Ministry of Education and Science of the Russian Federation
Saint Petersburg National Research University of Information
Technologies, Mechanics, and Optics

NANOSYSTEMS:

PHYSICS, CHEMISTRY, MATHEMATICS

2016, volume 7(5)

Наносистемы: физика, химия, математика
2016, том 7, № 5

NANO Ф&Х&М

NANOSYSTEMS:

PHYSICS, CHEMISTRY, MATHEMATICS

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Phone: +7(812)232-67-65, **Journal site:** http://nanojournal.ifmo.ru/,
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The scope of the journal includes all areas of nano-sciences. Papers devoted to basic problems of physics, chemistry, material science and mathematics inspired by nanosystems investigations are welcomed. Both theoretical and experimental works concerning the properties and behavior of nanosystems, problems of its creation and application, mathematical methods of nanosystem studies are considered.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 782–788

A distinguished mathematical physicist Boris S. Pavlov

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PACS 01.60.+q **DOI 10.17586/2220-8054-2016-7-5-782-788**

Keywords: mathematical physics.

Received: 10 September 2016

Revised: 1 October 2016

Professor Boris Pavlov passed away on 30 January 2016.

Boris Pavlov was born in Kronshtadt, Russia, 27 July 1936. He graduated from Physical faculty of Leningrad State University in 1958 and continued to work at the Department of Mathematical Physics. His PhD thesis (1964, Supervisor – M. S. Birman) was devoted to investigation the spectrum of non-self-adjoint operator $-y'' + qy$. Ten years later, his PhD Thesis was followed by a Doctoral dissertation in Mathematical Analysis: "Dilation Theory and Spectral Analysis of Nonselfadjoint Differential Operators". He was a Vice-rector (Research) of Leningrad University [1978–1981 and at the same time [1978–1982], he had a Chair of Mathematical Analysis at the Faculty of Mathematics and Mechanics of Leningrad State University. Later [1982–1995] he worked as a Professor at the department of Higher Mathematics and Mathematical Physics, Physics Faculty. The year 1995 was a branching point for him. He held a Personal Chair in Pure Mathematics at the University of Auckland from 1994 to 2007, however, he did not break his connections with Russia. From 1995 he was a Chief of Complex Systems Theory Laboratory at Physical Faculty. Since 2009, he was a member of the then newly formed Institute for Advanced Study at Massey University Albany.

B. S. Pavlov was well known for his high level of scholarship in diverse areas of analysis. He became a Fellow of the Royal Society of New Zealand in 2004 and a member of the Russian Academy of Natural Sciences in 2010. B. S. Pavlov leaves behind his wife Irina, a daughter and a son.

The highest scientific achievements of B. S. Pavlov (as he himself felt) are:

- Spectral theory of singular differential non-selfadjoint operators, 1962.
- Riesz-basis property of exponentials on a finite interval, 1979.
- Operator-theory interpretation of critical zeros of the Riemann zeta-function, 1972.
- Symmetric Functional Model for dissipative operators, 1979.
- Zero-range potentials with inner structure and solvable models, 1984.
- Theory of the shift operator on a Riemann surface, jointly with S. Fedorov. 1987.
- Modified analytic perturbation procedure ("Kick-start") for operators with eigenvalues embedded into continuous spectrum, 2005.
- Fitting of zero-range solvable model of a quantum network based on rational approximation of the Dirichle-to-Neumann map of the original Hamiltonian, 2007.
- Fitted solvable model of the stressed tectonic plate, in connection with prediction of powerful earthquakes, jointly with L. Petrova, 2008.
- Quasi-relativistic dispersion and high mobility of electrons in Si-B sandwich structures, jointly with N. Bagraev, 2009.
- Theoretical interpretation of the low-threshold field emission from carbon nano-clusters, jointly with Y. Fursey and A. Yafyasov, 2010.

He supervised more than 30 students. Among them were:

1. V. L. Oleinik, Master,PhD student 1965–1971 (Associate Professor, St. Petersburg University)

2. S. V. Petras, Master,PhD student 1965–1970 (Associate Professor, St. Petersburg University of Economics)

3. M. G. Suturin, Master,PhD student 1966–1971 (Associate Professor, St. Petersburg Institute for Airspace devices)

4. S. N. Naboko, Master, PhD student 1969–1976 (Full Professor, St. Petersburg University)

5. S. A. Avdonin, Master,PhD student 1969–1980 (Full Professor, the Univ. of Fairbancs, Alaska)

6. M. A.Shubova, Master,PhD student 1969–1982 (Full Professor, the University of New Hampshire, USA)

7. S. A. Ivanov, Master, PhD student 1972–1978 (Research worker at the Institute of Terrestrial Magnetism RAS, St. Petersburg)

8. I. Yu. Popov, Master, PhD student 1974–1978 (full Professor, Chair of Higher Mathematics, ITMO University, St. Petersburg)

9. Yu. A. Kuperin, Master student 1975–1978 (Doctor of Science, Full Professor, St. Petersburg University)

10. Y. E. Karpeshina, Master,PhD student 1975–1985 (Full Professor, Birmingham University, Alabama, USA)

11. K. A. Makarov, Master, PhD student 1976–1982 (Full professor, Univ. Missouri-Columbia)

12. S. E. Cheremshantsev, Master, PhD student 1976–1982 (Full Professor, Chair of Higher Mathematics, Orlean University, France)

13. A. V. Rybkin, Master, PhD student 1977–1982 (Full Professor, Univ. of Fairbancs, Alaska)

14. A. V. Strepetov, Master, PhD student 1978–1986 (St. Petersburg Institute of Airspace devices, St. Petersburg, Russia)

15. M. D. Faddeev, PhD student 1982–1985. (Associate Professor in St. Petersburg University)

16. P. B. Kurasov, Master, PhD student 1981–1987 (Associate Professor, Doctor of science, now in Lund University, Sweden)

17. A. E. Ryzhkov, Master, PhD student 1974–1980 (Associate Professor, ITMO University, St. Petersburg)

18. V. A. Evstratov, Master, PhD student 1984–1992 (Assistant Professor St. Petersbufg University till 1994. Now in business)

19. A. A. Shushkov, PhD student 1984–1987 (Assistant Professor St. Petersbufg University till 1991, now somewhere in Canada)

20. N. I. Gerasimenko, PhD student 1985–1987 (Associate Professor at the Higher Military School, St. Petersburg)

21. M. M. Pankratov, Master, PhD student 1987–1991 (Insurance Company, Switzerland.)

22. S. V. Frolov, Master, PhD student 1988–1993 (Doctor of Technology, Full Professor, ITMO University, St.Petersburg)

23. A. A. Pokrovski, Master, PhD student 1990–1995 (Research worker at the Institute for Physics of St. Petersburg University, St. Petersburg, Russia)

24. R. Killip, Master, PhD student, the Univ of Auckland 1994–1996 (Associate Professor, UCLA, Los-Angeles, USA)

25. J. Mac-Cormick, Master student, the Univ. of Auckland 1994–1995 (Research worker in Computer Design Laboratory UCLA)

26. A. Kraegeloh, Master thesis, the Univ. of Auckland 1995–1997 (Insurance company, Germany)

27. M. Harmer, Master,PhD student Auckland 1996–2000 (Post Doc., Prague)

28. A. B. Mikhailova, Master student 2000–2001, St-Petersburg Univ. (Research worker at the Institute for Physics of St. Petersburg University)

29. S. Mau, Master student, 1999–2002, the Univ of Auckland (PhD student, New York Univ., USA)

30. S. Marshall, Master student, the Univ of Auckland 2004–2006 (PhD student at Princeton)

31. S. Dillon, Master thesis, the Univ of Auckland, 2005–2007 (PhD at Massey Uni. NZ)

The scientific interests of B. S. Pavlov were very wide, ranging from quantum physics to earthquakes. But were not his only interests. He liked kayak travels and alpine skiing. Everybody knew him as a good painter. In this article, you can see his self-portrait. For his students, if they had a problem, they could visit Boris Sergeevich, as his door was always open and he would help them using all his abilities and talents. He was kind and wonderful person, a teacher in science and in life. We will never forget him.

To show particular remarkable features of B.S.Pavlov, we include here a few memories from his former students.

A. Kiselev. I had the good fortune to study with Boris Sergeevich Pavlov for several years after I transferred from LITMO to SPbGU in 1989. Boris Sergeevich had set my early direction in mathematics, suggesting problems to work on and topics to study. However, he did much more than that; he truly cared about his students, and provided support and advice not only professionally but in other aspects of life. More than anything, though, he influenced me through his personal example of doing mathematics. For him, mathematics was something to live and breathe, something to enjoy with friends and students. Boris Sergeevich treated his classes as performances, including a bit of occasional improvisation, making those instances some of the most inspiring moments I saw. He liked to say that mathematics is an experimental science. This way of thinking about mathematics – that one should build models, experiments, tirelessly explore the entire landscape surrounding the problem of interest – has become part of my mathematical DNA.

Boris Sergeevich was very generous and gentle with me, but he did not hesitate to provide precise feedback when something needed fixing. I remember my first ever presentation of research paper which I read in order to start working on my own problem. Within five minutes of the start Boris Sergeevich yawned and stopped me and explained that he does not need me to faithfully reproduce all the details. I am not at an exam now – what is the idea? This way my boring report quickly turned into a lively discussion. I am afraid that I could not tell the main idea, however Boris Sergeevich did not let us fail and helped me formulate it in the end (I am pretty sure now he figured it out long before I did but made me discover it myself). Every one of such interactions has been priceless for me. The friendly, supportive and wise guidance of Boris Sergeevich came at a key time in my education and truly helped me grow as a mathematician.

P. Kurasov. I would like to mention B. S. Pavlov's precepts for young scientists:

Do other things than other researchers;

Use other ways than other researchers;

Look sharp during your research;

Read, but do not read much, otherwise you will not be read;

Do not disregard negative results;

Do not "cram your results into explanation" before you have checked it carefully.

This article bibliography contains the papers of B. S. Pavlov in Refereed Journals.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 789–802

On resonances and bound states of Smilansky Hamiltonian

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PACS 02.30.Tb, 03.65.Db **DOI 10.17586/2220-8054-2016-7-5-789-802**

We consider the self-adjoint Smilansky Hamiltonian H_ε in $L^2(\mathbb{R}^2)$ associated with the formal differential expression $-\partial_x^2 - \frac{1}{2}(\partial_y^2 + y^2) - \sqrt{2}\varepsilon y\delta(x)$ in the sub-critical regime, $\varepsilon \in (0,1)$. We demonstrate the existence of resonances for H_ε on a countable subfamily of sheets of the underlying Riemann surface whose distance from the physical sheet is finite. On such sheets, we find resonance free regions and characterize resonances for small $\varepsilon > 0$. In addition, we refine the previously known results on the bound states of H_ε in the weak coupling regime ($\varepsilon \to 0+$). In the proofs we use Birman-Schwinger principle for H_ε, elements of spectral theory for Jacobi matrices, and the analytic implicit function theorem.

Keywords: Smilansky Hamiltonian, resonances, resonance free region, weak coupling asymptotics, Riemann surface, bound states.

Received: 1 July 2016. Revised: 28 July 2016.

In memory of B. S. Pavlov (1936–2016)

1. Introduction

In this paper we investigate resonances and bound states of the self-adjoint Hamiltonian H_ε acting in the Hilbert space $L^2(\mathbb{R}^2)$ and corresponding to the formal differential expression

$$-\partial_x^2 - \frac{1}{2}(\partial_y^2 + y^2) - \sqrt{2}\varepsilon y\delta(x) \qquad \text{on } \mathbb{R}^2, \tag{1.1}$$

in the sub-critical regime, $\varepsilon \in (0,1)$. The operator H_ε will be rigorously introduced in Section 1.1 below. Operators of this type were suggested by U. Smilansky in [1] as a model of *irreversible quantum system*. His aim was to demonstrate that the 'heat bath' need not have an infinite number of degrees of freedom. On a physical level of rigor he showed that the spectrum undergoes an abrupt transition at the critical value $\varepsilon = 1$. A mathematically precise spectral analysis of these operators and their generalizations has been performed by M. Solomyak and his collaborators in [2–8]. Time-dependent Schrödinger equation generated by Smilansky-type Hamiltonian is considered in [9].

By now many of the spectral properties of H_ε are understood. On the other hand, little attention has been paid so far to the fact that such a system can also exhibit resonances. The main aim of this paper is to initiate investigation of these resonances starting from demonstration of their existence. One of the key difficulties is that this model belongs to a class wherein the resolvent extends to a *Riemann surface* having uncountably many sheets. The same complication appears *e.g.* in studying resonances for quantum waveguides [10–13], [14, §3.4.2] and for general manifolds with cylindrical ends [15, 16].

In this paper, we prove the existence and obtain a characterization of resonances of H_ε on a countable subfamily of sheets whose distance from the physical sheet is finite in the sense explained below. On any such sheet we characterize a region which is free of resonances. As $\varepsilon \to 0+$, the resonances on such sheets are localized in the vicinities of the thresholds $\nu_n = n + 1/2$, $n \in \mathbb{N}$. We obtain a description of the subset of the thresholds in the vicinities of which a resonance exists for all sufficiently small $\varepsilon > 0$ and derive asymptotic expansions of these resonances in the limit $\varepsilon \to 0+$. No attempt has been made here to define and study resonances on the sheets whose distance from the physical sheet is infinite.

As a byproduct, we obtain refined properties of the bound states of H_ε using similar methods as for resonances. More precisely, we obtain a lower bound on the first eigenvalue of H_ε and an asymptotic expansion of the weakly coupled bound state of H_ε in the limit $\varepsilon \to 0+$.

Methods developed in this paper can also be useful to tackle resonances for the analog of Smilansky model with regular potential which is suggested in [17] and further investigated in [18, 19].

Notations

We use notations $\mathbb{N} := \{1, 2, \dots\}$ and $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ for the sets of positive and natural integers, respectively. We denote the complex plane by $\mathbb{C}$ and define its commonly used sub-domains: $\mathbb{C}^\times := \mathbb{C} \setminus \{0\}$, $\mathbb{C}_\pm := \{\lambda \in \mathbb{C}\colon \pm \operatorname{Im}\lambda > 0\}$ and $\mathbb{D}_r(\lambda_0) := \{\lambda \in \mathbb{C}\colon |\lambda - \lambda_0| < r\}$, $\mathbb{D}_r^\times(\lambda_0) := \{\lambda \in \mathbb{C}\colon 0 < |\lambda - \lambda_0| < r\}$, $\mathbb{D}_r := \mathbb{D}_r(0)$, $\mathbb{D}_r^\times := \mathbb{D}_r^\times(0)$ with $r > 0$. The principal value of the argument for $\lambda \in \mathbb{C}^\times$ is denoted by $\arg\lambda \in (-\pi, \pi]$. The branches of the square root are defined by:

$$\mathbb{C}^\times \ni \lambda \mapsto (\lambda)_j^{1/2} := |\lambda|^{1/2} e^{\mathrm{i}((1/2)\arg\lambda + j\pi)}, \qquad j = 0, 1.$$

If the branch of the square root is not explicitly specified, we understand the branch $(\cdot)_0^{1/2}$ by default. We also set $\mathbf{0} = (0, 0) \in \mathbb{C}^2$.

The L^2-space over $\mathbb{R}^d$, $d = 1, 2$, with the usual inner product is denoted by $(L^2(\mathbb{R}^d), (\cdot,\cdot)_{\mathbb{R}^d})$ and the L^2-based first order Sobolev space by $H^1(\mathbb{R}^d)$, respectively. The space of square-summable sequences of vectors in a Hilbert space $\mathcal{G}$ is denoted by $\ell^2(\mathbb{N}_0; \mathcal{G})$. In the case that $\mathcal{G} = \mathbb{C}$ we simply write $\ell^2(\mathbb{N}_0)$ and denote by $(\cdot,\cdot)$ the usual inner product on it.

For $\xi = \{\xi_n\} \in \ell^2(\mathbb{N}_0)$, we adopt the convention that $\xi_{-1} = 0$. *Kronecker symbol* is denoted by δ_{nm}, $n, m \in \mathbb{N}_0$, we set $\mathsf{e}_n := \{\delta_{nm}\}_{m\in\mathbb{N}_0} \in \ell^2(\mathbb{N}_0)$, $n \in \mathbb{N}_0$, and adopt the convention that $\mathsf{e}_{-1} := \{0\}$. We understand by $\operatorname{diag}(\{q_n\})$ the *diagonal matrix* in $\ell^2(\mathbb{N}_0)$ with entries $\{q_n\}_{n\in\mathbb{N}_0}$ and by $\mathsf{J}(\{a_n\}, \{b_n\})$ the *Jacobi matrix* in $\ell^2(\mathbb{N}_0)$ with diagonal entries $\{a_n\}_{n\in\mathbb{N}_0}$ and off-diagonal entries $\{b_n\}_{n\in\mathbb{N}}$[1]. We also set $\mathsf{J}_0 := \mathsf{J}(\{0\}, \{1/2\})$.

By $\sigma(\mathsf{K})$, we denote the spectrum of a closed (not necessarily self-adjoint) operator K in a Hilbert space. An isolated eigenvalue $\lambda \in \mathbb{C}$ of K having finite algebraic multiplicity is a point of the *discrete spectrum* for K; see [23, §XII.2] for details. The set of all the points of the discrete spectrum for K is denoted by $\sigma_{\mathrm{d}}(\mathsf{K})$ and the *essential spectrum* of K is defined by $\sigma_{\mathrm{ess}}(\mathsf{K}) := \sigma(\mathsf{K}) \setminus \sigma_{\mathrm{d}}(\mathsf{K})$. For a self-adjoint operator T in a Hilbert space, we set $\lambda_{\mathrm{ess}}(\mathsf{T}) := \inf\sigma_{\mathrm{ess}}(\mathsf{T})$ and, for $k \in \mathbb{N}$, $\lambda_k(\mathsf{T})$ denotes the k-th eigenvalue of T in the interval $(-\infty, \lambda_{\mathrm{ess}}(\mathsf{T}))$. These eigenvalues are ordered non-decreasingly with multiplicities taken into account. The number of eigenvalues with multiplicities of the operator T lying in a closed, open, or half-open interval $\Delta \subset \mathbb{R}$ satisfying $\sigma_{\mathrm{ess}}(\mathsf{T}) \cap \Delta = \varnothing$ is denoted by $\mathcal{N}(\Delta; \mathsf{T})$. For $\lambda \le \lambda_{\mathrm{ess}}(\mathsf{T})$ the *counting function* of T is defined by $\mathcal{N}_\lambda(\mathsf{T}) := \mathcal{N}((-\infty, \lambda); \mathsf{T})$.

1.1. Smilansky Hamiltonian

Define the *Hermite functions*:

$$\chi_n(y) := e^{-y^2/2} H_n(y), \qquad n \in \mathbb{N}_0. \tag{1.2}$$

Here, $H_n(y)$ is the *Hermite polynomial* of degree $n \in \mathbb{N}_0$ normalized by the condition $\|\chi_n\|_{\mathbb{R}} = 1$[2]. For more details on Hermite polynomials see [20, Chap. 22] and also [21, Chap. 5]. As it is well-known, the family $\{\chi_n\}_{n\in\mathbb{N}_0}$ constitutes an orthonormal basis of $L^2(\mathbb{R})$. Note also that the functions χ_n satisfy the three-term recurrence relation:

$$\sqrt{n+1}\chi_{n+1}(y) - \sqrt{2}y\chi_n(y) + \sqrt{n}\chi_{n-1}(y) = 0, \qquad n \in \mathbb{N}_0, \tag{1.3}$$

where we adopt the convention $\chi_{-1} \equiv 0$. The relation (1.3) can be easily deduced from the recurrence relation [20, eq. 22.7.13] for Hermite polynomials. By a standard argument any function $U \in L^2(\mathbb{R}^2)$ admits unique expansion:

$$U(x, y) = \sum_{n\in\mathbb{N}_0} u_n(x)\chi_n(y), \qquad u_n(x) := \int_{\mathbb{R}} U(x, y)\chi_n(y)\mathrm{d}y, \tag{1.4}$$

where $\{u_n\} \in \ell^2(\mathbb{N}_0; L^2(\mathbb{R}))$. Following the presentation in [7], we identify the function $U \in L^2(\mathbb{R}^2)$ and the sequence $\{u_n\}$ and write $U \sim \{u_n\}$. This identification defines a natural unitary transform between the Hilbert spaces $L^2(\mathbb{R}^2)$ and $\mathcal{H} := \ell^2(\mathbb{N}_0; L^2(\mathbb{R}))$. For the sake of brevity, we denote the inner product on $\mathcal{H}$ by $\langle\cdot,\cdot\rangle$. Note that the Hilbert space $\mathcal{H}$ can also be viewed as the tensor product $\ell^2(\mathbb{N}_0) \otimes L^2(\mathbb{R})$.

For any $\varepsilon \in \mathbb{R}$, we define the subspace $\mathcal{D}_\varepsilon$ of $\mathcal{H}$ as follows: an element $U \sim \{u_n\} \in \mathcal{H}$ belongs to $\mathcal{D}_\varepsilon$ *if, and only if*

(i) $u_n \in H^1(\mathbb{R})$ for all $n \in \mathbb{N}_0$;

(ii) $\{-(u_{n,+}'' \oplus u_{n,-}'') + \nu_n u_n\} \in \mathcal{H}$ with $u_{n,\pm} := u_n|_{\mathbb{R}_\pm}$ and $\nu_n = n + 1/2$ for $n \in \mathbb{N}_0$;

[1] We do not distinguish between Jacobi matrices and operators in the Hilbert space $\ell^2(\mathbb{N}_0)$ induced by them, since in our considerations all the Jacobi matrices are bounded, closed, and everywhere defined in $\ell^2(\mathbb{N}_0)$.

[2] This normalization means that $H_n(y)$ is, in fact, a product of what is usually called the *Hermite polynomial* of degree $n \in \mathbb{N}_0$ with a normalization constant which depends on n.

(iii) the boundary conditions

$$u_n'(0+) - u_n'(0-) = \varepsilon\big(\sqrt{n+1}u_{n+1}(0) + \sqrt{n}u_{n-1}(0)\big)$$

are satisfied for all $n \in \mathbb{N}_0$. For $n = 0$ only the first term is present on the right-hand side.

