obtain adiabatic approximations for the relevant resonant states, while producing a small perturbation of the dynamics on the scale h^{N_0}. According to these results, we finally suggest an alternative formulation of the adiabatic problem. An a posteriori justification of our method is obtained by considering an explicitly-solvable case.

Keywords: Schrödinger-Poisson equation, adiabatic evolution of resonances.

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1. Introduction

We consider the axial transport through resonant tunneling structures like highly doped p-n semiconductor heterojunctions (Esaki diodes), multiple barriers or quantum well diodes. In such systems, the conduction band edge-profile is described by a multiple-barrier potential (see e.g. in [7]). Due to the quantum tunneling, the charge carriers, at the resonant levels, interact with metastable states and, depending on the potential geometry, a local accumulation of charges may result. The corresponding repulsive effect, which can strongly modify the transport properties, have been described in the mean-field approximation by one-particle quantum Hamiltonians of Hartree-type with Poisson nonlinearity ([13]). In this framework, the barriers depth, fixing the time scale for the dispersion of the metastable states, can be rather large compared to the size of the wave packets. An unitarily equivalent description of the model then consists of replacing the kinetic part of the Hamiltonian with the 'semiclassical' 1D Laplacian, $-h^2\Delta$, while the potential is the superposition of a barrier, supported on a bounded interval $[a, b]$, and multiple potential wells with support of size h inside (a, b). The parameter h now corresponds to a rescaled Fermi length (see for instance [6]) fixing the quantum scale of the system and, coherently with the features of the physical

model, is assumed to be small. The resulting transport model is described by a double-scale Schrödinger-Poisson Hamiltonian:

$$H_{NL}^h = -h^2\Delta + \mathcal{V}^h + V_{NL}^h\,, \tag{1}$$

where the linear part of the potential is defined according to:

$$\mathcal{V}^h = V + W^h\,, \qquad \operatorname{supp} V = [a,b]\ , \tag{2}$$

and

$$W^h = -\sum_{n=1}^{N} w_n\left(\left(x-x_n\right)1/h\right)\ , \quad w_n \in \mathcal{C}^0\left(\mathbb{R},\mathbb{R}_+\right)\ , \quad \operatorname{supp}\, w_n = [-d,d]\ , \tag{3}$$

for some $d>0$. For a suitable choice of V, this fixes a semiclassical island with *quantum wells* supported around the collection of points $x_n \in (a,b)$, $n=1,...,N$. The nonlinear potential term, V_{NL}^h, solves a Poisson equation with a source given by the charge density of the system. The corresponding evolution problem is as follows:

$$\begin{cases} i\partial_t u^h\left(\cdot,t,k\right) = \left(-h^2\Delta + \mathcal{V}^h + V_{NL}^h\right)u^h\left(\cdot,t,k\right)\ , \\ \left(-h^2\Delta + \mathcal{V}^h + V_{NL}^h\big|_{t=0} - k^2\right)u^h\left(\cdot,0,k\right) = 0 \\ -\Delta V_{NL}^h = d^h\,, \\ d^h(x) = \int \frac{dk}{2\pi h} g(k)\ \left|u^h\left(x,t,k\right)\right|^2\ . \end{cases} \tag{4}$$

Here, $u^h\left(\cdot,t,k\right)$ denotes the nonlinear evolution of a generalized eigenfunction $u^h\left(\cdot,0,k\right)$ related to the Hamiltonian at $t=0$. The quantum state corresponding to this picture is described by a density matrix ρ^h defined by the momenta distribution $g(k)$, and whose kernel evolves in time according to

$$\rho_t^h(x,y) = \int \frac{dk}{2\pi h} g(k)\, u^h\left(x,t,k\right)\bar{u}^h\left(y,t,k\right)\ . \tag{5}$$

When $g(k)$ selects incoming waves (i.e.: $\operatorname{supp} g \subset \mathbb{R}_+$), the system is nourished by charges from the left, providing a non-equilibrium condition where, depending on the potential geometry, the particles may accumulate inside the wells. These systems – characterized by a very rich nonlinear characteristics, such as hysteresis phenomena and steadily oscillating currents – have attracted increasing interest, both for the challenging mathematical problems associated with them as well as the potential application perspectives.

Resonant energies, produced by the potential $\mathcal{V}^h$, naturally arise in this class of models and play a central role in the description of quantum tunneling. The incoming electrons, at resonant levels below $\sup_{(a,b)} V$, interact with resonant states which evolve in time according to a quasi-stationary dynamics. In particular, their L^2-mass remains concentrated in the vicinity of the wells support for a range of time exponentially large w.r.t. h. Depending on the position of the wells, this possibly induces a local charging process; then, the nonlinear coupling in (4) generates a positive response (depending upon the charge in the wells) which modifies the potential profile and reduces the tunneling rate.

This dynamics was considered in the works of G. Jona-Lasionio, C. Presilla and J. Sjöstrand ([13], [17], [18]), within a simplified framework where the Poisson potential is replaced by an affine function multiplied by a nonlinear charge density. Using slowly varying potential assumptions, WKB expansions and a one-mode approximation for the time evolution of the quantum state, the authors discuss the behavior of the sheet density

related to the accumulation of electrons in a single well determined by a flat double-barrier potential. Rephrasing the result of their work in our scaling, they show that the relevant time scale of the problem is on the order of $e^{\tau/h}$, corresponding to the imaginary part of the lowest resonance, and provide with an explicit equation for the evolution of the local charge density in the limit $h \to 0$ (eq. 9.7 in [17]).

It is worthwhile to note that these calculations have been shown to be relevant only in some specific cases. This concerns, in particular, the adiabatic approximation for the nonlinear evolution of generalized eigenfunctions, which appears to be an essential point of the analysis: the lack of an error bound in the adiabatic formulas for resonant states prevents the control of the possible remainder terms in the asymptotic limit. Moreover, the role played by the device's geometry in the emergence of nonlinear effects remains an open problem. This was pointed out by F.Nier, Y.Patel and V.Bonaillie-Nöel, in a series of works devoted to the steady state problem related to (4) under far-from-equilibrium assumptions. In [4]- [5], an accurate microlocal analysis of the tunneling effect as $h \to 0$ determines the limit occupation number of resonant states. This analysis leads to a simplified equation for the Poisson problem, where the limit charge density is described by a superposition of delta-shaped distributions centered in the points x_n (see the definition (3)).

The relevance of the adiabatic approximation, for the Schrödinger-Poisson equation in the regime of quantum wells, suggests that we consider as a preliminary step, a 'linearized' problem where the nonlinear term of H^h_{NL} is replaced by a potential supported on (a, b) and adiabatically dependent on time; namely we introduce the time dependent family of Schrödinger operators:

$$H^h_0(t) = -h^2\Delta + \mathcal{V}^h(t) \,, \tag{6}$$

where $\mathcal{V}^h(t) = V + W^h(t)$ fulfills the particular scaling (2)-(3) for all t. The adiabatic evolution of an observable χ (corresponding to a local charge) is described by the variable $A^h_0(t)$ solving the equation:

$$\begin{cases} A^h_0(t) = Tr\left[\chi\,\rho^h_0(t)\right] \,, \\ \rho^h_0(t) = \int \frac{dk}{2\pi h} g(k) \left|u^h(k,\cdot,t)\right\rangle \left\langle u^h(k,\cdot,t)\right| \,, \\ i\varepsilon\partial_t u^h(k,\cdot,t) = H^h_0(t) u^h(k,\cdot,t)\,, \\ \left(H^h_0(t=0) - k^2\right) u^h(k,\cdot,0) = 0\,. \end{cases} \tag{7}$$

In this framework, the relevant resonant energies for the transport problem are determined by the resonances of H^h_0 with the real part embedded in $\left(0, \inf_{[a,b]} V\right)$; these are usually referred to as *shape resonances*. In the asymptotic regime of quantum wells ($h \to 0$), it is known that the number of shape resonances is uniformly bounded w.r.t. h, while their imaginary part is on the order of $e^{\tau/h}$ for a suitable constant $\tau > 0$ depending on the potential geometry (for this point we refer to the analysis developed in [10]- [11]. Following [20], this quantity fixes the time scale for the dispersion of the corresponding resonant states. Hence, the effect of the accumulation of charges inside the wells can be investigated by choosing the adiabatic parameter ε, in (7), of size $e^{-\tau/h}$.

1.1. Detecting quantum resonances: the exterior complex dilation

The small-h analysis of the linearized problem (7), involves the following task: clarify, in an energy interval close to the shape resonances, the relation between the evolution of generalized eigenfunctions and of the resonant states in the adiabatic limit. Let us recall that

the resonances of a Schrödinger operator correspond (modulo a restriction to a dense subset of dilation-analytic functions) to the poles of the meromorphic extension of its resolvent to the second Riemann sheet (i.e.: $\operatorname{Im}\sqrt{z} < 0$). These are detected through the complex deformation method (see [12] for details), which can be adapted to our framework by using the exterior complex scaling: $x \to xe^{\theta 1_{\mathbb{R}\setminus(a,b)}(x)}$. When $\theta \in \mathbb{R}$, the related deformation is an unitary operator acting on $L^2(\mathbb{R})$ according to

$$U_\theta u(x) = \begin{cases} e^{\theta/2} u\left(e^\theta (x-b) - b\right), & x > b, \\ u(x), & (a,b), \\ e^{\theta/2} u\left(e^\theta (x-a) - a\right), & x < a. \end{cases} \tag{8}$$

For the Hamiltonian:

$$Q = -\Delta + \mathcal{V}, \qquad \text{with: } \mathcal{V} \in L^\infty(\mathbb{R}) \text{ and } supp\, \mathcal{V} = [a,b], \tag{9}$$

the corresponding deformed operator, next denoted with: $Q(\theta) = U_\theta Q U_\theta^{-1}$, is explicitly written as (see e.g. in [8]):

$$Q(\theta) = -e^{-2\theta 1_{\mathbb{R}\setminus(a,b)}} \Delta_\theta + \mathcal{V}, \tag{10}$$

where Δ_θ is the non-self-adjoint point perturbation of the Laplacian defined by the interface conditions:

$$\begin{cases} e^{-\frac{\theta}{2}} u(b^+) = u(b^-), \quad e^{-\frac{3}{2}\theta} u'(b^+) = u'(b^-), \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+), \quad e^{-\frac{3}{2}\theta} u'(a^-) = u'(a^+). \end{cases} \tag{11}$$

Namely, we have the following:

$$\Delta_\theta : \begin{cases} D(\Delta_\theta) = \{u \in H^2(\mathbb{R}\setminus\{a,b\}) \mid (11) \text{ holds}\}, \\ (\Delta_\theta u)(x) = -u''(x), \qquad x \in \mathbb{R}\setminus\{a,b\}. \end{cases} \tag{12}$$

When $\operatorname{Im}\theta > 0$, this deformation produces a rotation of the essential spectrum in the second Riemann sheet: $\sigma_{ess}(Q(\theta)) = e^{-2\operatorname{Im}\theta}\mathbb{R}_+$; in the cone spanned by $\mathbb{R}_+$ and $\sigma_{ess}(Q(\theta))$ the resonances of Q identify with the spectral points of $Q(\theta)$. This important result was first obtained by J. Aguilar, E. Baslev and J.M. Combes in [1], [3], where the case of analytic potentials w.r.t. the uniform complex dilation $x \to xe^\theta$ was considered (see also [12, Theorem 16.4]). For potentials which can be complex deformed only outside a compact region, the exterior complex scaling technique appeared in [19] in the singular version that we reconsider here.

Proposition 1.1. *Let Q be defined by (9); the resonances of Q in the cone*

$$K_\alpha = \{\arg z \in (-2\alpha, 0)\}, \qquad \text{with } \alpha < \frac{\pi}{4}, \tag{13}$$

are eigenvalues of the operators $Q(\theta)$ for $\alpha \leqslant \operatorname{Im}\theta$.

As a consequence, the resonant state associated with a resonance $E_{res} \in K_\alpha \cap \sigma(Q(\theta))$ can be defined as an eigenvector of $Q(\theta)$, with $\alpha \leqslant \operatorname{Im}\theta$, and we have

$$(Q(\theta) - E_{res})\,\psi_{E_{res}} = 0, \qquad \text{in } L^2(\mathbb{R}). \tag{14}$$

It is worth remarking that the resonances in K_α do not depend on the deformation, i.e.: if $E_{res} \in K_\alpha \cap \sigma(Q(\theta))$ for a given θ, then, $E_{res} \in K_\alpha \cap \sigma(Q(\theta'))$ for all $\theta' > \theta$ and $\alpha \leqslant \operatorname{Im}\theta'$. Nevertheless the solution $\psi_{E_{res}}$ of (14) possibly depends on θ in the exterior

region, while, according to the shape of U_θ, the cutoff $1_{(a,b)}(x)\,\psi_{E_{res}}$ (usually refferred to as the *quasi-resonant* state) is independent of θ.

1.2. An alternative approach to the adiabatic problem

The identification of the resonances for Q with the spectral points of the corresponding deformed operator $Q(\theta)$ suggest an alternative, and possibly more natural, framework to study the adiabatic problem (7). Let us define the observable χ according to

$$\chi \in \mathcal{C}^\infty(\mathbb{R}) , \qquad \operatorname{supp}\chi \subset\subset (a,b) . \tag{15}$$

With this choice, χ describes the charge accumulating in a region inside (a,b). Since χ commutes with the deformation map U_θ for all θ, making use of the properties of the trace operation we have:

$$A_0^h(t) = Tr\left[\chi\,\rho_0^h(t)\right] = Tr\left[U_\theta^*\chi U_\theta \rho_0^h(t)\right] = Tr\left[\chi U_\theta \rho_0^h(t)\,U_\theta^*\right] . \tag{16}$$

Here, $U_\theta\rho_0^h(t)\,U_\theta^*$ identifies with the evolution at time t of a deformed density matrix, when the dynamical system is generated by $H_0^h(t,\theta) = U_\theta H_0^h(t)\,U_\theta^{-1}$. This allows us to rephrase (7) in the equivalent form:

$$\begin{cases} A_0^h(t) = Tr\left[\chi\rho_0^h(t,\theta)\right] , \\ \rho_0^h(t,\theta) = \int \frac{dk}{2\pi h} g(k)\,\left|u_\theta^h(k,\cdot,t)\right\rangle\left\langle u_\theta^h(k,\cdot,t)\right| , \\ i\varepsilon\partial_t u_\theta^h(k,\cdot,t) = H_0^h(t,\theta)\,u_\theta^h(k,\cdot,t) , \\ \left(H_0^h(t=0,\theta) - k^2\right) u_\theta^h(k,\cdot,0) = 0 . \end{cases} \tag{17}$$

When g selects energies close to the shape resonances, the relevant information about the solution $u_\theta^h(k,\cdot,t)$ of the adiabatic problem in (17) are related to the evolution of the resonant states. To fix this point, assume that, for a suitable choice of $\mathcal{V}^h(t)$ in (6), the linearized operator $H_0^h(t)$ has a shape resonance $E^h(t)$ remaining close for all time to a limit energy λ^0 (in a sense which will be specified later with an explicit example). According to Proposition 1.1, we have: $E^h(t) \in K_\alpha \cap \sigma\left(H_0^h(t,\theta)\right)$ for some $\pi/4 \geqslant \alpha > 0$ and $\alpha \leqslant \operatorname{Im}\theta$, and the corresponding instantaneous resonant state $\psi_{E^h(t)}$ solves the eigenvalue equation (14) with $Q(\theta) = H_0^h(t,\theta)$. As far as $\operatorname{supp} g = \left\{k>0\,,\ k^2 \sim \operatorname{Re} E_{res}^h(t) \sim \lambda^0\right\}$, it is expected that

$$1_{(a,b)}(x)\,u_\theta^h(k,x,t) \sim 1_{(a,b)}(x)\,\psi^h(t) , \tag{18}$$

where $\psi^h(t)$ is the solution of the problem

$$\begin{cases} i\varepsilon\partial_t\psi^h(t) = H_0^h(t,\theta)\,\psi^h(t) , \\ \psi^h(0) = \psi_{E^h(0)} . \end{cases} \tag{19}$$

For $\varepsilon = e^{-\tau/h}$, the small-$h$ asymptotics of this dynamic is related to the adiabatic evolution of an eigenvector of the initial operator $H_0^h(t=0,\theta)$ and standard results in adiabatic perturbation theory (see e.g. in [16]) would suggest to identify $\psi^h(t)$ with the instantaneous resonant state $\psi_{E^h(t)}$ (multiplied by a suitable modulation factor), with an error of size $e^{-\tau/h}$. Such an adiabatic approximation and the relation (18) could be implemented in (10) to study the asymptotic behavior of $A_0^h(t)$ as $h \to 0$.

The main difficulty in this approach is due to the fact that the complex scaling does not preserve the m-accretivity of the operator, i.e.: the quadratic form associated with $H_0^h(t,\theta)$ has an imaginary part with undetermined sign (see the eq. (1.5) in [8]); as a

consequence, the deformed dynamics may exhibit exponential growth w.r.t. t. Since uniform-in-time estimates for the dynamical system are necessary to prove the adiabatic theorem, the lack of this condition in our case, prevents us from developing a rigorous approach to the study of (19) in the small-h limit.

2. A modified model

A possible strategy to overcome the lack of uniform-in-time estimates occurring in the study of the dynamical system (19) consists of modifying the physical Hamiltonian H_0^h according to the following:

$$H_\theta^h : \begin{cases} D\left(H_\theta^h\right) = \{u \in H^2\left(\mathbb{R}\backslash\{a,b\}\right) \mid (11) \text{ holds}\}\,, \\ \\ \left(H_\theta^h\, u\right)(x) = -h^2 u''(x) + \mathcal{V}^h(x)\, u(x)\,, \qquad x \in \mathbb{R}\backslash\{a,b\}\,, \end{cases} \tag{20}$$

where, as before, the potential is formed by the superposition of a barrier supported on $[a,b]$, and a collection of quantum wells W^h defined by (3). It worthwhile to remark that, for $\theta \neq 0$, H_θ^h is neither self-adjoint nor symmetric and identifies with an extension of the symmetric restriction

$$H_{0,0}^h = H_0^h \upharpoonright \left\{u \in H^2\left(\mathbb{R}\right) \mid u(\alpha) = u'(\alpha) = 0\,,\ \alpha = a,b\right\}\,. \tag{21}$$

In this connection, H_θ^h is an explicitly solvable model w.r.t. H_0^h and relevant quantities, as its resolvent or generalized eigenfunctions, can be expressed in terms of corresponding non-modified quantities, related to the selfadjoint operator H_0^h, through non-perturbative formulas. This well-known property of point perturbations (see e.g. in [2]) provides us with a usefull tool for spectral analysis and allows us to consider the pair $\left\{H_\theta^h, H_0^h\right\}$ as a scattering system. In particular, if $1_{[a,b]}\mathcal{V}^h > 0$, it has been shown that H_θ^h has a purely continuous spectrum coinciding with $\mathbb{R}_+$, provided that θ is small (depending on h; see [14]). A detailed analysis concerned with operators of this class has been developed (in a slightly more general framework) in [8]- [15]. In what follows, we resume their main features.

2.1. Shape resonances in the regime of quantum wells

Let: $\mathcal{V}^h = V + W^h$, with V and W^h defined as in (2)-(3) and fufilling the following constraints:

$$1_{[a,b]}V \geqslant c\,, \quad \sup\left\{\|V\|_{L^\infty(\mathbb{R})}\,, \left\|W^h\right\|_{L^\infty(\mathbb{R})}\right\} \leqslant \frac{1}{c}\,, \quad \text{supp } W^h \subset\subset (a,b)\,, \tag{22}$$

for some $c > 0$, uniformly w.r.t. $h \in (0, h_0]$. It is known that this particular potential's shape prevents the accumulation of the possible eigenvalues of the corresponding 'Dirichlet operator', H_D^h,

$$H_D^h = -h^2\partial_x^2 + \mathcal{V}^h\,, \qquad D\left(H_D^h\right) = H^2\left([a,b]\right) \cap H_0^1\left([a,b]\right)\,, \tag{23}$$

in the energy region $\left(c, \inf_{[a,b]} V\right)$ when the limit $h \to 0$ is considered (e.g. in [4]). Then, we assume $\mathcal{V}^h$ to verify the following spectral condition.