By [7, Thm. 2.1], the operator:

$$\operatorname{dom} \mathsf{H}_\varepsilon := \mathcal{D}_\varepsilon, \qquad \mathsf{H}_\varepsilon\{u_n\} := \{-(u_{n,+}'' \oplus u_{n,-}'') + \nu_n u_n\}, \tag{1.5}$$

is self-adjoint in $\mathcal{H}$. It corresponds to the formal differential expression (1.1). Further, we provide another way of defining H_ε which makes the correspondence between the operator H_ε and the formal differential expression (1.1) more transparent. To this aim, we define the straight line $\Sigma := \{(0, y) \in \mathbb{R}^2 \colon y \in \mathbb{R}\}$. Then, the Hamiltonain H_ε, $\varepsilon \in (-1, 1)$, can be alternatively introduced as the unique self-adjoint operator in $L^2(\mathbb{R}^2)$ associated via the first representation theorem [22, Thm. VI.2.1] with a closed, densely defined, symmetric, and semi-bounded quadratic form:

$$\begin{aligned} \mathfrak{h}_\varepsilon[u] &:= \|\partial_x u\|^2_{\mathbb{R}^2} + \frac{1}{2}\|\partial_y u\|^2_{\mathbb{R}^2} + \frac{1}{2}(yu, yu)_{\mathbb{R}^2} + \varepsilon\sqrt{2}\left(\operatorname{sign}(y)|y|^{1/2}u|_\Sigma, |y|^{1/2}u|_\Sigma\right)_{\mathbb{R}}, \\ \operatorname{dom}\mathfrak{h}_\varepsilon &:= \left\{u \in H^1(\mathbb{R}^2) \colon yu \in L^2(\mathbb{R}^2), |y|^{1/2}(u|_\Sigma) \in L^2(\mathbb{R})\right\}. \end{aligned} \tag{1.6}$$

For more details and for the proof of equivalence between the two definitions of H_ε, see [7, §9]. Since H_ε commutes with the parity operator in y-variable, it is unitarily equivalent to $\mathsf{H}_{-\varepsilon}$. We remark that the case $\varepsilon = 0$ admits separation of variables. Thus, it suffices to study H_ε with $\varepsilon > 0$.

In the following proposition, we collect fundamental spectral properties of H_ε, $\varepsilon \in (0, 1)$, which are of importance in the present paper.

Proposition 1.1. *Let the self-adjoint operator H_ε, $\varepsilon \in (0, 1)$, be as in* (1.5)*. Then the following claims hold:*

(i) $\sigma_{\mathrm{ess}}(\mathsf{H}_\varepsilon) = [1/2, +\infty)$;

(ii) $\inf \sigma(\mathsf{H}_\varepsilon) \geq \dfrac{1-\varepsilon}{2}$;

(iii) $1 \leq \mathcal{N}_{1/2}(\mathsf{H}_\varepsilon) < \infty$;

(iv) $\mathcal{N}_{1/2}(\mathsf{H}_\varepsilon) = 1$ *for all sufficiently small* $\varepsilon > 0$.

Items (i)–(iii) follow from [6, Lem 2.1] and [7, Thm. 3.1 (1),(2)]. Item (iv) is a consequence of [6, Thm. 3.2] and [7, §10.1]. Although we only deal with the sub-critical case, $\varepsilon \in (0, 1)$, we remark that in the critical case, $\varepsilon = 1$, the spectrum of H_1 equals to $[0, +\infty)$ and that in the sup-critical case, $\varepsilon > 1$, the spectrum of H_ε covers the whole real axis. Finally, we mention that in most of the existing literature on the subject not $\varepsilon > 0$ itself but $\alpha = \sqrt{2}\varepsilon$ is chosen as the coupling parameter. We choose another normalization of the coupling parameter in order to simplify formulae in the proofs of the main results.

1.2. Main results

While we are primarily interested in the resonances, as indicated in the introduction, we have also a claim to make about the discrete spectrum which we present here as our first main result and which complements the results listed in Proposition 1.1.

Theorem 1.2. *Let the self-adjoint operator H_ε, $\varepsilon \in (0, 1)$, be as in* (1.5)*. Then the following claims hold.*

(i) $\lambda_1(\mathsf{H}_\varepsilon) \geq 1 - \sqrt{\dfrac{1}{4} + \varepsilon^4}$ *for all* $\varepsilon \in (0, 1)$.

(ii) $\lambda_1(\mathsf{H}_\varepsilon) = \nu_0 - \dfrac{\varepsilon^4}{16} + \mathcal{O}(\varepsilon^5)$ *as* $\varepsilon \to 0+$.

Theorem 1.2 (i) is proven by means of Birman–Schwinger principle. The bound in Theorem 1.2 (i) is non-trivial for $\varepsilon^4 < 3/4$. This bound is better than the one in Proposition 1.1 (ii) for small $\varepsilon > 0$.

For the proof of Theorem 1.2 (ii) we combine Birman-Schwinger principle and the analytic implicit function theorem. We expect that the error term $\mathcal{O}(\varepsilon^5)$ in Theorem 1.2 (ii) can be replaced by $\mathcal{O}(\varepsilon^6)$ because the operator H_ε has the same spectral properties as $\mathsf{H}_{-\varepsilon}$ for any $\varepsilon \in (0, 1)$. Therefore, the expansion of $\lambda_1(\mathsf{H}_\varepsilon)$ must be invariant with respect to interchange between ε and $-\varepsilon$. In Lemma 4.1 given in Section 4 we derive an implicit scalar equation on $\lambda_1(\mathsf{H}_\varepsilon)$. This equation gives analyticity of $\varepsilon \mapsto \lambda_1(\mathsf{H}_\varepsilon)$ for small ε. It can also be used to compute higher order terms in the expansion of $\lambda_1(\mathsf{H}_\varepsilon)$. However, these computations might be quite tedious.

Our second main result concerns the resonances of H_ε. Before formulating it, we need to define the resonances rigorously. Let us consider the sequence of functions:

$$r_n(\lambda) := (\nu_n - \lambda)^{1/2}, \qquad n \in \mathbb{N}_0. \tag{1.7}$$

Each of them has two branches $r_n(\lambda, l) := (\nu_n - \lambda)_l^{1/2}$, $l = 0, 1$. The vector-valued function $R(\lambda) = (r_0(\lambda), r_1(\lambda), r_2(\lambda), \dots)$ naturally defines the Riemann surface $\widehat{Z}$ with uncountably many sheets. With each sheet of $\widehat{Z}$ we associate the set $E \subset \mathbb{N}_0$ and the *characteristic vector* l^E defined as:

$$l^E := \{l_0^E, l_1^E, l_2^E, \dots\}, \qquad l_n^E := \begin{cases} 0, & n \notin E, \\ 1, & n \in E. \end{cases} \tag{1.8}$$

We adopt the convention that $l_{-1}^E = 0$. The respective sheet of $\widehat{Z}$ is convenient to denote by Z_E. Each sheet Z_E of $\widehat{Z}$ can be identified with the set $\mathbb{C} \setminus [\nu_0, +\infty)$ and we denote by $Z_E^\pm$ the parts of Z_E corresponding to $\mathbb{C}_\pm$. With the notation settled, we define the realization of $R(\cdot)$ on Z_E as:

$$R_E(\lambda) := (r_0(\lambda, l_0^E), r_1(\lambda, l_1^E), r_2(\lambda, l_2^E), \dots). \tag{1.9}$$

The sheets Z_E and Z_F are *adjacent* through the interval $(\nu_n, \nu_{n+1}) \subset \mathbb{R}$, $n \in \mathbb{N}_0$, ($Z_E \sim_n Z_F$), if their characteristic vectors l^E and l^F satisfy:

$$\begin{aligned} l_k^F &= 1 - l_k^E, \qquad \text{for } k = 0, 1, 2, \dots, n \\ l_k^F &= l_k^E, \qquad \text{for } k > n. \end{aligned}$$

We set $\nu_{-1} = -\infty$ and note that any sheet Z_E is adjacent to itself through (ν_{-1}, ν_0). In particular, the function $\lambda \mapsto R_E(\lambda)$ turns out to be componentwise analytic on the Riemann surface $\widehat{Z}$.

The sequence $\mathfrak{E} = \{E_1, E_2, \dots, E_N\}$ of subsets of $\mathbb{N}_0$ is called a *path* if for any $k = 1, 2, \dots, N-1$ the sheets Z_{E_k} and $Z_{E_{k+1}}$ are adjacent. The following discrete metric:

$$\rho(E, F) := \inf\{N \in \mathbb{N}_0 \colon \mathfrak{E} = \{E_1, E_2, \dots, E_N\}, E_1 = E, E_N = F\}, \tag{1.10}$$

turns out to be convenient. The value $\rho(E, F)$ equals the number of sheets in the shortest path connecting Z_E and Z_F. Note that for some sheets Z_E and Z_F a path between them does not exist and in this case we have $\rho(E, F) = \infty$. We identify the *physical sheet* with the sheet $Z_\varnothing$ (for $E = \varnothing$). A sheet Z_E of $\widehat{Z}$ is *adjacent* to the physical sheet $Z_\varnothing$ if $\rho(E, \varnothing) = 1$ and it can be characterised by existence of $N \in \mathbb{N}_0$ such that $l_n^E = 1$ *if, and only if* $n \le N$. Also, we define the component:

$$\widetilde{Z} := \cup_{E \in \mathcal{E}} Z_E \subset \widehat{Z}, \qquad \mathcal{E} := \{E \subset \mathbb{N}_0 \colon \rho(E, \varnothing) < \infty\}, \tag{1.11}$$

of $\widehat{Z}$ which plays a distinguished role in our considerations. Any sheet in $\widetilde{Z}$ is located on a finite distance from the physical sheet with respect to the metric $\rho(\cdot, \cdot)$. The component $\widetilde{Z}$ of $\widehat{Z}$ in (1.11) can alternatively be characterized as:

$$\widetilde{Z} = \cup_{F \in \mathcal{F}} Z_F, \qquad \mathcal{F} := \{F \subset \mathbb{N}_0 \colon \sup\{n \in \mathbb{N}_0 \colon l_n^F = 1\} < \infty\}. \tag{1.12}$$

The number of the sheets in $\widetilde{Z}$ is easily seen to be countable. In order to define the resonances of H_ε on $\widetilde{Z}$, we show that the resolvent of H_ε admits an extension to $\widetilde{Z}$ in a certain weak sense.

Proposition 1.3. *For any $u \in L^2(\mathbb{R})$ and $n \in \mathbb{N}_0$ the function:*

$$\lambda \mapsto \mathfrak{r}_{n,\varepsilon}^{\varnothing}(\lambda; u) := \big\langle (\mathsf{H}_\varepsilon - \lambda)^{-1} u \otimes \mathsf{e}_n, u \otimes \mathsf{e}_n \big\rangle \tag{1.13}$$

admits unique meromorphic continuation $\mathfrak{r}_{n,\varepsilon}^{E}(\cdot; u)$ from the physical sheet $Z_\varnothing$ to any sheet $Z_E \subset \widetilde{Z}$.

The proof of Proposition 1.3 is postponed until Appendix. Now we have all the tools to define resonances of H_ε on $\widetilde{Z}$.

Definition 1.4. *Each resonance of H_ε on $Z_E \subset \widetilde{Z}$ is identified with a pole of $\mathfrak{r}_{n,\varepsilon}^{E}(\cdot; u)$ for some $u \in L^2(\mathbb{R})$ and $n \in \mathbb{N}_0$. The set of all the resonances for H_ε on the sheet Z_E is denoted by $\mathcal{R}_E(\varepsilon)$.*

Our definition of resonances for H_ε is consistent with [23, §XII.6], see also [14, Chap. 2] and [24] for multi-threshold case. It should be emphasized that by the spectral theorem for self-adjoint operators the eigenvalues of H_ε are also regarded as resonances in the sense of Definition 1.4 lying on the physical sheet $Z_\varnothing$. This allows us to treat the eigenvalues and 'true' resonances on the same footing. Needless to say, bound states and true resonances correspond to different physical phenomena and their equivalence in this paper is merely a useful mathematical abstraction.

According to Remark 2.5 below, the set of the resonances for H_ε on Z_E is symmetric with respect to the real axis. Thus, it suffices to analyze resonances on Z_E^-. Now, we are prepared to formulate the main result on resonances.

Theorem 1.5. *Let the self-adjoint operator H_ε, $\varepsilon \in (0,1)$, be as in* (1.5)*. Let the sheet $Z_E \subset \widetilde{Z}$ of the Riemann surface $\widehat{Z}$ be fixed. Define the associated set by:*

$$\mathcal{S}(E) := \big\{ n \in \mathbb{N} \colon (l^E_{n-1}, l^E_n, l^E_{n+1}) \in \{(1,0,0),(0,1,1)\} \big\}.$$

Let $\mathcal{R}_E(\varepsilon)$ be as in Definition 1.4 and set $\mathcal{R}_E^-(\varepsilon) := \mathcal{R}_E(\varepsilon) \cap \mathbb{C}_-$. Then, the following claims hold:

(i) $\mathcal{R}_E^-(\varepsilon) \subset \mathcal{U}(\varepsilon) := \big\{ \lambda \in \mathbb{C}_- \colon |\nu_{n-1} - \lambda||\nu_n - \lambda| \le \varepsilon^4 n^2, \ \forall n \in \mathbb{N} \big\}$.

(ii) *For any $n \in \mathcal{S}(E)$ and sufficiently small $\varepsilon > 0$ there is exactly one resonance $\lambda_n^E(\mathsf{H}_\varepsilon) \in \mathbb{C}_-$ of H_ε on Z_E^- lying in a neighbourhood of ν_n, with the expansion*

$$\lambda_n^E(\mathsf{H}_\varepsilon) = \nu_n - \frac{\varepsilon^4}{16}\big[(2n+1) + 2n(n+1)\mathrm{i}\big] + \mathcal{O}(\varepsilon^5), \qquad \varepsilon \to 0+. \tag{1.14}$$

(iii) *For any $n \in \mathbb{N} \setminus \mathcal{S}(E)$ and all sufficiently small $\varepsilon, r > 0$*

$$\mathcal{R}_E^-(\varepsilon) \cap \mathbb{D}_r(\nu_n) = \varnothing.$$

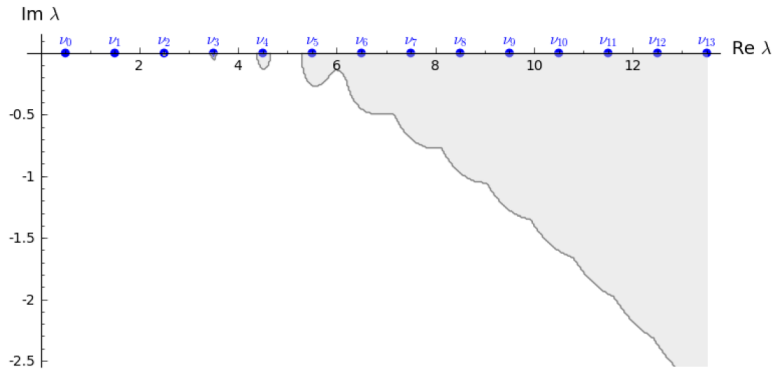

FIG. 1.1. The region $\mathcal{U}(0.12)$ (for $\varepsilon = 0.12$) from Theorem 1.5 (i) (in grey) consists of 6 connected components. The components located in the neighbourhoods of the points ν_0, ν_1, ν_2, ν_3, are not visible because of being too small. The plot is performed with the aid of *Sagemath*.

In view of Theorem 1.5 (i) for sufficiently small $\varepsilon > 0$, the resonances of H_ε on any sheet of $\widetilde{Z}$ are located in some vicinity of the thresholds ν_n (see Figure 1.1). Such behavior is typical for problems with many thresholds; see *e.g.* [11, 13] and [14, §2.4, 3.4.2]. Note also that the estimate in Theorem 1.5 (i) reflects the correct order in ε in the weak coupling limit $\varepsilon \to 0+$ given in Theorem 1.5 (ii). However, the coefficient of ε^4 in the definition of $\mathcal{U}(\varepsilon)$ can be probably improved. Observe also that $\mathcal{R}_E^-(\varepsilon) \subset \mathcal{U}(1)$ for any $\varepsilon \in (0,1)$.

According to Theorem 1.5 (ii)–(iii), the existence of a resonance near the threshold ν_n, $n \in \mathbb{N}$, on a sheet Z_E for small $\varepsilon > 0$ depends only on the branches chosen for $r_{n-1}(\lambda)$, $r_n(\lambda)$, $r_{n+1}(\lambda)$ on Z_E. Although, one cannot exclude that higher order terms in the asymptotic expansion (1.14) depend on the branches chosen for other square roots. By exactly the same reason as in Theorem 1.2 (ii), we expect that the error term $\mathcal{O}(\varepsilon^5)$ in Theorem 1.5 (ii) can be replaced by $\mathcal{O}(\varepsilon^6)$. Theorem 1.5 (ii)–(iii) are proven by means of the Birman-Schwinger principle and the analytic implicit function theorem. The implicit scalar equation on resonances derived in Lemma 4.1 gives analyticity of $\varepsilon \mapsto \lambda_n^E(\mathsf{H}_\varepsilon)$ for small $\varepsilon > 0$ and, as in the bound state case, it can be used to compute further terms in the expansion of $\lambda_n^E(\mathsf{H}_\varepsilon)$.

We point out that according to numerical tests that we performed, some resonances emerge from the inner points of the intervals (ν_n, ν_{n+1}), $n \in \mathbb{N}_0$, as $\varepsilon \to 1-$. The mechanism for the creation of these resonances is unclear at the moment.

Example 1.6. *Let $E = \{1,2,4,5\}$. In this case $l^E = \{0,1,1,0,1,1,0,0,0,0,0,\dots\}$ and we get that $\mathcal{S}(E) = \{1,4,6\}$. By Theorem 1.5 (ii)–(iii) for all sufficiently small $\varepsilon > 0$ there will be exactly one resonance on Z_E^- near ν_1, ν_4, ν_6 and no resonances near the thresholds ν_n with $n \in \mathbb{N} \setminus \{1,4,6\}$. We confirm this result by numerical tests whose outcomes are shown in Figures 1.2 and 1.3.*

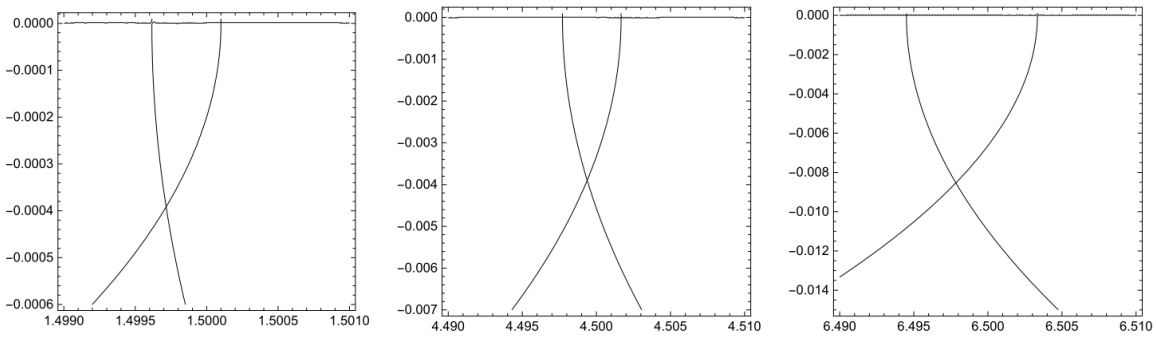

FIG. 1.2. Resonances of H_ε with $\varepsilon = 0.2$ lying on Z_E^- with $E = \{1, 2, 4, 5\}$ are computed numerically with the help of *Mathematica*. Unique weakly coupled resonances near the thresholds $\nu_1 = 1.5$, $\nu_4 = 4.5$, $\nu_6 = 6.5$ are located at the intersections of the curves.

To plot Figure 1.2, we used the condition on resonances in Theorem 2.4 below. The infinite Jacobi matrix in this condition was truncated up to a reasonable finite size. Along the curves, respectively, the real and the imaginary part of the determinant of the truncated matrix vanishes. At the points of intersection of the curves the determinant itself vanishes. These points are expected to be close to true resonances[3]*. We have also numerically verified that resonances do not exist near other low-lying thresholds ν_n with $n \in \mathbb{N} \setminus \{1, 4, 6\}$, which corresponds well to Theorem 1.5. In Figure 1.3 we summarize the results of all the numerical tests.*

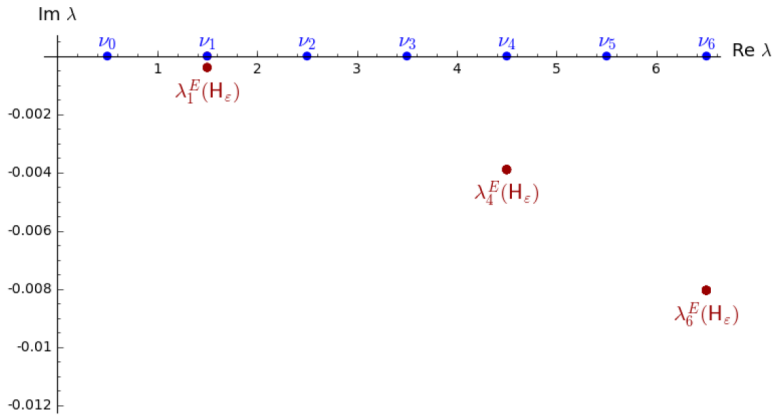

FIG. 1.3. Resonances of H_ε with $\varepsilon = 0.2$ lying on Z_E^- with $E = \{1, 2, 4, 5\}$.

Finally, we mention that no attempt has been made here to analyze the multiplicities of the resonances and to investigate resonances lying on $\widehat{Z} \setminus \widetilde{Z}$.

Structure of the paper

Birman-Schwinger-type principles for the characterization of eigenvalues and resonances of H_ε are provided in Section 2. Theorem 1.2 (i) on a lower bound for the first eigenvalue and Theorem 1.5 (i) on resonance free region are proven in Section 3. The aim of Section 4 is to prove Theorem 1.2 (ii) and Theorem 1.5 (ii)–(iii) on weakly coupled bound states and resonances. The proofs of technical statements formulated in Proposition 1.3 and Theorem 2.4 are postponed until Appendix.

2. Birman-Schwinger-type conditions

The Birman–Schwinger principle is a powerful tool for analyzing the discrete spectrum of a perturbed operator in the spectral gaps of the unperturbed one. This principle also has other various applications. Frequently, it can be generalized to detect resonances, defined as the poles of a meromorphic continuation of the (sandwiched)

[3]The analysis of convergence of the numerical method is beyond our scope.

resolvent from the physical sheet to non-physical sheet(s) of the underlying Riemann surface. In the model under consideration, we encounter yet another manifestation of this principle.

In order to formulate a Birman-Schwinger-type condition on the bound states for H_ε, we introduce the sequence of functions:

$$b_n(\lambda) := \frac{n^{1/2}}{2(\nu_n - \lambda)^{1/4}(\nu_{n-1} - \lambda)^{1/4}}, \qquad n \in \mathbb{N}, \tag{2.1}$$

and the off-diagonal Jacobi matrix:

$$\mathsf{J}(\lambda) = \mathsf{J}\left(\{0\}, \{b_n(\lambda)\}\right), \qquad \lambda \in (0, \nu_0)\,. \tag{2.2}$$

Recall that we use the same symbol $\mathsf{J}(\lambda)$ for the operator in $\ell^2(\mathbb{N}_0)$ generated by this matrix. It is straightforward to check that the operator $\mathsf{J}(\lambda)$ is bounded and self-adjoint. It can be easily verified that the difference $\mathsf{J}(\lambda) - \mathsf{J}_0$ is a compact operator. Therefore, one has $\sigma_{\rm ess}(\mathsf{J}(\lambda)) = \sigma_{\rm ess}(\mathsf{J}_0) = [-1, 1]$. Moreover, the operator $\mathsf{J}(\lambda)$ has simple eigenvalues $\pm\mu_n$, $\mu_n > 1$, with the only possible accumulation points at $\mu = \pm 1$.