Condition 2.1. *There exists a real* λ^0 *and a cluster of eigenvalues* $\left\{\lambda_j^h\right\}_{j=1}^{\ell} \subset \sigma\left(H_D^h\right)$ *such that the conditions*

$$\begin{aligned} &i) \qquad c \leqslant \lambda^0 \leqslant \inf_{[a,b]} V - c \leqslant \|V\|_{L^\infty(\mathbb{R})} \leqslant \tfrac{1}{c}\,, \\ &ii) \qquad d\left(\lambda^0, \sigma\left(H_D^h\right) \setminus \left\{\lambda_j^h\right\}_{j=1}^{\ell}\right) \geqslant c\,, \\ &iii) \qquad \max_{1\leqslant j\leqslant \ell} \left|\lambda_j^h - \lambda^0\right| \leqslant \tfrac{h}{c}\,. \end{aligned} \tag{24}$$

hold for all $h \in (0, h_0]$.

Under the action of an exterior dilation $U_{i\gamma}$ with $\gamma > 0$ (see the definition 8), the modified Hamiltonian H_θ^h transforms according to (e.g. in [8])

$$H_\theta^h(i\gamma) = -h^2 \eta(x)\, \Delta_{\theta+i\gamma} + \mathcal{V}^h\,, \qquad \eta(x) = e^{-2i\gamma 1_{\mathbb{R}\setminus(a,b)}(x)}\,, \tag{25}$$

where the operator's domain is obtained from (20) by replacing θ by $\theta + i\gamma$ in the interface conditions (11). In the exterior domain, the solution φ_{res} of the eigenvalue problem corresponding to a resonance $z_{res} \in \{p \in \mathbb{C} \mid \arg p \in (-2\gamma, 0)\}$

$$\left(H_\theta^h(i\gamma) - z_{res}\right)\varphi_{res} = 0\,, \qquad \varphi_{res} \in L^2(\mathbb{R})\,, \tag{26}$$

exhibits the exponential modes

$$\begin{cases} \varphi_{res}(x) = c_+ e^{i\frac{(z_{res})^{1/2}e^{i\gamma}}{h}(x-b)}\,, & x > b\,, \\ \varphi_{res}(x) = c_- e^{i\frac{(z_{res})^{1/2}e^{i\gamma}}{h}(a-x)}\,, & x < a\,. \end{cases} \tag{27}$$

Let $\mathcal{P}_z^h(\theta) = \left(-h^2\Delta_\theta + \mathcal{V}^h\right)$

$$D(\mathcal{P}_z^h(\theta)) = \left\{u \in H^2((a,b))\,,\ \left(h\partial_x + iz^{1/2}e^{-\theta}\right)u(a) = 0\,,\ \left(h\partial_x - iz^{1/2}e^{-\theta}\right)u(b) = 0\right\}\,, \tag{28}$$

where $(z)^{1/2}$ is determined according to $\arg z \in \left[-\frac{\pi}{2}, \frac{3}{2}\pi\right)$. Using (27), the resonance equation (26) is re-termed as a non-linear eigenvalue problem for the operator $\mathcal{P}_z^h(\theta)$

$$\left(\mathcal{P}_{z_{res}}^h(\theta) - z_{res}\right)\varphi_{res} = 0\,. \tag{29}$$

It is worthwhile to note that this equation does not depend on the deformation, but only on the interface conditions in (20). Following the approach of Helffer-Sjöstrand (see [11], [21]), the resonances for the full Hamiltonian $H_\theta^h(i\gamma)$ can be investigated after reducing the Grushin problem modeled from the Dirichlet operator H_D^h for the boundary value operator $\mathcal{P}_{z_{res}}^h(\theta)$. This analysis, developed in [8], shows that, for potentials fulfilling the conditions (24), the shape resonances are localized in small regions of the corresponding Dirichlet's eigenvalues λ_j^h as $h \to 0$. In particular, let ω_δ denotes the regions:

$$\omega_\delta = \left\{z \in \mathbb{C}\,,\ d\left(z, \left\{\lambda_j^h\right\}_{j=1}^{\ell}\right) \leqslant \delta\right\}\,, \tag{30}$$

and $d_{Ag}(x, y, \mathcal{V}, \lambda)$

$$d_{Ag}(x, y, \mathcal{V}, \lambda) = \int_y^x \sqrt{(\mathcal{V}(s) - \lambda)_+}\, ds\,, \qquad x \geqslant y\,, \tag{31}$$

the *Agmon distance* between x and y related to a potential $\mathcal{V}$ and an energy $\lambda \in \mathbb{R}_+$.

Proposition 2.1. *Let $\mathcal{V}^h = V + W^h$ be defined according to (2)-(3), (22), and assume the conditions (24) to hold. Then, for all $h \in (0, h_0]$ and $|\theta| \leqslant \frac{c^2 h}{8}$, the operator H^h_θ has exactly ℓ resonances in $\omega_{\frac{ch}{2}}$, $\left\{z^h_j\right\}_{j=1}^{\ell}$, possibly counted with multiciplicities. Considered as functions of h, after the proper labelling w.r.t. j, these fulfill the relations:*

$$z^h_j(\theta) - \lambda^h_j = \mathcal{O}\left(h^{-3} e^{-\frac{2S_0}{h}}\right). \tag{32}$$

where $S_0 = d_{Ag}\left(\{a,b\}, \cup_{k=1}^N \{x_k\}, V, \lambda^0\right)$ is the Agmon distance between the asymptotic support of W^h and the barrier's boundary. Under the additional condition

$$\lim_{h\to 0} h^3 e^{\frac{2S_0}{h}} \min_{j\neq j'} \left|\lambda^h_j - \lambda^h_{j'}\right| = +\infty, \tag{33}$$

the variations of $z^h_j(\theta) - z^h_j(0)$ is estimated by the following:

$$\max_{j\in\{1\dots\ell\}} \left|z^h_j(\theta) - z^h_j(0)\right| = \mathcal{O}\left(|\theta| h^{-3} e^{-\frac{2S_0}{h}}\right), \tag{34}$$

for all $e^{-\frac{2S_0}{h}} < |\theta| < \frac{c^2 h}{8}$.

As a consequence of (32), the size of the imaginary part of the shape resonances is: $\left|\operatorname{Im} z^h_j(\theta)\right| \lesssim h^{-3} e^{-\frac{2S_0}{h}}$. When the quantum evolution generated by H^h_θ is considered for initial states with energies close to $z^h_j(\theta)$, it is important to have a lower bound for $\operatorname{Im} z^h_j(\theta)$ as $h \to 0$. Providing such a lower bound is a standard result in semiclassical analysis; in [5]-[8] this problem is analyzed for Schrödinger operators depending on the scaling parameter h according to the rules prescribed for $\mathcal{V}^h$. Under some additional spectral assumptions, it is shown that:

$$\left|\operatorname{Im} z^h_j(\theta)\right| \gtrsim e^{-\frac{2S_0}{h}}. \tag{35}$$

In what follows we will assume that this lower bound holds.

2.2. The quantum evolution problem

We next consider the time propagator generated by the operator H^h_θ. In a slightly more general framework, a detailed analysis of this problem has been developed in [15], where the modified dynamics is defined through a similarity, between H^h_θ and the corresponding self-adjoint model H^h_0, holding in some spectral subspace under the assumption that the parameters θ and h are small.

The generalized eigenfunctions of H^h_θ, next denoted with $\psi^h_\theta(\cdot, k, \mathcal{V}^h)$, solve of the boundary value problem (we refer to [14]- [15])

$$\begin{cases} \left(-h^2\partial_x^2 + \mathcal{V}^h\right) u = k^2 u, \qquad x \in \mathbb{R}\backslash\{a,b\}\ ,\ k \in \mathbb{R}, \\ \\ e^{-\frac{\theta}{2}} u(b^+) = u(b^-), \quad e^{-\frac{3}{2}\theta} u'(b^+) = u'(b^-), \\ \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+), \quad e^{-\frac{3}{2}\theta} u'(a^-) = u'(a^+), \end{cases} \tag{36}$$

and fulfill the exterior conditions

$$\psi^h_\theta(x,k,\mathcal{V}^h)\Big|_{\substack{x<a\\k>0}} = e^{i\frac{k}{h}x} + R^h(k,\theta)e^{-i\frac{k}{h}x}, \quad \psi^h_\theta(x,k,\mathcal{V}^h)\Big|_{\substack{x>b\\k>0}} = T^h(k,\theta)e^{i\frac{k}{h}x}, \tag{37}$$

$$\psi^h_\theta(x,k,\mathcal{V}^h)\Big|_{\substack{x<a\\k<0}} = T^h(k,\theta)e^{i\frac{k}{h}x}, \quad \psi^h_\theta(x,k,\mathcal{V}^h)\Big|_{\substack{x>b\\k<0}} = e^{i\frac{k}{h}x} + R^h(k,\theta)e^{-i\frac{k}{h}x}, \tag{38}$$

describing an incoming wave function of momentum k with reflection and transmission coefficients R^h and T^h. In the case $\theta = 0$, the generalized Fourier transform associated with $\mathcal{H}_0^h(\mathcal{V}^h)$ is defined by:

$$\left(\mathcal{F}^h\varphi\right)(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi h)^{1/2}} \left(\psi_0^h(x,k,\mathcal{V}^h)\right)^* \varphi(x)\,, \qquad \varphi \in L^2(\mathbb{R})\,. \tag{39}$$

Recall that $\mathcal{F}^h$ is a bounded operator on $L^2(\mathbb{R})$ with a right inverse coinciding with the adjoint $\left(\mathcal{F}^h\right)^*$

$$\left(\mathcal{F}^h\right)^* f(x) = \int \frac{dk}{(2\pi h)^{1/2}}\, \psi_0^h(x,k,\mathcal{V}^h) f(k)\,. \tag{40}$$

In particular, it results: $\mathcal{F}^h\left(\mathcal{F}^h\right)^* = \mathbb{I}$ in $L^2(\mathbb{R})$, while the product $\left(\mathcal{F}^h\right)^*\mathcal{F}^h$ defines the projector on the absolutely continuous subspace of $\mathcal{H}_0^h(\mathcal{V}^h)$ (cf. [22]).

We are interested in the quantum evolution for initial states residing in a spectral subspace of energies close to λ^0 (the eccumulation point of the resonances); let assume the interval $[\Lambda_1, \Lambda_2] \subset \mathbb{R}$ such that:

$$c \leqslant \Lambda_1 < \Lambda_2 \leqslant \inf_{[a,b]} V - c\,, \quad \sigma\left(H_D^h\right) \cap [\Lambda_1, \Lambda_2] = \left\{\lambda_j^h\right\}_{j=1}^{\ell}\,, \tag{41}$$

uniformly w.r.t. $h \in (0, h_0]$. The spectral projector on $[\Lambda_1, \Lambda_2]$ associated to H_0^h is next denoted with $\Pi_{[\Lambda_1,\Lambda_2]}$; this is explicitly given by:

$$\Pi_{[\Lambda_1,\Lambda_2]}\varphi = \int_{\mathbb{R}} \frac{dk}{(2\pi h)^{1/2}}\, 1_{[\Lambda_1,\Lambda_2]}\left(k^2\right) \psi_0^h(x,k,\mathcal{V}^h) \left(\mathcal{F}_{\mathcal{V}^h}^h\varphi\right)(k)\,. \tag{42}$$

The similarity between H_θ^h and H_0^h on the subspace $\Pi_{[\Lambda_1,\Lambda_2]}\varphi L^2(\mathbb{R})$ is provided by the operators $\mathcal{W}_\theta^h$ defined through the integral kernel:

$$\mathcal{W}_\theta^h(x,y) = \int_{\mathbb{R}} \frac{dk}{2\pi h}\, 1_{[\Lambda_1,\Lambda_2]}\left(k^2\right) \psi_\theta^h(x,k,\mathcal{V}^h) \left(\psi_0^h(x,k,\mathcal{V}^h)\right)^*\,. \tag{43}$$

The next proposition rephrases in our case the result presented in [15] .

Proposition 2.2. *Let $\mathcal{V}^h = V + W^h$ satisfy the conditions (24) and $|\theta| \lesssim h^{N_0}$, with $N_0 \geqslant 4$. If the interval $[\Lambda_1, \Lambda_2]$ verifies (41) and the lower bound (35) holds, then there exists $\eta > 0$ such that: $\left\{\mathcal{W}_\theta^h\,,\ \theta \in \mathbb{C}\,, \mathcal{B}\ |\theta| < \eta\, h^{N_0}\right\}$ form an analytic family of bounded operators in $L^2(\mathbb{R})$ fulfilling the expansion:*

$$\mathcal{W}_\theta^h - \Pi_{[\Lambda_1,\Lambda_2]}\varphi = \mathcal{O}\left(h^{N_0-2}\right)\,, \tag{44}$$

in the $\mathcal{L}\left(L^2(\mathbb{R})\right)$ operator norm. For $|\theta| < \eta\, h^{N_0}$, the operators $\mathcal{W}_\theta^h$, $\mathcal{W}_\theta^h H_0^h$ and $H_\theta^h\mathcal{W}_\theta^h$ map $L^2(\mathbb{R})$ into $D\left(H_\theta^h\right)$, and it results

$$H_\theta^h\mathcal{W}_\theta^h = \mathcal{W}_\theta^h H_0^h\,. \tag{45}$$

As a consequence of (44)-(45), the modified quantum evolution can be defined through the unitary propagator $e^{-itH_0^h}$ by conjugation as far as the initial state is considered in $\Pi_{[\Lambda_1,\Lambda_2]}L^2(\mathbb{R})$.

Theorem 2.1. *Let $h \in (0, h_0]$ and $|\theta| \lesssim h^{N_0}$, with $N_0 \geqslant 4$. Under the assumptions of the proposition 2.2, iH_θ^h generates a strongly continuous group of bounded operators on $\Pi_{[\Lambda_1,\Lambda_2]}L^2(\mathbb{R})$. For a fixed t, $e^{-itH_\theta^h}$ is analytic w.r.t. θ and the expansion:*

$$\left(e^{-itH_\theta^h} - e^{-itH_0^h}\right)\Pi_{[\Lambda_1,\Lambda_2]} = \tilde{\mathcal{R}}^h(t,\theta)\,, \tag{46}$$

holds with:

$$\sup_{t\in\mathbb{R}} \left\| \tilde{\mathcal{R}}^h(t) \right\|_{\mathcal{L}(L^2(\mathbb{R}))} = \mathcal{O}\left(h^{N_0-2}\right) . \tag{47}$$

2.3. Adiabatic evolution of shape resonances

We next consider a non-autonomous Hamiltonian defined by (20) through a time dependent potential $\mathcal{V}^h(t)$ such that the spectral profile of $H^h_\theta(t)$ corresponds to the pitcure given in the Proposition 2.1 for any time. In particular, the potential is assigned according to the following conditions:

Condition 2.2. *$\mathcal{V}^h(t) = V(t)+W^h(t)$, with $V, W^h \in \mathcal{C}^K(\mathbb{R}, L^\infty(\mathbb{R}))$ for $K \geqslant 2$, supp $V(t) = [a,b]$ and*

$$W^h(t) = -\sum_{n=1}^{N} w_n\left(t, (x-x_n)\,1/h\right) , \quad supp\ w_n(t) = [-d,d] . \tag{48}$$

We assume that for all t the estimates (22) and the conditions (24) hold with $\lambda^0 \in \mathcal{C}^K(\mathbb{R})$ and $c > 0$ fixed.

Under these assumptions, $H^h_\theta(t)$ has a cluster of time dependent shape resonances $\left\{z^h_j(\theta,t)\right\}_{j=1}^{\ell}$ which, for $\gamma > 0$ large enough, belong to $\sigma\left(H^h_\theta(i\gamma,t)\right)$, with $H^h_\theta(i\gamma,t)$ denoting the exterior complex-dilation of $H^h_\theta(t)$. Since $\sigma_{ess}\left(H^h_\theta(i\gamma)\right) = e^{-2i\gamma}\mathbb{R}_+$, due to the semiclassical estimates (32) and the assumption (ii)-(24), $\left\{z^h_j(\theta,t)\right\}_{j=1}^{\ell}$ is an isolated part of the spectrum of $H^h_\theta(i\gamma,t)$. Denoting with $\Pi_{z^h_j(\theta,t)}$ the corresponding time-dependent (non-orthogonal) projetcor, the adiabatic problem for this cluster of spectral points is written as:

$$\begin{cases} i\varepsilon\partial_t u^h_t = H^h_\theta(i\gamma,t)u^h_t , \\ \\ u^h_{t=0} \in \Pi_{z^h_j(\theta,t)}L^2(\mathbb{R}) . \end{cases} \tag{49}$$

If the dynamical system generated by $H^h_\theta(i\gamma,t)$ allows uniform-in-time estimates, this problem can be analyzed following the standard approach of the adiabatic theorem with spectral gap condition. For a particular choice of the deformation, the modification introduced by the θ-dependent interface conditions allows to obtain such a result. Indeed, the deformation $H^h_\theta(i\gamma)$ is characterized as follows (Lemma 3.1 in [8]):

Lemma 2.2. *Let $\theta = i\gamma$, $\gamma > 0$. Then: $iH^h_{i\gamma}(i\gamma)$ is maximal accretive.*

It follows that, for each fixed t, $e^{-isH^h_{i\gamma}(i\gamma,t)}$ is a semigroup of contractions; then, the regularity-in-time of the potential allows us to conclude that the non-autonomous Hamiltonian $H^h_{i\gamma}(i\gamma,t)$ generates a quantum dynamical system of contractions (see [8, Proposition 3.7]). In the application perspectives, we need to minimize the error produced by modification of the Hamiltonian; hence, we next assume γ to be polynomially small w.r.t. h. In this framework, the resonances $z^h_j(i\gamma,t)$ are close to the essential spectrum (located in $e^{-i2\gamma}\mathbb{R}_+$) and the spectral gap condition depends on h. Then the estimates of $\partial^k_t\left(H^h_\theta(i\gamma,t)-z\right)$ in the region: $\left|z-z^h_j(\theta,t)\right| \sim \gamma$, behave as γ^{-1}. This entails a loss of some power for h (depending on γ) in the adiabatic formula. Nevertheless, assuming $\varepsilon = e^{-\tau/h}$ for some $\tau > 0$, it is still possible to obtain an error bound exponentially small w.r.t. h. Next, we recall, in the simplified case of a single shape resonance, the result of the adiabatic theorem provided with in [8, Theorem 7.1] (see also [9] for the explicit form of the modulation factor $\mu(t)$ below).

Theorem 2.3. *Let $\mathcal{V}^h(t)$ fulfill the Condition 2.2 with $\ell = 1$, and let $E^h(t)$, $\psi_{E^h(t)}$ respectively denote the shape resonance end the resonant state related to $H^h_{ih^N}(ih^N, t)$ in the neighbourhood of size h of the limit energy λ^0. We set $\varepsilon = e^{-\tau/h}$ with $\tau > 0$, and assume that*

$$\left\| \psi_{E^h(t)} - \psi^*_{E^h(t)} \right\|_{L^2(\mathbb{R})} \leqslant \varepsilon^{1-\delta}\,, \tag{50}$$

holds for any $\delta \in (0,1)$. Then, the solution $\psi^h(t)$ of the problem: $0 \leqslant t \leqslant T$

$$\begin{cases} i\varepsilon\partial_t\psi^h(t) = H^h_{ih^N}(ih^N,t)\psi^h(t)\,, \\ \\ \psi^h(0) = \psi_{E^h(0)}\,, \end{cases} \tag{51}$$

fulfills the estimate:

$$\max_{t\in[0T]} \left\| \psi^h(t) - v^h(t) \right\|_{L^2(\mathbb{R})} \leqslant C_{a,b,c,\delta,T}\,\varepsilon^{1-\delta} \left\| \psi_{E^h(0)} \right\|_{L^2(\mathbb{R})}\,, \tag{52}$$

where the auxiliary dynamics $v^h(t)$ is expressed as:

$$v^h(t) = \mu(t)\, e^{-\frac{i}{\varepsilon}\int_0^t E^h(s)\,ds}\psi_{E^h(t)}\,, \tag{53}$$

with

$$\mu(t) = \exp\left(\int_0^t \frac{\left\langle \psi_{E^h(s)}, \partial_s \psi_{E^h(t)} \right\rangle}{\left\| \psi_{E^h(s)} \right\|^2_{L^2(\mathbb{R})}}\, ds \right) + \mathcal{O}\left(\varepsilon^{1-\delta}\right)\,, \tag{54}$$

while the positive constant $C_{a,b,c,\delta,T}$ possibly depends on the data.