Theorem 2.1. *[6, Thm. 3.1] Let the self-adjoint operator H_ε, $\varepsilon \in (0, 1)$, be as in* (1.5) *and let the Jacobi matrix $\mathsf{J}(\lambda)$ be as in* (2.2)*. Then, the relation:*

$$\mathcal{N}((0, \lambda); \mathsf{H}_\varepsilon) = \mathcal{N}((1/\varepsilon, +\infty); \mathsf{J}(\lambda)), \tag{2.3}$$

holds for all $\lambda \in (0, \nu_0)$.

Remark 2.2. A careful inspection of the proof of [6, Thm 3.1] yields that Theorem 2.1 can also be modified, replacing (2.3) by:

$$\mathcal{N}((0, \lambda]; \mathsf{H}_\varepsilon) = \mathcal{N}([1/\varepsilon, +\infty); \mathsf{J}(\lambda)). \tag{2.4}$$

In other words, the right endpoint of the interval $(0, \lambda)$ and the left endpoint of the interval $(1/\varepsilon, +\infty)$ can be simultaneously included.

The following consequence of Theorem 2.1 and of the above remark will be useful further.

Corollary 2.3. *Let the assumptions be as in Theorem 2.1. Then the following claims hold:*

(i) *$\varepsilon \mapsto \lambda_k(\mathsf{H}_\varepsilon)$ are continuous non-increasing functions;*

(ii) *$\dim\ker\left(\mathsf{H}_\varepsilon - \lambda\right) = \dim\ker\left(\mathsf{I} + \varepsilon\mathsf{J}(\lambda)\right)$ for all $\lambda \in (0, \nu_0)$. In particular, since the eigenvalues of $\mathsf{J}(\lambda)$ are simple, the eigenvalues of H_ε are simple as well.*

Proof. (i) Let $\varepsilon_1 \in (0, 1)$. For $\lambda = \lambda_k(\mathsf{H}_{\varepsilon_1})$, $k \in \mathbb{N}$, we have by Theorem 2.1 and Remark 2.2

$$\mathcal{N}([1/\varepsilon_1, +\infty); \mathsf{J}(\lambda)) = \mathcal{N}((0, \lambda]; \mathsf{H}_{\varepsilon_1}) \geq k.$$

Hence, for any $\varepsilon_2 \in (\varepsilon_1, 1)$, we obtain:

$$\mathcal{N}((0, \lambda]; \mathsf{H}_{\varepsilon_2}) = \mathcal{N}([1/\varepsilon_2, +\infty); \mathsf{J}(\lambda)) \geq \mathcal{N}([1/\varepsilon_1, +\infty); \mathsf{J}(\lambda)) \geq k.$$

Therefore, we get $\lambda_k(\mathsf{H}_{\varepsilon_2}) \leq \lambda = \lambda_k(\mathsf{H}_{\varepsilon_1})$. Recall that H_ε represents the quadratic form $\mathfrak{h}_\varepsilon$ defined in (1.6). Continuity of the eigenvalues follows from [22, Thms. VI.3.6, VIII.1.14] and from the fact that the quadratic form:

$$\operatorname{dom}\mathfrak{h}_\varepsilon \ni u \mapsto \varepsilon\sqrt{2}\left(\operatorname{sign} y|y|^{1/2}u|_\Sigma, |y|^{1/2}u|_\Sigma\right)_{\mathbb{R}}, \qquad \varepsilon \in (0, 1),$$

is relatively bounded with respect to

$$\operatorname{dom}\mathfrak{h}_\varepsilon \ni u \mapsto \|\partial_x u\|^2_{\mathbb{R}^2} + \frac{1}{2}\|\partial_y u\|^2_{\mathbb{R}^2} + \frac{1}{2}(yu, yu)_{\mathbb{R}^2}$$

with a bound less than one; *cf.* [6, Lem. 2.1].

(ii) By Theorem 2.1, Remark 2.2, and using symmetry of $\sigma(\mathsf{J}(\lambda))$ with respect to the origin we get:

$$\begin{aligned}\dim\ker\left(\mathsf{H}_\varepsilon - \lambda\right) &= \mathcal{N}((0, \lambda]; \mathsf{H}_\varepsilon) - \mathcal{N}((0, \lambda); \mathsf{H}_\varepsilon)\\ &= \mathcal{N}([1/\varepsilon, +\infty); \mathsf{J}(\lambda)) - \mathcal{N}((1/\varepsilon, +\infty); \mathsf{J}(\lambda)) = \dim\ker\left(\mathsf{I} + \varepsilon\mathsf{J}(\lambda)\right).\end{aligned}$$

□

For resonances of H_ε, one can derive a Birman-Schwinger-type condition analogous to the one in Corollary 2.3 (ii). For the sheet $Z_E \subset \widetilde{Z}$ of the Riemann surface $\widehat{Z}$, we define the Jacobi matrix:

$$\mathsf{J}_E(\lambda) := \mathsf{J}(\{0\}, \{b_n^E(\lambda)\}), \qquad \lambda \in \mathbb{C} \setminus [\nu_0, +\infty), \tag{2.5}$$

where

$$b_n^E(\lambda) := \frac{1}{2}\left(\frac{n}{r_n(\lambda, l_n^E)r_{n-1}(\lambda, l_{n-1}^E)}\right)^{1/2}, \qquad n \in \mathbb{N}. \tag{2.6}$$

The Jacobi matrix $\mathsf{J}_E(\lambda)$ in (2.5) is closed, bounded, and everywhere defined in $\ell^2(\mathbb{N}_0)$, but in general non-selfadjoint. For $E = \varnothing$ and $\lambda \in (0, \nu_0)$ the Jacobi matrix $\mathsf{J}_\varnothing(\lambda)$ coincides with $\mathsf{J}(\lambda)$ in (2.2). In what follows it is also convenient to set $b_0^E(\lambda) = 0$. In the next theorem, we characterize resonances of H_ε lying on the sheet Z_E.

Theorem 2.4. *Let the self-adjoint operator H_ε, $\varepsilon \in (0,1)$, be as in* (1.5)*. Let the sheet $Z_E \subset \widetilde{Z}$ be fixed, let $\mathcal{R}_E(\varepsilon)$ be as in Definition 1.4 and the associated operator-valued function $\mathsf{J}_E(\lambda)$ be as in* (2.5)*. Then, the following equivalence holds:*

$$\lambda \in \mathcal{R}_E(\varepsilon) \qquad \Longleftrightarrow \qquad \ker\big(\mathsf{I} + \varepsilon \mathsf{J}_E(\lambda)\big) \neq \{0\}. \tag{2.7}$$

For $E = \varnothing$, the claim of Theorem 2.4 follows from Corollary 2.3 (ii). The proof of the remaining part of Theorem 2.4 is postponed until Appendix. The argument essentially relies on Krein-type resolvent formula [7] for H_ε and on the analytic Fredholm theorem [25, Thm. 3.4.2].

Remark 2.5. Thanks to compactness of the difference $\mathsf{J}_E(\lambda) - \mathsf{J}_0$ we get by [23, Lem. XIII.4.3] that $\sigma_{\mathrm{ess}}(\varepsilon \mathsf{J}_E(\lambda)) = \sigma_{\mathrm{ess}}(\varepsilon \mathsf{J}_0)) = [-\varepsilon, \varepsilon]$. Therefore, the equivalence (2.7) can be rewritten as:

$$\lambda \in \mathcal{R}_E(\varepsilon) \qquad \Longleftrightarrow \qquad -1 \in \sigma_{\mathrm{d}}(\varepsilon \mathsf{J}_E(\lambda)).$$

Identity $\mathsf{J}_E(\lambda)^* = \mathsf{J}_E(\overline{\lambda})$ combined with [22, Rem. III.6.23] and with Theorem 2.4 yields that the set $\mathcal{R}_E(\varepsilon)$ is symmetric with respect to the real axis.

3. Localization of bound states and resonances

In this section we prove Theorem 1.2 (i) and Theorem 1.5 (i). The idea of the proof is to estimate the norm of $\mathsf{J}_E(\lambda)$ and to apply Corollary 2.3 (ii) and Theorem 2.4.

Proof of Theorem 1.2 (i) and Theorem 1.5 (i). The square of the norm of the operator $\mathsf{J}_E(\lambda)$ in (2.5) can be estimated from above by:

$$\begin{aligned} \|\mathsf{J}_E(\lambda)\|^2 &\leq \sup_{\xi \in \ell^2(\mathbb{N}_0), \|\xi\|=1} \|\mathsf{J}_E(\lambda)\xi\|^2 \leq \sup_{\xi \in \ell^2(\mathbb{N}_0), \|\xi\|=1} \bigg(\sum_{n \in \mathbb{N}_0} |b_n^E(\lambda)\xi_{n-1} + b_{n+1}^E(\lambda)\xi_{n+1}|^2 \bigg) \\ &\leq \sup_{\xi \in \ell^2(\mathbb{N}_0), \|\xi\|=1} \bigg(2 \sum_{n \in \mathbb{N}_0} \big(|b_n^E(\lambda)|^2 |\xi_{n-1}|^2 + |b_{n+1}^E(\lambda)|^2 |\xi_{n+1}|^2 \big) \bigg) \\ &\leq 4 \sup_{n \in \mathbb{N}_0} |b_n^E(\lambda)|^2 \sup_{\xi \in \ell^2(\mathbb{N}_0), \|\xi\|=1} \|\xi\|^2 = 4 \sup_{n \in \mathbb{N}} |b_n^E(\lambda)|^2, \end{aligned} \tag{3.1}$$

where $b_n^E(\lambda)$, $n \in \mathbb{N}_0$, are defined as in (2.6).

If $\|\varepsilon \mathsf{J}_E(\lambda)\| < 1$ holds for a point $\lambda \in \mathbb{C}_-$, then the condition $\ker\big(\mathsf{I} + \varepsilon \mathsf{J}_E(\lambda)\big) \neq \{0\}$ is not satisfied. Thus, λ cannot by Theorem 2.4 be a resonance of H_ε lying on Z_E^- in the sense of Definition 1.4. In view of estimate (3.1) and of (2.6) to fulfil $\|\varepsilon \mathsf{J}_E(\lambda)\| < 1$, it suffices to satisfy:

$$\frac{n}{|\nu_{n-1} - \lambda|^{1/2} |\nu_n - \lambda|^{1/2}} < \frac{1}{\varepsilon^2}, \qquad \forall\, n \in \mathbb{N},$$

or, equivalently,

$$|\nu_n - \lambda| \cdot |\nu_{n-1} - \lambda| > \varepsilon^4 n^2, \qquad \forall\, n \in \mathbb{N}.$$

Thus, the claim of Theorem 1.5 (i) is proven. If $\|\varepsilon \mathsf{J}_\varnothing(\lambda)\| < 1$ holds for a point $\lambda \in (0, 1/2)$ then the condition $\ker\big(\mathsf{I} + \varepsilon \mathsf{J}_\varnothing(\lambda)\big) \neq \{0\}$ is not satisfied. Thus, by Corollary 2.3 (ii), λ is not an eigenvalue of H_ε. In view of (3.1) and (2.6) to fulfil $\|\varepsilon \mathsf{J}_\varnothing(\lambda)\| < 1$, it suffices to satisfy:

$$\big(\nu_{n-1} - \lambda\big)\big(\nu_n - \lambda\big) = \lambda^2 - 2n\lambda + n^2 - 1/4 > n^2 \varepsilon^4, \qquad \forall\, n \in \mathbb{N}. \tag{3.2}$$

The roots of the equation $\lambda^2 - 2n\lambda + n^2 - 1/4 - n^2\varepsilon^4 = 0$ are given by $\lambda_n^\pm(\varepsilon) = n \pm \sqrt{1/4 + n^2\varepsilon^4}$. Since $\lambda_n^+(\varepsilon) > 1/2$ for all $n \in \mathbb{N}$, the condition (3.2) yields $\lambda_1(\mathsf{H}_\varepsilon) \geq \min\limits_{n \in \mathbb{N}} \lambda_n^-(\varepsilon)$. For $n \in \mathbb{N}$ we have:

$$\lambda_{n+1}^-(\varepsilon) - \lambda_n^-(\varepsilon) = 1 - \frac{(2n+1)\varepsilon^4}{\big(\frac{1}{4} + n^2\varepsilon^4\big)^{1/2} + \big(\frac{1}{4} + (n+1)^2\varepsilon^4\big)^{1/2}} \geq 1 - \frac{(2n+1)\varepsilon^4}{(2n+1)\varepsilon^2} = 1 - \varepsilon^2 > 0.$$

Hence, $\min\limits_{n \in \mathbb{N}} \lambda_n^-(\varepsilon) = \lambda_1^-(\varepsilon)$ and the claim of Theorem 1.2 (i) follows. □

4. The weak coupling regime: $\varepsilon \to 0+$

In this section, we prove Theorem 1.2 (ii) and Theorem 1.5 (ii)–(iii). Intermediate results of this section given in Lemmata 4.1 and 4.3 are of an independent interest.

First, we introduce some auxiliary operators and functions. Let $n \in \mathbb{N}_0$ and the sheet $Z_E \subset \widetilde{Z}$ be fixed. We make use of notation $\mathsf{P}_{kl} := \mathsf{e}_{n+k-2}(\cdot, \mathsf{e}_{n+l-2})$ with $k, l \in \{1,2,3\}$. Note that for $n = 0$ we have $\mathsf{P}_{k1} = \mathsf{P}_{1k} = 0$ for $k = 1,2,3$. It will also be convenient to decompose the Jacobi matrix $\mathsf{J}_E(\lambda)$ in (2.5) as:

$$\mathsf{J}_E(\lambda) = \mathsf{S}_{n,E}(\lambda) + \mathsf{T}_{n,E}(\lambda), \tag{4.1}$$

where the operator-valued functions $\lambda \mapsto \mathsf{T}_{n,E}(\lambda), \mathsf{S}_{n,E}(\lambda)$ are defined by:

$$\mathsf{T}_{n,E}(\lambda) := b^E_{n+1}(\lambda)\left[\mathsf{P}_{23} + \mathsf{P}_{32}\right] + b^E_n(\lambda)\left[\mathsf{P}_{21} + \mathsf{P}_{12}\right], \qquad \mathsf{S}_{n,E}(\lambda) := \mathsf{J}_E(\lambda) - \mathsf{T}_{n,E}(\lambda). \tag{4.2}$$

Clearly, the operator-valued function $\mathsf{S}_{n,E}(\cdot)$ is uniformly bounded on $\mathbb{D}_{1/2}(\nu_n)$. Moreover, for sufficiently small $r = r(n) \in (0, 1/2)$ the bounded operator $\mathsf{I} + \varepsilon\mathsf{S}_{n,E}(\lambda)$ is at the same time boundedly invertible for all $(\varepsilon, \lambda) \in \Omega_r(n) := \mathbb{D}_r \times \mathbb{D}_r(\nu_n)$. Thus, the operator-valued function:

$$\mathsf{R}_{n,E}(\varepsilon, \lambda) := \big(\mathsf{I} + \varepsilon\mathsf{S}_{n,E}(\lambda)\big)^{-1}, \tag{4.3}$$

is well-defined and analytic on $\Omega_r(n)$ and, in particular, $\mathsf{R}_{n,E}(0, \nu_n) = \mathsf{I}$. Furthermore, we introduce auxiliary scalar functions $\Omega_r(n) \ni (\varepsilon, \lambda) \mapsto f^E_{kl}(\varepsilon, \lambda)$ by:

$$f^E_{kl}(\varepsilon, \lambda) := \big(\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{e}_{n+k-2}, \mathsf{e}_{n+l-2}\big), \qquad k, l \in \{1,2,3\}. \tag{4.4}$$

Thanks to $\mathsf{R}_{n,E}(0, \nu_n) = \mathsf{I}$ we have $f^E_{kl}(0, \nu_n) = \delta_{kl}$. Finally, we introduce 3×3 matrix-valued function:

$$\mathbb{D}_r \times \mathbb{D}^{\times}_r(\nu_n) \ni (\varepsilon, \lambda) \mapsto \mathsf{A}_{n,E}(\varepsilon, \lambda) := \big(a^E_{kl}(\varepsilon, \lambda)\big)^{3,3}_{k,l=1} \tag{4.5}$$

with the entries given for $k, l = 1,2,3$ by:

$$a^E_{kl}(\varepsilon, \lambda) := b^E_n(\lambda)\big(f^E_{1k}(\varepsilon, \lambda)\delta_{2l} + f^E_{2k}(\varepsilon, \lambda)\delta_{1l}\big) + b^E_{n+1}(\lambda)\big(f^E_{2k}(\varepsilon, \lambda)\delta_{3l} + f^E_{3k}(\varepsilon, \lambda)\delta_{2l}\big). \tag{4.6}$$

We remark that $\operatorname{rank}\mathsf{A}_{n,E}(\varepsilon, \lambda) \leq 2$ due to linear dependence between the first and the third columns in $\mathsf{A}_{n,E}(\varepsilon, \lambda)$.

In the first lemma, we derive an implicit scalar equation which characterizes those points $\lambda \in \mathbb{C} \setminus [\nu_0, +\infty)$ near ν_n for which the condition $\ker\left(\mathsf{I} + \varepsilon\mathsf{J}_E(\lambda)\right) \neq \{0\}$ is satisfied under additional assumption that $\varepsilon > 0$ is small enough. This equation can be used to characterize the 'true' resonances for H_ε as well as the weakly coupled bound state if $n = 0$ and $E = \varnothing$.

Lemma 4.1. *Let the self-adjoint operator H_ε, $\varepsilon \in (0,1)$, be as in* (1.5)*. Let $n \in \mathbb{N}_0$ and the sheet $Z_E \subset \widetilde{Z}$ be fixed. Let $r = r(n) > 0$ be chosen as above. Then for all $\varepsilon \in (0, r)$ a point $\lambda \in \mathbb{D}_r(\nu_n) \setminus [\nu_0, \infty)$ is a resonance of H_ε on Z_E if, and only if*

$$\det\big(\mathsf{I} + \varepsilon\mathsf{A}_{n,E}(\varepsilon, \lambda)\big) = 0.$$

Proof. Using the decomposition (4.1) of $\mathsf{J}_E(\lambda)$ and the auxiliary operator in (4.3), we find:

$$\dim\ker\left(\mathsf{I} + \varepsilon\mathsf{J}_E(\lambda)\right) = \dim\ker\left(\mathsf{I} + \varepsilon\mathsf{S}_{n,E}(\lambda) + \varepsilon\mathsf{T}_{n,E}(\lambda)\right) = \dim\ker\left(\mathsf{I} + \varepsilon\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right). \tag{4.7}$$

Note that:

$$\operatorname{rank}\left(\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right) \leq \operatorname{rank}\left(\mathsf{T}_{n,E}(\lambda)\right) \leq 3$$

and, hence, using [26, Thm. 3.5 (b)], we get:

$$\dim\ker\left(\mathsf{I} + \varepsilon\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right) \geq 1 \qquad \Longleftrightarrow \qquad \det\left(\mathsf{I} + \varepsilon\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right) = 0. \tag{4.8}$$

For the orthogonal projector $\mathsf{P} := \mathsf{P}_{11} + \mathsf{P}_{22} + \mathsf{P}_{33}$ the identity $\mathsf{T}_{n,E}(\lambda) = \mathsf{T}_{n,E}(\lambda)\mathsf{P}$ is straightforward. Hence, employing [27, IV.1.5] we find:

$$\det\left(\mathsf{I} + \varepsilon\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right) = \det\left(\mathsf{I} + \varepsilon\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\mathsf{P}\right) = \det\left(\mathsf{I} + \varepsilon\mathsf{P}\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\right). \tag{4.9}$$

For $k, l \in \{1,2,3\}$ we can write the following identities:

$$\begin{aligned}
\mathsf{P}_{kk}\mathsf{P}\mathsf{R}_{n,E}(\varepsilon, \lambda)\mathsf{T}_{n,E}(\lambda)\mathsf{P}_{ll} &= \mathsf{P}_{kk}\mathsf{R}_{n,E}(\varepsilon, \lambda)\Big(b^E_n(\lambda)\left[\mathsf{P}_{21} + \mathsf{P}_{12}\right] + b^E_{n+1}(\lambda)\left[\mathsf{P}_{23} + \mathsf{P}_{32}\right]\Big)\mathsf{P}_{ll} \\
&= \mathsf{P}_{kk}\mathsf{R}_{n,E}(\varepsilon, \lambda)\Big(b^E_n(\lambda)\left[\mathsf{P}_{2l}\delta_{1l} + \mathsf{P}_{1l}\delta_{2l}\right] + b^E_{n+1}(\lambda)\left[\mathsf{P}_{2l}\delta_{3l} + \mathsf{P}_{3l}\delta_{2l}\right]\Big) \\
&= \mathsf{P}_{kl}b^E_n(\lambda)\left[f^E_{2k}(\varepsilon, \lambda)\delta_{1l} + f^E_{1k}(\varepsilon, \lambda)\delta_{2l}\right] + \mathsf{P}_{kl}b^E_{n+1}(\lambda)\left[f^E_{2k}(\varepsilon, \lambda)\delta_{3l} + f^E_{3k}(\varepsilon, \lambda)\delta_{2l}\right] \\
&= a^E_{kl}(\varepsilon, \lambda)\mathsf{P}_{kl}
\end{aligned}$$

with f_{kl}^E as in (4.4), and as a result we get

$$\mathsf{PR}_{n,E}(\varepsilon,\lambda)\mathsf{T}_{n,E}(\lambda)=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{kl}^E(\varepsilon,\lambda)\mathsf{P}_{kl},$$

with $a_{kl}^E(\varepsilon,\lambda)$ as in (4.6). Hence, the determinant in (4.9) can be expressed as:

$$\det\left(\mathsf{I}+\varepsilon\mathsf{R}_{n,E}(\varepsilon,\lambda)\mathsf{T}_{n,E}(\lambda)\right)=\det(\mathsf{I}+\varepsilon\mathsf{A}_{n,E}(\varepsilon,\lambda))$$

where on the right-hand side we have the determinant of the 3×3 matrix $\mathsf{I}+\varepsilon\mathsf{A}_{n,E}(\varepsilon,\lambda)$; *cf.* (4.5). The claim of lemma then follows from (4.7), (4.8), and Theorem 2.4. □

In the second lemma, we establish the existence and investigate properties of solutions of the scalar equation in Lemma 4.1. To this aim it is natural to try to apply the *analytic implicit function theorem*. The main obstacle that makes a direct application of the implicit function theorem difficult lies in the fact that $\lambda\mapsto\det(\mathsf{I}+\varepsilon\mathsf{A}_{n,E}(\varepsilon,\lambda))$ is not analytic near ν_n due to the cut on the real axis. We circumvent this obstacle by applying the analytic implicit function theorem to an auxiliary function which is analytic in the disc and has values in different sectors of this disc that are in direct correspondence with the values of $\lambda\mapsto\det(\mathsf{I}+\varepsilon\mathsf{A}_{n,E}(\varepsilon,\lambda))$ on the four different sheets in $\widetilde{Z}$ which are mutually adjacent in a proper way.

Assumption 4.2. *Let $n\in\mathbb{N}_0$ and the sheet $Z_E\subset\widetilde{Z}$ be fixed. Let the sheets Z_F, Z_G and Z_H be such that $Z_E\sim_{n-1}Z_F$, $Z_F\sim_n Z_G$ and $Z_G\sim_{n-1}Z_H$. For $r>0$ let the matrix-valued function $\mathbb{D}_r\times\mathbb{D}_r^\times\ni(\varepsilon,\kappa)\mapsto\mathsf{B}_{n,E}(\varepsilon,\kappa)$ be defined by:*

$$\mathsf{B}_{n,E}(\varepsilon,\kappa):=\begin{cases}\mathsf{A}_{n,E}(\varepsilon,\nu_n-\kappa^4), & \arg\kappa\in\Phi_E:=(-\pi,-\frac{3\pi}{4}]\cup(0,\frac{\pi}{4}],\\ \mathsf{A}_{n,F}(\varepsilon,\nu_n-\kappa^4), & \arg\kappa\in\Phi_F:=(-\frac{3\pi}{4},-\frac{\pi}{2}]\cup(\frac{\pi}{4},\frac{\pi}{2}],\\ \mathsf{A}_{n,G}(\varepsilon,\nu_n-\kappa^4), & \arg\kappa\in\Phi_G:=(-\frac{\pi}{2},-\frac{\pi}{4}]\cup(\frac{\pi}{2},\frac{3\pi}{4}],\\ \mathsf{A}_{n,H}(\varepsilon,\nu_n-\kappa^4), & \arg\kappa\in\Phi_H:=(-\frac{\pi}{4},0]\cup(\frac{3\pi}{4},\pi].\end{cases}$$

Tracing the changes in the characteristic vector along the path $Z_E\sim_{n-1}Z_F\sim_n Z_G\sim_{n-1}Z_H$, one easily verifies that $Z_H\sim_n Z_E$. Thus, $\mathsf{B}_{n,E}$ is analytic on $\mathbb{D}_r\times\mathbb{D}_r^\times$ for sufficiently small $r>0$ which is essentially a consequence of componentwise analyticity in $\mathbb{D}_r$ of vector-valued function:

$$\kappa\mapsto R_\bullet(\nu_n-\kappa^4),\qquad \bullet\in\{E,F,G,H\}\quad\text{for}\quad\arg\kappa\in\Phi_\bullet,$$

where $R_\bullet$ is as in (1.9).

Lemma 4.3. *Let $n\in\mathbb{N}_0$ and the sheet $Z_E\subset\widetilde{Z}$ be fixed. Set $(\mathfrak{p},\mathfrak{q},\mathfrak{r}):=(l_{n-1}^E,l_n^E,l_{n+1}^E)$. Let the matrix-valued function $\mathsf{B}_{n,E}$ be as in Assumption 4.2. Then the implicit scalar equation:*

$$\det\left(\mathsf{I}+\varepsilon\mathsf{B}_{n,E}(\varepsilon,\kappa)\right)=0$$

has exactly two solutions $\kappa_{n,E,j}(\cdot)$ analytic near $\varepsilon=0$ such that $\kappa_{n,E,j}(0)=0$, satisfying $\det(\mathsf{I}+\varepsilon\mathsf{B}_{n,E}(\varepsilon,\kappa_{n,E,j}(\varepsilon)))=0$ pointwise for sufficiently small $\varepsilon>0$, and having asymptotic expansions:

$$\kappa_{n,E,j}(\varepsilon)=\varepsilon\frac{(z_{n,E})_j^{1/2}}{2}+\mathcal{O}(\varepsilon^2),\qquad\varepsilon\to0+,\tag{4.10}$$

where $z_{n,E}=(-1)^{\mathfrak{q}+\mathfrak{r}}(n+1)+(-1)^{\mathfrak{p}+\mathfrak{q}+1}n\mathrm{i}$.

Proof. First, we introduce the shorthand notations:

$$u(\kappa):=b_n^\bullet(\nu_n-\kappa^4),\quad v(\kappa):=b_{n+1}^\bullet(\nu_n-\kappa^4),\qquad\bullet\in\{E,F,G,H\}\quad\text{for}\quad\arg\kappa\in\Phi_\bullet.$$

Let b_{kl} with $k,l\in\{1,2,3\}$ be the entries of the matrix-valued function $\mathsf{B}_{n,E}$. Furthermore, we define the scalar functions $X=X(\varepsilon,\kappa)$, $Y=Y(\varepsilon,\kappa)$, and $Z=Z(\varepsilon,\kappa)$ by:

$$\begin{aligned}X&:=b_{11}+b_{22}+b_{33},\\ Y&:=b_{11}b_{22}+b_{22}b_{33}+b_{11}b_{33}-b_{13}b_{31}-b_{12}b_{21}-b_{23}b_{32},\\ Z&:=b_{11}b_{22}b_{33}+b_{13}b_{32}b_{21}+b_{12}b_{23}b_{31}-b_{13}b_{31}b_{22}-b_{12}b_{21}b_{33}-b_{11}b_{23}b_{32}.\end{aligned}\tag{4.11}$$

Employing an elementary formula for the determinant of 3×3 matrix, the equation $\det(\mathsf{I}+\varepsilon\mathsf{B}_{n,E}(\varepsilon,\kappa))=0$ can be equivalently written as:

$$1+\varepsilon X(\varepsilon,\kappa)+\varepsilon^2Y(\varepsilon,\kappa)+\varepsilon^3Z(\varepsilon,\kappa)=0.\tag{4.12}$$

By a purely algebraic argument, one can derive from (4.6) that $Z = 0$. Hence, (4.12) simplifies to $1 + \varepsilon X(\varepsilon, \kappa) + \varepsilon^2 Y(\varepsilon, \kappa) = 0$. Introducing new parameter $t := \varepsilon/\kappa$, we can further rewrite this equation as:

$$1 + t\kappa X(\varepsilon, \kappa) + t^2 \kappa^2 Y(\varepsilon, \kappa) = 0. \tag{4.13}$$

Note also that the coefficients $(\varepsilon, \kappa) \mapsto \kappa X(\varepsilon, \kappa), \kappa^2 Y(\varepsilon, \kappa)$ of the quadratic equation (4.13) are analytic in $\mathbb{D}_r^2$. For each fixed pair (ε, κ) the equation (4.13) has (in general) two distinct roots $t_j(\varepsilon, \kappa)$, $j = 0, 1$. The condition $\det(\mathsf{I} + \varepsilon \mathsf{B}_{n,E}(\varepsilon, \kappa)) = 0$ with $\kappa \neq 0$ holds *if, and only if* at least one of the two conditions:

$$f_j(\varepsilon, \kappa) := \varepsilon - \kappa t_j(\varepsilon, \kappa) = 0, \qquad j = 0, 1, \tag{4.14}$$

is satisfied. Using analyticity of $u(\cdot)$ and $v(\cdot)$ near $\kappa = 0$, we compute:

$$\lim_{\kappa\to 0} \kappa u = \lim_{r\to 0+} re^{\mathrm{i}\pi/8} u(re^{\mathrm{i}\pi/8}) = \lim_{r\to 0+} \frac{n^{1/2}}{2} \frac{re^{\mathrm{i}\pi/8}}{((-1+\mathrm{i}r^4)_{\mathfrak{p}}^{1/2} (\mathrm{i}r^4)_{\mathfrak{q}}^{1/2})^{1/2}} = \frac{n^{1/2} e^{\mathrm{i}\pi/8}}{2((-1)^{\mathfrak{p}+\mathfrak{q}} \mathrm{i} e^{\mathrm{i}\pi/4})^{1/2}},$$

$$\lim_{\kappa\to 0} \kappa v = \lim_{r\to 0+} re^{\mathrm{i}\pi/8} v(re^{\mathrm{i}\pi/8}) = \lim_{r\to 0+} \frac{(n+1)^{1/2}}{2} \frac{re^{\mathrm{i}\pi/8}}{((\mathrm{i}r^4)_{\mathfrak{q}}^{1/2} (1+\mathrm{i}r^4)_{\mathfrak{r}}^{1/2})^{1/2}} = \frac{(n+1)^{1/2} e^{\mathrm{i}\pi/8}}{2((-1)^{\mathfrak{q}+\mathfrak{r}} e^{\mathrm{i}\pi/4})^{1/2}}.$$

Hence, we get:

$$\begin{aligned}
\lim_{\varepsilon,r\to 0+} re^{\mathrm{i}\pi/8} b_{kl}(\varepsilon, re^{\mathrm{i}\pi/8}) &= \lim_{r\to 0+} re^{\mathrm{i}\pi/8} u(re^{\mathrm{i}\pi/8}) \big(f_{2k}^E(\mathbf{0}) \delta_{3l} + f_{3k}^E(\mathbf{0}) \delta_{2l} \big) \\
&\quad + \lim_{r\to 0+} re^{\mathrm{i}\pi/8} v(re^{\mathrm{i}\pi/8}) \big(f_{1k}^E(\mathbf{0}) \delta_{2l} + f_{2k}^E(\mathbf{0}) \delta_{1l} \big) \\
&= \frac{n^{1/2} e^{\mathrm{i}\pi/8} \big(\delta_{2k}\delta_{3l} + \delta_{3k}\delta_{2l} \big)}{2((-1)^{\mathfrak{p}+\mathfrak{q}} \mathrm{i} e^{\mathrm{i}\pi/4})^{1/2}} + \frac{(n+1)^{1/2} e^{\mathrm{i}\pi/8} \big(\delta_{1k}\delta_{2l} + \delta_{2k}\delta_{1l} \big)}{2((-1)^{\mathfrak{q}+\mathfrak{r}} e^{\mathrm{i}\pi/4})^{1/2}}.
\end{aligned}$$

Combining this with (4.11) we end up with:

$$\begin{aligned}
\lim_{(\varepsilon,\kappa)\to\mathbf{0}} \kappa X &= \lim_{\varepsilon,r\to 0+} re^{\mathrm{i}\pi/8} X(\varepsilon, re^{\mathrm{i}\pi/8}) = \lim_{\varepsilon,r\to 0+} re^{\mathrm{i}\pi/8} \big[b_{11} + b_{22} + b_{33} \big](\varepsilon, re^{\mathrm{i}\pi/8}) = 0, \\
\lim_{(\varepsilon,\kappa)\to\mathbf{0}} \kappa^2 Y &= \lim_{\varepsilon,r\to 0+} r^2 e^{\mathrm{i}\pi/4} Y(\varepsilon, re^{\mathrm{i}\pi/8}) \\
&= \lim_{\varepsilon,r\to 0+} r^2 e^{\mathrm{i}\pi/4} \big[b_{11}b_{22} + b_{22}b_{33} + b_{11}b_{33} - b_{13}b_{31} - b_{12}b_{21} - b_{23}b_{32} \big](\varepsilon, re^{\mathrm{i}\pi/8}) \\
&= \lim_{\varepsilon,r\to 0+} r^2 e^{\mathrm{i}\pi/4} \big[- b_{12}b_{21} - b_{23}b_{32} \big](\varepsilon, re^{\mathrm{i}\pi/8}) \\
&= - \left(\frac{n^{1/2} e^{\mathrm{i}\pi/8}}{2((-1)^{\mathfrak{p}+\mathfrak{q}} \mathrm{i} e^{\mathrm{i}\pi/4})^{1/2}} \right)^2 - \left(\frac{(n+1)^{1/2} e^{\mathrm{i}\pi/8}}{2((-1)^{\mathfrak{q}+\mathfrak{r}} e^{\mathrm{i}\pi/4})^{1/2}} \right)^2 \\
&= - \frac{(-1)^{\mathfrak{p}+\mathfrak{q}+1} n \mathrm{i}}{4} - \frac{(-1)^{\mathfrak{q}+\mathfrak{r}} (n+1)}{4} = - \frac{z_{n,E}}{4}.
\end{aligned}$$

Hence, the roots $t_j(\varepsilon, \kappa)$ of (4.13) converge in the limit $(\varepsilon, \kappa) \to \mathbf{0}$ to the roots $2\big[(z_{n,E})_j^{1/2}\big]^{-1}$, $j = 0, 1$, of the quadratic equation $z_{n,E} t^2 - 4 = 0$. Moreover, analyticity of the coefficients in equation (4.13), the above limits, and the formula for the roots of a quadratic equation imply analyticity of the functions $(\varepsilon, \kappa) \mapsto t_j(\varepsilon, \kappa)$ near $\mathbf{0}$.

Step 2. The partial derivatives of f_j in (4.14) with respect to ε and κ are given by $\partial_\varepsilon f_j = 1 - \kappa \partial_\varepsilon t_j$ and $\partial_\kappa f_j = -t_j - \kappa \partial_\kappa t_j$. Analyticity of t_j near $\mathbf{0}$ implies $(\partial_\varepsilon f_j)(\mathbf{0}) = 1$ and $(\partial_\kappa f_j)(\mathbf{0}) = -t_j$. In particular, we have shown that $(\partial_\kappa f_j)(\mathbf{0}) \neq 0$. Since the functions $f_j(\cdot)$ are analytic near $\mathbf{0}$ and satisfy $f_j(\mathbf{0}) = 0$, we can apply the analytic implicit function theorem [25, Thm. 3.4.2] which yields existence of a unique function $\kappa_j(\cdot)$, analytic near $\varepsilon = 0$ such that $\kappa_j(0) = 0$ and that $f_j(\varepsilon, \kappa_j(\varepsilon)) = 0$ holds pointwise. Moreover, the derivative of κ_j at $\varepsilon = 0$ can be expressed as:

$$\kappa_j'(0) = - \frac{(\partial_\varepsilon f_j)(\mathbf{0})}{(\partial_\kappa f_j)(\mathbf{0})} = \frac{1}{t_j(\mathbf{0})}. \tag{4.15}$$

Hence, we obtain Taylor expansion for κ_j near $\varepsilon = 0$:

$$\kappa_j(\varepsilon) = \kappa_j(0) + \kappa_j'(0)\varepsilon + \mathcal{O}(\varepsilon^2) = \frac{\varepsilon}{t_j(\mathbf{0})} + \mathcal{O}(\varepsilon^2) = \varepsilon \frac{(z_{n,E})_j^{1/2}}{2} + \mathcal{O}(\varepsilon^2) \qquad \varepsilon \to 0+ .$$

The functions κ_j, $j = 0, 1$, satisfy all the requirements in the claim of the lemma. □

Now we are prepared to prove Theorem 1.2 (ii) and Theorem 1.5 (ii)–(iii) from the introduction.

Proof of Theorem 1.2 (ii). By Proposition 1.1 (iv) we have $\mathcal{N}_{1/2}(\mathsf{H}_\varepsilon) = 1$ for all sufficiently small $\varepsilon > 0$. Recall that we denote by $\lambda_1(\mathsf{H}_\varepsilon)$ the corresponding unique eigenvalue. Thus, we have by Lemma 4.1:

$$\det(\mathsf{I} + \varepsilon \mathsf{A}_{0,\varnothing}(\varepsilon, \lambda_1(\mathsf{H}_\varepsilon))) = 0.$$

Using the construction of Assumption 4.2 for the physical sheet and $n = 0$, we obtain

$$\det(\mathsf{I} + \varepsilon \mathsf{B}_{0,\varnothing}(\varepsilon, (\nu_0 - \lambda_1(\mathsf{H}_\varepsilon))^{1/4})) = \det(\mathsf{I} + \varepsilon \mathsf{A}_{0,\varnothing}(\varepsilon, \lambda_1(\mathsf{H}_\varepsilon))) = 0,$$

where we have chosen the principal branch for $(\cdot)^{1/4}$. Thus, by Lemma 4.3, we get:

$$(\nu_0 - \lambda_1(\mathsf{H}_\varepsilon))^{1/4} = \frac{\varepsilon}{2} + \mathcal{O}(\varepsilon^2), \qquad \varepsilon \to 0+,$$

where we have used the fact that $z_{0,\varnothing} = 1$. Hence, taking the fourth power of the left and right hand sides in the above equation we arrive at:

$$\lambda_1(\mathsf{H}_\varepsilon) = \nu_0 - \frac{\varepsilon^4}{16} + \mathcal{O}(\varepsilon^5), \qquad \varepsilon \to 0 + . \qquad \square$$

Proof of Theorem 1.5 (ii)–(iii). Let $n \in \mathbb{N}$ and the sheet $Z_E \subset \widetilde{Z}$ be fixed. Let us repeat the construction of Assumption 4.2. By Lemma 4.3 we infer that there exist exactly two analytic solutions $\kappa_{n,E,j}$, $j = 0, 1$ of the implicit scalar equation $\det(\mathsf{I} + \varepsilon \mathsf{B}_{n,E}(\varepsilon, \kappa)) = 0$ such that $\kappa_{n,E,j}(0) = 0$. It can be checked that both solutions correspond to the same resonance and it suffices to analyze the solution $\kappa_{n,E} := \kappa_{n,E,0}$ only.

For all small enough $\varepsilon > 0$ the asymptotics (4.10) yields:

$$\arg(\kappa_{n,E}(\varepsilon)) = \frac{1}{2}\arg(z_{n,E}) \in \Phi_E, \quad \textit{if, and only if} \quad n \in \mathcal{S}(E).$$

Hence, if $n \in \mathbb{N} \setminus \mathcal{S}(E)$, Lemmata 4.1 and 4.3 imply that there will be no resonances in the vicinity of the point $\lambda = \nu_n$ lying on Z_E^- for sufficiently small $\varepsilon > 0$. Thus, we have proven Theorem 1.5 (iii). While if $n \in \mathcal{S}(E)$ we get by Lemmata 4.1 and 4.3 that there will be exactly one resonance

$$\lambda_n^E(\mathsf{H}_\varepsilon) = \nu_n - (\kappa_{n,E}(\varepsilon))^4,$$

in the vicinity of the point $\lambda = \nu_n$ lying on Z_E^- for sufficiently small $\varepsilon > 0$ and its asymptotic expansion is a direct consequence of the asymptotic expansion (4.10) given in Lemma 4.3. Thus, the claim of Theorem 1.5 (ii) follows. $\square$

APPENDIX

A. Krein's formula, meromorphic continuation of resolvent, and condition on resonances

In this appendix, we use Krein's resolvent formula for Smilansky Hamiltonian to prove Proposition 1.3 and Theorem 2.4 on meromorphic continuation of $(\mathsf{H}_\varepsilon - \lambda)^{-1}$ to $\widetilde{Z}$. The proposed continuation procedure is of an iterative nature wherein, we first extend $(\mathsf{H}_\varepsilon - \lambda)^{-1}$ to the sheets adjacent to the physical sheet, then to the sheets which are adjacent to the sheets being adjacent to the physical sheet and so on.

To this aim, we define for $n \in \mathbb{N}_0$ the scalar functions $\mathbb{C}\setminus[\nu_0, +\infty) \mapsto y_n(\lambda)$ and $(\mathbb{C}\setminus[\nu_0, +\infty))\times\mathbb{R} \mapsto \eta_n(\lambda; x)$ by:

$$y_n(\lambda) := r_n(\lambda)\sqrt{\nu_n}, \qquad \eta_n(\lambda; x) := \nu_n^{1/4}\exp(-r_n(\lambda)|x|), \tag{A.1}$$

where $r_n(\cdot)$, $n \in \mathbb{N}_0$, is as in (1.7). Next, we introduce the following operator-valued function:

$$\mathsf{T}(\lambda)\colon \ell^2(\mathbb{N}_0) \to \mathcal{H}, \qquad \mathsf{T}(\lambda)\{c_n\} := \{c_n\eta_n(\lambda; x)\}.$$

For each fixed $\lambda \in \mathbb{C} \setminus [\nu_0, +\infty)$ the operator $\mathsf{T}(\lambda)$ is bounded and everywhere defined and the adjoint of $\mathsf{T}(\overline{\lambda})$ acts as:

$$\mathsf{T}(\overline{\lambda})^*\{u_n\} \sim \{I_n(\lambda; u_n)\}_{n\in\mathbb{N}_0}, \qquad I_n(\lambda; u) := \int_{\mathbb{R}} \eta_n(\lambda; x)u(x)\mathrm{d}x.$$

With these preparations, the resolvent difference of H_ε and H_0 can be expressed by [7, Thm. 6.1] (see also [4, Sec. 6]) as follows:

$$(\mathsf{H}_\varepsilon - \lambda)^{-1} = (\mathsf{H}_0 - \lambda)^{-1} + \mathsf{T}(\lambda)\mathsf{Y}(\lambda)\big[\big(\mathsf{I} + \varepsilon\mathsf{J}_\varnothing(\lambda)\big)^{-1} - \mathsf{I}\big]\mathsf{Y}(\lambda)\mathsf{T}(\overline{\lambda})^*, \quad \lambda \in \mathbb{C} \setminus [\nu_0, +\infty), \tag{A.2}$$

where H_0 is the Smilansky Hamiltonian with $\varepsilon = 0$, $\mathsf{Y}(\lambda) = \operatorname{diag}\{(2y_n(\lambda))^{-1/2}\}$ and $\mathsf{J}_\varnothing(\lambda)$ is as in (2.5). The formula (A.2) can be viewed as a particular case of abstract Krein's formula (see *e.g.* [29–31]) for the resolvent difference of two self-adjoint extensions of their common densely defined symmetric restriction.

Proof of Proposition 1.3 and Theorem 2.4. Let us fix $n \in \mathbb{N}_0$ and a sheet $Z_E \subset \widetilde{Z}$. We denote by $\mathsf{R}_n(\lambda)$ the resolvent of the self-adjoint operator $H^2(\mathbb{R}) \ni f \mapsto -f'' + \nu_n f$ in the Hilbert space $L^2(\mathbb{R})$. We can express the function $\mathfrak{r}^{\varnothing}_{n,\varepsilon}(\cdot\,; u)$ in (1.13) using Krein's formula (A.2) as:

$$\begin{aligned}
\mathfrak{r}^{\varnothing}_{n,\varepsilon}(\lambda; u) &= \big\langle (\mathsf{H}_\varepsilon - \lambda)^{-1} u \otimes \mathsf{e}_n, u \otimes \mathsf{e}_n \big\rangle \\
&= \big\langle (\mathsf{H}_0 - \lambda)^{-1} u \otimes \mathsf{e}_n, u \otimes \mathsf{e}_n \big\rangle + \Big(\mathsf{Y}(\lambda) \Big[\big(\mathsf{I} + \varepsilon \mathsf{J}_{\varnothing}(\lambda)\big)^{-1} - \mathsf{I} \Big] \mathsf{Y}(\lambda) \mathsf{T}(\overline{\lambda})^* u \otimes \mathsf{e}_n, \mathsf{T}(\lambda)^* u \otimes \mathsf{e}_n \Big) \\
&= (\mathsf{R}_n(\lambda) u, u)_{\mathbb{R}} + I_n(\lambda; u) \overline{I_n(\overline{\lambda}; u)} \Big(\big[\big(\mathsf{I} + \varepsilon \mathsf{J}_{\varnothing}(\lambda)\big)^{-1} - \mathsf{I} \big] \mathsf{Y}(\lambda) \mathsf{e}_n, \mathsf{Y}(\lambda)^* \mathsf{e}_n \Big) \\
&= (\mathsf{R}_n(\lambda) u, u)_{\mathbb{R}} + \frac{I_n(\lambda; u) I_n(\lambda; \overline{u})}{2 y_n(\lambda)} \Big[\Big(\big(\mathsf{I} + \varepsilon \mathsf{J}_{\varnothing}(\lambda)\big)^{-1} \mathsf{e}_n, \mathsf{e}_n \Big) - 1 \Big].
\end{aligned}$$

Since $(\mathsf{R}_n(\lambda) u, u)_{\mathbb{R}}$, $y_n(\lambda)$, $I_n(\lambda; u)$, and $I_n(\lambda; \overline{u})$ can be easily analytically continued to $\widetilde{Z}$, to extend $\mathfrak{r}^{\varnothing}_{n,\varepsilon}(\cdot\,; u)$ meromorphically to the other sheets of the component $\widetilde{Z}$ it suffices to extend:

$$\mathfrak{s}^{\varnothing}_{n,\varepsilon}(\lambda) := \Big(\big(\mathsf{I} + \varepsilon \mathsf{J}_{\varnothing}(\lambda)\big)^{-1} \mathsf{e}_n, \mathsf{e}_n \Big),$$

meromorphically from $Z_{\varnothing}$ to $\widetilde{Z}$. The poles of the meromorphic extension of $\mathfrak{s}^{\varnothing}_{n,\varepsilon}(\cdot)$ can be identified with the resonances of H_ε in the sense of Definition 1.4.