3. A conjecture for the linearized transport problem

We finally reconsider the linearized verion of the transport problem introduced in (7). According to the result of Theorem 2.1, for initial states characterized by energies close to a cluster of resonaces allowing the lower bound (35), the distance between the propagators $\exp\left(-itH^h_{ih^{N_0}}\right)$ and $\exp\left(-itH^h_0\right)$ is controlled uniformely-in-time in the L^2-operator norm by $\mathcal{O}\left(h^{N_0-2}\right)$ for $N_0 \geqslant 4$. In the non-autonomous case, this suggests that, under the same initial conditions, the quantum dynamical systems generated by $H^h_{ih^{N_0}}(t)$ and $H^h_0(t)$ remain close to each other. In particular, we conjecture that on the adiabatic time-scale, the result of Theorem 2.1 extends according to:

$$\sup_{t\in[0,T]} \left\| u^h(t) - u^h_0(t) \right\|_{L^2(\mathbb{R})} = \mathcal{O}\left(h^{N_0-2}\right)\,, \tag{55}$$

where $u^h(t)$ and $u^h_0(t)$ solve the equations: $i\varepsilon\partial_t u^h(t) = H^h_{ih^{N_0}}(t)u^h(t)$ and $i\varepsilon\partial_t u^h_0(t) = H^h_0(t)u^h_0(t)$ with $u^h_0(0) = u^h(0) \in \Pi_{[\Lambda_1,\Lambda_2]}L^2(\mathbb{R})$. When $\operatorname{supp} g = \{k > 0\,,\ |k^2 - \lambda^0| = \mathcal{O}(h)\}$, this initial condition is *almost* fufilled by the modified problem

$$\begin{cases} A^h(t) = Tr\left[\chi\,\rho^h(t)\right]\,, \\ \\ \rho^h(t) = \int \frac{dk}{2\pi h} g(k)\, \left|u^h(k,\cdot,t)\right\rangle \left\langle u^h(k,\cdot,t)\right|\,, \\ \\ i\varepsilon\partial_t u^h(k,\cdot,t) = H^h_{ih^{N_0}}(t)u^h(k,\cdot,t)\,, \\ \\ \left(H^h_{ih^{N_0}}(t=0) - k^2\right) u^h(k,\cdot,0) = 0\,, \end{cases} \tag{56}$$

and the solution $A^h_0(t)$ in (7) is expected to be related to $A^h(t)$ by:

$$A^h_0(t) = A^h(t) + \mathcal{O}\left(h^{N_0-2}\right)\,. \tag{57}$$

Let the observable χ be defined by (15); proceeding as in (16), we have:

$$A^h(t) = Tr\left[\chi\,\rho^h(t)\right] = Tr\left[U_\theta^*\chi U_\theta \rho^h(t)\right] = Tr\left[\chi U_\theta \rho^h(t)\,U_\theta^*\right]\,. \tag{58}$$

Noticing that $U_\theta\rho^h(t)\,U_\theta^*$ identifies with the time evolution generated by the deformed operators $H^h_{ih^{N_0}}(ih^{N_0},t) = U_\theta H^h_{ih^{N_0}}(t)U_\theta^{-1}$, the problem (56) is rewritten as

$$\begin{cases} A^h(t) = Tr\left[\chi\,\tilde\rho^h(t)\right]\,, \\ \tilde\rho^h(t) = \int \frac{dk}{2\pi h} g(k)\,\left|\tilde u^h(k,\cdot,t)\right\rangle\left\langle\tilde u^h(k,\cdot,t)\right|\,, \\ i\varepsilon\partial_t\tilde u^h(k,\cdot,t) = H^h_{ih^{N_0}}(ih^{N_0},t)\tilde u^h(k,\cdot,t)\,, \\ \left(H^h_{ih^{N_0}}(ih^{N_0},t=0) - k^2\right)\tilde u^h(k,\cdot,0) = 0\,. \end{cases} \tag{59}$$

In this equivalent formulation, the result of Theorem 2.3 applies and the evolution of resonant states related to shape resonances is properly described by adiabatic formulas of the type (52). This clarifies the idea of our approach: the modification of the physical model (9) by h-dependent artificial interface conditions, although introducing a small error on the solution $A_0^h(t)$ (controlled by a power of h), allows us to work in the complex deformed setting (59) where, under the condition (18), an adiabatic approximation holds for the deformed dynamics $\tilde u^h(k,\cdot,t)$.

3.1. An explicit example and final remarks

A rigorous justification of the method described in this work is still an open problem which mainly concerns the validity of conjecture (55), allowing one to compare the modified variable $A^h(t)$ and the physical one $A_0^h(t)$.

In [9], the small-h behavior of the solution of (56) has been investigated for a time dependent potential formed by a flat barrier of height $V_0 > 0$ plus an attractive, time-dependent delta interaction acting in $x_0 \in (a,b)$ and preserving the quantum-well scaling. Explicitly, we consider the model:

$$H^h_{ih^{N_0}}(t) = -h^2\Delta_{ih^{N_0}} + 1_{[a,b]}(x)\,V_0 + h\alpha(t)\,\delta_{x_0}\,. \tag{60}$$

Under suitable assumptions on $\alpha(t)$ (corresponding to the Condition 2.2), these operators have a single shape resonance $E^h(t)$ localized close to a positive energy below V_0. In this framework, an explicit formula for the deformed dynamics $\tilde u^h(k,\cdot,t)$ and direct computations allow us to prove that the relations (18), (50) hold; then, the asymptotic behavior of $A^h(t)$ as $h \to 0$ can be analyzed using the result (52). In a configuration where the scattering involves only incoming from the left wave functions and the interaction point x_0 is closer to the l.h.s. of the barrier (i.e.: $|x_0 - a| < |x_0 - b|$), $A^h(t)$ exhibits the decomposition:

$$A^h(t) = a(t) + \mathcal{J}(t) + \mathcal{O}\left(h^{N_0}\right)\,, \tag{61}$$

where the main term $a(t) = \mathcal{O}(1)$ solves a limit equation describing the charging process of the well, while the first error term is $\mathcal{J}(t) = \mathcal{O}(h^2)$ (we refer to [9, Theorem 2.1]). In particular, our limit equation is coherent with the nonlinear reduced model obtained in [13], while the interface conditions do not affect the main contributions to $A^h(t)$ when N_0 is large enough. Hence, this result appears as an indirect confirmation of the validity of the expansion conjectured in (55).

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TUNNELING IN MULTIDIMENSIONAL WELLS

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A full asymptotic series for low eigenvalues and eigenfunctions of a stationary Schrödinger operator with a nondegenerate well was constructed in [29]. This allowed us to describe the tunneling effect for a potential with two or more identical wells with sufficient accuracy. The procedure is described in the following discussion. Some formulae are obtained and corresponding problems are discussed.

Keywords: Shrödinger operator, potential, tunneling, eigenvalues and eigenfunctions.

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1. Introduction

Consider the Schrödinger equation:

$$-\frac{h^2}{2}\triangle u + Vu = Eu, \tag{1.1}$$

where $\Delta = \sum_{i=1}^{d} \partial^2/\partial {x_i}^2$ is the Laplace operator, V is a real valued function defined on $\mathbb{R}^d$ having nondegenerate minima (wells) with some mode of symmetry.

If V has a finite number of identical wells which differ only by space translations and $V(x) > C$ beyond the region of the wells where C exceeds the value of V at minimum, the lower part of the spectrum of the corresponding Schrödinger operator is organized in the following way. There is a set of finite groups of eigenvalues (each connected with some quantum vector $n \in \mathbb{N}^d$), the distance between the groups being of the order h, and the distance between eigenvalues in each group, the splitting, being exponentially small with respect to h.

It is possible to find explicit formulae for the widths of these splittings using semiclassical asymptotics for each well. The problem was considered in different ways by different authors and almost completely solved in the one dimensional case [1–11]. The case $d > 1$ seems much more complicated. There are many results obtained in this area (see [11–20] and the list is far from complete). Still, the picture is not so complete as when $d = 1$. The semiclassical asymptotics of the discrete spectrum and strict estimates of the splittings are described in [11–13] and other works of these authors (using the theory of pseudo differential operators). The semiclassical expansion for the eigenfunctions and the rigorous asymptotics for the splitting widths in the lowest levels ($n = 0$) were obtained in [18–20] (with the use of a Maslov's canonical operator). Still, there are no effective (as when $d = 1$) splitting asymptotic formulae in terms of the potential for a set of arbitrary levels ($|n| = 1, 2, 3, \ldots$). The possibility of solving this problem in that case was discussed on the Diffraction Day Conference this spring in the talk of A. Anikin and M. Rouleux. These results have not been published yet.

My approach to this problem is different. In order to write down strict asymptotic formulae for splittings in the d-dimensional case, one has to develop methods of [9]. To do

so, it is necessary to find a sufficiently accurate semiclassical approximation to eigenstates for a single well in some vicinity of a minimum, independent of h. Such an approximation was constructed in [29]. The formal series on powers of h was obtained. Coefficients in all terms were found in some domain independent of h. Terms for eigenfunctions are analytic for analytic potential. If we truncate the series at the N-th term, the remaining sums satisfy the equation (1.1) with an error on the order of $h^{N+1}\exp(-S/h)$, where S is a nonnegative function defined in [29]. They give us so called *quasi-modes* [21]. The possibility to take N as large as we like and exponential decreasing of all terms beyond some vicinity of a minimum allows one, with the help of *quasi-modes*, to find real eigenfunctions and eigenvalues approximately, with exponentially small errors, smaller than the widths of the splittings. (The program was realized in [9] for $d = 1$.) The constructed series allow us to investigate the set of zeros for the eigenfunctions. The latter is interesting by itself and may be essentially used while finding the splitting asymptotics for $|n| > 1$.

2. Asymptotic expansions for the eigenstates in one well

We look for eigenfunctions u_n and eigenvalues E_n of (1.1) where V is a real valued function defined on $\mathbb{R}^d$ having a nondegenerate minimum at the origin in the form of the following series:

$$E_n = \sum_{j=1}^{\infty} E_{nj} h^j, \tag{2.1}$$

$$u_n = \exp\left\{-\frac{S}{h}\right\} \sum_{j=0}^{\infty} u_{nj} h^j, \tag{2.2}$$

where $E_{nj} \in \mathbb{R}$, $n = (n_1, n_2, \ldots, n_d) \in \mathbb{N}^d$ is a quantum vector, $S = S(x)$, $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, $u_{nj} = u_{nj}(x)$, $j = 0, 1, 2, \ldots$, are functions independent of h.

One can find u_{n0} in the following form:

$$u_{n0} = \psi^n e^{P_n(x)}, \tag{2.3}$$

where:

$$\psi = \psi(x) = (\psi_1(x), \psi_2(x), \ldots, \psi_d(x)), \qquad \psi^n = \prod_{i=1}^{d} \psi_i^{n_i},$$

the functions $\psi_i(x)$, $i = 1, 2, \ldots, d$, and $S(x)$ satisfy the following equations:

$$S(x) = S^0(x) = \frac{1}{2}\sum_{i=1}^{d} \psi_i^2, \tag{2.4}$$

$$S^J = \frac{1}{2}\sum_{i=1}^{d} (1 - 2\delta_{ij})\psi_i^2, \quad j = 1, \ldots, d, \quad \delta_{ij} = \begin{cases} 1, & if\ i = j, \\ 0, & if\ i \neq j. \end{cases} \tag{2.5}$$

$$\left(\nabla S^j\right)^2 = 2V, \qquad j = 0, 1, \ldots, d, \tag{2.6}$$

$$\langle \nabla\psi_i, \nabla\psi_j \rangle = \delta_{ij} (\nabla\psi_j)^2. \tag{2.7}$$

Symbols ∇ and $\langle \cdot, \cdot \rangle$ denote a *gradient* and a *scalar product* in $\mathbb{R}^d$ respectively.

We put the series (2.1) and (2.2) into the Schrödinger equation (1.1) and equate coefficients of each power of h to zero. The equation for power 0 is satisfied automatically because

of (2.6). The requirement for the coefficient of first degree in h to be equal to zero, gives us the following equation for the function P_n and the number E_{n1}:

$$\left\langle \nabla S^0, \nabla P_n \right\rangle = E_{n1} - \frac{\Delta S^0}{2} - \sum_{i=1}^{d} n_i (\nabla \psi_i)^2. \tag{2.8}$$

The analogous requirement for the coefficient of h^2 gives the equation for u_{n1} and E_{n1}:

$$\left\langle \nabla S^0, \nabla u_{n1} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{n1} \right) u_{n1} = \left\{ F_1 + \psi^n \left[\frac{\triangle P_n + (\nabla P_n)^2}{2} + E_{n2} \right] \right\} e^{P_n}, \tag{2.9}$$

where

$$F_1 = \sum_{i=1}^{d} \frac{n_i(n_i-1)}{2} \psi_i^{n_i-1} (\nabla \psi_i)^2 \prod_{j \neq i} \psi_j^{n_i} + \sum_{i=1}^{d} \frac{n_i}{2} \psi_i^{n_i-1} \Delta \psi_i + \sum_{i=1}^{d} n_i \psi_i^{n_i-1} \left\langle \nabla \psi_i, \nabla P_n \right\rangle \prod_{j \neq i} \psi_j^{n_i}.$$

So on, for each $j \geq 2$ we obtain the equation:

$$\left\langle \nabla S^0, \nabla u_{nj} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{n1} \right) u_{nj} = - \frac{\triangle u_{n,j-1}}{2} + \sum_{l=1}^{j-1} E_{n,l+1} u_{n,j-1} + \psi^n \mathrm{e}^{P_n(x)} E_{n,j+1}. \tag{2.10}$$

In [29], a procedure of constructing solutions for these equations was described and the following theorems were proven.

3. The phase theorem for the analytic potential

Let V be analytic with the following Taylor series:

$$V(x) = \frac{1}{2} \sum_{i=1}^{d} \omega_i^2 x_i^2 + \sum_{|k| \geq 3} v_k x^k, \qquad k = (k_1, k_2, \ldots, k_d) \in \mathbb{N}^d, \qquad |k| = \sum_{i=1}^{d} k_i \ , \tag{3.1}$$

convergent in a polydisk $|x_i| \leq r$, $i = 1, 2, \ldots, d$ with the numbers $\omega_i > 0$, $i = 1, 2, \ldots, d$.

We search for solutions for equation (2.6) in the form of a power series:

$$S^j(x) = \frac{1}{2} \sum_{i=1}^{d} \omega_i \left(1 - 2\delta_{ij}\right) x_i^2 + \sum_{|k| \geq 3} \left(S^j\right)_k x^k, \qquad j = 0, 1, \ldots, d, \tag{3.2}$$

and comparing coefficients of x^k , we find the following recurrent formulae for $\left(S^j\right)_k$:

$$\left(S^j\right)_k = \frac{\tilde{v}_k}{\langle k, I_j \omega \rangle}, \tag{3.3}$$

where $\omega = (\omega_1, \omega_2, \ldots, \omega_d)$; I_0 is a unitary matrix of order d; I_j, $j = 1, \ldots, d$, is a diagonal matrix of the order d with -1 standing at the j-th place of the diagonal and 1 at the others, $\tilde{v}_k = v_k$ for $|k| = 3$ and $\tilde{v}_k = v_k + \text{terms, depending on } \left(S^j\right)_l$, $|l| < |k|$, for $|k| \geq 4$.

It is easy to see that for the positive numbers ω_i, $i = 1, 2, \ldots, d$, the denominators in expressions (3.3) for $j = 1, 2, \ldots, d$, can be equal to zero. So, even to formally construct these series, we have to impose some additional conditions on the potential V.

Simultaneously, we construct a change of variables:

$$\Phi^j : y_j = (y_{j1}, \ldots, y_{jn}) \quad \mapsto \quad \left(x_1 = \Phi_1^j(y_j), \ldots, x_d = \Phi_d^j(y_j)\right), \tag{3.4}$$

which transforms the vector field $\langle \nabla S^j,\ \nabla \cdot \rangle$ into the normal form:

$$L_0^j = \sum_{i=1}^{d} \omega_i \left(1 - 2\delta_{ij}\right) y_{ij} \frac{\partial}{\partial y_{ij}}. \tag{3.5}$$

We search the functions $\Phi_i^j(y)$, $i = 1, 2, \ldots, d$, in the following form:

$$\Phi_1^j(y_j) = y_{ij} + \sum_{|k| \geq 2} \left(\Phi_i^j\right)_k y_j^k,. \tag{3.6}$$

In order to find the coefficients $\left(\Phi_i^j\right)_k$, we replace $x_i,\ i = 1, 2, \ldots, d$, in $\langle \nabla S^j,\ \nabla \cdot \rangle$ by $\Phi_1^j(y_j)$ of the form (3.6) and equate the obtained series (in variables y) to L_0^j. Hence, we find the following expressions for the coefficients:

$$\left(\Phi_i^j\right)_k = \frac{\tilde{S}_{i,j,k}}{\langle k - ort_i\ ,\ I_j \omega \rangle}\ , \quad j = 0, 1, .., d, \quad |k| \geq 2, \tag{3.7}$$

where:

$$\tilde{S}_{i,j,k} = (k_i + 1)\left(S^j\right)_{k + ort_i} + \text{terms, depending on } \left(\Phi_l^j\right)_m\ , \quad l = 1, 2, \ldots, d, \quad |m| < |k|\ ,$$

ort_i is an element of a standard basis $\{ort_i\}_1^d$ having all components equal to 0 except of the i-th one, which is equal to 1.

We see here that some denominators are equal to zero for some values of ω. We have to exclude these values.

Let us make the following definitions:

(1) we say, that the positive numbers $\omega_1, \omega_2, \ldots, \omega_d$ are *nonresonant*- if they are linearly independent over integers;

(2) positive numbers $\omega_1, \omega_2, \ldots, \omega_d$ are said to be *Diophantine* if there exist positive numbers α and C such that for any $k \in \mathbb{Z}^d$, $k \neq 0$,

$$|\langle k, \omega \rangle| \geq \frac{C}{|k|^\alpha}; \tag{3.8}$$

(3) we denote the set of vectors $\omega = (\omega_1, \omega_2, \ldots, \omega_d)$ with positive components by Ω, the set of ω with nonresonant components by Ω_{nr}, the set of ω with *Diophantine* components by Ω_D.

Theorem A. *Let the potential V be analytic, represented by a series of the form (3.1) convergent in the vicinity of the origin.*

(1) *If $\in \Omega_{nr}$, then there exists a pair: a unique positive analytic function S^0 which can be represented by convergent series of the form (3.2) for $j = 0$ in some vicinity of the origin and satisfies the equation (2.6); and a unique analytic diffeomorphism Φ^0 which transforms the vector field $\langle \nabla S^j,\ \nabla \cdot \rangle$ to the normal form L_0^0 given by (3.5).*

(2) *If $\in \Omega_D$, then for each $j \in \{1, 2, \ldots, d\}$ there exists a pair: a unique analytic function S^j which can be represented by convergent series of the form (3.2) in some vicinity of the origin and satisfies the equation (2.6); and a unique analytic, diffeomorphism Φ^j which transforms the vector field $\langle \nabla S^j,\ \nabla\ \rangle$ to the normal form L_0^j given by (3.5).*

The proof of this theorem is published in [29].

Remark 3.1. Normal forms of the vector fields (i.e. of Hamiltonian systems of differential equations) are described in literature on classical mechanics e.g. [22–25]. A typical situation there is that given a vector field, one has to find the simplest form for it in suitable variables. Here, we have no given vector fields. We are looking for vector fields which are solutions for the nonlinear Eiconal equation (2.6). The normal forms (3.5) are used as an auxiliary tool.

Remark 3.2. In case (1), the nonresonance condition is necessary to construct Φ^0 (not S^0). There are no small denominators in (3.3) for $j = 0$. The existence of analytic S^0 was established in [26] in a more general situation.

Remark 3.3. One can give the following geometrical interpretation for the results of the *Theorem A*. The functions S^j are the generating functions for Lagrangian manifolds, which are invariant with respect to the classical dynamical system with the potential $-V(x)$. The potential $-V(x)$ has a 'hunch' at the origin (instead of a 'well' of $V(x)$). So our quantum mechanical problem 'at the bottom of a well' is equivalent to a classical problem 'near the top of a hill'. The origin is a point of singularity in this problem, a point of infinite time in classical dynamics, a point of vanishing energy of the Lagrangian manifolds. The theorem gives the existence of the generating functions S^J for the invariant Lagrangian manifolds in a small vicinity of that point.

The geometrical aspects of the problem were considered in [27]. In addition to the proof of *Theorem A*, the following lemma was proven.