To this aim, we set by definition:

$$\mathfrak{s}^{E}_{n,\varepsilon}(\lambda) := \Big(\big(\mathsf{I} + \varepsilon \mathsf{J}_{E}(\lambda)\big)^{-1} \mathsf{e}_n, \mathsf{e}_n \Big),$$

for any $\lambda \in \mathbb{C} \setminus [\nu_0, +\infty)$ such that $-1 \notin \sigma(\varepsilon \mathsf{J}_E(\lambda))$. In what follows, we let Z_E and Z_F be two sheets of $\widetilde{Z}$ such that $Z_E \sim_{n-1} Z_F$ with $n \in \mathbb{N}_0$[4]. Suppose that $\lambda \mapsto \mathfrak{s}^{E}_{n,\varepsilon}(\cdot)$ is well defined and meromorphic either on Z_E^+ or on Z_E^-. Next, we extend $\lambda \mapsto \mathfrak{s}^{E}_{n,\varepsilon}(\cdot)$ meromorphically from $Z_E^{\pm}$ to $Z_F^{\mp}$. Without loss of generality, we restrict our attention to the case that $\lambda \mapsto \mathfrak{s}^{E}_{n,\varepsilon}(\cdot)$ is meromorphic on Z_E^+ and extend it meromorphically to Z_F^-. On the open set $\Omega_n := \mathbb{C}_+ \cup \mathbb{C}_- \cup (\nu_{n-1}, \nu_n)$, the operator-valued function:

$$\mathsf{J}_{EF}(\lambda) := \begin{cases} \mathsf{J}_E(\lambda), & \lambda \in \mathbb{C}_+, \\ \mathsf{J}_F(\lambda), & \lambda \in \Omega_n \setminus \mathbb{C}_+, \end{cases}$$

is analytic which is essentially a consequence of analyticity on Ω_n of the entries $b^{\bullet}_m(\lambda)$ (with $\bullet = E$ for $\lambda \in \mathbb{C}_+$ and $\bullet = F$ for $\lambda \in \mathbb{C}_-$) for the underlying Jacobi matrix. Thus, the operator-valued function:

$$\Omega_n \ni \lambda \mapsto \mathsf{A}^{EF}_{\varepsilon}(\lambda) := \varepsilon \, (\mathsf{I} + \varepsilon \mathsf{J}_0)^{-1} \, (\mathsf{J}_{EF}(\lambda) - \mathsf{J}_0)$$

is also analytic on Ω_n because of the analyticity of $\mathsf{J}_{EF}(\lambda)$. Furthermore, the values of $\mathsf{A}^{EF}_{\varepsilon}(\cdot)$ are compact operators thanks to compactness of the difference $\mathsf{J}_{EF}(\lambda) - \mathsf{J}_0$. Taking into account that:

$$\Big(\big(\mathsf{I} + \mathsf{A}^{EF}_{\varepsilon}(\lambda)\big)^{-1} \mathsf{e}_n, (\mathsf{I} + \varepsilon \mathsf{J}_0)^{-1} \mathsf{e}_n \Big) = \begin{cases} \mathfrak{s}^{E}_{n,\varepsilon}(\lambda), & \lambda \in \mathbb{C}_+, \\ \mathfrak{s}^{F}_{n,\varepsilon}(\lambda), & \lambda \in \Omega_n \setminus \mathbb{C}_+, \end{cases}$$

we obtain from the analytic Fredholm theorem [28, Thm. VI.14] that $\mathbb{C}_- \ni \lambda \mapsto \mathfrak{s}^{F}_{n,\varepsilon}(\lambda)$ is a meromorphic continuation of $\mathbb{C}_+ \ni \lambda \mapsto \mathfrak{s}^{E}_{n,\varepsilon}(\lambda)$ across the interval (ν_{n-1}, ν_n) and that the poles of $\mathbb{C}_- \ni \lambda \mapsto \mathfrak{s}^{F}_{n,\varepsilon}(\lambda)$ satisfy the condition:

$$\ker \, (\mathsf{I} + \varepsilon \mathsf{J}_F(\lambda)) \neq \{0\}, \qquad \lambda \in \mathbb{C}_-.$$

Starting from the physical sheet $Z_{\varnothing}$, we use the above procedure iteratively to extend $\mathfrak{s}^{\varnothing}_{n,\varepsilon}(\cdot)$ meromorphically to the whole of $\widetilde{Z}$ thus proving Proposition 1.3 and Theorem 2.4. □

Acknowledgements

This research was supported by the Czech Science Foundation (GAČR) within the project 14-06818S.

[4]Recall that for any sheet Z_E holds $Z_E \sim_{-1} Z_E$.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 803–815

Spectral properties of a symmetric three-dimensional quantum dot with a pair of identical attractive δ-impurities symmetrically situated around the origin II

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PACS 02.30.Gp, 02.30.Hq, 02.30.Hq, 02.30.Lt, 02.30.Sa, 02.30.Tb, 03.65.Db, 03.65.Ge, 68.65.Hb

DOI 10.17586/2220-8054-2016-7-5-803-815

In this note, we continue our analysis (started in [1]) of the isotropic three-dimensional harmonic oscillator perturbed by a pair of identical attractive point interactions symmetrically situated with respect to the origin, that is to say, the mathematical model describing a symmetric quantum dot with a pair of point impurities. In particular, by making the coupling constant (to be renormalized) dependent also upon the separation distance between the two impurities, we prove that it is possible to rigorously define the unique self-adjoint Hamiltonian that, differently from the one introduced in [1], behaves smoothly as the separation distance between the impurities shrinks to zero. In fact, we rigorously prove that the Hamiltonian introduced in this note converges in the norm-resolvent sense to that of the isotropic three-dimensional harmonic oscillator perturbed by a single attractive point interaction situated at the origin having double strength, thus making this three-dimensional model more similar to its one-dimensional analog (not requiring the renormalization procedure) as well as to the three-dimensional model involving impurities given by potentials whose range may even be physically very short but different from zero. Moreover, we show the manifestation of the Zeldovich effect, known also as level rearrangement, in the model investigated herewith. More precisely, we take advantage of our renormalization procedure to demonstrate the possibility of using the concept of 'Zeldovich spiral', introduced in the case of perturbations given by rapidly decaying potentials, also in the case of point perturbations.

Keywords: level crossing, degeneracy, point interactions, renormalisation, Schrödinger operators, quantum dots, perturbed quantum oscillators, Zeldovich effect, level rearrangement.

Received: 27 June 2016

Revised: 25 July 2016

1. Introduction

The main purpose of this note is to extend the results of [1] by fixing the problematic behavior of the Hamiltonian $H_{\{\beta,\vec{x}_0\}}$ studied therein in the limit $x_0 = |\pm\vec{x}_0| \to 0_+$, that is to say as the distance between the two twin point perturbations shrinks to zero. As was noticed in [1], the Hamiltonian $H_{\{\beta,\vec{x}_0\}}$, the self-adjoint energy operator of the three-dimensional isotropic harmonic oscillator perturbed by a pair of identical point interactions symmetrically situated around the origin defined rigorously by means of a 'coupling constant renormalization', does not converge to $H_{2\beta}$, the one of the three-dimensional isotropic harmonic oscillator perturbed by a single point interaction situated at the origin having double strength. Such a singular behavior manifested by singular double wells with point interactions in three dimensions is in sharp contrast with conventional double wells generated by potentials, whose range may even be very short but non-zero. By citing [1] it is important to recall that *'as is well known to Quantum Chemistry students, three-dimensional interactions with a nonzero range do not manifest this singular behavior in the limit of the distance between the two centers shrinking to zero, as the classical textbook example of* H_2^+ *smoothly approaching* He^+ *in the limit* $R \to 0_+$ *clearly shows'* (see [2–4]). The same phenomenon had been observed in [5] (see also [6–10]) dealing with another model involving a pair of identical point interactions symmetrically situated around the origin defined rigorously by using a 'coupling constant renormalization' as well, namely the one-dimensional energy operator in which the kinetic component is given by the Salpeter free Hamiltonian $\sqrt{p^2+m^2}$, $m > 0$.

As was fully proved in [10], this singular behavior does not occur in the one-dimensional analog of the model given that the Dirac distribution is an infinitesimally small perturbation of the Laplacian in one dimension, which

implies that the renormalization procedure is not required at all in that case to define a self-adjoint Hamiltonian (obtained instead by means of the KLMN theorem, see [11]).

Here, in the next section, we adopt the same strategy used in [5] to regularize the behavior in the limit $x_0 \to 0_+$: we make the coupling constant to be renormalized dependent also on x_0, in addition to the two standard parameters, namely the positive integer labeling the ultraviolet energy cut-off and the real number whose reciprocal represents the extension parameter (see [5–7]). The new self-adjoint Hamiltonian $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, clearly dependent on x_0 and obtained as the norm resolvent limit after removing the energy cut-off (Theorem 2.1), is shown to approach smoothly $H_{2\beta}$ in the norm resolvent limit as $x_0 \to 0_+$ (Theorem 2.2). We would like to stress that, although this is exactly the strategy employed also in papers such as [12–14] to obtain the self-adjoint operator with the δ'-interaction perturbing either the negative Laplacian or the Hamiltonian of the harmonic oscillator in one dimension as the norm resolvent limit of Hamiltonians with the perturbation consisting of a triple of δ-interactions, the dependence on x_0 is completely different.

We also carry out the detailed spectral analysis of the lowest lying eigenvalues of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ as functions of α, the parameter labeling the self-adjoint extensions. Although the analysis could be extended to higher eigenvalues at the conceptual level, we have decided to restrict our investigation because of its increasing operational complexity (the same restriction had also been adopted in [1, 8–10, 15, 16]). The latter analysis shows that the spectrum of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, similarly to that of the operator $H_{\{\beta,\vec{x}_0\}}$ investigated in [1], exhibits the rather remarkable phenomenon of having a range of values of the parameter where the $2S$ state is more tightly bound than the $2P$ one.

In the third section, we revisit the spectral analysis of the lowest lying eigenvalues by regarding them as functions of β, the parameter appearing explicitly in the coupling constant to be renormalized. Our main motivation for this further analysis has been the fact that, following [17], the latter parameter is the conventional one used to study the manifestation of the Zeldovich effect (see [18]), widely known also as level rearrangement. We are going to show that the phenomenon, studied by the authors of that article when the perturbation of the three-dimensional isotropic harmonic oscillator is represented by a potential whose range is physically very short but different from zero, does manifest itself also in the case of point perturbations. In particular, it is our intention to demonstrate that the structure of the discrete spectrum of operators like $H_{2\beta}$ and $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ can be better understood by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R}\times S^1$, with E, the energy parameter, drawn along the real line (the symmetry axis of the cylinder) and the extension parameter along the unit circle identifying $\pm\infty$, instead of the traditional $\mathbb{R}^2$. This alternative representation was first introduced in [19], in which the rather intriguing concept of 'Zeldovich spiral' was proposed investigating the 3D-isotropic harmonic oscillator perturbed by three rapidly decaying potentials, even though their plots are of the type E vs. $\alpha = 1/\beta$. In the third section of the current note, we will show that, as a result of our renormalization procedure (which is different from the one adopted in [20] and leads to the spectral requirement $E_0(\alpha = 0, x_0) = 0 = E_0(\beta = +\infty, x_0)$ for the ground state energy of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$), the Zeldovich spiral can also be visualized in the case of point perturbations of the three-dimensional isotropic harmonic oscillator directly on plots of the type E vs. β.

Finally, in the last section we review the key results of this note and outline prospective avenues of further research work.

2. The regularized three-dimensional isotropic harmonic oscillator perturbed by two twin attractive point perturbations symmetrically situated with respect to the origin

Given that all the steps preceding the introduction of the coupling constant are identical to those from (3.1) up to (3.10) in [1], we omit them here and refer the reader to that paper. As anticipated earlier and following the strategy used in [5], the coupling constant will be made dependent on the magnitude of the position vectors of the twin point impurities, namely $x_0 = |\pm\vec{x}_0|$, $x_0 = (x_0, 0, 0)$, $x_0 > 0$, as follows:

$$\frac{1}{\mu(\ell,\beta;x_0)} = \frac{1}{\beta} + 2\sum_{|\vec{n}|=0}^{\ell}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}}, \tag{2.1}$$

or equivalently

$$\mu(\ell,\beta;x_0) = \beta\left[1 + 2\beta\sum_{|\vec{n}|=0}^{\ell}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}}\right]^{-1} \tag{2.1b}$$

with $\beta \in \mathbb{R}^3\backslash\{0\}$.

In perfect accordance with the use of the term 'attractive' in [1, 5, 8, 9], it is clear that $\mu(\ell,\beta;x_0) > 0$ for the large values of ℓ involved in the limit $\ell \to +\infty$ regardless of the sign of β, making the singular interaction attractive because of the presence of the negative sign in the second term in (3.2) in [1].

Hence, for any $E < 3/2$:

$$\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_s^{-1}(\vec{x}_0,\vec{x}_0) = \frac{1}{2\beta} + \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}-E} \tag{2.2}$$

and

$$\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\vec{x}_0) = \frac{1}{2\beta} + \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\psi(x_0)_{2n_1+1}^2\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1+2n_2+2n_3+\frac{5}{2}-E}. \tag{2.3}$$

Therefore, we need only mimic what was done in [1] to get that, after removing the ultraviolet cut-off, i.e. in the limit $\ell \to +\infty$, the norm resolvent limit of our net of Hamiltonians

$$\begin{aligned}\left(\mathrm{H}_{\{\ell,\beta,\vec{x}_0\}} - E\right)^{-1} &= (H_0-E)^{-1} \\ &+ \frac{1}{\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_s^{-1}(\vec{x}_0,\vec{x}_0)} \left|(H_0^\ell - E)_s^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0^\ell - E)_s^{-1}(\vec{x}_0,\cdot)\right| \\ &+ \frac{1}{\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\vec{x}_0)} \left|(H_0^\ell - E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\cdot)\right|\end{aligned} \tag{2.4}$$

is given by:

$$\begin{aligned}&(H_0-E)^{-1} + \frac{\left|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta} + \lim\limits_{\ell\to+\infty}\left[\sum\limits_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum\limits_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}-E}\right]} \\ &\quad + \frac{\left|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta} + \lim\limits_{\ell\to+\infty}\left[\sum\limits_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum\limits_{|\vec{n}|=0}^{\ell}\frac{\psi(x_0)_{2n_1+1}^2\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1+2n_2+2n_3+\frac{5}{2}-E}\right]} \\ &\quad = (H_0-E)^{-1} + \frac{\left|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta} - E\sum\limits_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}} \\ &\quad\quad + \frac{\left|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta} + \lim\limits_{\ell\to+\infty}\left[\sum\limits_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum\limits_{|\vec{n}|=0}^{\ell}\frac{\psi(x_0)_{2n_1+1}^2\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1+2n_2+2n_3+\frac{5}{2}-E}\right]}.\end{aligned} \tag{2.5}$$

As can be immediately noticed, the series in the denominator of the second term on the right hand side is convergent for any fixed $x_0 > 0$ and any $E < 3/2$ as an easy consequence of an estimate similar to (3.8) in [1] (see also (2.2) in [9]).

We can also analyze the limits appearing in both denominators in (2.5) by means of a suitable modification of the method used in [1] (essentially based on the properties of the semigroup of the three-dimensional harmonic oscillator, as seen in [1, 9, 20]). In fact, for any $E < 3/2$, the limit in the first denominator of (2.5) is given by:

$$\begin{aligned}-E\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)} &= \lim_{\ell\to+\infty}\left[\sum_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}-E}\right] = \\ &\frac{1}{2\pi^{3/2}}\left[\int_0^1 \frac{\xi^{\frac{1}{2}}}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right] = \\ &\frac{1}{2\pi^{3/2}}\int_0^1 \frac{(\xi^{\frac{1}{2}} - \xi^{\frac{1}{2}-E})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi < \infty.\end{aligned} \tag{2.6}$$

The second one, well defined even for any $E < 5/2$, is instead equal to:

$$\frac{1}{2\pi^{3/2}}\left[\int_0^1 \frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right] < \infty. \tag{2.7}$$

Hence, for any $E < 3/2$, the norm limit of the resolvents for $\ell \to +\infty$ (i.e after removing the ultraviolet cut-off) can be written as:

$$\begin{aligned}(H_0-E)^{-1} &+ \frac{\left|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta}+\frac{1}{2\pi^{3/2}}\int_0^1 \frac{(\xi^{\frac{1}{2}}-\xi^{\frac{1}{2}-E})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi} \\ &+ \frac{\left|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta}+\frac{1}{2\pi^{3/2}}\left[\int_0^1 \frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right]}.\end{aligned} \tag{2.8}$$

The final part of the proof meant to show that the limiting operator (2.8) is indeed the resolvent of a self-adjoint operator is omitted, as was also done in the case of its counterpart in [1], since it is exactly along the same lines of its analogs in the aforementioned papers [5, 8, 9].

The results obtained so far can thus be summarized in the following theorem.

Theorem 2.1. *The Hamiltonian of the three-dimensional isotropic oscillator perturbed by two identical attractive point interactions situated symmetrically with respect to the origin at the points* $\pm\vec{x}_0 = (\pm x_0, 0, 0)$, $x_0 = |\pm\vec{x}_0| > 0$, *making sense of the merely formal expression*

$$\mathrm{H}_{\{\mu(\beta;x_0),\vec{x}_0\}} = H_0 - \mu(\beta;x_0)\left[\delta(\vec{x}-\vec{x}_0)+\delta(\vec{x}+\vec{x}_0)\right]$$

with

$$\mu(\beta;x_0) = \beta\left[1+2\beta\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}}\right]^{-1}$$

is the self-adjoint operator $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ *whose resolvent is given by the bounded operator (2.8). The latter is the limit of the resolvents of the Hamiltonians (with the energy cut-off* ℓ *defined by (2.4)) in the norm topology of bounded operators on* $L^2(\mathbb{R}^3)$ *once the energy cut-off is removed, i.e. for* $\ell \to +\infty$. *Furthermore,* $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ *regarded as a function of* β *is an analytic family in the sense of Kato.*

Before moving forward, it may be worth noticing the close analogy between the denominator of the second term in (2.5) (and its other representation in (2.8)) and its counterpart in the case of the spherically symmetric quantum dot with a single point impurity centered at the origin appearing in (2.4) in [1] (see also (2.5) in [9]). As a result of this analogy, even before getting into the detailed spectral analysis of the operator, we can already anticipate that, as was pointed out in [1, 9] for the spectrum of the Hamiltonian of the isotropic harmonic oscillator perturbed by a single point impurity, also in the case of the operator introduced in Theorem 2.1 the ground state energy for $\alpha = 0$, where $\alpha = 1/\beta$ (corresponding to the limiting case of point impurities of infinite strength), is equal to zero for any $x_0 > 0$ (α is sometimes called, in the literature on point interactions, see e.g. [6], 'extension parameter').

The ground state energy of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, denoted by $E_0(\alpha;x_0)$, can be determined for any fixed value of $x_0 > 0$ by solving the equation:

$$\frac{\alpha}{2} = E\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}, \tag{2.9}$$

solving with respect to E, or equivalently:

$$\alpha = \frac{1}{\pi^{3/2}}\int_0^1 \frac{(\xi^{\frac{1}{2}-E}-\xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi. \tag{2.9a}$$

The plot of $E_0(\alpha; x_0 = 0.2)$, shown below in Fig. 1, can be compared with both Fig. 1 in [1], the one of the ground state energy of the Hamiltonian of the 3D-isotropic harmonic oscillator perturbed by a single point impurity centered at the origin, and Fig. 3 in the same paper, the corresponding one of the ground state energy

of the operator with the symmetrical configuration of point impurities investigated therein obtained for the same value of the separation distance ($x_0 = 0.2$). As was to be expected, the anticipated similarity of the ground state energy of the Hamiltonian introduced in the above theorem with the one considered in the second section of [1] and in [9] is rather striking: both curves intersect the vertical axis at the origin, in agreement with the spectral requirement mentioned earlier at the end of the introduction.

The asymptotic approach to $E_0 = 3/2$, as $\alpha = 1/\beta \to +\infty$, is a straightforward consequence of the fact that the operator converges to the Hamiltonian of the unperturbed harmonic oscillator in the norm resolvent sense.

In the graph shown below (Fig. 2), we also provide the analogous graph for the other value of the distance between each center and the origin considered in [1], that is to say $x_0 = 0.4$.

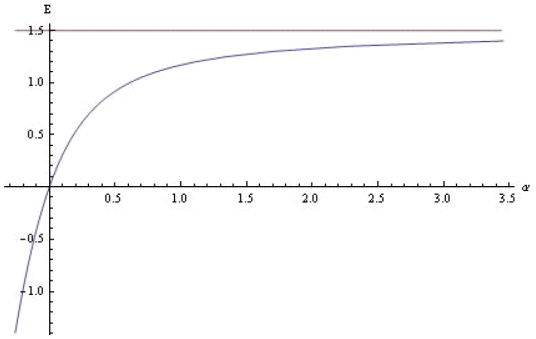

FIG. 1. The ground state energy E_0 of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as a function of the extension parameter $\alpha = 1/\beta$

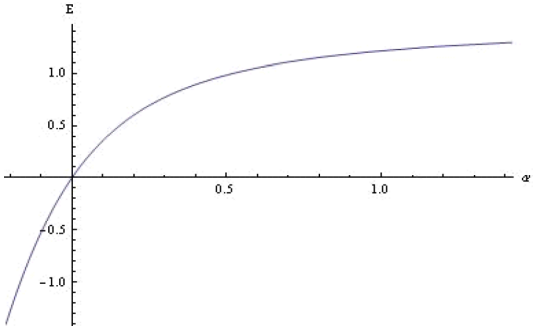

FIG. 2. The ground state energy E_0 of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.4$, as a function of the extension parameter $\alpha = 1/\beta$

In Fig. 3, in order to make more evident the role played by the separation distance x_0, we provide a visual comparison between $E_0(\alpha; x_0 = 0.2)$ and $E_0(\alpha; x_0 = 1)$.

Finally, we show the comparison between $E_0(\alpha; x_0 = 0.2)$ and $E_0(\alpha; x_0 = 0))$ in Fig. 4.

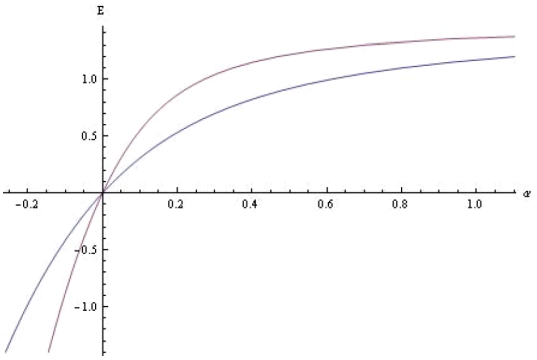

FIG. 3. Comparison between $E_0(\alpha; x_0 = 0.2)$ (blue curve) and $E_0(\alpha; x_0 = 1)$ (violet curve)

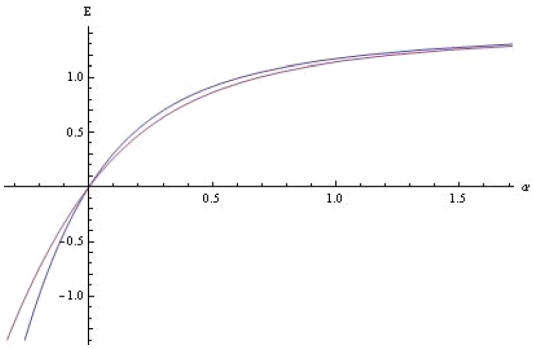

FIG. 4. Comparison between $E_0(\alpha; x_0 = 0.2)$ (blue curve) and $E_0(\alpha; x_0 = 0)$ (violet curve)

As can be noticed from the last two graphs, the behavior of the ground state energy $E_0(\alpha; x_0)$ as a function of x_0 changes remarkably in the vicinity of $\alpha = 0$ ($E = 0$): whilst for positive parameter values, the energy increases as the distance increases, conforming to the expected pattern in terms of the 'positional disorder' (see [1, 20]), the opposite occurs for negative values of α.

Therefore, it is worth computing the derivative of $E_0(\alpha; x_0)$ with respect to x_0 in order to get a better understanding of this phenomenon. By means of implicit differentiation, we can write for any $E < 3/2$:

$$\frac{dE}{dx_0} = -\frac{\dfrac{\partial}{\partial x_0}\displaystyle\int_0^1 \frac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}} d\xi}{\dfrac{\partial}{\partial E}\displaystyle\int_0^1 \frac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}} d\xi}, \tag{2.10}$$

having simplified the factor $1/\pi^{3/2}$.

After computing the two partial derivatives (by moving the derivatives inside the integrals, using dominated convergence) we get:

$$\frac{dE}{dx_0} = -\frac{2x_0\displaystyle\int_0^1 \frac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[\frac{1-\xi}{1+\xi}e^{-x_0^2\frac{1-\xi}{1+\xi}} + \frac{1+\xi}{1-\xi}e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}} d\xi}{\displaystyle\int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]\ln\xi}{(1-\xi^2)^{3/2}} d\xi}. \tag{2.11}$$

Given that $\ln\xi \leq 0$ over the interval $(0, 1]$, the denominator is always negative. With regard to the sign of the numerator, we notice that for $\alpha > 0$ (resp. $\alpha < 0$) the energy belongs to the interval $(0, 3/2)$ (resp. $(-\infty$,0)), so that the integral, and therefore the numerator, is positive (resp. negative). Hence, the whole expression on the right hand side is positive for $\alpha > 0$ and negative for $\alpha < 0$.

The lowest antisymmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, created by the twin point perturbations and emerging out of the eigenvalue $5/2$ (which stays in the spectrum but with its degeneracy lowered to two) will be denoted by $E_1(\alpha; x_0) < 5/2$. It can be determined for any fixed value of $x_0 > 0$ by solving the equation:

$$\alpha = \frac{1}{\pi^{3/2}}\int_0^1 \frac{\left(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}}\right)e^{-x_0^2\frac{1-\xi}{1+\xi}} - \left(\xi^{\frac{1}{2}-E} + \xi^{\frac{1}{2}}\right)e^{-x_0^2\frac{1+\xi}{1-\xi}}}{(1-\xi^2)^{3/2}} d\xi \tag{2.12}$$

with $E = E_1(\alpha; x_0)$.

The resulting graph of $E_1(\alpha; x_0 = 0.2)$ is provided below in Fig. 5.

As can be noticed, the asymptotic approach to the unperturbed antisymmetric energy level $E = 5/2$, as the parameter $\alpha = 1/\beta \to \infty$, is a straightforward consequence of the fact that the operator converges to the Hamiltonian of the unperturbed harmonic oscillator in the norm resolvent sense.

The lowest excited symmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, created by the twin point perturbations and emerging out of the eigenvalue $7/2$ (which stays in the spectrum but with its degeneracy lowered to five) will be denoted by $E_2(\alpha; x_0) < 7/2$ (see [1, 9]).

By essentially mimicking again what was done in [1] to determine the equation enabling us to compute the second symmetric eigenvalue, which was in turn based on the techniques used in [8–10, 15, 16], we get that $E_2(\alpha; x_0)$ is the solution of the following equation:

$$\alpha = \frac{4Ee^{-x_0^2}}{3\,(3-2E)\,\pi^{3/2}} + \frac{1}{\pi^{3/2}}\int_0^1 \frac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}} - 2e^{-x_0^2}(1-\xi^2)^{3/2}\right]}{(1-\xi^2)^{3/2}} d\xi \tag{2.13}$$

with $E = E_2(\alpha; x_0)$.

In Fig. 6 shown below, we have plotted the three lowest eigenvalues created by the twin point perturbations, namely $E_0(\alpha; 0.2)$, $E_1(\alpha; 0.2)$ and $E_2(\alpha; 0.2)$, as well as the two other eigenvalues $E = 5/2$ and $E = 7/2$ still present in the spectrum but with their degeneracy lowered by one due to the emergence of $E_1(\alpha; 0.2)$ and $E_2(\alpha; 0.2)$. The energy level $E = 3/2$ is no longer in the spectrum but has nevertheless been plotted since it is the lower horizontal asymptote of $E_2(\alpha; 0.2)$ in addition to being the upper one of the ground state energy $E_0(\alpha; 0.2)$.

As is evident from the graph, the striking spectral feature observed in [1] for the Hamiltonian $H_{\{1/\alpha,\vec{x}_0\}}$ studied therein, that is to say the existence of a range of values of the extension parameter for which the lowest excited symmetric eigenstate is more tightly bound than the lowest excited antisymmetric one due to the double level crossing between $E_1(\alpha; 0.2)$ and $E_2(\alpha; 0.2)$, is present also in the spectrum of our 'regularized' operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$. We avoid producing the analog of Table 1 in [1] since it would be perfectly identical apart from the numerical values of the points $\alpha_i, i = 1, 2, 3, 4$. However, it is certainly worth making a comparison between the

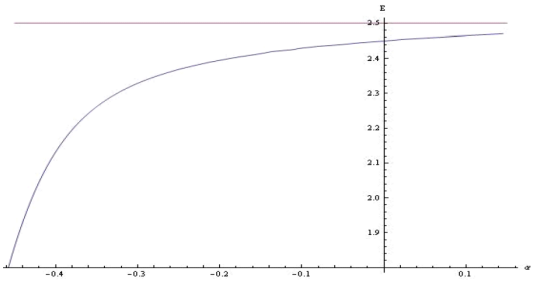

FIG. 5. The lowest antisymmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as a function of the extension parameter $\alpha = 1/\beta$

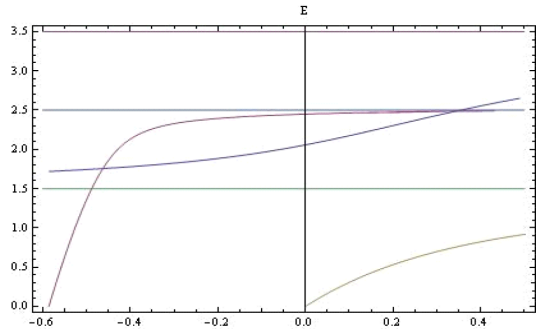

FIG. 6. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as functions of the extension parameter $\alpha = 1/\beta$

interval $[\alpha_2, \alpha_3]$ (the range of values of the parameter over which $2S < 2P$, adopting the widely used notation adopted in atomic physics, as is done in [17]), for $\sigma\left(H_{\{1/\alpha,0.2\}}\right)$ investigated in [1] and for $\sigma\left(\mathrm{H}_{\{1/\alpha,0.2\}}\right)$ being studied here: whilst in the former case the interval was approximately $[-0.126478, 0.309201]$, here the interval has expanded to become $[-0.462637, 0.339]$. We will come back to this point in the next section of this note.

On the other hand, as was the case for the operator $H_{\{1/\alpha,\vec{x}_0\}}$ studied in [1], the increase of the separation distance between the two centers leads to the 'disentanglement' between the two spectral curves in the sense that the two level crossings disappear and $E_1(\alpha; 0.2) < E_2(\alpha; 0.2)$ for any value of the extension parameter α and any value of x_0 beyond a certain threshold X_0. In Fig. 7 shown below we provide the reader with the visualization of the latter spectral phenomenon for $x_0 = 0.45$.

Therefore, in complete analogy with what was done in [1], it is entirely possible to determine the solution of the system:

$$\begin{cases} E_1(\alpha, x_0) = E_2(\alpha, x_0), \\ \dfrac{\partial}{\partial\alpha} E_1(\alpha, x_0) = \dfrac{\partial}{\partial\alpha} E_2(\alpha, x_0). \end{cases} \tag{2.14}$$

in order to locate the value of x_0 and the corresponding coordinates (α, E) of the point where we have the tangential contact between the two spectral curves. The numerical solution of (2.14) is the point with coordinates $E = E_t$ (approximately equal to 2.17509732), $x_0 = X_t$ (approximately equal to 0.31558276), and $\alpha = \alpha_t$ (approximately equal to 0.04957412). The plot of the tangential contact between the two spectral curves for $x_0 = X_t$ is provided below in Fig. 8.

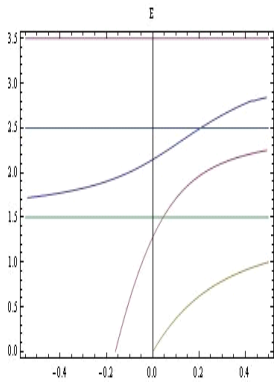

FIG. 7. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.45$, as functions of the extension parameter $\alpha = 1/\beta$

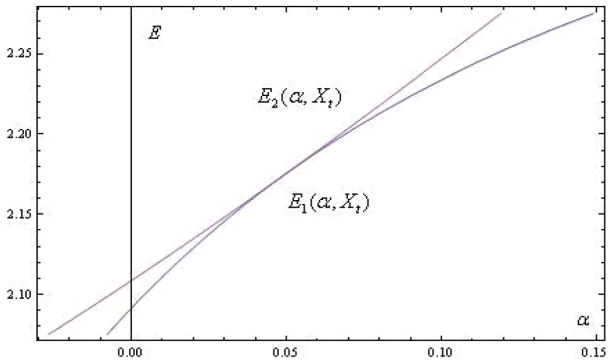

FIG. 8. The curves of the two eigenenergies $E_1(\alpha, X_t)$ and $E_2(\alpha, X_t)$ (X_t being approximately equal to 0.31558276) intersecting each other tangentially at $\alpha = \alpha_t$ (approximately equal to 0.04957412)

We can also visualize the intersection between the two eigenenergies as three-dimensional surfaces (Fig. 9).

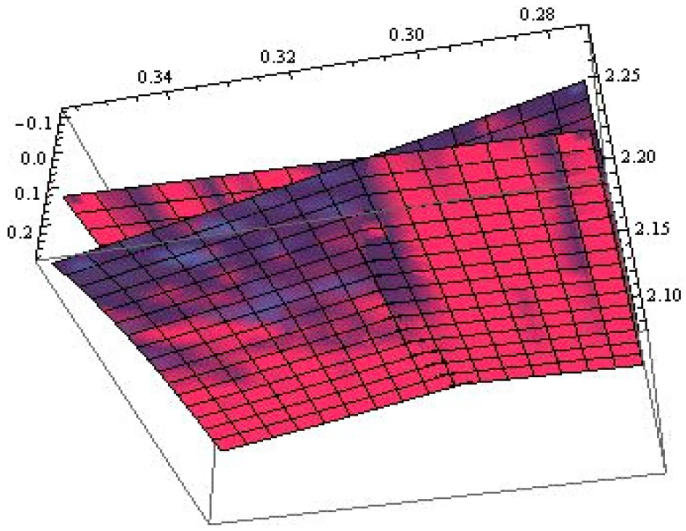

FIG. 9. The two eigenenergies $E_1(\alpha; x_0)$ and $E_2(\alpha; x_0)$ as three-dimensional surfaces

Before ending this section, we wish to state and prove the theorem showing that the singular double well Hamiltonian, defined in the previous theorem, differently from the one considered in [1], behaves smoothly as the distance between the two attractive point interactions shrinks to zero, which fully explains our extensive use of the term 'regularization' throughout this note.

Theorem 2.2. *The resolvents of the self-adjoint Hamiltonians*

$$\mathrm{H}_{\{\beta,\vec{x}_0\}}$$

converge, as the distance $x_0 \to 0_+$ (the magnitude of the vectors giving the location of the centres of the twin point impurities), in the norm topology of bounded operators on $L^2(\mathbb{R}^3)$ to

$$(H_{2\beta} - E)^{-1} = (H_0 - E)^{-1} + \frac{\big|(H_0 - E)^{-1}(\cdot, 0)\big\rangle\big\langle(H_0 - E)^{-1}(0, \cdot)\big|}{(2\beta)^{-1} - E\sum\limits_{|\vec{n}|=0}^{\infty} \dfrac{\Psi^2_{2\vec{n}}(0)}{(|2\vec{n}| + 3/2)(|2\vec{n}| + 3/2 - E)}}, \tag{2.15}$$

namely the one of the self-adjoint Hamiltonian of the three-dimensional isotropic harmonic with an attractive point interaction centred at the origin having double strength.

Proof. We start by noting that, because of the local nature of the limit procedure, it is not restrictive at all to consider only those values of x_0 in a suitable right neighbourhood of zero, i.e. $(0, X_0]$. Moreover, without any loss of generality, we may also restrict the proof to $\beta > 0$.

As shown earlier, for any $\beta > 0$, $E_0(\beta; x_0)$ is an increasing function of x_0, which implies that $E_0(\beta; 0) < E_0(\beta; x_0)$. Furthermore, given that for both operators $E_0(+\infty; 0) = 0$ and $E_0(\infty; x_0) = 0$, any negative E will belong to the resolvent set of both operators.

Therefore, by referring to (2.5), what is to be shown here for all $E < 0$ is simply:

$$\big\|(H_{2\beta} - E)^{-1} - (\mathrm{H}_{\{\beta,\vec{x}_0\}} - E)^{-1}\big\|_\infty \leq \big\|(H_{2\beta} - E)^{-1} - (\mathrm{H}_{\{\beta,\vec{x}_0\}} - E)^{-1}\big\|_p =$$

$$\left\| \left[\frac{\big|(H_0-E)^{-1}(\cdot,0)\big\rangle\big\langle(H_0-E)^{-1}(0,\cdot)\big|}{(2\beta)^{-1}-E\displaystyle\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}} - \frac{\big|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\big|}{(2\beta)^{-1}-E\displaystyle\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}} \right] \right.$$

$$\left. \oplus \frac{\big|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\big|}{(2\beta)^{-1}+\lim\limits_{\ell\to+\infty}\left[\displaystyle\sum_{|\vec{n}|=0}^{\ell}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}|+3/2}-\sum_{|\vec{n}|=0}^{\ell}\frac{\psi(x_0)^2_{2n_1+1}\psi^2_{2n_2}(0)\psi^2_{2n_3}(0)}{2n_1+2n_2+2n_3+5/2-E}\right]} \right\|_p \to 0, \quad (2.16)$$

as $x_0 \to 0_+$, for any Schatten norm of index $p > 3$ (the fact that the resolvent of H_0 belongs to any Schatten ideal with index $p > 3$ is shown in [9]). Since both direct summands inside the norm are operators of finite rank, the left hand side of (2.16) is bounded from above by:

$$\left\| \frac{\big|(H_0-E)^{-1}(\cdot,0)\big\rangle\big\langle(H_0-E)^{-1}(0,\cdot)\big|}{(2\beta)^{-1}-E\displaystyle\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}} - \frac{\big|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\big|}{(2\beta)^{-1}-E\displaystyle\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}} \right\|_1$$

$$+ \left\| \frac{\big|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\big|}{(2\beta)^{-1}+\lim\limits_{\ell\to+\infty}\left[\displaystyle\sum_{|\vec{n}|=0}^{\ell}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}|+3/2}-\sum_{|\vec{n}|=0}^{\ell}\frac{\psi(x_0)^2_{2n_1+1}\psi^2_{2n_2}(0)\psi^2_{2n_3}(0)}{2n_1+2n_2+2n_3+5/2-E}\right]} \right\|_1 . \quad (2.17)$$

Let us deal with the limit of the first summand. Of course, if we can prove that the second term inside the norm converges to the first one in $T_1(L^2(\mathbb{R}^3))$ (the norm on the trace class operators acting on $L^2(\mathbb{R}^3)$), then the norm of their difference will necessarily converge to zero.

As can be guessed, the proof is bound to be rather similar to the one of Theorem 2.2(b) in [10] for the one-dimensional analog of the model since the behavior of the following series will play a crucial role:

$$\big((H_0)_s^{-1}(\vec{x}_0,\cdot),(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\big) = \sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}, \quad (2.18)$$

$$\big\|(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\big\|_2^2 = \sum_{|\vec{n}|=0}^{\infty}\frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{(|2\vec{n}|+3/2-E)^2} = (H_0-E)_s^{-2}(\vec{x}_0,\vec{x}_0). \quad (2.19)$$

As a consequence of the estimate (3.8) in [1], it is evident that, in order to take advantage of the dominated convergence theorem, it will not be possible to use the square of the uniform norm $\|\psi_{2n}\|_\infty^2$, as was done in the one-dimensional case, since the latter decays only like $1/(2n)^{1/6}$ (see [21, 22]), a decay not sufficiently rapid to ensure the convergence of

$$\sum_{n=0}^{\infty}\frac{\|\psi_{2n}\|_\infty^2}{(2n+1/2)^{2/3}}.$$

However, given that the limit procedure involves only those x_0's in $(0, X_0]$ for some suitable $X_0 > 0$, we need not use the global maximum of ψ_{2n} in our quest for a dominating ℓ_1-sequence but rather the one over such a right vicinity of zero. Then, we can take advantage of the estimates (21) in [23] in order to state that, by choosing any $X_0 \le \sqrt{3}-1$, we are guaranteed that there exists a constant C such that:

$$\sum_{n=0}^{\infty}\frac{\psi^2_{2n}(x_0)}{(2n+1/2)^{2/3}} \le \frac{2^{2/3}}{\sqrt{\pi}} + \sum_{n=1}^{\infty}\frac{C^2}{(2n)^{1/2}(2n+1/2)^{2/3}} < \infty, \quad (2.20)$$

which ensures, together with the fact that

$$\sum_{n=0}^{\infty} \frac{\psi^2_{2n}(0)}{(2n+1/2)^{2/3}} < \infty,$$

the possibility of exploiting the dominated convergence for the three-dimensional series (2.18) and (2.19). Having established this technical subtlety, the remainder of the proof can mimic the aforementioned one for the one-dimensional analog almost word by word. As to the second summand of (2.17), since

$$\left\|(H_0-E)^{-1}_{as}(\vec{x}_0,\cdot)\right\|^2_2 = \sum_{|\vec{n}|=0}^{\infty} \frac{\psi^2_{2n_1+1}(x_0)\psi^2_{2n_2}(0)\psi^2_{2n_3}(0)}{\left(2n_1+2n_2+2n_3+\frac{5}{2}-E\right)^2} = (H_0-E)^{-2}_{as}(\vec{x}_0,\vec{x}_0), \tag{2.21}$$

it is clear that a dominating ℓ_1-sequence can be found also in this case such that:

$$\left|(H_0-E)^{-1}_{as}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)^{-1}_{as}(\vec{x}_0,\cdot)\right| \to 0_+$$

in $T_1(L^2(\mathbb{R}^3))$ as $x_0 \to 0_+$. The latter convergence to zero is further enhanced by the divergence of the denominator since, as $x_0 \to 0_+$, we have:

$$\int_0^1 \frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi \to 2\int_0^1 \frac{\xi^{\frac{1}{2}}}{(1-\xi^2)^{3/2}}d\xi = +\infty,$$

differently from its one-dimensional counterpart which stays finite. This concludes the proof of the theorem.

3. Manifestation of the Zeldovich effect (level rearrangement)

Although we might return to the issue in a separate paper in the near future, we cannot help anticipating here that it is possible to reinterpret the results of the spectral analysis carried out in this note from a slightly different point of view in order to discuss the manifestation of the Zeldovich effect (see [18]) in the case of the three lowest eigenvalues of the self-adjoint operator being analyzed in this note taking account of the results outlined in [17,19].

By citing [17], *'in 1959, Zeldovich discovered an interesting phenomenon while considering an excited electron in a semiconductor. The model describing the electron-hole system consists of a Coulomb attraction modified at short-distance. A similar model is encountered in the physics of exotic atoms: if an electron is substituted by a negatively charged hadron, this hadron feels both the Coulomb field and the strong interaction of the nucleus'*. Moreover, *'Zeldovich and later Shapiro and his collaborators look at how the atomic spectrum evolves when the strength of the short-range interaction is increased, so that it becomes more and more attractive. The first surprise, when this problem is encountered, is that the atomic spectrum is almost unchanged even though the nuclear potential at short distance is much larger than the Coulomb one. When the strength of the short-range interaction reaches a critical value, the ground state of the system leaves suddenly the domain of typical atomic energies, to become a nuclear state, with large negative energy. The second surprise is that, simultaneously, the first radial excitation leaves the range of values very close to the pure Coulomb 2S energy and drops towards (but slightly above) the 1S energy. In other words, the "hole" left by the 1S atomic level becoming a nuclear state is immediately filled by the rapid fall of the 2S. Similarly, the 3S state replaces the 2S, etc. This is why the process is named level rearrangement'*.

In their paper, the authors extend their analysis from exotic atoms to quantum dots which are mathematically modelled by Hamiltonians with the harmonic confinement perturbed by an attractive interaction whose action is strong only in the short range.

Although only attractive perturbations of the 3D-isotropic harmonic oscillator represented by square wells are considered, the authors of [17] observe, in addition to the aforementioned level rearrangement (Zeldovich effect), the same remarkable spectral phenomenon noticed by us in this note and its predecessor [1] dealing with point perturbations, namely the double level crossing because of which the level ordering becomes $1S < 2S < 2P$ over a certain range of values of the appropriate parameter, the coupling constant (resp. the extension parameter) in the case of [17] (resp. our model with point interactions).