We denote by B_r a Banach space of analytic functions in $B(r) = y \in \mathbb{C}^d : |y_i| < r$, $i = 1, 2, \ldots, d$ with the norm $\|f\| = \sup_{y \in B(r)} |f(y)|$, by $B_{r,M,n,0}$ the subspace of B_r which is the set of functions having the Taylor series, which contains only the terms with power $|k| \geq M \geq 0$ and coefficient at power n equal to zero, by $\omega_0 = min_{i \in \{1,\ldots,d\}} \omega_i$.

Lemma 1. *Given $r' < r$, there exists a bounded operator $\{L_n^j\}^{-1}$: $B_{r,M,n,0} \to B_{r',M,n,0}$ which solves the equation $L_n^j = f|_{B(r')}$, $u \in B_{r',M,n,0}$, $f \in B_{r,M,n,0}$, in the following cases:*

(1) *for any $\omega \in \Omega$, $j = 0$, $n = (0, \ldots, 0)$;*

(2) *for $\omega \in \Omega_{nr}$, $j = 0$, n arbitrary;*

(3) *for $\omega \in \Omega_D$, $j = 1, \ldots, d$, n arbitrary,*

and there exists a positive constant $c_1 = c_1(M, d, \omega, r)$ such that in both cases (1), (2):

$$\left\| \left\{ L_n^0 \right\}^{-1} \right\| \leq \frac{c_1}{(r - r')^{d-1}},$$

in case (3) there exists a positive constant $c_2 = c_2(\alpha, M, d, \omega, r)$ such that:

$$\left\| \left\{ L_n^0 \right\}^{-1} \right\| \leq \frac{c_2}{(r - r')^{\alpha + d}}.$$

4. Constructing the series (2.1), (2.2)

In order to construct the whole series (2.1) and (2.2), we have to find at first (after solving (2.6)) all the functions $\psi_j(x)$ which satisfy the following equations:

$$\psi_j^2(x) = S^0(x) - S^j(x), \qquad j = 1,\ 2,\ \ldots\ , d\ . \tag{4.1}$$

Lemma 2. *Let $S^j(x)$, $j = 0,\ \ldots,\ 1,\ d$, be taken from Theorem A.*

Then, the right hand sides in the formulae (4.1) are the full squares, i.e. there exist d unique analytic functions ψ_j, $j = 1, 2..., d$, which satisfy the equations (4.1) and have the following convergent series:

$$\psi_j = \sqrt{\omega_j} x_j + \sum_{|k|\geq 2} (\psi_j)_k x^k, \qquad j = 1,\ 2,\ \ldots\ , d, \tag{4.2}$$

in some vicinity of the origin.

After changing the variables of (3.4), the equation (2.8) satisfies the conditions of *Lemma 1*, case (1), $M = 1$, if we choose E_{n1} in the following way:

$$E_{n1} = \sum_{i=1}^{d} \left(n_i + \frac{1}{2} \right) \omega_i. \tag{4.3}$$

According to *Lemma 1*, there exists an analytic solution, which after returning back to coordinates x, gives us in some polydisk an analytic solution for (2.8) which vanishes at the origin.

Each of the equations (2.9) and (2.11) has the following form:

$$\left\langle \nabla S^0, \nabla u_{n1} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{n1} \right) u_{n1} = F. \tag{4.4}$$

We search for the solution of (5.7) in the form of the product:

$$u = U e^{P_0}, \tag{4.5}$$

where P_0 is a solution of equation (2.8) for $n = 0$. This means that:

$$\left\langle \nabla S^0, \nabla e^{P_0} \right\rangle + \left(\frac{\triangle S^0}{2} - E_{01} \right) e^{P_0} \equiv 0. \tag{4.6}$$

After putting (4.5) into (4.4) we obtain the following equation for the unknown function U:

$$L_0 \tilde{U} - \langle n, \omega \rangle \tilde{U} = \tilde{F} e^{-\tilde{P}_0}, \tag{4.7}$$

where $L_0 = L_0^0$ is the normal form of the operator $\langle \nabla S^0, \nabla \cdot \rangle$ in coordinates y, 'tilde' means the change of variables: $F(x) = \tilde{F}(y)$. Now the left hand side operator is that of *Lemma 1*, case (2).

The condition of solvability for equation (4.7) is the following:

$$\left(\tilde{F} e^{-\tilde{P}_0} \right)_n = 0, \tag{4.8}$$

$(F)_n$ is noting the Taylor coefficient at y^n of the function F.

Hence, we obtain the following expressions for all the terms of the series (2.1), i.e.:

$$E_{n2} = -\frac{1}{2} \left(\left[\triangle \tilde{P}_n + \left(\nabla \tilde{P}_n \right)^2 \right] \right)_0 - \omega^{-\frac{n}{2}} \left(\tilde{F}_1 e^{\tilde{P}_n - \tilde{P}_0} \right)_n, \tag{4.9}$$

$$E_{nj} = \omega^{-\frac{n}{2}} \left(\left[\frac{\triangle \tilde{u}_{j-1}}{2} - \sum_{l=1}^{j-1} E_{n,l+1} \tilde{u}_{n,j-1} \right] e^{-\tilde{P}_0} \right)_n, \qquad j \geq 2; \tag{4.10}$$

and find all the functions u_{nj}, $j = 1, 2, \ldots$ in form (4.5).

5. Main theorem and concluding remarks

Results from paper [29] are summarized in the following theorem.

Theorem B. *Let the potential V in Schrödinger equation (1.1) be analytic, represented in a vicinity of the origin by Taylor series (3.1) with positive Diophantine numbers $\omega_1, \omega_2, \ldots, \omega_d$.*

Then for any $\in \mathbb{N}^d$, $0 \leq |n| \leq n^*$, $N \in \mathbb{N}$, one can construct the following pair:

a number:

$$E_n = \sum_{j=1}^{N} E_{nj} h^j,$$

and an analytic function:

$$u_n = \exp\left\{-\frac{S^0}{h}\right\} \sum_{j=0}^{N-1} u_{nj} h^j,$$

which satisfies the Schrödinger equation (1.1) up to terms of the order $h^{N+1}\exp\{-S^0/h\}$ in some vicinity of the origin independent of h. Here: $S^0(x)$ is the positive analytic solution of (2.6) with Taylor series (3.2) (see Theorem A), analytic functions $u_{nj}(x)$ $(j = 0, 1, ..., N-1)$ and numbers $u_{nj}(x)$ $(j = 1, 2, ..., N)$ have the form given by formulae (2.3), (4.2), (4.5) and (4.3), (4.9), (4.10).

Remark 5.1. One can lengthen the functions S^J analytically onto a larger domain by the formulae $S^j = \int \sum_{i=1}^{d} p_i^j dx_i^j$, $j = 1, 2, \ldots, d$, where for each j the integral is taken along the trajectory of the corresponding Hamiltonian system. Hence, one can lengthen the functions $\psi_j(x)$, $j = 1, 2, \ldots, d$, and u_{nj}, $j = 0, 1, 2, \ldots$ in a similar way. Thus, one can construct sufficient *quasi-modes* in a rather large domain containing the point of a minimum. Then, in the problem with many identical wells, situated so that the distances between the points of the minima are finite, one can do the following. Construct *quasi-modes* for each well in such a domain, that the two neighboring domains intersect. Then multiply those *quasi-modes* on the cutting functions equal to zero beyond the mentioned domains. The approximation for the eigenfunctions of the problem can be taken as a linear combination of these cut-off *quasi-modes*. It is then possible to write the rigorous splitting formulae following the ideology of [9] for an arbitrary $n \in \mathbb{N}$ in the form as it was obtained in [18–20] for $n = 0$.

Thus, one can find:

$$\Delta E_n = a_n e^{-b_n/h} \left(1 + O(h)\right),$$

where, in the case $d = 1$, $\quad b_n = \int_{x_1}^{x_2} \sqrt{2V(x)}dx$,

in the case $d \geq 2$, $\quad b_n = \int_{M_1 \breve{} M_2} \sqrt{2V(x)}dl$,

the last integral is taken along the extreme line of the functional in the right hand side of the last formula.

It is important to note that to find the pre-exponential coefficient in the splitting formula for $|n| > 0$, one has to be sure that on the trajectory of the corresponding Hamiltonian system the corresponding eigenfunction is not equal to zero. Hence, one has to investigate the zero-sets of the eigenfunctions. Some examples in a one-dimensional case were considered by my student N. Homchenko and published in [30].

Remark 5.2. In order to find the zero-sets of the eigenfunctions, one can also use expansions of the form (2.2). It is more convenient, however, to construct for this purpose an *ansatz* with Hermite polynomials, namely:

$$u_n = \left[e^{P_n} \prod_{i=1}^{d} H_{n_i}\left(\frac{\psi_i}{\sqrt{h}}\right) + \sum_{j=1}^{\infty} h^j G_j \right] \exp\left\{ -\frac{S^0}{h} \right\}, \tag{5.1}$$

where S^0 and ψ_i, $i \in (1, \ldots, d)$, are the above-described functions, $H_{n_i}(t) = (-1)^{n_i} e^{t^2} \left(e^{-t^2}\right)^{(n_i)}$ are Hermite polynomials which satisfy the following differential equation:

$$H''_{n_i}(t) - 2tH'_{n_i}(t) + 2n_i H_{n_i}(t) = 0. \tag{5.2}$$

If we put series (5.1) and (2.1) into the Schrödinger equation (1.1) and equate coefficients at each power of h to zero (taking into account (5.2)), we will obtain problems for G_j quite similar to those described in Section 4. Solving them, we will construct all the functions G_j. In zero approximation the eigenfunction u_n has the form of an exponent multiplied by a product of Hermite polynomials. Hence, in the zero approximation, we find a set of zeros of the function u_n as a net of intersecting surfaces $\Sigma_i : \psi_i(x) = t_{ij}$, $i = 1, 2, \ldots, d$, $t_{ij} \in R_i$, R_i is a set of roots of $H_{n_i}(t)$. The first term of (5.1) depends on third and fourth derivatives of the potential V at the origin. It does not vanish if they are not equal to zero. In this case, one can already find in the first approximation, that Σ_i do not intersect. They have quasi-intersections. A more detailed description of this *ansatz* and some examples were published in [31] and [32].

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POLARIZATION CHARACTERISTICS OF RADIATION OF ATOMIC ENSEMBLE UNDER COHERENT EXCITATION IN THE PRESENCE OF A STRONG MAGNETIC FIELD

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Numerical solutions of the Liouville equation are used to study of the polarization characteristics of an ensemble of He atoms in 3^3S_1 state in the presence of the strong magnetic field when the coherent population of this level is realized from 2^3P state.

Keywords: Coherens excitation, evolution of density matrix, interference effects.

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1. Introduction

Coherent excitation of levels belonging to a particular state, can lead to a number of interesting phenomena, for example – coherent population trapping (CPT) and electromagnetically-induced transparency, which have been extensively studied for decades. Continuing interest in these phenomena is related not so much to the phenomena themselves, but rather their applications – lasing without inversion [1], laser cooling [2] and stored light [3]. If the system under consideration is not in the CPT state, the polarization characteristics of its radiation can be used for the diagnostics of the anisotropy of the processes occurring in that system. Previously, these characteristics have been used for diagnostics of ions drift velocities in gas discharge plasma [4], the proton and electron beams of the sun's chromosphere and the earth's atmosphere [5], [6], the magnetic fields of Z-pinch [7] and tokamak [8] hot plasma and cold plasma of the upper layers of Earth's atmosphere [9].

In general, for the investigation of CPT phenomena, the lower superfine levels of alkali atoms are used. According to the our viewpoint the polarization characteristics of other atoms for instance helium are of interest. The emission of helium can be observed in the solar atmosphere and if the observation take place nearby the sun spots strong magnetic field should be imposed on the system of observation [10].

Due to the fact that the considered phenomena are associated with coherent processes, a satisfactory description of these processes is only possible using the apparatus of the density matrix, allowing one to take into account correlation in the initial conditions.

Polarization characteristics of the system's radiation are related to its internal ordering, which can be changed by an external magnetic field. Studies of the effect of the magnetic field on the system can be done in two ways, for the first one, the field is turned on during registration of systems radiation [11], [12], in the second , as it will be assumed in this paper, the system is constantly under the influence of the field. In the latter case, the role of the constant magnetic field is reduced to the splitting of the fine or hyperfine structures levels, and

to changing the symmetry of the problem in question. The result of these two factors will be discussed below.

2. Description of polarization phenomena

To describe the polarization phenomena, it's convenient to expand the system density operator over the irreducible tensor operators:

$$\rho = \sum_{k,q} \rho_q^k T_q^{k\dagger}. \tag{1}$$

The coefficients of this expansion are known as a polarization moments and can be defined by the following formula:

$$\rho_q^k(j) = \sum_{m,m'} (-1)^{j-m'} \begin{bmatrix} j & j & k \\ m & -m' & q \end{bmatrix} (\rho)_{m,m'}, \tag{2}$$

where j denotes the magnitude of the angular momentum of the system under consideration, m is the magnetic quantum number and the expression in square brackets is known as the Clebsch-Gordan coefficients [13].

The physical meaning of the polarization moments is that they determine the ordering of the angular momenta of the ensemble of particles, i.e. the ensemble average of the linear combinations of the components of the tensor, which is comprised of the components of the angular momentum. For example, such averages of first and second rank tensors can be implied [10]:

$$\begin{aligned}
\langle j_z \rangle &= \frac{\sqrt{2j(2j+1)(2j+2)}}{2\sqrt{3}} \rho_0^1, \\
\langle j_\pm \rangle &= \pm \frac{\sqrt{2j(2j+1)(2j+2)}}{\sqrt{6}} \rho_\mp^1, \\
\left\langle 3j_z^2 - j^2 \right\rangle &= \frac{\sqrt{(2j-1)2j(2j+1)(2j+2)(2j+3)}}{2\sqrt{5}} \rho_0^2, \\
\langle j_z j_\pm + j_\pm j \rangle &= \mp \frac{\sqrt{(2j-1)2j(2j+1)(2j+2)(2j+3)}}{2\sqrt{15}} \rho_{\mp 1}^2, \\
\left\langle j_\pm^2 \right\rangle &= \frac{\sqrt{(2j-1)2j(2j+1)(2j+2)(2j+3)}}{\sqrt{30}} \rho_{\pm 2}^2.
\end{aligned} \tag{3}$$

Conversely, the polarization moments define intensity of the radiation polarized along the unit vector $\overrightarrow{e}_\lambda$ emitted by the transition from the excited level with angular momentum j to the lower-lying state with angular momentum j_0

$$I_\lambda = I_0 Sp\left(d_\lambda \rho d_\lambda^*\right) = I_0 \sum_{k,q} (-1)^k \left|\langle j_0 \| 1 \| j \rangle\right|^2 \begin{Bmatrix} 1 & 1 & k \\ j & j & j_0 \end{Bmatrix} \Phi_{k,q}\left(\overrightarrow{e}_\lambda\right) \rho_{-q}^k(j), \tag{4}$$

where I_0 is a factor that depends on fundamental constants and frequency, d_λ is the projection of the atomic dipole moment on the direction of the oath $\overrightarrow{e}_\lambda$, $\langle j_0 \| 1 \| j \rangle$ – reduced matrix element, an expression in the figure braces $6j$-symbol [13], and $\Phi_{k,q}\left(\overrightarrow{e}_\lambda\right)$ denotes the so-called polarization tensor, which is determined by observation conditions and depends on $s_q^{(\lambda)}$ –

expansion coefficients of the unit vector of the polarization direction of detected radiation by circular unit vectors:

$$\Phi_{k,q}(\overrightarrow{e}_\lambda) = \sum_{q_1,q_2}(-1)^{1-q_1} s_{q_1}^{(\lambda)*} s_{q_2}^{(\lambda)} \begin{bmatrix} 1 & 1 & k \\ -q_2 & q_1 & q \end{bmatrix}. \tag{5}$$

In particular, if I_x, I_y, I_z would denote the intensities of the radiation polarized in three mutually perpendicular directions defined by the axes OX, OY and OZ respectively , from formula (4) can be obtained:

$$I_x + I_y + I_z = I_0 \left|[j_0 \left|1\right| j]\right|^2 \frac{1}{\sqrt{2j+1}} \rho_0^0(j). \tag{6}$$

In the same manner, for the difference between the intensities of radiation polarized in two mutually perpendicular directions (e.g., OZ and OY) and observed along the third direction (in this case OX), we have:

$$\left(I_z - I_y\right)_x = I_0 \left|[j_0 \left|1\right| j]\right|^2 (2j+1)(-1)^{j+j_0+1} \begin{Bmatrix} 1 & 1 & 2 \\ j & j & j_0 \end{Bmatrix} \left[\frac{3}{\sqrt{6}} \rho_0^2(j) + Re\left(\rho_2^2(j)\right)\right]. \tag{7}$$

For the difference between the intensities of radiation polarized along the right and left circle when observed along the axis OZ, we have:

$$\left(I_+ - I_-\right)_z = I_0 \left|[j_0 \left|1\right| j]\right|^2 (2j+1)(-1)^{j+j_0+1} \begin{Bmatrix} 1 & 1 & 1 \\ j & j & j_0 \end{Bmatrix} \rho_0^1(j). \tag{8}$$

From the last three expressions, it can be seen, that the sum of the intensities of radiation polarized in three mutually perpendicular directions is defined by polarization moment of zero rank, the anisotropy of the radiation which is linearly polarized in two mutually perpendicular directions is determined by the components of the moment of the second rank, and, finally, the anisotropy of the circularly polarized radiation - by the components of the moment of the first rank. The polarization moment of the second rank is called alignment tensor, while the polarization moment of the first rank, which has three components – the orientation vector. Components ρ_0^2 of the alignment tensor is often named as longitudinal, whereas components ρ_1^2 and ρ_2^2 are known as uncleaned alignment and transverse ones. Based on the above, one can say that the polarization moments define the ordering of the angular momenta of the ensemble of particles and the anisotropy of the dipole radiation of that ensemble.

3. Statement of the problem and discussion of the results of the numerical calculations

In this paper, we consider the time dependance of 3^3S_1 state of the atom He, the excitation of which is performed from 2^3P multiplet of this atom. It is assumed that the system is placed into a strong magnetic field sufficient to break the thin bond of P-multiplet under consideration. We will also assume that state 2^3P is populated from the ground state of this atom by a proton or electron impact or other axially symmetric excitation sufficient to tear up the fine bound, and which the symmetry axis makes an angle θ with the axis OZ of the laboratory frame of reference. As a result of this excitation in the frame of reference associated with the anisotropy axis, on the 2^3P – levels, ordering of the angular moments of the population T_0^0 and longitudinal alignment T_0^2 will be induced. Then, by introducing a parameter $\alpha = T_0^2/T_0^0$, which may be called the anisotropy parameter, for efficiencies of populations of the magnetic sublevels of 2^3P_j state in the laboratory frame of reference XYZ, one can write the following:

$$\sigma_{j,m;j',m'} = \frac{1}{2j+1}A^{(0)}(j,j',l,s) + \alpha\sum_q (-1)^{j'+m'}\begin{bmatrix} j & j' & 2 \\ m & -m' & q \end{bmatrix} D^{(2)}_{0,q}(\theta)A^{(2)}(j,j',l,s), \quad (9)$$

where l and s are the orbital and the spin moments, $D^2_{m,m'}(\theta)$ elements of three-dimensional rotation [13], and $A^{(k)}_j$ depends on coefficients of vector addition of moments:

$$A^{(k)}(j,j',l,s) = (-1)^{j'+s+k+l}\sqrt{(2j+1)(2j'+1)}\begin{Bmatrix} l & l & k \\ j & j' & s \end{Bmatrix}. \quad (10)$$

The Hamiltonian operator of the atomic system placed in a strong magnetic field of strength $\mathcal{H}$ is defined by the orbital $\hat{l}$ angular momenta and $\hat{s}$ the spin ones

$$\hat{H} = \hat{H}_F + \hat{W}, \quad (11)$$

where $\hat{H}_F = \hat{H}_0 + \mu_0\hat{\mathcal{H}}(\hat{l} + 2\hat{s})$ depends on the value of the moments, μ_0 – the Bohr magneton and on the value and direction of magnetic field. Furthermore, we expect that the direction of magnetic field makes an angle χ with the OZ axis of the laboratory frame of reference.

Operator $\hat{W}$ describes the interaction of the system with the electromagnetic field, performing the excitation from 2^3P state to 3^3S ones (hereafter referred to as the state of 'a' and 'b', respectively (see Fig. 1)). Then, if we assume that the exciting field is linearly polarized along the axis OZ of the laboratory frame of reference, in the basis of eigenfunctions of the square momentum and its projection for the matrix element of operator $\hat{W}$, it can be written as follows:

$$(W_{ab})_{j_a,m_a;j_b,m_b} = \langle j_a m_a | d_z | j_b m_b \rangle =$$
$$= \hbar\Omega(-1)^{l_a+s+j_b+l_b+1}\sqrt{(2l_b+1)(2j_b+1)}\begin{bmatrix} j_b & 1 & j_a \\ m_b & 0 & m_a \end{bmatrix}\begin{Bmatrix} l_b & l_a & 1 \\ j_a & j_b & s \end{Bmatrix}\begin{bmatrix} l_b & 1 & l_a \\ 0 & 0 & 0 \end{bmatrix}, \quad (12)$$

where $\Omega = \mathcal{E}\langle j_a \parallel r \parallel j_b\rangle/\hbar$ is the Rabi frequency, which depends on the electric field intensity $\mathcal{E}$ and irreducible matrix element of operator r. The evolution of the density matrix for a system of two states is described by the Liouville equation, which for the blocks of the density matrix $\widetilde{\rho}_{i,j}$ $i,j = a,b$ may be written in form:

$$\begin{aligned} \frac{d}{dt}\widetilde{\rho}_{aa}(t) &= \Gamma\widetilde{\rho}_{bb}(t) - i(W_{ab}(t)\widetilde{\rho}_{ba}(t) - \widetilde{\rho}_{ab}(t)W_{ba}(t)), \\ \frac{d}{dt}\widetilde{\rho}_{bb}(t) &= -\Gamma\widetilde{\rho}_{bb}(t) - i(W_{ba}(t)\widetilde{\rho}_{ab}(t) - \widetilde{\rho}_{ba}(t)W_{ab}(t)), \\ \frac{d}{dt}\widetilde{\rho}_{ab}(t) &= -\frac{\Gamma}{2}\widetilde{\rho}_{ab}(t) - \frac{i}{\hbar}(E_a - E_b)\widetilde{\rho}_{ab}(t) - i(W_{ab}(t)\widetilde{\rho}_{bb}(t) - \widetilde{\rho}_{aa}(t)W_{ab}(t), \\ \widetilde{\rho}_{ba}(t) &= \widetilde{\rho}^{\dagger}_{ab}(t), \end{aligned} \quad (13)$$

where Γ is a matrix that describes relaxation processes.The solution of this system should be found according to initial conditions $\widetilde{\rho}_{bb}(0) = 0$, $\widetilde{\rho}_{ab}(0) = 0$, $\widetilde{\rho}_{ba}(0) = 0$. As to density matrix of the state 'a', in the base of the eigenfunctions of the square of the momentum and its projection this matrix is proportional to the matrix $\sigma_{j,m;j',m'}$, which is specified by relation (9). In order to reduce the system (13) to a more convenient form for numerical computation, first, it is necessary to introduce dimensionless time $\tau = t/\tau_0$, where τ_0 – the

lifetime of the excited 3^3S_1 state, and secondly, to move from the basis of eigenfunctions of the square of the momentum and its projection to the basis on which operator H_F of (11) is diagonal (M-basis). Then, if we introduce density matrices $\rho_{i,j}(t)$ $(i,j=a,b)$, connected with the similar matrices introduced earlier with the help of relations $(\rho_{ij}(\tau))_{M,M_1} = (\widetilde{\rho}_{ii}(\tau))_{M,M_1}$ $(i=a,b)$, $(\rho_{ba}(\tau))_{M,M_1} = (\widetilde{\rho}_{ba}(\tau))_{M,M_1}\exp[-i\tau((E_b)_M-(E_a)_{M_1}/\hbar)]$ $(\rho_{i,j}(\tau) = (\rho_{j,i}(\tau))^{\dagger})$, then the dimensionless energy levels $(E_a)_M = E_a + (\varepsilon_a)_M$ and $(E_b)_M = E_b + \hbar\omega + (\varepsilon_b)_M$ are expressed through $(\varepsilon_i)_M$ $(i=a,b)$ – the eigenvalues of operator $\hat{H}_F$ and $\omega = (E_b - E_a)/\hbar$ – transition frequency between the levels of b and a with the energies E_b and E_a respectively (see Fig. 1) and, at last the laser frequency $\omega_{ex} = \omega + \widetilde{\delta}/\hbar$. The eigenvalues $(\varepsilon_a)_M$ and $(\varepsilon_b)_M$ here possess the values $\pm n\mu_0\mathcal{H}$, whereas $(n=0,1,2,3)$ and $(n=0,2)$ for the states 'a' and 'b' respectively. It should be mentioned that eigenvalue $n=1$ of the state 'a' is twice degenerate.

Using these new notations, the system (13) takes the form:

$$\begin{aligned}
\frac{d}{d\tau}\rho_{aa}(\tau) &= \gamma_a\rho_{bb}(\tau) + \frac{i}{2\hbar}e^{-i\tau\delta}\rho_{ab}(\tau)\,(W_{ba})_I\,(\tau) - \frac{i}{2\hbar}e^{i\tau\delta}\,(W_{ab}(\tau))_I\,\rho_{ba}(\tau),\\
\frac{d}{d\tau}\rho_{bb}(\tau) &= -\gamma\rho_{bb}(\tau) - \frac{i}{2\hbar}e^{-i\tau\delta}(W_{ba})_I\rho_{ab}(\tau) + \frac{i}{2\hbar}e^{i\tau\delta}\rho_{ba}(\tau)(W_{ab})_I,\\
\frac{d}{d\tau}\rho_{ab}(\tau) &= -\frac{\gamma}{2}\rho_{ab}(\tau) + \frac{i}{2\hbar}e^{i\tau\delta}\rho_{aa}(\tau)(W_{ab})_I - \frac{i}{2\hbar}e^{i\tau\delta_a}(W_{ab})_I\rho_{bb}(\tau),\\
\frac{d}{d\tau}\rho_{ba}(\tau) &= -\frac{\gamma}{2}\rho_{ba}(\tau) - \frac{i}{2\hbar}e^{-i\tau\delta}(W_{ba})_I\rho_{aa}(\tau) + \frac{i}{2\hbar}e^{-i\tau\delta_a}\rho_{bb}(\tau)(W_{ba})_I,
\end{aligned} \tag{14}$$

where the subscript 'I' indicates that this operator is recorded in the interaction representation $((Wab)_I)_{M,N} = (W_{ab})_{M,N}\exp[i((\varepsilon_a)_M - (\varepsilon_b)_N)\tau]$ and δ is the dimensionless laser detuning $\delta = \widetilde{\delta}\tau_0/\hbar$.

It should be noted that the 2^3P state, owing to the transition from the level with $j=1$ (when level with $j=2$ is metastable one [15]), is characterized by the finite value of the lifetime. This leads an exponential decrease in the value $\sigma_{j,m;j',m'}$ (9) and for additional exponential decreasing of the solution of the system (13), that did no connect with the coherence process. Therefore, one can say that the decrease in the population of the 2^3P state is connected with the presence of magnetic field, that mixes the levels of this multiplet. This exponential decay will not be considered in this article.

With regard to the integration of the system of matrix equations, the left side of which contains a matrix of order n, it should be noted, that the universal method in this case is a method of reducing this system to the system of ordinary differential equations of order n^2. In the case when the matrix coefficients of the right part do not depend on the time, the system can be integrated using the Laplace transform or the transition from the matrix $\widetilde{\rho_{i,j}}$ $i,j=a,b$, to the matrix $\rho = U^{\dagger}\widetilde{\rho}U$ [16], where the matrix U – is the matrix of the eigenvectors of the Hamiltonian operator (11). In the present paper, system (13) was integrated by the series expansion, the implementation of which may be briefly described as following. Due to the fact that the density matrix does not depend explicitly on the time, the derivative of the matrix $\widetilde{\rho}_{i,j}$ of order n, can be obtained from the derivative of order $n-1$ of this matrix by using the commutation of the latter matrix with the Hamiltonian operator (11). After this, for the derivative of $\widetilde{\rho}^{(n)}_{i,j}$, expressions similar to (13), with the difference that the right side contains derivatives of $\widetilde{\rho}^{(n-1)}_{i,j}$ will be obtained. After this, performing replacements similar to those mentioned above, leads to expressions for the derivatives of the matrix $\rho_{i,j}$ $i,j=a,b$, that are similar to (14). Using such procedure, at a fixed time, one can calculate the first four derivatives

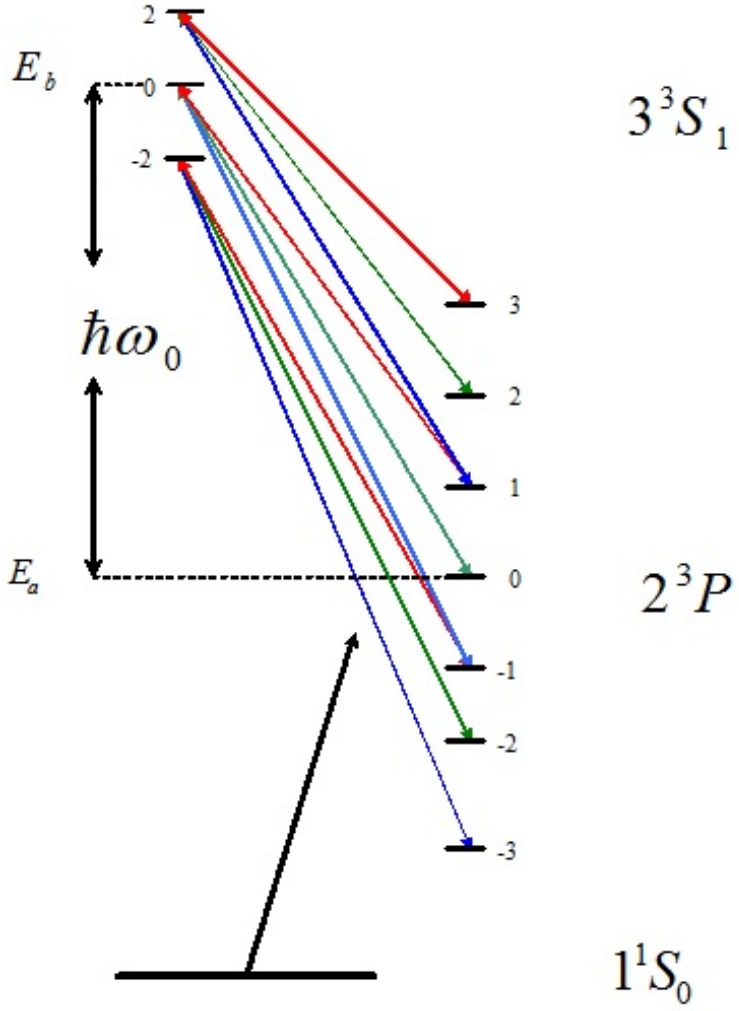

FIG. 1. Splitting scheme of 3^3S and 2^3P states of the He atom in a strong magnetic field ($M-$ base). (Eigenvalues ± 1 of state 'a' are doubly-degenerate).

of the matrix $\rho_{i,j}$, and then determine the value of this matrix at the incremented point using the Taylor formula. As for the relaxation terms, they were considered in accordance with the Pauli equation [15]: as the level 3^3S_1 decays incrementally into multiplet levels of 2^3P, a term describing the relaxation of state 'b' has the form of $\frac{1}{3}I_3\rho_{bb}$, where I_3 is the identity matrix of the third order. (The time is measured in units of the time of life of 3^3S_1 state and therefore the time interval equal to the lifetime of this state is equal to one). As for the density matrix of the multiplet 2^3P (state 'a'), because of the proposed isolation of the 3^3S_1 and 2^3P states, the term in equation (14) describing the relaxation of the state 'a' has the form $\frac{1}{9}I_9\rho_{aa}$, where I_9 is the identity matrix of the ninth order. With regards to the correlation density matrices, in this paper it is assumed that their relaxation constants are $\gamma/2$.

At Fig. 2 the dependency of the population of 3^3S_1 state of He atom on the dimensionless time for several values of the detuning of the laser frequency $\delta = 0, 1, 2, 3$, the intensity of magnetic field $H = 5000\ G$ and the angle of inclination of magnetic field direction $\chi = \pi/4$ is represented. From this picture, it can be inferred that the CPT state is achieved for sufficiently large frequency deviations ($\delta \geq 2$). The latter fact is clear from the above, since the entire chain of $\Lambda-$ schemes 'opens' only for sufficiently high δ.

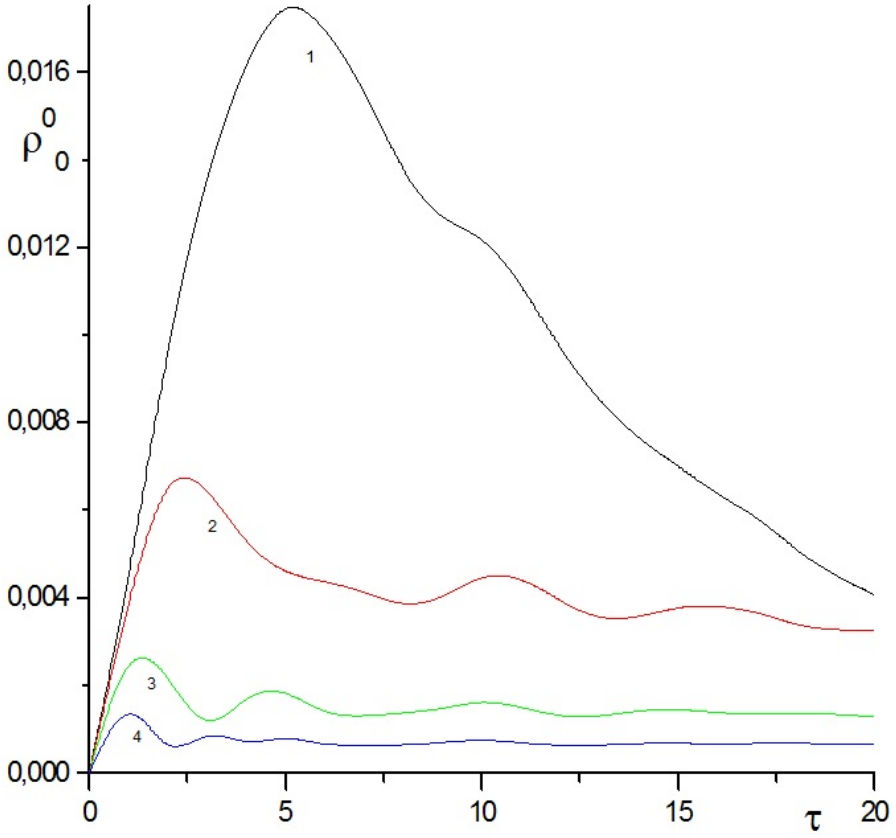

FIG. 2. The dependence of the 3^3S state population of the He atom on dimensionless time at $\mathcal{H} = 5000\ G$ and $\chi = \pi/4$ for $\delta = 0, 1, 2, 3$ (lines $1 - 4$ respectively)

We note further, that under the axially symmetric impact excitation of 2^3P multiplet, at the $^3S_1$ level, alignment is not at all induced for all values of the angles χ and θ. This result seems complex: the 3^3S_1 state is populated from levels of the 2^3P multiplet, where the impact alignment is induced, and therefore, the anisotropy of the lower state population should be transferred to the upper states.

Such a situation is shown in Fig. 3, where the dependence of the alignment induced in the 3^3S_1 state while separate isotropic population of the 2^3P_1 and 2^3P_2 levels when $\delta = 2$ is illustrated. The last figure shows that alignment, which is induced on the $^3S_1$ state, is of different sign when population of the 2^3P_2 or 2^3P_1 state is occurring. Dependence of the alignment induced from the $^3P_2$ state on time changes sign from negative to positive, however, the case is reversed for the $^3P_1$ state. It is interesting that for each population mean, the sign will change at the very same instant. From the above, it can be concluded that the signal of alignment becoming zero is due to both the symmetry of the impact-excited 2^3P state and that of the W_{ab} matrix, which describes the excitation process of the upper 3^3S_1 level. It should be mentioned, that the above-represented reasoning only illustrates the inputs of states with $j = 1$ and $j = 2$ of multiplet 2^3P into alignment induced on the3^3S_1 state: in the presence of a strong magnetic field, states with different j are mixed and separate excitation from these states is impossible.

Figure 4, shows the dependency of the 3^3S_1 state population on dimensionless time at a fixed detuning, intensity of the magnetic field and for the several values of angle χ. The figure

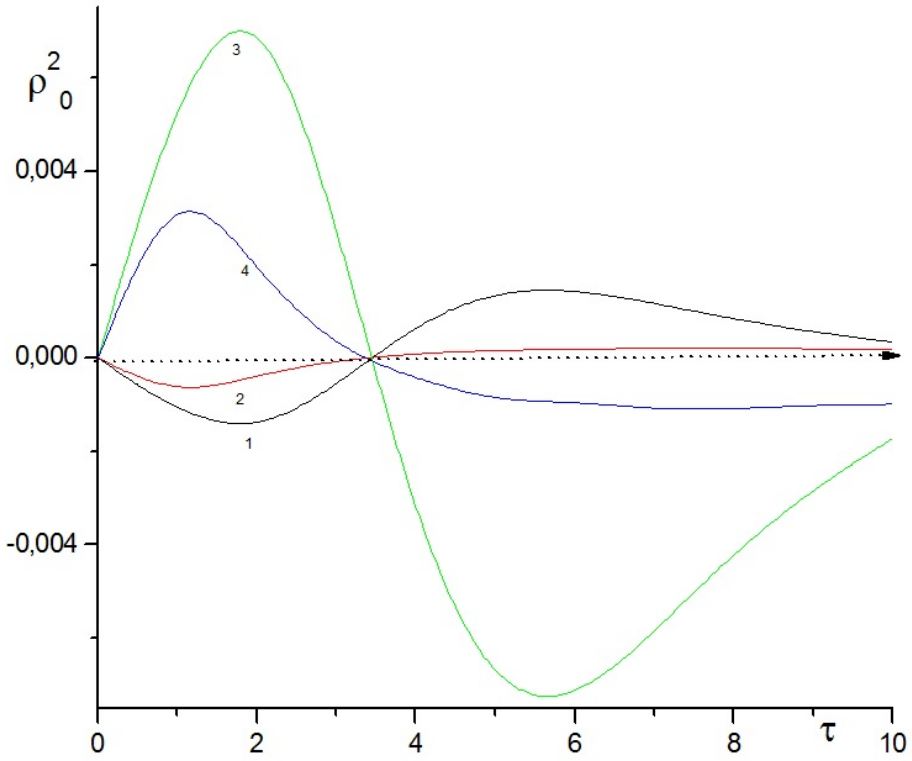

FIG. 3. The dependence of the alignment induced on 3^3S_1 state, when population happens individually for the 2^3P_2 (curves 1 and 2) and 2^3P_1 (curves 3 and 4) levels ($\delta = 1, 2$, $\mathcal{H} = 5000\ G$ and $\chi = \pi/4$).

shows that the population increases with the angle χ increasing from 0 to $\pi/4$, but then begins to decrease. This decreasing becomes faster the closer the angle χ is to the value of $\pi/2$. When $\chi = \pi/2$, the population turns to zero. Note that a similar result was obtained in [17] in the framework of approximate solutions for the Schrodinger equation with the use of perturbation theory over the Rabi frequency. Using a similar method for the approximate solution of system (14) has led to the following expression for the matrix elements ρ_{bb}:

$$\left(\rho_{bb}\right)_{M,M_1} = \hbar^2 \sum_{\xi,\mu} \left(W_{ba}\right)_{M,\xi} \left(\rho_{aa}\left(0\right)\right)_{\xi,\mu} \left(W_{ab}\right)_{\mu,M_1}$$
$$\left[\exp\left(\frac{\left(-\gamma\hbar - 2i\left(\delta + \left(\varepsilon_a\right)_\xi - \left(\varepsilon_b\right)_M\right)\right.}{2\hbar}t\right) + \exp\left(\frac{\left(-\gamma\hbar + 2i\left(\delta + \left(\varepsilon_a\right)_\mu - \left(\varepsilon_b\right)_{M_1}\right)\right.}{2\hbar}t\right) - \right.$$
$$\left.\exp\left(\frac{\left(-\gamma\hbar + 2i\left(+\left(\varepsilon_a\right)_\mu - \left(\varepsilon_a\right)_\xi + \left(\varepsilon_b\right)_M - \left(\varepsilon_b\right)_{M_1}\right)\right.}{2\hbar}t\right)\right], \tag{15}$$

which, due to cumbersome analytical expressions for W_{ab} and $\rho_{aa}(0)$ in $M-$basis, is rather short at only $\chi = \pi/2$, when for the population of level b one can write the following:

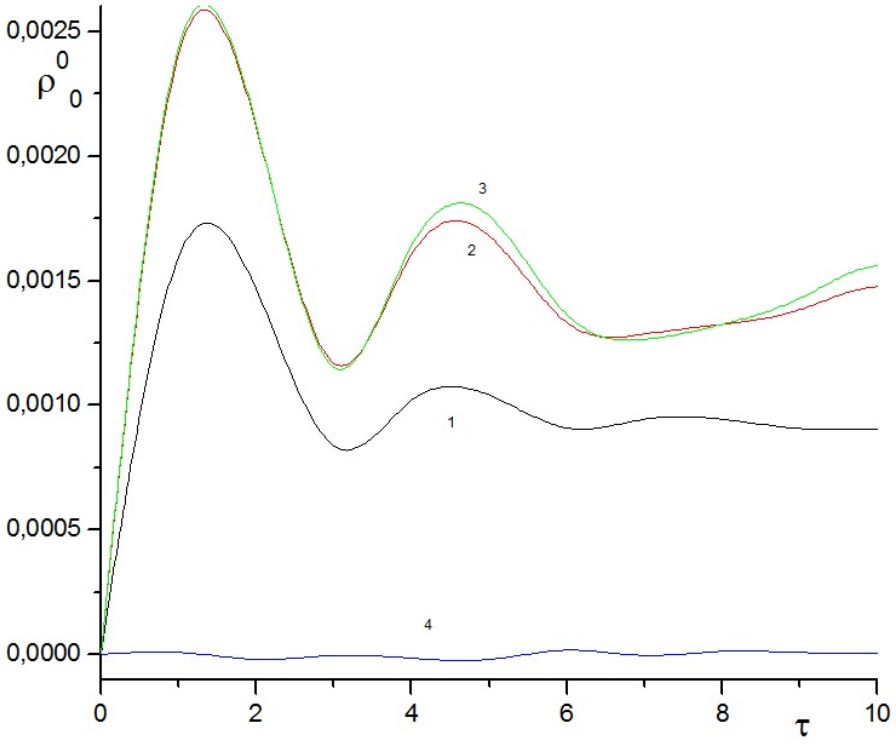

FIG. 4. The dependence of the population of 3^3S He atom on the dimensionless time at $\mathcal{H} = 5000\ G$, $\delta = 2$ and $\chi = 0, \pi/6, \pi/4, \pi/2$ (lines $1-4$ respectively).

$$(\rho_{bb})_0^0(t) = \frac{\hbar^2}{288\sqrt{3}\left(\Omega_L^2 - \delta^2\right)^2}\left[-11\delta^2 - 17\Omega_L^2 + 4\left(5\Omega_L^2 + 2\delta^2\right)\cos\left(\frac{\delta t}{\hbar}\right)\cos\left(\frac{\Omega_L t}{\hbar}\right) + 3\left(\delta^2 - \Omega_L^2\right)\cos\left(\frac{2\Omega_L t}{\hbar}\right) + 28\delta\Omega_L \sin\left(\frac{\delta t}{\hbar}\right)\sin\left(\frac{\Omega_L t}{\hbar}\right)\right]. \tag{16}$$

From the last expression, where, for brevity, we set $\gamma = 0$, one can see that for large values of the magnetic field intensity $(\rho_{bb})_0^0 \sim 1/\Omega_L^2$, which is consistent with the results of numerical calculation, which, let us recall, provides the populations turning to zero at $\chi = \pi/2$. Regarding the alignment, the approximate calculation according to equation (16) shows that at the point $\chi = \pi/2$, it has the highest infinitesimal order than $1/\Omega_L^2$, which is also consistent with the results of numerical calculations.

We further note that when $\chi \neq 0$, the magnetic field reduces the symmetry of the problem, resulting in the possibility of induction at the 3^3S level, the ordering of types different from the populations and longitudinal alignment discussed above. Numerical calculations showed that the character of the of the uncleaned and transverse alignment dependencies, $(\rho_{bb})_1^2$ and $(\rho_{bb})_2^2$, respectively are the same: they first increase and then decrease while remaining positive over the $0 < \chi < \pi/2$ interval, and are equal to zero at the ends of this interval. An example of an uncleaned alignment depending on the time for several values of the detuning of the laser frequency is shown in Fig. 5. As for orientation, it also becomes zero at the ends of said interval, whereas on the inside it is about two orders of magnitude smaller than the alignment.

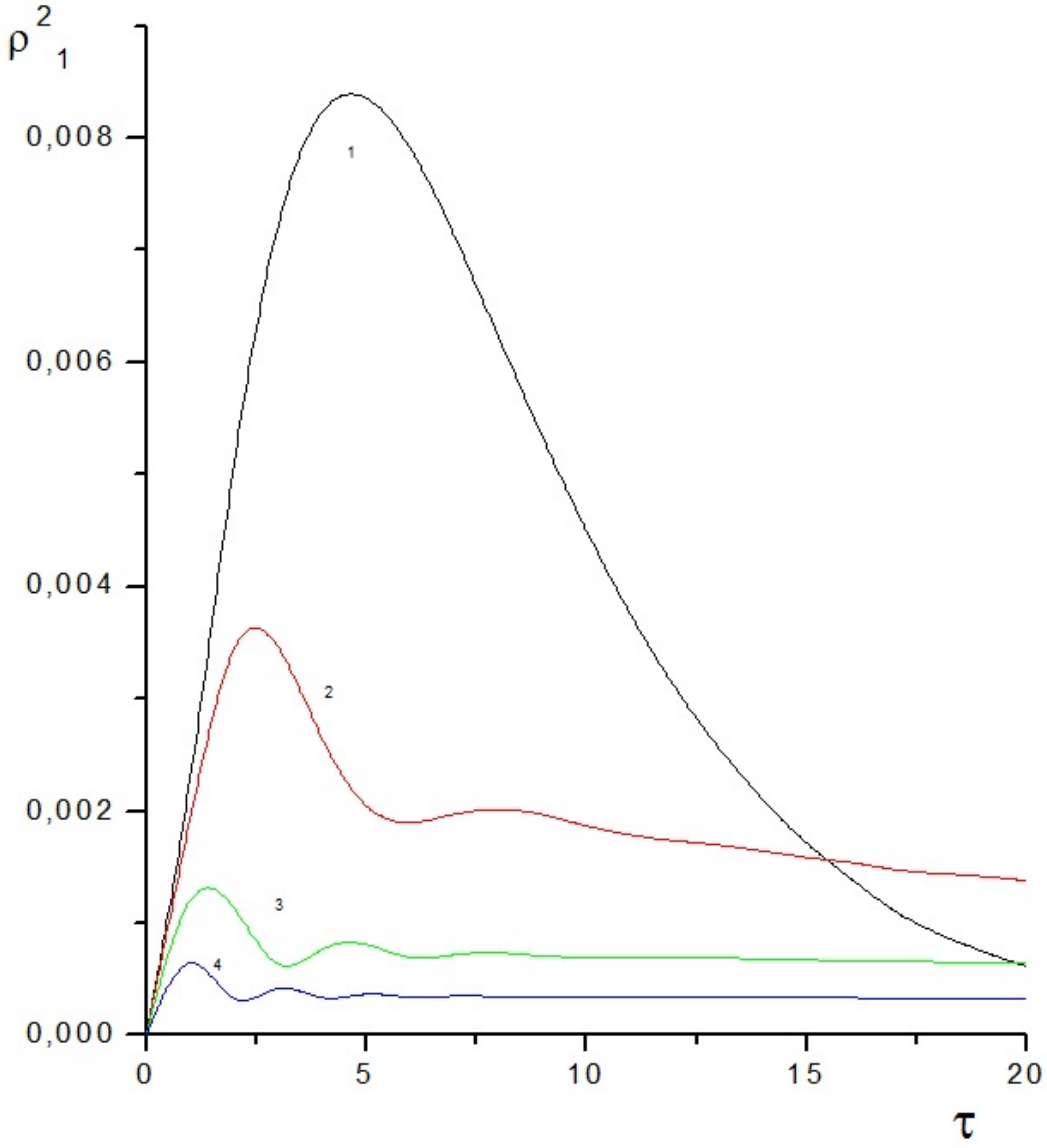

FIG. 5. The dependence on the uncleaned alignment of dimensionless time at $\mathcal{H} = 5000\ G$, $\chi = \pi/4$ and $\delta = 0, 1, 2, 3$ (lines $1 - 4$ respectively)

4. Conclusion

In this paper, the helium atom is used as an example for investigation of the influence of a strong magnetic field on the polarization characteristics of the radiation of a multi-level system, a set of lower levels of which are populated from the ground state by an axially symmetric excitation, while the upper levels are populated from lower levels in a coherent manner. With the help of numerical solutions of the Liouville equation, it has been shown that the system achieves the CPT state for large enough detunings of the laser frequency. For lower detunings at the excited state of the system, angular momenta ordering of population type is induced, whereas the ordering of alignment type is absent. In cases when the direction of the excitation processes anisotropies are orthogonal to the magnetic field direction, the system reaches a state of CPT, i.e. population, and hence the alignment of the system turns to zero.

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BORDER EFFECT, FRACTAL STRUCTURES AND BRIGHTNESS OSCILLATIONS IN NON-SILVER PHOTOGRAPHIC MATERIALS

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A brief review of effects in information recording systems based on complex compounds of polyvinyl alcohol (PVA) with metals (Au, Cu, Pt, Bi) is presented. As the result of irradiation, the chain reaction process of decomposition causes the aggregation of metal atoms or metal salts molecules to point centers or dendritic crystals. Some features of these processes are outlined.

Keywords: Non-silver photography, chain process, diffusion, aggregation, fractal dimension.

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1. Introduction

In this paper, we want to present a brief review of works performed in the 1980's – early 1990's, mainly at the Leningrad Mechanical Institute and Khabarovsk Pedagogical Institute. This research was devoted to the investigation of photoinitiated and radiation-initiated processes in thin films of polyvinyl alcohol (PVA) with complex ions of gold, copper, platinum, bismuth and other metals inserted into the polymer chain. These investigations were stimulated by fast depletion of silver supplies used in photomaterials. In these circumstances, the search for alternative media of photographic information recording seemed a very practical task. Now, the technological development in the field of the digital photography has radically reduced the severity of this problem. Nevertheless, in some fields the traditional method of image recording still remains preferable, and new materials based on results obtained in this research in question may appear useful. At the same time, we want to underline, that physical processes found in investigated materials, in our view, are of great interest themselves, as for some of these processes and we have no satisfactory explanation for some of these processes. We hope that this article will perhaps invite the attention of the contemporary generation of researchers to these questions.

2. Chain process of light-induced decomposition of complex ions of heavy metals

As was established in [1–3], the light-induced (and also radiation-induced) decomposition of halogen-containing compounds of certain metals in PVA films, such as solid solution $H\,[AuCl_4]$–PVA, is carried out in accordance with a chain reaction process. The process is initiated by excitation of a halogen in the auric complex ion:

$$[AuCl_4]^- + h\nu \rightarrow \left\{[AuCl_4]^-\right\}^* \rightarrow AuCl + 2Cl^{\cdot} + Cl^- \,. \tag{1}$$

As a result of this primary reaction (1), we obtain chlorine radicals $Cl^{\cdot}$ which propagate along polymer chains and cause further decomposition of ions:

$$[AuCl_4]^- + Cl^{\cdot} \rightarrow AuCl + Cl^{\cdot} + Cl_2 + Cl^- \,. \tag{2}$$

The chain continuation reaction (2) repeats over and over again. The chain length appears not less than 10^3. This process can be facilitated by reactions between $Cl^{\cdot}$-radicals with PVA, these reactions also have chain character.

During propagation, the chlorine radicals can be captured by traps or two radicals can form the Cl_2 molecule. These reactions lead to chain termination.

After decomposition of complex metal ions, some additional reactions can follow. Products of these reactions, metal atoms or salt molecules, diffuse and aggregate:

$$AuCl \rightarrow phase$$
$$3AuCl \rightarrow 2Au + AuCl_3$$
$$Au \rightarrow phase$$
$$\ldots$$

Analogous processes take place in PVA films containing complex ions of other metals.

3. Bordering effect

If the film is lightened uniformly, then metal or metal salts aggregate at point centers, which are also uniformly distributed, see Fig 1. When the concentration of metal (or salt) increases, then the concentration of phase centers also increases, while at the same time, the sizes of centers decrease, because the probability of the center formation increases nonlinearly with metal concentration.

When the irradiation is not uniform, then, as a rule, the concentration of the precipitated metal (salt) increases with an increase in the irradiation density. Nevertheless, if we have a large difference in this density, so that it is very high in the light-affected area, and it is negligible in the shadow area, we can observe the additional enlargement of point centers near the boundary of these areas (border effect) [4], see Fig 2. At the same time, the concentration of point centers near the boundary remains approximately the same as inside the irradiated zone. There are also some rare, large centers in shadow area near the boundary.

To explain this effect, the following model was proposed. After high-intensity irradiation, almost all complex ions in irradiated area decompose, and atoms of metal (salt molecules) aggregate to phase centres with uniform size and concentration. At the same time, $Cl^{\cdot}$-radicals which appear in the primary reaction (1), move to the shadow zone and cause the secondary reaction (2) here. The metal (salt), which appears in this reaction, begins to diffuse. As the rate of the reaction (2) is rather small, then the concentration of metal (salt) is also small. Under these conditions, the majority of the metal do not form

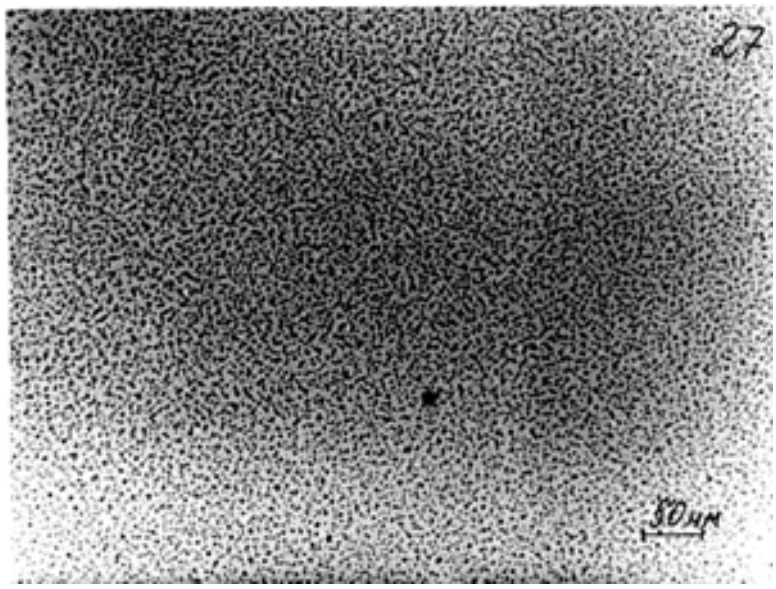

FIG. 1. Centres of Cu-phase aggregation

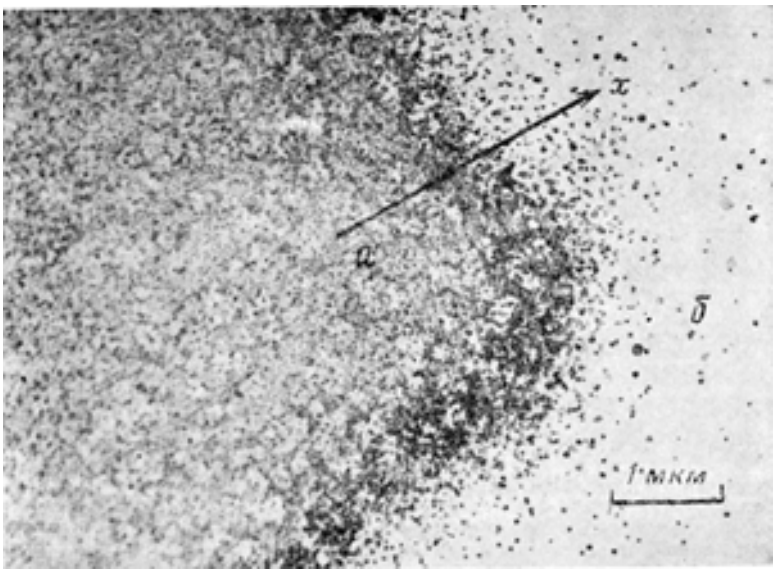

FIG. 2. Centers of $AuCl$-phase aggregation near the boundary between lightened and shadow areas in the PVA-H $[AuCl_4]$ film

centers in the shadow area, but diffuse to irradiated region and cause the growth of phase centers near the boundary.

To describe this process, a simplified mathematical model was proposed and explicit formulae were obtained. The results of calculations are in satisfactory agreement with experimental data.

4. Fractal structures

When the primary reaction is induced not by light, but by a high-energetic electron beam, then under some additional conditions (e.g., initial concentration of complex ions must belong to some diapason), then it can aggregate not to point centers, but to dendritic

crystals [5]. Fig. 3 and 4 show that the growth of such crystals begins from the boundary of the film or from some impurities, e.g. point centers which were formed earlier.

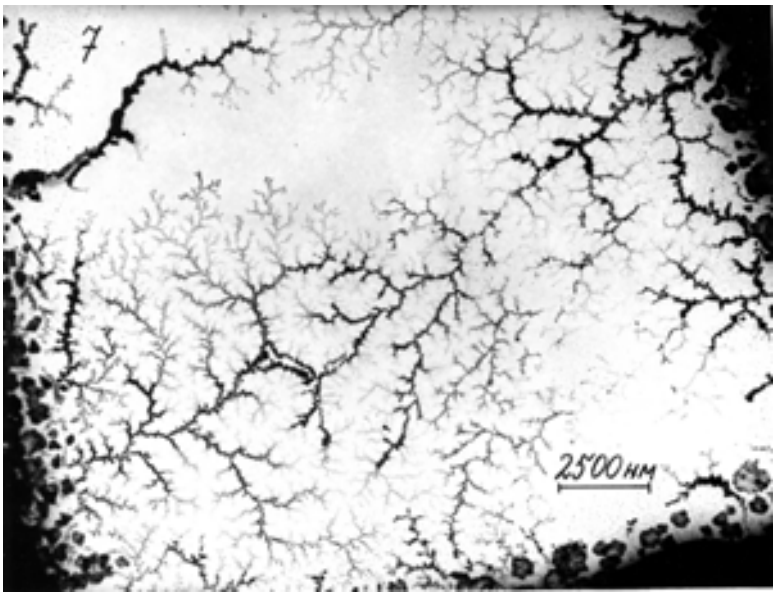

Fig. 3. Dendritic crystal of *AuCl* near the boundary of the film

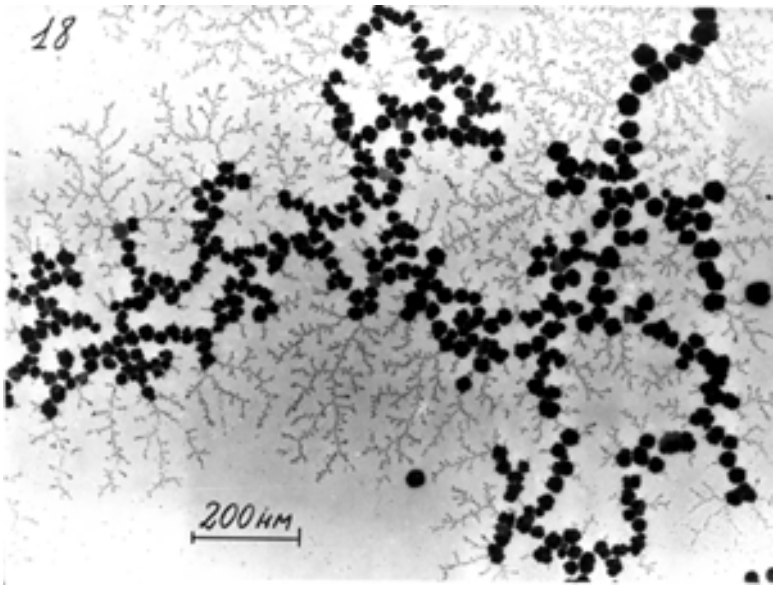

Fig. 4. Point centres and dendritic crystal of *AuCl*

In a wide range of sizes, such dendritic crystals can be considered as fractal structures. Those fractal dimensions were found by direct calculation using an electron microscope. It was surprising that these dimensions do not coincide for *AuCl* and *Cu* dendrites, see Fig. 5, 6.