Therefore, in order to investigate the manifestation of the Zeldovich effect in our model, it makes sense to plot the curves representing the energy levels as functions of the parameter β instead of α, the extension parameter. By citing [1], we wish to remind the reader that the latter '*is physically characterized by being proportional to the inverse scattering length*'.

We first plot the equivalent of Fig. 2 in [1], that is to say the graph of the ground state energy and the eigenenergy pertaining to the next symmetric bound state ($2S$) created by the point perturbation of the Hamiltonian H_β, the one of the 3D-isotropic harmonic oscillator perturbed by a single attractive point perturbation centred

at the origin, as functions of the parameter β. Of course, if $\beta = 0$, we have the unperturbed Hamiltonian H_0 of the 3D-isotropic harmonic oscillator. We have also plotted the horizontal lines $E = 3/2$, no longer in the spectrum except for $\beta = 0$, and $E = 5/2$, the eigenenergy of the $2P$ state, clearly not affected by the central point perturbation.

Furthermore, we draw the reader's attention to the two horizontal asymptotes appearing in the plot, the lower one for the ground state $(1S)$ energy obviously situated at $E = 0$, and the upper one for the energy of the next symmetric bound state $(2S)$ located approximately at 2.307876 (Fig. 10(a)).

By comparing the above graph to Fig. 2 in [1], in which the energy is plotted against the extension parameter α, we cannot refrain from pointing out the analysis carried out in [19] to the interested reader. Although the spectral analysis therein pertains to three Hamiltonians with potentials whose range is short but different from zero (the finite square well, the modified Poshl-Teller potential and an exponential one), the ideas put forward in that article are relevant also in the case of point perturbations of the isotropic harmonic oscillator in three dimensions.

First of all, as is stressed in that note, from the point of view of the experimental observation of this intriguing physical phenomenon '*currently available experimental techniques in cold-atoms research offer an exciting opportunity for a direct observation of the Zeldovich effect without the difficulties imposed by conventional condensed matter and nuclear physics studies'*.

It is important to remind the reader that the typical graphs used to describe the level rearrangement phenomenon are drawn assuming the presence of the negative sign multiplying the coupling constant in the interaction term of the Hamiltonian so that the interaction becomes increasingly attractive as the coupling goes from negative to positive infinity, which might look a bit unusual since it is exactly the opposite of the standard plots based on the presence of the positive sign in front of the coupling constant in the interaction term of the Hamiltonian.

By looking at the above graph, it is crucial to realize that, differently from the plots in [17, 19] and because of our renormalization, the manifestation of the Zeldovich effect occurs in the vicinity of $\beta = 0$ whilst the left boundary of the graph is instead $\beta = -\infty$.

As stated at the beginning of this section, here, it is not our intention to dwell on an extensive discussion of the level rearrangement phenomenon based on the ideas proposed in [19]. We simply wish to stress that we certainly agree with the authors that the Zeldovich effect implied by the plots of the energy versus either α or β can be better understood by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R} \times S_1$, with the energy E drawn along the real line (the symmetry axis of the cylinder) and either parameter along the unit circle identifying $\pm\infty$, which naturally leads them to the introduction of the denomination 'Zeldovich spiral'.

In order to show the 'flow' of the spectrum along the Zeldovich spiral, we plot again the above graph with the arrows showing that in the E vs. β plot the spectral flow goes from top to bottom vertically and counter clockwise along S_1 (Fig. 10(b)).

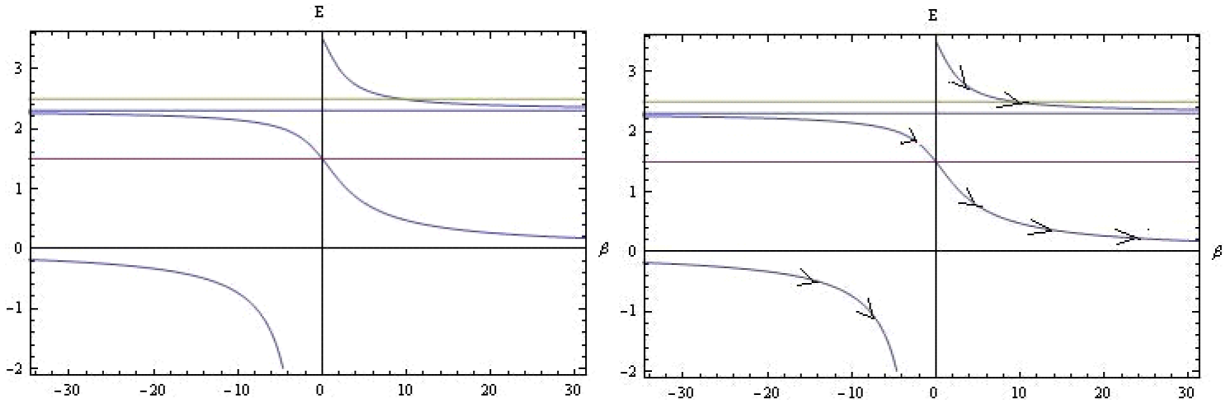

FIG. 10. The ground state energy and the next eigenenergy of the Hamiltonian H_β as functions of the strength parameter β

The analogous graph of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, with $x_0 = 0.2$, shows, in addition to similar features, the presence of the curve pertaining to the $2P$ eigenenergy with its horizontal asymptote located slightly below the energy level $5/2$ at approximately 2.450008. The horizontal asymptote of the curve of the $2S$ eigenenergy is situated instead at approximately 2.058391.

Furthermore, as pointed out in the comments on the E vs. α plot, there is a range of values of the parameter over which the $2S$ eigenenergy falls below the $2P$ eigenenergy, namely $(-\infty, \beta_2)$ (with $\beta_2 = 1/\alpha_2$ approximately

equal to -2.161522) along the negative semiaxis and $(\beta_3, +\infty)$ (with $\beta_3 = 1/\alpha_3$ approximately equal to 2.949853) along the positive one.

Hence, we can infer that, as we rotate counter clockwise along the Zeldovich spiral from the angle corresponding to β_3 to the one corresponding to β_2, the $2S$ state is more tightly bound than the $2P$ one (Fig. 11).

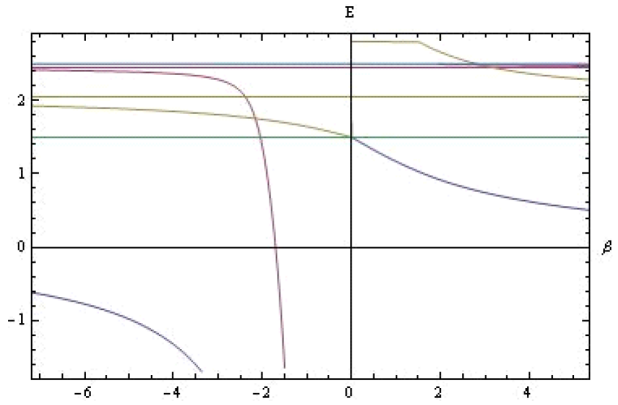

FIG. 11. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, with $x_0 = 0.2$, as functions of the parameter β

4. Final remarks

The main goal of this note has been to show that, by renormalizing the coupling constant in a way that is dependent on x_0 (the distance between each point interaction center and the origin), the self-adjoint Hamiltonian modeling an isotropic three-dimensional harmonic oscillator perturbed by two twin attractive point interactions symmetrically situated around the origin can be rigorously defined in such a way to avoid the problem encountered in our previous paper [1]: the self-adjoint Hamiltonian investigated therein did not converge to the one with a single point interaction located at the origin having double strength.

By citing [1], it is important to recall that *'as is well known to Quantum Chemistry students, three-dimensional interactions with a nonzero range do not manifest this singular behavior in the limit of the distance R between the two centers shrinking to zero, as the classical textbook example of* H_2^+ *smoothly approaching* He^+ *in the limit* $R \to 0_+$ *clearly shows*' (see [2–4]). Hence, the regularization being proposed here should make such singular double wells more similar to conventional double wells generated by rapidly decaying potentials.

We remind the reader that this singular behavior seems to be a general feature of models with double singular wells represented by point interactions requiring the renormalization of the coupling constant, as has also recently been noticed in the case of the one-dimensional Salpeter Hamiltonian studied in [5].

Furthermore, we have carried our spectral analysis not only in terms of α, the extension parameter physically related to the inverse scattering length, but also in terms of β, the strength parameter directly involved in the renormalization procedure. Our main motivation for this further analysis has been the fact that, following [17], the latter parameter is the conventional one used to study the manifestation of the Zeldovich effect, known also as level rearrangement. We have been able to show that the phenomenon, studied by the authors when the perturbation of the three-dimensional isotropic harmonic oscillator is represented by a potential whose range is physically very short but different from zero, does manifest itself also in the case of point perturbations.

We wish to stress that a remarkable advantage resulting from our renormalization procedure, uniquely associated to the fundamental spectral condition $E_0(\alpha = 0, x_0) = 0 = E_0(\beta = +\infty, x_0)$, is that the Zeldovich spiral, introduced by Farrell et al. in [19] by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R} \times S^1$, with E along the real line (the symmetry axis of the cylinder) and the parameter α along the unit circle identifying $\pm\infty$, can be visualized directly in a plot of the energy vs. β as well.

Acknowledgements

We wish to thank Prof. Igor Yu. Popov (Chair of Higher Mathematics, ITMO University, St. Petersburg, Russian Federation) for his kind invitation to contribute to this special issue dedicated to the memory of our dear friend Boris Pavlov. The first author had the great luck to meet him in the 80s, first during a meeting in Dubna, and was greatly impressed by his bright mind, his contagious enthusiasm for mathematics, that he transmitted to a large

number of students. One of the topics we discussed was the subject of point interactions. He gave fundamental contributions to this area and, more generally, to spectral theory. The contacts with him and his research associates happily accompanied our further scientific life.

The second author had the privilege of meeting him in February 1991 as we were both visiting Prof. Albeverio in Bochum. It was a great pleasure, shared also by the third author, to see him twenty-four years later in St. Petersburg on the occasion of the international conference 'Mathematical Challenge of Quantum Transport in Nanosystems', held at ITMO University, St. Petersburg, Russian Federation (9–11 September 2015). It is with great gratitude that we acknowledge his scientific legacy and dedicate this work to his memory.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 816–834

Resonance scattering across the superlattice barrier and the dimensional quantization

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DOI 10.17586/2220-8054-2016-7-5-816-834

Carbon nano-cluster cathodes exhibit a low threshold electron emission, which is 2–3 orders lower than on metals and semiconductors. We confirm the effect by direct experiments with graphene structures. We are suggesting a model based on the interference electrons wave function in 3D-space charge region of carbon structure interface with vacuum. The low-threshold emission is explained, in frames of the model, by the resonance properties of the barrier formed on the interface. Also in the following topics: interpretation of recent experimental findings for saturation of the field emission; local spectral analysis of multidimensional periodic lattices: dispersion via DN-map; examples of iso-energetic surfaces associated with solvable models of periodic lattice; Lagrangian version of the operator extension algorithm; solvable models of selected one-body spectral problems; quantum dot attached to the node of a quantum graph; a solvable model of a discrete lattice and spectral structure of a 1D superlattice via analytic perturbation procedure.

Keywords: periodic interface, carbon cover, Weyl-Titchmarsh function, resonance, field emission, DN-map.

Received: 23 August 2016

Revised: 1 September 2016

1. An example: resonance concepts of the low-threshold field emission

In numerous recent experiments, see for instance [1–7] extremely low-threshold field emission from metallic cathodes under carbon deposit was observed for electric fields $(10^4 - 10^5 V/cm)$. This is a surprisingly strong effect, because the field initiating a noticeable emission $(10^{-10} - 10^{-9} A)$ from these materials is by 2-3 orders of magnitude less than the field required for the field-emission from the traditional metals and semiconductors. Despite an obviously unusual nature of the effect, numerous authors, see for instance [5, 6] attempted to explain the low-threshold phenomenon trivially with use of the classical Fowler-Nordheim techniques, based on enhancing of the field at the micro-protrusions. They assume that the local field F_s near the emitting center is calculated as $F_0 = \gamma F_0$, where γ is the field enhancement coefficient, defined by the micro-geometry, and F_0 is the field of the equivalent flat capacitor. This completely classical explanation of the low-threshold emission phenomenon is not universal, and certainly non-valid for deposit, considered in our recent papers [3, 7] because the surface of the carbon flakes, obtained by the detonation synthesis, are perfectly smooth, see the flakes (see Fig. 1) under maximal magnifications.

with rare and relatively small protrusions. These protrusions are able to lower the threshold 5-fold, while 10^2 times lowering is observed in our experiments. We suggested in in [3, 7] an alternative explanation of the threshold lowering (field enhancement) based on the dimensional (size-) quantization in the under-surface space-charge region. The classical Fowler-Nordheim techniques for calculating the transmission coefficient T for simple rectangular potential barrier, see [8], gives an exponentially small value $T \approx e^{-qa}$ with $q = \sqrt{v - 2mE\hbar^{-2}}$ for the under-barrier tunneling with $v >> 2mE\hbar^{-2}$ and the width of the barrier equal to a. The resonance modification of the classical Fowler-Nordheim algorithm for calculating the transmission coefficient across a rectangular barrier, in presence of the energy levels of the size-quantization, meets some technical complications which can be avoided while substituting the rectangular barrier with delta-barrier supplied with an inner structure, attached to the barrier by Datta and Das-Sarma boundary condition, see [9, 10] for discussion of this phenomenological boundary condition and the derivation of it from the first principles in [11]. The program of resonance interpretation of the low-threshold field emission, based on zero-range model barrier with an inner structure, is developed in [7]. Where the zero-dimensional metal-carbon interface is substituted by the 1+0 solvable model for electron transmission from the metallic cathode to vacuum through the 0D barrier, supplied with an inner structure, emulation of the discrete levels of the size quantization is interpreted as the Tamm surface state. Based on this model, we developed a resonance version of the classical Fowler-Nordheim machinery, considering the complex Tamm levels as resonances which serve as bridges helping electrons with Fermi energy to exit from the metallic cathode into

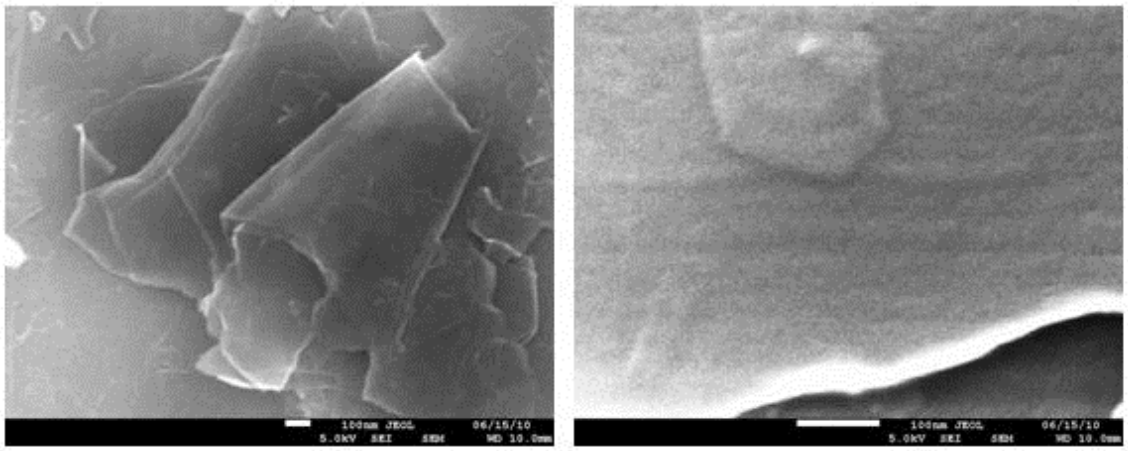

FIG. 1. Images of carbon Nano-clusters obtained via scanning electron microscope

vacuum across the carbon deposit. The role of the field enhancing factor in [7] was played by the small effective mass of electron in the carbon structure. Indeed, the field is measured by the steepness of the potential slope. But the effective steepness is calculated with respect to the De-Broghlie wavelength which is m/m_e times bigger than the conventional De-Broghlie wavelength at the same energy. The corresponding formula for the transmission coefficient was derived for the general 1D model of the space-charge region, with complex discrete spectrum of Tamm surface levels. The presence of these **resonance details** in the barrier may result in much larger value of the transmission coefficient values T for electrons with certain energy. In [7] we substitute the inner structure by a finite matrix, which is fit based on experimental data on size quantization, emulating the barrier barrier with inner structure by equivalent T-junction with the generalized Datta and Das Sarma boundary conditions, see [9–11]. The 1D model of the contact zone of the emitter in the form of a T-junction consisting of the cathode (1) $-\infty < x < 0$, the vacuum (2) $0 < x < \infty$, and the deposit (3) attached at the origin. The components u_s, $s = 1, 2, 3$ of the wave-function of the electron satisfy on the intervals $(-\infty, 0), (0, \infty)$ the Schrödinger equations with appropriate potentials, see [7]:

$$u(x) = \begin{cases} u_1(x) = & e^{-ip_1 x} + Re^{ip_1 x}, & -\infty < x < 0 \\ u_2(x) = & Te^{-ip_2 x}, & a < x < \infty. \end{cases} \tag{1}$$

In [7], we model the component u^3 of the wave-function on the barrier by the finite vector and, correspondingly, substitute the barrier by a zero-range model with an inner structure, see [12, 13], defined by the finite Hermitian matrix A. Interaction between components u_1, u_2, u_3 is defined via imposing boundary conditions onto the boundary data $u_1(0.u_1'(0))$ and $u_2(0.u_2'(0))$ and abstract boundary data $\xi_{c,s}$ of the inner structure, with regard of vanishing of the sum of corresponding boundary forms with $u = u^3$, $v = v^3$:

$$-\frac{\hbar^2}{2m_1}\left[\frac{du^1}{dx}\bar{v}^1 - u^1\frac{d\bar{v}^1}{dx}\right]\Big|_{x=-0} + \frac{\hbar^2}{2m_1}\left[\frac{du^2}{dx}\bar{v}^2 - u^2\frac{d\bar{v}^1}{dx}\right]\Big|_{x=+0} +$$

$$+\xi_c^u\bar{\xi}_s^v - \xi_s^u\bar{\xi}_c^v = J^1(u^1, v^1) + J^2(u^2, v^2) + J^3(u, v).$$

see Appendix 1 and [12]. In particular, the sum vanishes while Datta-Das Sarma boundary conditions are imposed at the contact $x = 0$ between the deposit and vacuum (on the barrier). Those boundary conditions are defined, similarly to Datta-Das Sarma, [9], by the vector parameter $\vec{\beta} = (\beta_1, \beta_2, \beta_3)$ as:

$$\frac{u^1}{\beta_1} = \frac{u^2}{\beta_2} = \frac{\xi_-^u}{\beta_1}, \quad \frac{\hbar^2}{2m_1}u_1'\bar{\beta}_1 + \frac{\hbar^2}{2m_2}u_2'\bar{\beta}_2 + \xi_+^u\bar{\beta} = 0, \tag{2}$$

The quantum-mechanical meaning of the similar parameter $\vec{\beta}$ in the case of the T-junction is revealed in [11]. It is defined by the spectral properties of the inner structure and the corresponding eigenfunction, [11]. Assuming that the wave-function of the electron in the carbon layer and in vacuum is a scattered wave, we represent the components of it in the deposit and in vacuum as $u^1 = e^{ip_1x_1} + e^{-ip_1x_1}R_1(\lambda)$, $u^2 = Te^{-ip_2x_2}$. Substituting this scattering Ansatz into the above boundary conditions, we obtain an expression for the transmission coefficient T

from the deposit into vacuum $T(\lambda) =:$

$$\frac{\bar{\beta}_1\beta_2\, m_1^{-1/2}}{|\beta_1^2|{m_1}^{-1/2} + |\beta_2^2|{m_2}^{-1/2} + i|\beta_3|^2\left[\hbar\,\mathcal{M}\sqrt{2E}\right]^{-1}}. \tag{3}$$

In the non-resonance situation, $\mathcal{M} \approx$ Const, the Datta-Das Sarma parameter $(1, 1, e^{qa/2})$ defines the exponential small transmission rate $T \approx e^{-aq}$. Then, in the resonance situation, $\mathcal{M} = \mathcal{M}(\lambda)$ the transmission is exponentially small on the complement of the set of poles of $\mathcal{M}$, but is essentially greater at the poles λ_p $\mathcal{M}(\lambda_p) = \infty$, where $\mathcal{M}^{-1} = 0$. In particular, for $m_1 << m_2$ we have at the poles, that

$$T = \frac{\bar{\beta}_1\beta_2\, m_1^{-1/2}}{|\beta_1|^2{m_1}^{-1/2} + |\beta_2|^2{m_2}^{-1/2}} \approx \frac{\beta_2}{\beta_1},$$

which can be essentially greater than exponential estimate $T \approx e^{-2av}$. Then, in the resonance situation, $\mathcal{M} = \mathcal{M}(\lambda)$ based on $\beta_3 \approx e^{vd}$ we see the peak of the transmission coefficient at the eigenvalues of the matrix A which play a role of the levels of the size quantization on the barrier (with special boundary conditions on the contact of the barrier with the inner part of the deposit and the vacuum. This condition is compatible with unitarity of the full scattering matrix on the interface deposit-vacuum, if the weights m_1^{-1}, m_2^{-1} are taken into account.

In our case, we have:

$$j = -\frac{2ev_F}{\hbar^2}\int \frac{\bar{\beta}_1\,\beta_2\; m_1^{-1/2}\;[f(E) - f(E+eV)]\;EdE}{|\beta_1|^2 m_1^{-1/2} + |\beta_2|^2 m_2^{-1/2} + i|\beta_2|^2[\hbar\sqrt{2E}\mathcal{M}]^{-1}},$$

where $\mathcal{M} = \mathcal{M}(E)$, is the Weyl-Titchmarsh function of the inner structure, see Appendix 1. just the value of T at the Fermi level, with a trivial coefficient.

But in fact, the estimation of the emission current requires taking into account the density of states $|\frac{\partial\lambda}{\partial p}|^{-1}$ which requires continuity of the spectrum of surface states, while the 1D model of surface state provides only discrete resonances.

One more competing viewpoint on field emission presented , in particular, in [14] is essentially quantum, but not trivially spectral as one in [3, 7]. In [14], the field emission from negative electron affinity sites on the atmosphere-GaAs interface is accompanied by optically stimulated process of oxygen adsorption. The corresponding optically induced pinning of the Fermi level leads to quenching and subsequent regeneration of the emission, which is connected in [14] with the presence of antisite defects in GaAs, formed due to the reconstruction of gallium dangling bonds on the GaAs - atmosphere interface. A possibility of the optical manipulation (monochromatic irradiation) the charges of the metastable antisite defects formed by the Ga dangling bonds is an extremely interesting aspect of the electron emission from GaAs, including enhancing the emission current due to monochromatic irradiation of the cathode under fixed exterior field. One may guess that the resonance optical excitation may generate beats of the oscillation modes which may help electrons energy to overcome the limits laid by the work function for given exterior field.