As we can see on Fig. 7, the branches of dendrites consist of microcrystals with diameters ~ 10 nm.

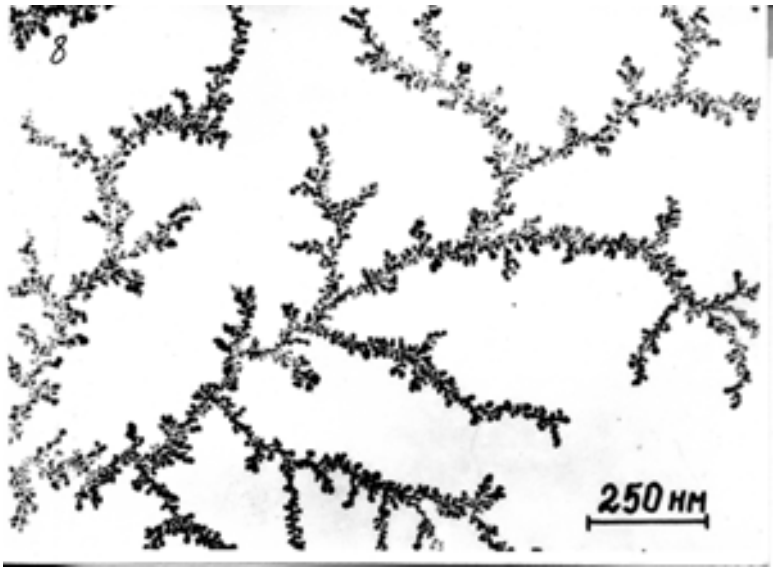

FIG. 5. Dendritic crystal of $AuCl$, the fractal dimension is 1.63 ± 0.04

FIG. 6. Dendritic crystal of Cu, the fractal dimension is 1.76 ± 0.05

5. Evolution of dendrites

In these experiments, the electron microscope was the source of electrons which caused the decomposition of complex ions, and the same microscope was used to observe results of this reaction. Further observation also caused additional irradiation of previously-formed dendrites. As a result, the dissolution of dendritic crystals take place. This process is accompanied by pulsations of crystal density in channels, branches and those parts disappear and restore at the same places repeatedly. At the end of this process, the crystal eventually disappears, Fig. 8 demonstrating its trace as a cavity in the film.

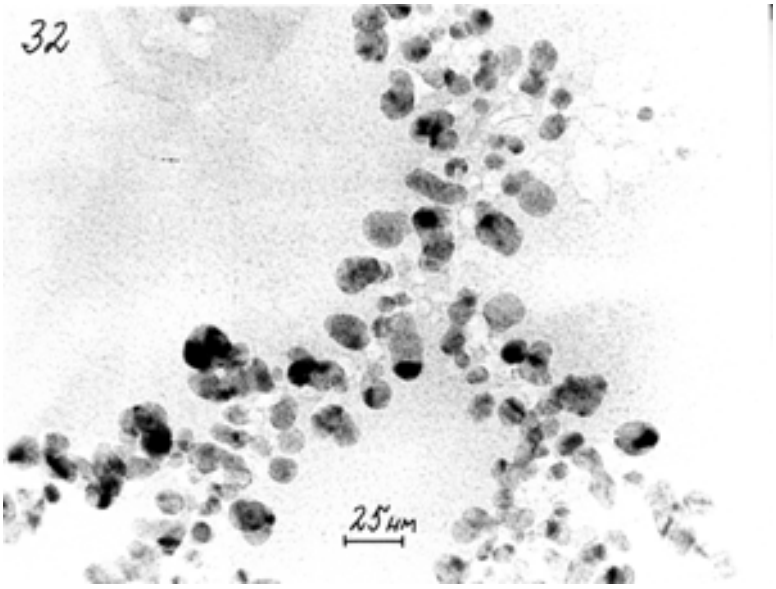

FIG. 7. Microcrystals of Cu

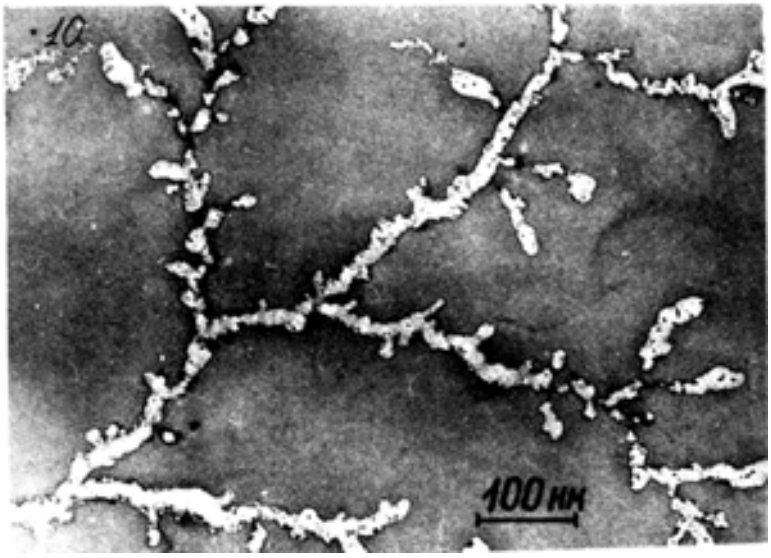

FIG. 8. The cavity at the place of dendritic crystal of $AuCl$

6. Conclusion

In this paper, we only briefly outlined some results of research concerning light-induced and radiation-induced reactions in compounds of PVA with complex ions of heavy metals. The authors intend to return to problems discussed here and represent them in detail in subsequent publications.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 140–145

ON THE STOKES FLOW COMPUTATION ALGORITHM BASED ON WOODBURY FORMULA

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The Stokes approximation is used for the description of flow in nanostructures. An algorithm for Stokes flow computation in cases when there is great variation in the viscosity over a small spatial region is described. This method allows us to overcome computational difficulties of the finite-difference method. The background of the approach is using the Woodbury formula - a discrete analog of the Krein resolvent formula. The particular example of a rectangular domain is considered in detail. The inversion of the discrete Stokes operator is made in analytic form for the case of constant viscosity.

Keywords: nanotube, Stokes flow, finite-difference method.

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1. Introduction

Flow in nanostructures have many peculiarities which are not explained by the conventional theory of fluid flow [1, 2]. At present, there is no general theory of nanoflows. We can only mention a few specific models [3–5]. Experiments show that nano-sized confinement leads to strong variation of liquid viscosity within the nanostructure [6–8]. One observes a similar situation when dealing with flow with nanoparticles or with singularities (see, e.g., [9, 10]). Additionally, there is a fraction separation effect [11]. This is an indirect confirmation of the crystalline model of nanoflow which is based on assumption that nanoliquid contains solid-like inclusions. To describe such flow in the framework of the model it is necessary to solve the Stokes equation with strong variation in viscosity. This creates difficulties for computations, particularly for the finite difference scheme [12–15]. To overcome these obstacles an approach based on the Woodbury formula was suggested [16]. The formula reduces the inversion of the discrete Stokes operator with small inclusions having strong viscosity contrast to the inversion of the operator with constant (or slowly varying) viscosity and the inversion of small rank operator. In the present paper, we consider in detail the first step.

In more detail, the governing equations in d-dimensional (d=2,3) case (i.e. the Stokes and continuity equations for velocity v and pressure p under the action of force F) can be written as follows:

$$\frac{\partial}{\partial x_j}\left(\eta\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)\right)-\frac{\partial p}{\partial x_i}=F_i,\ \frac{\partial v_i}{\partial x_i}=0. \tag{1}$$

We assume that the viscosity η has strong variation in small spatial domain and is constant outside of it. We use finite-difference discretization on non-staggered grid:

$$\begin{cases} h_j^{-1}\Delta_j(\eta(h_j^{-1}\nabla_j v_i + h_i^{-1}\nabla_i v_j)) - h_i^{-1}\nabla_i p = F_i, \\ h_i^{-1}\Delta_i v_i = 0, \end{cases} \tag{2}$$

where h_i is a mesh size, Δ_i is a forward difference, ∇_i is a backward difference,

$$\Delta_j f(x_1, \ldots, x_d) = f(x_1, \ldots, x_i + h_i, \ldots, x_d) - f(x_1, \ldots, x_i, \ldots, x_d),$$

$$\nabla_j f(x_1, \ldots, x_d) = f(x_1, \ldots, x_i, \ldots, x_d) - f(x_1, \ldots, x_i - h_i, \ldots, x_d).$$

The Woodbury formula allows us to improve the procedure of solving equations (2) in the case of strong viscosity variation.

2. Woodbury formula

Let us briefly describe the finite-difference approach based on the Woodbury formula (as for details, see [16]). Consider the discrete Stokes operator S on the lattice:

$$SV_i = \triangle_j(\eta(\nabla_j V_i + \nabla_i V_j)),$$

where V is the liquid velocity, η is the viscosity. Symbols Δ_p and ∇_p are used, correspondingly, for the forward and the backward finite differences for coordinate p where we assume for simplicity (it is not a limitation) that the lattice has a unit step. We use the following operator representation:

$$S = S_a + S_p^T, \quad S_a := \eta S_0,$$

where S_0 is the Stokes operator with the viscosity equals one:

$$S_0 V_i = \sum_j (\triangle_j \nabla_j V_i + \triangle_j \nabla_i V_j),$$

and:

$$S_p^T V_i = (\triangle_j \eta) T_j (\nabla_j V_i + \nabla_i V_j).$$

Here T_i is the translation operator:

$$T_i f(x_1, \ldots, x_d) = f(x_1, \ldots, x_i + h_i, \ldots, x_d).$$

Note that the operator S_p has small rank due to the property of the viscosity η, i.e. the corresponding matrix has many zero entries. We would like to solve the following equation:

$$SV = G,$$

where G is preassigned vector. To find a solution in our case it is convenient to use the Woodbury formula:

$$V_i = S^{-1}G_i = (\eta S_0 + S_p)^{-1}G = [1 - (\eta S_0)^{-1}(1 + S_p^T(\eta S_0)^{-1})^{-1}S_p^T](\eta S_0)^{-1}G$$

One can see that we have real computational improvement (due to small rank of S_p^T) if we can find the inverse operator $(\eta S_0)^{-1}$ without high computational complexity. It is really so. We can find the inverse operator for the case of constant viscosity, e.g., by using of the discrete Fourier transform. Namely, let:

$$X = (\eta S_0)^{-1}G = S_0^{-1}\eta^{-1}G.$$

To find X one should solve the equation:

$$\eta S_0 X = G.$$

After the Fourier transformation we obtain:

$$\hat{S_0}\hat{X} = \hat{\eta^{-1}}G \Leftrightarrow \hat{X} = (\hat{S_0})^{-1}\hat{\eta^{-1}}G$$

These operations are not associated with high complexity.

In the next section we consider in detail how to use the discrete Fourier transform in a particular case.

3. Discrete Stokes operator inversion for the case of constant viscosity in a rectangle

To find the inverse matrix we use the discrete Fourier transform. To introduce it we need the corresponding system of eigenfunctions. Let us choose the system.

Consider the discrete Stokes equations coupled with the discrete continuity equation for the case of constant viscosity $\eta = 1$:

$$\begin{cases} -2\Delta_1\nabla_1 V_1 - \Delta_2(\nabla_2 V_1 + \nabla_1 V_2) + \nabla_1 P = F_1, \\ -2\Delta_2\nabla_2 V_2 - \Delta_1(\nabla_1 V_2 + \nabla_2 V_1) + \nabla_2 P = F_2, \\ \Delta_1 V_1 + \Delta_2 V_2 = 0. \end{cases} \tag{3}$$

We deal with vector fields V and F and scalar field P, determined on a two-dimensional lattice with $N = L^2$ nodes. The nodes are numbered by vectors with integer terms $x = (x_1, x_2)$, $x_k \in \mathcal{D} = [0, L] \cap \mathbb{Z}$. Symbols Δ_p and ∇_p are used, correspondingly, for the forward and the backward finite differences for coordinate p:

$$\Delta_1 f(x) = f(x_1 + 1, x_2) - f(x), \quad \nabla_1 f(x) = f(x) - f(x_1 - 1, x_2),$$
$$\Delta_2 f(x) = f(x_1, x_2 + 1) - f(x), \quad \nabla_2 f(x) = f(x) - f(x_1, x_2 - 1),$$

where we assume for simplicity (it is not a limitation) that the lattice has a unit step. We will solve the system (3) with the free slip boundary condition:

$$\begin{cases} V_k\big|_{x_k=\pm L} = 0 \\ \nabla_j V_k\big|_{x_j=\pm L} = 0, \quad j \neq k. \end{cases} \tag{4}$$

Consider a one-dimensional lattice $\mathcal{D}$ and the family of functions ϕ_n, $n = 1..L-1$ determined on the lattice by the following expressions:

$$\phi_n(t) = \sin\frac{\pi n t}{L}, \quad t \in \mathcal{D}.$$

One can verify that the functions ϕ_n form a basis in the space of functions on the lattice $\mathcal{D}$, satisfying the conditions:

$$\phi_j(0) = \phi_j(L) = 0. \tag{5}$$

Consider the operator:

$$\Delta\nabla f(t) = \nabla f(t+1) - \nabla f(t) = f(t+1) - 2f(t) + f(t-1).$$

It is simple to verify that $\Delta\nabla = \nabla\Delta$). Direct calculation gives us:

$$\Delta\nabla\phi_j(t) = \Delta\nabla\sin\frac{\pi j t}{L} = \sin\frac{\pi j(t+1)}{L} - 2\sin\frac{\pi j t}{L} + \sin\frac{\pi j(t-1)}{L} = 2\sin\frac{\pi j t}{L}(\cos\frac{\pi j}{L} - 1),$$

hence,

$$\Delta\nabla\phi_j = \nabla\Delta\phi_j = \alpha_j\phi_j, \quad \alpha_j = 2\left(\cos\frac{\pi j}{L} - 1\right). \tag{6}$$

We introduce the notation:

$$\theta_j = \Delta\phi_j. \tag{7}$$

Then,

$$\nabla\theta_j = \nabla\Delta\phi_j = \alpha_j\phi_j. \tag{8}$$

Particularly,

$$\nabla\theta_j(d) = \alpha_j\phi_j(d) = 0, \quad \nabla\theta_j(0) = 0. \tag{9}$$

One can verify that θ_j is also the eigenvector of the operator of second symmetric finite difference corresponding to the same eigenvalue as ϕ_j. Actually,

$$\Delta\nabla\theta_j = \Delta\nabla\Delta\phi_j = \Delta\alpha_j\phi_j = \alpha_j\theta_j. \tag{10}$$

We additionally determine $\theta_0 \equiv 1$ and $\phi_0 \equiv 0$, which satisfy all the above-described properties.

Consider the family of functions Ψ_j, where the vector index $j = (j_1, j_2)$ has coordinates $j_p = 0..L-1$:

$$\Psi^j(x) = \theta_{j_1}(x_1)\theta_{j_2}(x_2).$$

Let us seek the solution of equation (3) in the form:

$$V_k(x) = \sum_j V_k^j \nabla_k \Psi^j(x), k = 1, 2, \quad P(x) = \sum_j P^j \Psi^j(x), \tag{11}$$

for some real coefficients V_k^j, P^j. One can see that the expression of such type satisfies the boundary conditions (4). One can show that any vector field V satisfying the conditions (4) can be represented in the form of (11). But arbitrary pressure field P, generally speaking, can not be presented in such form. Now we consider the component related to the velocity field only.

Substituting (11) into the Stokes equation from (3), one obtains:

$$-\sum_{p=1}^{2}\Delta_p\left(\nabla_p\sum_j V_k^j\nabla_k\Psi^j + \nabla_k\sum_j V_p^j\nabla_p\Psi^j\right) + \nabla_k\sum_j P^j\Psi^j = \sum_j F_k^j\nabla_k\Psi^j, \quad k = 1, 2,$$

where F_k^j is the projection of F_k on Ψ^j. Changing the order of summation, one gets:

$$\sum_j\left[P^j\nabla_k\Psi^j - F_k^j\nabla_k\Psi^j - \sum_{p=1}^{N}\left(V_k^j\Delta_p\nabla_p\nabla_k\Psi^j - V_p^j\Delta_p\nabla_k\nabla_p\Psi^j\right)\right] = 0.$$

Using the commutativity $\Delta_n\nabla_m = \nabla_m\Delta_n$ and the property $\Delta_p\nabla_p\Psi^j = \alpha_{j_p}\Psi^j$, One finds that

$$\sum_j\left[P^j - F_k^j - \sum_{p=1}^{2}\alpha_{j_p}\left(V_k^j - V_p^j\right)\right]\nabla_k\Psi^j = 0.$$

Due to linear independence of the vectors $\nabla_k\Psi^j$, the Stokes equation is equivalent to a set of systems:

$$P^j - \sum_{p=1}^{2}\alpha_{j_p}\left(V_k^j - V_p^j\right) = F_k^j, \quad k = 1, 2, \forall j.$$

Substituting (11) into the continuity equation from (3), we come to the equation:

$$\sum_{p=1}^{2}\Delta_p\sum_j V_p^j\nabla_p\Psi^j(x) = 0.$$

After simplification one gets:

$$\sum_j \sum_{p=1}^{2} \alpha_{j_p} V_p^j \Psi^j(x) = 0.$$

Due to linear independence of Ψ^j, the system is equivalent to the following one:

$$\sum_{p=1}^{2} \alpha_{j_p} V_p^j = 0 \quad \forall j.$$

Finally, the problem (3) with the boundary conditions (4) is reduced to the set of systems:

$$\begin{cases} P^j - \sum_{p=1}^{2} \alpha_{j_p} \left(V_k^j - V_p^j\right) = F_k^j \quad k = 1, 2, \forall j, \\ \sum_{p=1}^{2} \alpha_{j_p} V_p^j = 0 \quad \forall j. \end{cases}$$

Using the second equation, one can simplify the first one:

$$\begin{cases} P^j - V_k^j \sum_{p=1}^{2} \alpha_{j_p} = F_k^j \quad k = 1, 2, \forall j, \\ \sum_{p=1}^{2} \alpha_{j_p} V_p^j = 0 \quad \forall j. \end{cases}$$

Multiplying the first equation by α_{j_k} and making a summation by k, one gets:

$$P^j \left(\sum_k \alpha_{j_k}\right) - \left(\sum_k \alpha_{j_k} V_k^j\right) \left(\sum_{p=1}^{2} \alpha_{j_p}\right) = \left(\sum_k \alpha_{j_k} F_k^j\right) \quad \forall j,$$

Due to the second equation of the system, one has:

$$P^j = \frac{\sum_{p=1}^{2} \alpha_{j_p} F_p^j}{\sum_{p=1}^{2} \alpha_{j_p}} \quad \forall j.$$

Hence, the first equation gives us the velocity field:

$$V_k^j = \frac{P^j - F_k^j}{\sum_{p=1}^{2} \alpha_{j_p}} \quad k = 1, 2, \forall j.$$

Thus, for this particular case we obtained the solution in an explicit form. As for more complicated domain, one can follow the suggested procedure if the system of eigenfunctions is known. In this case the approach described allows one to obtain essential acceleration and guaranteed convergence of the computations for strongly varying viscosity.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (1), P. 146–153

STRONG SOLUTIONS AND THE INITIAL DATA SPACE FOR SOME NON-UNIFORMLY PARABOLIC EQUATIONS

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This paper is devoted to strong solutions of the first and second initial-boundary problems for non-uniformly parabolic equations. These equations are used in mechanics, glaciology, rheology, image processing as well as for nanosystem modeling. The initial data space for these problems was explicitly described as Orlicz—Sobolev spaces.

Keywords: non-uniformly parabolic equation, strong solution, initial data space, Orlicz—Sobolev space.

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1. Introduction

Let us consider the abstract Cauchy problem for the parabolic equation:

$$u'(t) + A(u(t)) = 0, \quad t > 0, \tag{1}$$

$$u(0) = u_0. \tag{2}$$

The solution for this problem can be considered in different meanings, for example, a classical solution, strong solution, weak (or mild) solution, entropy solution, etc. This paper is devoted to a strong solution for this problem.

If A is an unbounded linear operator in Hilbert space H, then it is proved that there does not exist a strong solution for all $u_0 \in H$ (see [2, 11]). It is proved in [13] that there exists a strong solution if and only if $u_0 \in [D(A), H]_{1/2}$, where $[D(A), H]_{1/2}$ is an interpolation space (see [9, 15]).

If A is a nonlinear operator, the weak solutions of these problems is often investigated. We consider the case where the operator A has the form:

$$A(u) = -\operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right],$$

with the Dirichlet and Neumann boundary conditions for the first and second initial-boundary problem respectively. Here, $\Phi\colon \mathbb{R} \to \mathbb{R}_+$ is an N-function that satisfies Δ_2-condition, therefore, it is natural to investigate these problems in Orlicz and Orlicz–Sobolev spaces. For these problems, we obtain the necessary and sufficient conditions for the existence and uniqueness of the strong solution.

Non-uniformly parabolic equations are used in mechanics, glaciology, rheology, image processing (e.g., see [4, 6, 8, 12]) as well as for nanosystem modeling (see [14, 16]).

Now, we consider some examples of the function $\Phi(\xi)$ and corresponding nonlinear equations.

If $\Phi(\xi) = \xi^p/p$, $p > 1$, then the nonlinear equation has the form:

$$u_t - \Delta_p u = 0,$$

where $\Delta_p u = \operatorname{div}(|\nabla u|^{p-2}\nabla u)$ is the p-Laplace operator. The p-Laplacian type equations have many applications in fluid mechanics, glaciology, and rheology, etc. (see [4] and [8, Chapter 2]).

If $\Phi(\xi) = \xi \log(1+\xi)$, then we obtain the equation related to image processing. This special case has been investigated thoroughly in [17] as a model that developed Perona and Malik's concept in [12].

If $\Phi(\xi) = \xi \log(1 + L_k(\xi))$, where $L_i(\xi) = \log(1 + L_{i-1}(\xi))$ $(i = 1, 2, \ldots, k)$ and $L_0(\xi) = \log(1 + \xi)$, for $\xi \geq 0$, then we obtain the parabolic equation such that the corresponding elliptic problems are introduced in Prandtl–Eyring fluids and plastic materials with a logarithmic hardening law (see [6]).

2. Functional Spaces

In this section, we introduce functional spaces that are called Orlicz spaces and Orlicz–Sobolev spaces. The spaces $L_\Phi(\Omega)$, called *Orlicz spaces*, are studied in depth in the monograph by Krasnosel'skii and Rutickii [7] and also in the doctoral thesis by Luxemburg [10]. If the role played by $L_p(\Omega)$ in the definition of Sobolev space $W_p^m(\Omega)$ is assigned instead to an Orlicz space $L_\Phi(\Omega)$, the resulting space is denoted by $W^m L_\Phi(\Omega)$ and called an *Orlicz–Sobolev space*. Many properties of Sobolev spaces have been extended to Orlicz–Sobolev spaces, mainly by Donaldson and Trudinger [5].

Let ϕ be a real-valued function defined on $[0, \infty)$ and having the following properties:

(a) $\phi(0) = 0$, $\phi(t) > 0$ if $t > 0$, $\lim\limits_{t\to\infty} \phi(t) = \infty$;

(b) ϕ is nondecreasing;

(c) ϕ is right continuous.

Then, the real-valued function $\Phi(\xi)$ is defined on $[0, \infty)$ by:

$$\Phi(\xi) = \int_0^\xi \phi(t)dt,$$

which is called an *N-function*. It can be proved that any N-function is continuous, strictly increasing, and convex.

We set:

$$\Phi^*(\eta) = \max_{\xi\geq 0}(\xi\eta - \Phi(\xi)).$$

If Φ is an N-function, then Φ^* is also an N-function. The function Φ^* is called the *polar function*.

An N-function Φ is said to satisfy *Δ_2-condition near infinity* if there exists $\xi_0 > 0$ and a positive constant M such that for every $\xi > \xi_0$:

$$\Phi(2\xi) \leq M\Phi(\xi). \tag{3}$$

Let Ω be a bounded domain and Φ be an N-function. The Orlicz class is the set of all (equivalence classes modulo equality a.e. in Ω of) measurable functions $u(x)$ defined on Ω and satisfying:

$$\int_\Omega \Phi(|u(x)|)dx < \infty.$$

If Ω is a bounded domain, then the Orlicz class is a linear space (under pointwise addition and scalar multiplication) if and only if Φ satisfies Δ_2-condition near infinity. Below, we

consider only the case where Φ satisfies Δ_2-condition near infinity. Note that the case where Φ does not satisfy Δ_2-condition near infinity is more complicated.

If the Orlicz class is a linear space, then we can consider it as the *Orlicz space* $L_\Phi(\Omega)$ with the norm:

$$\|u\|_{L_\Phi(\Omega)} = \inf\left\{k : \int_\Omega \Phi\left(\frac{|u(x)|}{k}\right) dx \le 1\right\}, \tag{4}$$

(this norm is due to Luxemburg [10]). The space $L_\Phi(\Omega)$ is a Banach space.

We also introduce the space $W^1L_\Phi(\Omega)$ as completion of $C^\infty(\Omega)$ with respect to the norm:

$$\|u\|_{W^1L_\Phi(\Omega)} = \|u\|_{L_2(\Omega)} + \||\nabla u|\|_{L_\Phi(\Omega)}. \tag{5}$$

By $\mathring{W}^1L_\Phi(\Omega)$, we denote completion of $C_0^\infty(\Omega)$ with respect to the norm (5). Here, $C^\infty(\Omega)$ is the set of infinitely differentiable functions in Ω and $C_0^\infty(\Omega)$ is the set of infinitely differentiable functions in Ω with compact support. The space $W^1L_\Phi(\Omega)$ can be called an *Orlicz–Sobolev space*, but in our case, $W^1L_\Phi(\Omega) \subset L_2(\Omega)$. In the general case, it is not true (for example, see [1, Chapter VIII]).

3. The First Initial-Boundary Problem

Let Ω be a bounded domain in $\mathbb{R}^n$ ($n \ge 2$) with Lipschitz boundary $\partial\Omega$ and $T > 0$. We denote $\Omega_T = \Omega \times (0,T)$ and $\Gamma = \partial\Omega \times (0,T)$. We consider the following parabolic equation

$$u_t - \operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right] = 0 \qquad \text{in } \Omega_T, \tag{6}$$

with the initial-boundary conditions

$$u\big|_\Gamma = 0 \qquad \text{on } \Gamma, \tag{7}$$

$$u(x,0) = u_0(x) \qquad \text{in } \Omega. \tag{8}$$

here $\Phi\colon \mathbb{R} \to \mathbb{R}_+$ is an N-function, $\Phi'\colon \mathbb{R} \to \mathbb{R}$ is the derivative of the function $\Phi(\xi)$ with respect to ξ, and ∇u is the gradient of the function $u(x,t)$ with respect to the spatial variables x. Problem (6)–(8) is called the first initial-boundary problem for a nonlinear equation.

Our main assumption is that $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition. We study the existence and uniqueness of a strong solution for problem (6)–(8). We assume that $u_0 \in L_2(\Omega)$.

Definition 1. The function $u(x,t)$ is called a *strong solution* of problem (6)–(8) if the following conditions are met:

(1) $u \in L_2(\Omega_T) \cap L_1(0,T;W_1^1(\Omega))$,

$$\int_0^T \int_\Omega \Phi'(|\nabla u|)|\nabla u|\, dxdt < +\infty,$$

and $u\big|_\Gamma = 0$;

(2) $u_t \in L_2(\Omega_T)$;

(3) for every $v \in C^1(\overline{\Omega}_T)$ such that $v|_{t=T} = 0$ and $v|_\Gamma = 0$, we have:

$$\int_0^T \int_\Omega \left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u \cdot \nabla v - uv_t\right] dxdt = \int_\Omega u_0(x)v(x,0)dx. \tag{9}$$

Remark 1. If $u(x,t)$ is a strong solution of problem (6)–(8), then:

$$\operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right] \in L_2(\Omega_T)$$

as well and the function $u(x,t)$ satisfies equation (6) a.e. in Ω_T and the initial condition (8) (in the sense of trace).

In [3], the uniqueness and existence of the weak solution were proven. In [18], the uniqueness and existence of the entropy solution were proven. These results were obtained if the function Φ satisfies weaker conditions than Δ_2-condition.

Now we formulate the result concerning the strong solution.

Theorem 1. *Let $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition near infinity. Then problem* (6)–(8) *has a strong solution if and only if*

$$u_0 \in \mathring{W}^1 L_\Phi(\Omega). \tag{10}$$

The strong solution of problem (6)–(8) *is unique.*

Proof.

1. It is easy to show that the solution of problem (6)–(8) is unique (because the function $\Phi(\xi)$ is convex).

2. To prove an existence of a strong solution, we use the Faedo–Galerkin method. Let the system of functions $\{e_k\}_{k=1}^{\infty}$, $e_k \in C^1(\overline{\Omega})$, $e_k|_\Gamma = 0$ be linearly independent and full in $\mathring{W}^1 L_\Phi(\Omega)$ (and in $L_2(\Omega)$ respectively).

We set $w_N(x,t) = \sum\limits_{k=1}^{N} c_{Nk}(t)e_k(x)$ $(N = 1,2,\ldots)$. The functions $w_N(x,t)$ are called the *Faedo–Galerkin approximations* and the coefficients $c_{Nk}(t)$ can be found from the corresponding relations.

We obtain the following estimate for $w_N(x,t)$:

$$\int_\Omega |w_N(x,\tau)|^2 dx \le \|u_0\|^2_{L_2(\Omega)} \quad (\tau \in (0,T)), \tag{11}$$

$$\int_0^\tau \int_\Omega \Phi'(|\nabla w_N|)|\nabla w_N|\, dxdt \le \frac{1}{2}\|u_0\|^2_{L_2(\Omega)}. \tag{12}$$

Using (11), we also have:

$$\|w_N\|^2_{L_2(\Omega_T)} \le T\|u_0\|^2_{L_2(\Omega)}. \tag{13}$$

From (12), (13) it follows that we can choose a subsequence (we also denote it by w_N for simplicity) such that:

$$w_N \rightharpoonup u \quad \text{weakly in } L_2(0,T;\mathring{W}^1 L_\Phi(\Omega)).$$

Moreover:

$$\|u\|^2_{L_2(\Omega_T)} \le T\|u_0\|^2_{L_2(\Omega)},$$

$$\int_0^\tau \int_\Omega \Phi'(|\nabla u|)|\nabla u|\, dxdt \le \frac{1}{2}\|u_0\|^2_{L_2(\Omega)}.$$

We also have the following estimate for $\|w_{Nt}\|_{L_2(\Omega_T)}$:

$$\|w_{Nt}\|^2_{L_2(\Omega_T)} \le \int_\Omega \Phi(\nabla w_N(x,0))dx.$$

We have that $w_N(x,0) \rightharpoonup u_0(x)$ as $N \to \infty$ weakly in $L_2(\Omega)$. Therefore, $\nabla w_N(x,0) \rightharpoonup \nabla u_0(x)$ as $N \to \infty$ weakly in $L_2(\Omega)$, i.e.:

$$\int_\Omega \nabla w_N(x,0)\eta(x)dx \to \int_\Omega \nabla u_0(x)\eta(x)dx,$$

as $N \to \infty$ for an arbitrary function $\eta \in C(\overline{\Omega})$. Since the functions $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition, we obtain that $w_N(x,0) \rightharpoonup u_0(x)$ as $N \to \infty$ weakly in $\mathring{W}^1 L_\Phi(\Omega)$. Thus:

$$\int_\Omega \Phi(\nabla w_N(x,0))dx \le C,$$

where C does not depend on N, and:

$$\|w_{Nt}\|^2_{L_2(\Omega_T)} \le C.$$

Therefore, we can choose a subsequence (we also denote it by w_N for simplicity) such that:

$$w_{Nt} \rightharpoonup u_t \quad \text{weakly in } L_2(\Omega_T).$$

3. Now we need to verify that $u(x,t)$ is a solution for problem (6)–(8). This can be done by using the standard technique for the Faedo–Galerkin method.

4. We need to prove that if there exists a strong solution $u(x,t)$ of problem (6)–(8), then the function $u_0(x)$ satisfies condition (10). It follows from these estimates:

$$\|u_0\|^2_{L_2(\Omega)} \le C\left(\|u\|^2_{L_2(\Omega_T)} + \int_0^T \int_\Omega \Phi'(|\nabla u|)|\nabla u|\, dxdt\right), \tag{14}$$

$$\int_\Omega \Phi(\nabla u_0(x))dx \le C\left(\|u_t\|^2_{L_2(\Omega_T)} + \|u\|^2_{L_2(\Omega_T)} + \left\|\operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right]\right\|^2_{L_2(\Omega_T)}\right), \tag{15}$$

where the constant C does not depend on $u(x,t)$.

Theorem 1 is thus proved. □

4. The Second Initial-Boundary Problem

Let Ω be a bounded domain in $\mathbb{R}^n$ ($n \ge 2$) with Lipschitz boundary $\partial\Omega$ and $T > 0$. We denote $\Omega_T = \Omega \times (0,T)$ and $\Gamma = \partial\Omega \times (0,T)$. We consider the following parabolic equation:

$$u_t - \operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right] = 0 \qquad \text{in } \Omega_T \tag{16}$$

with the initial-boundary conditions:

$$\left.\frac{\partial u}{\partial \mathbf{n}}\right|_\Gamma = 0 \qquad \text{on } \Gamma, \tag{17}$$

$$u(x,0) = u_0(x) \qquad \text{in } \Omega. \tag{18}$$

Here, $\Phi\colon \mathbb{R} \to \mathbb{R}_+$ is an N-function, $\Phi'\colon \mathbb{R} \to \mathbb{R}$ is the derivative of the function $\Phi(\xi)$ with respect to ξ, and ∇u is the gradient of the function $u(x,t)$ with respect to the spatial variables x, $\mathbf{n}$ is the unit normal vector of Γ. Problem (16)–(18) is called the second initial-boundary problem for nonlinear equation.

Our main assumption is that $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition near infinity. We study the existence and uniqueness of a strong solution for problem (16)–(18). We assume that $u_0 \in L_2(\Omega)$.

Definition 2. The function $u(x,t)$ is called a *strong solution* of problem (16)–(18) if the following conditions are met:

(1) $u \in L_2(\Omega_T) \cap L_1(0,T;W_1^1(\Omega))$,

$$\int_0^T \int_\Omega \Phi'(|\nabla u|)|\nabla u|\,dxdt < +\infty;$$

(2) $u_t \in L_2(\Omega_T)$;

(3) for every $v \in C^1(\overline{\Omega}_T)$ such that $v|_{t=T} = 0$, we have:

$$\int_0^T \int_\Omega \left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u \cdot \nabla v - uv_t\right] dxdt = \int_\Omega u_0(x)v(x,0)dx. \tag{19}$$

Remark 2. If $u(x,t)$ is a strong solution of problem (16)–(18), then:

$$\operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right] \in L_2(\Omega_T),$$

as well and the function $u(x,t)$ satisfies equation (16) a.e. in Ω_T and the initial condition (18) (in the sense of trace).

In [17], the uniqueness and existence of the weak solution were proven if the function $\Phi(\xi) = \xi\log(1+\xi)$. This problem is related to image analysis.

Now, we formulate the results concerning the strong solution.

Theorem 2. *Let $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition. Then problem* (16)–(18) *has a strong solution if and only if:*

$$u_0 \in W^1L_\Phi(\Omega). \tag{20}$$

The strong solution of problem (16)–(18) *is unique.*

Proof.

1. It is easy to show that the solution of problem (16)–(18) is unique (because the function $\Phi(\xi)$ is convex).

2. To prove an existence of a strong solution, we use the Faedo–Galerkin method. Let the system of functions $\{e_k\}_{k=1}^\infty$, $e_k \in C^1(\overline{\Omega})$, $e_k|_\Gamma = 0$ be linearly independent and full in $W^1L_\Phi(\Omega)$ (and in $L_2(\Omega)$ respectively).

We set $w_N(x,t) = \sum\limits_{k=1}^N c_{Nk}(t)e_k(x)$ $(N = 1,2,\ldots)$. The functions $w_N(x,t)$ are called the *Faedo–Galerkin approximations* and the coefficients $c_{Nk}(t)$ can be found from the corresponding relations.

We obtain the following estimate for $w_N(x,t)$:

$$\int_\Omega |w_N(x,\tau)|^2dx \le \|u_0\|^2_{L_2(\Omega)} \quad (\tau \in (0,T)), \tag{21}$$

$$\int_0^\tau \int_\Omega \Phi'(|\nabla w_N|)|\nabla w_N|\,dxdt \le \frac{1}{2}\|u_0\|^2_{L_2(\Omega)}. \tag{22}$$

Using (21), we also have:

$$\|w_N\|^2_{L_2(\Omega_T)} \le T\|u_0\|^2_{L_2(\Omega)}. \tag{23}$$

From (22) and (23) it follows that we can choose a subsequence (we also denote it by w_N for simplicity) such that:

$$w_N \rightharpoonup u \quad \text{weakly in } L_2(0,T;\mathring{W}^1L_\Phi(\Omega)).$$

Moreover:

$$\|u\|^2_{L_2(\Omega_T)} \le T\|u_0\|^2_{L_2(\Omega)},$$
$$\int_0^\tau \int_\Omega \Phi'(|\nabla u|)|\nabla u|\,dxdt \le \frac{1}{2}\|u_0\|^2_{L_2(\Omega)}.$$

We also have the following estimate for $\|w_{Nt}\|_{L_2(\Omega_T)}$:

$$\|w_{Nt}\|^2_{L_2(\Omega_T)} \le \int_\Omega \Phi(\nabla w_N(x,0))dx.$$

We have that $w_N(x,0) \rightharpoonup u_0(x)$ as $N \to \infty$ weakly in $L_2(\Omega)$. Therefore, $\nabla w_N(x,0) \rightharpoonup \nabla u_0(x)$ as $N \to \infty$ weakly in $L_2(\Omega)$, i.e.:

$$\int_\Omega \nabla w_N(x,0)\eta(x)dx \to \int_\Omega \nabla u_0(x)\eta(x)dx,$$

as $N \to \infty$ for an arbitrary function $\eta \in C(\overline{\Omega})$. Since the functions $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition, we obtain that $w_N(x,0) \rightharpoonup u_0(x)$ as $N \to \infty$ weakly in $W^1L_\Phi(\Omega)$. Thus:

$$\int_\Omega \Phi(\nabla w_N(x,0))dx \le C,$$

where C does not depend on N, and:

$$\|w_{Nt}\|^2_{L_2(\Omega_T)} \le C.$$

Therefore, we can choose a subsequence (we also denote it by w_N for simplicity) such that:

$$w_{Nt} \rightharpoonup u_t \quad \text{weakly in } L_2(\Omega_T).$$

3. Now we need to verify that $u(x,t)$ is a solution of problem (16)–(18). This can be done using the standard technique for the Faedo–Galerkin method.

4. We need to prove that if there exists a strong solution $u(x,t)$ for problem (16)–(18), then the function $u_0(x)$ satisfies condition (20). It follows from these estimates:

$$\|u_0\|^2_{L_2(\Omega)} \le C\left(\|u\|^2_{L_2(\Omega_T)} + \int_0^T \int_\Omega \Phi'(|\nabla u|)|\nabla u|\,dxdt\right), \tag{24}$$

$$\int_\Omega \Phi(\nabla u_0(x))dx \le C\left(\|u_t\|^2_{L_2(\Omega_T)} + \|u\|^2_{L_2(\Omega_T)} + \left\|\operatorname{div}\left[\frac{\Phi'(|\nabla u|)}{|\nabla u|}\nabla u\right]\right\|^2_{L_2(\Omega_T)}\right), \tag{25}$$

where the constant C does not depend on $u(x,t)$.

Theorem 2 is thus proved. □

5. The Initial Data Space

We define the *initial data space* as the space of the initial data such that there exists a strong solution only for them.

Theorem 3 (Main Result)**.** *If $\Phi(\xi)$ and $\Phi^*(\xi)$ satisfy the Δ_2-condition, then:*

(1) $\mathring{W}^1L_\Phi(\Omega)$ *is the initial data space for the first initial-boundary problem* (6)–(8)*;*
(2) $W^1L_\Phi(\Omega)$ *is the initial data space for the second initial-boundary problem* (16)–(18).

Proof. The proof clearly follows from Theorems 1 and 2. □

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