In fact, the emission current depends on the density of states $|\frac{d\lambda}{dp}|^{-1}$ – the inverse derivative of the energy with respect to the quasi-momentum, which does not arise in the 1D model. Fortunately, the spectrum of the size quantization in the quasi-2D periodic space charge layer is not discrete, but continuous, and consists of a sequence of spectral bands $\frac{d\lambda}{dp} \approx 0$ with a nontrivial dispersion. Attempting to explain the low threshold phenomenon, we have to develop the spectral approach for 2D periodic lattices , with regard of calculation the dispersion $\lambda(p^{\|} = \lambda(p_1, p_2))$ on the spectral bands responsible for the transmission electrons from the space-charge region 3 to vacuum 2, involving, together with the orthogonal to the interface (2,3) component $p^{\perp}$ of the momentum, the tangential component $p^{\|}$. Planning to develop the scattering machinery for calculation of the corresponding transmission coefficient, we call the ultimate modification of the Fowler-Nordheim technique, involving the continuous spectrum with 2D quasi- momentum $p^{\|}$ (1 + 2), contrary to the original Fowler-Nordheim scattering approach (1 + 0) based on scalar Schrödinger equation with 0D interface. We speculate that the continuity of spectrum arises due to the contribution of the electron flow in the carbon layer to the ultimate current. While the structure and period of the crystalline lattice in metal M may differ from the period and (hexagonal) structure of the carbon (graphene) G- layer, the problem becomes too difficult mathematically. But fortunately in our case, the metal can be considered as a bath filled with electrons, with some of natural orbitals disrupted on the metal/carbon interface. It is known, that the disrupted orbitals – the dangling bonds, see for instance [14], are restructured, transforming the interface into a quasi-2D lattice parallel to the GM interface, with a period defined by the graphene (G)-lattice , see (see Fig. 2). The calculation of resulting band-gap structure for the interacting

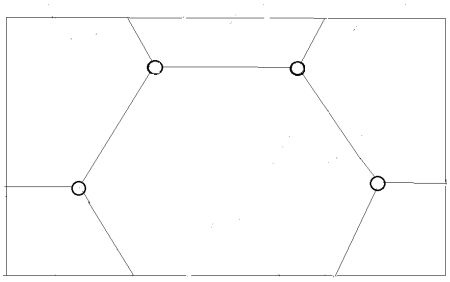

FIG. 2. Due to exterior electric field, the space-charge layer (SC) on the interface of the carbon and metal is restructured into periodic quasi-2D lattice with a rectangular period, as shown. The horizontal periodicity of the structure is not affected by the exterior electric field, normal to the interface, but the total band-gap structure is perturbed due to interaction of two periodic lattices, with equal periods, on the interface: one in metal $\mathcal{M}$, another in carbon, $\mathcal{G}$, resulting in the arisal of flat thin spectral bands of the size quantization

quasi-2D M and G lattices requires special analytical techniques using the Dirichlet-to-Neumann map, which is presented in section 3 below.

2. Interpretation of recent experimental findings for saturation of the field emission

Contrary to the basic (2 + 1) model of the cathode, see Fig. 2. DN formalism, see below, section 4, allows us to calculate the dispersion function of the spectral band of the size quantization in terms of the structure of the space-charge region and the electric field applied.

But in fact the estimation of the emission current requires taking into account the density of states $|\frac{\partial\lambda}{\partial p}|^{-1}$, which can't be introduced properly in the 1D model. Fortunately, the spectrum of the size quantization in the quasi 2D **periodic** space charge layer is continuous, and consists of a sequence of flat spectral bands, with nontrivial dispersion $\lambda = \lambda(p)$. The ultimate version of explanation of the low threshold phenomenon, we suggest in this paper, takes into account both size quantization of electrons in the space-charge layer **cv** due to perturbation of the periodic structure in the space-charge layer in 1D vertical direction $p^{\perp}$ and the continuity of the corresponding spectrum due to periodicity of the quasi 2D structure in horizontal direction $p^{\parallel} = (p_1, p_2)$. We call the ultimate modification *the "2+1" model* of the cathode, see Fig. 1.

DN formalism, see below, section 4, allows calculation of the dispersion function of the spectral band of the size quantization in terms of the structure of the space-charge period and electric field applied. We are able to calculate the the gradient of the dispersion function $dE = |\nabla_p E(\vec{p})|dp_{\perp}$ with $E = p^2/2m$. Then, for the 2-D system, the density of states in the 2-D is calculated as an integral on the surface S of the cathode [15]:

$$\rho(E) = \frac{1}{(2\pi\hbar)^2} \int \frac{dS}{|\nabla_p E|} = \frac{1}{2\pi\hbar^2}\frac{p}{\frac{\partial E}{\partial p}} = \frac{m}{2\pi\,\hbar^2}. \tag{4}$$

Recent experiments done by our group confirm the continuity of spectrum 2D-size quantization and allow us to estimate the effective mass m^* and the de Broglie wavelength in space-charge region depending on electron's concentration $n_{ex} = \frac{1}{q}\int_0^{\tau} J(t)dt$, where $j = I/S$, $I = 80$ A is the current and $S \approx 0.75$ cm^2 – the area of the cathode, $\tau \approx 2 \times 10^{-9}$ s. Monitoring of the current density allows us to estimate the experimental density of charges $Q = 2.4 \times 10^{-7}$ Coul/cm^2, which corresponds to density of electrons $n \approx 1.3 \times 10^{12}$ cm^{-2}.

On another hand, from the size-quantization theory [15] the 2D density of electrons is estimated as:

$$n_{2D} = \frac{m^* kT}{2\pi\hbar^2} \ln\left(1 + \exp\frac{E_0 - E_F}{kT}\right) \tag{5}$$

Here, m^* is the effective electron mass, E_0—the size-quantization level, E_F—the Fermi level. In our case

$$E_0 \approx E_F, \quad n_{\exp} = n_{2D} = \frac{m^* kT}{2\pi\hbar^2}\ln 2 \tag{6}$$

The de Broglie electron wavelength [15] in graphene flakes is:

$$\lambda = \frac{2\pi\hbar}{\sqrt{2m^*\,(kT)}}. \tag{7}$$

Based on the preceding Equations (6) and (7), we estimate the electron effective mass and the de Broglie electron

$$m^* = \frac{(2\pi\hbar)^2}{2(kT)} \tag{8}$$

At room temperature, we have $\lambda \approx 18$ nm, $m^* \leq 10^{-2}\ m_0$.

The potential on the space-charge region of the cathode, covered with carbon flakes is defined by the electric double layers formed by the electric field applied on the metal-carbon and carbon-vacuum interface and oriented by the outer normal looking toward vacuum. The horizontal periodicity of the cover is not affected by the field, but the vertical periodicity is perturbed by the potential well defined by the electric field, see Fig. 2. We assume that the depth of penetration of the field into the carbon layer defines the width of the potential well and the steepness of its wall. The hexagonal lattice can be represented as a periodic lattice with rectangular periods, 4 carbon atoms in each minimal period.

3. Resonance scattering on a low-dimensional superlattice and field emission from the metal-carbon interface

The above criticism of the resonance 0+1 scenario of the low-threshold field emission may be resolved based on a combination of Bagraev's findings in [14] on the periodic reconstruction of dangling bonds and recent results of our experimentalists [16], revealing the role of the continuous spectrum of the size quantization. Hereafter, we construct a solvable (2 + 1) model of a periodic 2D lattice on an interface of the Luttinger bath in metal and vacuum and calculate the scattering amplitude depending on resonance properties of the lattice period. The model can be used not only for analysis of the low-threshold emission, but also for studying the properties and dynamics stability of electric contact as a detail of a nano-device, or, generally, a quantum network. While simplest zero-range models of 2D lattices in 3D have been thoroughly investigated neglecting the "inner structure" see [17], the use of similar models with inner structure allows to interpret various instabilities of the contacts based on resonance properties of the of the inner structure.

Consider a flat 2D periodic lattice situated on the plane $z = 0$. Periods $\Omega_{\vec{l}} = \left\{a_{l^1} < x^1 < a_{l^1} + a\right\} \times \left\{a_{l^2} < x^2 < a_{l^2} + a\right\}$ in model problem [17] contain a singular points in the corners. The lattice of singular points is invariant with respect to the shifts by $a\vec{l}$. According to [17], the Laplacian restricted onto the domain D_0 of smooth functions vanishing near singular points $\left\{a_{\vec{l}}\right\}$ can be extended to Laplacian with singular zero-range potential defined by a boundary condition at the singular points imposed onto elements from the union of the domain D_0 of the restricted operator A_0 and deficiency elements selected as Green functions $G(x, a_l, \lambda_0)$, $\Im\lambda_0 \neq 0$ of the Laplacian. Disregarding the inner structure, one can find the scattered waves and the waveguide eigenfunction based on the Ansatzes:

$$\Psi^S(x, \nu, \lambda) = e^{ip\langle p,x\rangle} + \sum_{a_{\vec{l}}} G(x, a_{\vec{l}}, \lambda) A^S_{\vec{l}}, \tag{9}$$

$$\Psi^W(x, \nu, \lambda) = \sum_{a_{\vec{l}}} G(x, a_{\vec{l}}, \lambda) A^W_{\vec{l}}\,. \tag{10}$$

The above ansatzes possess the asymptotics at the singular points:

$$\Psi^S(x, \nu, \lambda) = u^S = \frac{A^S_{\vec{l}}}{4\pi|x - a_{\vec{l}}|} + B^S_{\vec{l}} + o(1). \tag{11}$$

$$\Psi^W(x, \nu, \lambda) = u^W = \frac{A^W_{\vec{l}}}{4\pi|x - a_{\vec{l}}|} + B^W_{\vec{l}} + o(1). \tag{12}$$

They define the boundary forms on the domain D_0^+ of the adjoint operator $-\Delta_0^+$:

$$J(u, v) = \langle -\Delta_0^+ u, v\rangle + \langle u, \Delta_0^+ v\rangle = \sum_{\vec{l}} \left[\langle B_{\vec{l}}(u), A_{\vec{l}}(v)\rangle - \langle A_{\vec{l}}(u), B_{\vec{l}}(v)\rangle\right], \tag{13}$$

which vanish under "local" boundary condition, see [17] (with $\alpha = -4\pi\mathcal{G}$):

$$B_{\vec{l}} + \mathcal{G} A_{\vec{l}} = 0. \tag{14}$$

with an Hermitian (real) parameter $\mathcal{G}$. The eigenfunctions (9, 10) are found in [17] from equations obtained via substitution of the coefficients $A^S_{\vec{l}} = f(\nu, \lambda) e^{ip\langle \nu, a_{\vec{L}}\rangle}$, $A^W_{\vec{l}} = e^{i\langle q, a_{\vec{l}}\rangle}$. The quasi-momentum $q(\lambda)$ for flat square

lattice $a_{\vec{L}}$, see [17]:

$$\mathcal{G} + \frac{i\sqrt{\lambda}}{4\pi} + \sum_{\vec{L}\neq 0} \frac{e^{i\sqrt{\lambda}|\vec{L}a|}}{4\pi|\vec{L}a|} e^{i\langle q, a\vec{l}\rangle} = 0. \tag{15}$$

Similarly, the scattering amplitude is found from the Ansatz (9 substituted to the above boundary condition:

$$\Psi^S(x,\nu,\lambda) = e^{ip\langle p,x\rangle} + f(\nu,\lambda)\sum_{a_{\vec{l}}} G(x, a_{\vec{l}}, \lambda) e^{i\sqrt{\lambda}\langle \nu, a_{\vec{l}}\rangle}$$

which implies an equation for the amplitude f:

$$f = -\left[\mathcal{G} + \frac{i\sqrt{\lambda}}{4\pi} + \sum_{\vec{L}\neq 0} G(x, a_{\vec{l}}, \lambda) e^{i\sqrt{\lambda}\langle \nu, a\vec{L}\rangle}\right]^{-1} \tag{16}$$

In [17], the ultimate formulae are simplified, for flat rectangular lattices, based on the Poisson identity $\sum_{n\in Z} e^{i\tau n} = 2\pi\sum_{n\in Z}\delta(\tau + 2\pi n)$ and explicit calculations of the lattice sums are involved. Notice that the resonance features of the amplitude at the waveguide spectral bands arise when $\sqrt{\lambda}\langle\nu, a\vec{L}\rangle = \langle q, a\vec{L}\rangle$. For the square flat lattices with no inner structure, the resonance properties and effective masses on the waveguide spectral band are defined only by the geometry of the lattice, see [17] .

In this paper, we consider flat periodic square lattice situated on the plane $z = 0$, **with inner structure**. The presence of the inner structure defines the resonance properties of the lattice and may help to interpret instabilities of the scattering amplitude depending of properties of atoms filling the period. Consider countable set of equivalent finite-dimensional spaces $K_{\vec{l}} \equiv K$ and a virtual lattice $\oplus\sum_{\vec{L}} A_{\vec{L}}$ of equivalent operators $A_{\vec{L}} \equiv A$. We use the virtual lattice, based on operator extension procedure, to emulate the inner structure of the set of periods $\Omega_{\vec{L}}$. Selecting non-overlapping deficiency subspaces $\frac{A+iI}{A-iI}N_i \equiv N_{-i}$, we introduce in the defect $N \equiv N_i + N_{-i}$ a basis $\{W_c^r, W_s^r\}_r$, see Appendix 1, and calculate the boundary form of the (formal) adjoint operator A_0^+ in terms of the decomposition coefficients $u, v \in D(A_0^+)$:

$$u = u_0 + \sum_r W_c^r\,\xi_c^r + W_s^r\,\xi_s^r = u_0 + \sum_r \frac{A}{A-iI}\Xi_c^r - \frac{I}{A-iI}\Xi_s^r,$$

with $\Xi_c^r,\ \Xi_s^r \in N_i,\ u_0 \in D(A_0)$ and the boundary form for $u = u_0 + \frac{A}{A-iI}\Xi_c^u - \frac{I}{A-iI}\Xi_s^u$, $v = v_0 + \frac{A}{A-iI}\Xi_c^v - \frac{I}{A-iI}\Xi_s^v$:

$$J^A(u,v) = \langle A_0^+ u, v\rangle - \langle u, A_0^+ v\rangle = \langle \Xi_c^u,\, \Xi_s^v\rangle - \langle \Xi_s^u(u),\, \Xi_c^v\rangle. \tag{17}$$

The components of the solution $u = u_0 + \frac{A}{A-iI}\Xi_c^u - \frac{I}{A-iI}\Xi_s^u$ of the homogeneous equation $A_0^+ u - \lambda u = 0$ are connected by the Weyl-Titchmarsh function $\mathcal{M} = P_{N_i}\frac{I+\lambda A}{A-\lambda I}P_{N_i}$:

$$P_{N_i}\frac{I+\lambda A}{A-\lambda I}P_{N_i}\ \Xi_c^u + \Xi_s^u = 0. \tag{18}$$

Self-adjoint extensions of the restricted operator A_0 are parametrized by Hermitian matrices $\mathcal{G} : N_i \to N_i$, which define the domain of the corresponding extensions as restriction of $D(A_0^+)$ onto the Lagrangian plane:

$$\mathcal{L}^{\mathcal{B}} = \left\{ u_0 + \left[\frac{A}{A-iI}\Xi_c^u - \frac{I}{A-iI}\,\Xi_s^u)\right]\right\},\ \text{where}\ \ \Xi_s(u) + \mathcal{B}\Xi_c(u) = 0, \tag{19}$$

see Appendix 1 and more details in [12]. The spectrum of the extension is defined from the dispersion equation:

$$[\mathcal{M} - \mathcal{B}]\,\Xi_c^u = 0. \tag{20}$$

Attaching the quantum dots $A_{\vec{l}}$ to the periods $\Omega_{\vec{l}}$ of the lattice $\left\{a_{\vec{l}}\right\}$ we supply the lattice in $L_2(R_3)$ with an inner structure so that we could consider the corresponding resonance scattering problem in $L_2(R_3) \oplus \sum_{vecL} K_{\vec{L}}$, with regard of the waveguide branch of spectrum, associated with the inner structure.

4. Local spectral analysis of multidimensional periodic lattices: dispersion via DN-map

The Bloch function and dispersion of the one-dimensional periodic Schrödinger operator is found based on transfer matrix constructed of standard solutions of the Cauchy problem on the period.

$$-\chi'' + q(x)\chi = \lambda\chi, \quad q(x+a) = q(x), \quad \chi(x+a) = \mu\chi(x),$$
$$\mu \equiv e^{ipa}, \quad \lambda = \lambda(p).$$
$$\chi = \theta + m\varphi, \quad \theta(0) = 1, \quad \theta'(0) = 0, \quad \varphi(0) = 0, \quad \varphi'(0) = 1.$$
$$-\theta'' + q\theta = \lambda\theta, \quad -\varphi'' + q\varphi = \lambda\varphi. \tag{21}$$

The spectral bands σ_s are defined by the condition $-1 \le \frac{1}{2}\mathcal{T}(\lambda) \le 1$ imposed on the trace $\operatorname{Tr}\mathcal{T}(\lambda) = \theta(a) + \varphi'(a)$ of the transfer matrix:

$$\mathcal{T} = \begin{pmatrix} \theta(a) & \varphi(a) \\ \theta'(a) & \varphi'(a) \end{pmatrix}: \quad \mathcal{T}\begin{pmatrix} \chi(0) \\ \chi'(0) \end{pmatrix} = \begin{pmatrix} \chi(a) \\ \chi'(a) \end{pmatrix} = \mu \begin{pmatrix} \chi(0) \\ \chi'(0) \end{pmatrix}.$$

The dispersion $\lambda = \lambda(p)$ and the positions of the spectral bands $\sigma : |\mu| = 1$ are defined $-2 \le \mu + \mu^{-1} = \operatorname{Tr}\mathcal{T} < 2$, see Fig. 3.

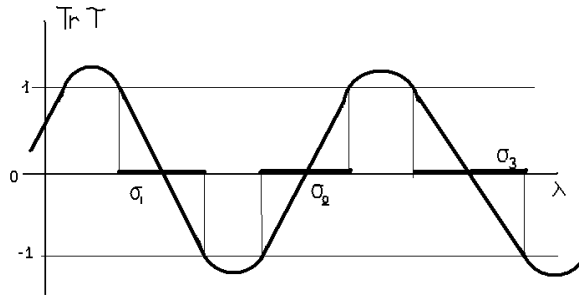

FIG. 3. The spectral bands σ_s of the 1D periodic problem are found from the condition $-1 \le \operatorname{Tr}\mathcal{T}/2 \le 1$.

One can also obtain Bloch solutions from analysis of a boundary problem, by considering, instead of the standard solutions θ, φ of the Cauchy problem, another pair of solutions ψ_0, ψ_a of the same Schrödinger equation $-\psi'' + q\psi = \lambda\psi$, with the boundary data $\psi_0(0) = 1, \psi_0(a) = 0$ and, respectively $\psi_a(0) = 0, \psi_a(a) = 1$. These solutions ψ_0, ψ_a of the Schrödinger equation are linearly independent if λ is not an eigenvalue of the corresponding Dirichlet problem on the period (see Fig. 4):

$$W(\psi_0, \psi_a)\Big|_0 = -\psi_a{}'(0) = W(\psi_0, \psi_a)\Big|_a = \psi_0{}'(a) = W(\psi_0, \psi_a)\Big|_a.$$

Then the Bloch solution can be found as a linear combination of ψ_0, ψ_a in the form:

$$\chi(x) = \chi(0)\psi_0(x) + \chi(a)\psi_a(x) = \chi(0)\left[\psi_0(x) + e^{ipa}\psi_a(x)\right] \tag{22}$$

which implies:

$$\chi'(a) = \chi(0)\left[\psi_0'(a) + e^{ipa}\psi_a'(a)\right] = e^{ipa}\,\chi(0)\,\left[\psi_0'(0) + e^{ipa}\psi_a'(0)\right].$$

The quasi-momentum exponential $e^{ipa} = \mu$ is found from the quadratic equation:

$$[\psi_0'(a) + \mu\psi_a'(a)] = \mu\,[\psi_0'(0) + \mu\psi_a'(0)]$$

which can be re-written as:

$$\mu^2 + \frac{\psi_0'(0) - \psi_a'(a)}{\psi_a'(0)}\,\mu - \frac{\psi_0'(a)}{\psi_a'(0)} = 0. \tag{23}$$

Here, the coefficient in front of $-\mu$ is equal again to the trace $\operatorname{Tr}\mathcal{T}$ of the transfer-matrix:

In the multidimensional case the roles of the basic solutions ψ_0, ψ_a of the boundary problems for the Schrödinger equation on the square 2D period are played by solutions associated with the boundary data forming an orthogonal basis $\{\psi_s^\Gamma\} \in L_2(\Gamma)$ on the boundary of the period $\Omega : \partial\Omega = \Gamma$:

$$-\triangle\,\psi_s + q\psi_s = \lambda\psi_s, \;\; \psi_s\Big|_\Gamma = \psi_s^\Gamma, \; \langle\psi_s^\Gamma, \psi_t^\Gamma\rangle_{L_2(\Gamma)} = \delta_{st}.$$

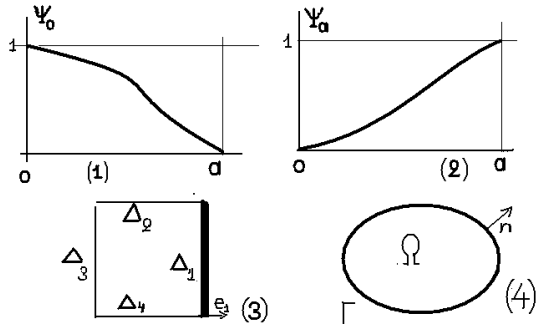

FIG. 4. Standard solutions ψ_0 (1) of the 1D boundary problem. Standard solutions ψ_{Δ^1} of the 2D boundary problem on the square.

Due to the uniqueness theorem for these elliptic equations the solutions $\{\psi_s\}$ are linearly independent, and their linear combinations approximate a solution of any boundary problem with the boundary data u_Γ decomposed on the boundary basis.

$$\mathcal{DN} : u_\Gamma \longrightarrow \left.\frac{\partial u}{\partial n}\right|_\Gamma . \tag{24}$$

Then, the Green's formula allows us to transform the matrix element into the bilinear form of the Schrödinger operator:

$$\langle u_l, \mathcal{DN} u_m \rangle = \int\limits_\Omega [\nabla \bar{u}_l \nabla u_m + q \bar{u}_l \, u_m - \lambda \bar{u}_l \, u_m] \, d\Omega. \tag{25}$$

Beginning from the solution of a sequence of Neumann problems for a smooth orthogonal basis $\{\rho_s\}$ in $L_2(\Gamma)$:

$$-\triangle v_s + q v_s = \lambda v_s, \ \left.\frac{\partial v_s}{\partial n}\right|_\Gamma = \rho_s,$$

we obtain the following expression for the matrix elements of the Neumann-to-Dirichlet map:

$$\mathcal{ND} : \left.\frac{\partial u}{\partial n}\right|_\Gamma \longrightarrow \left. v \right|_\Gamma ,$$

$$\langle \mathcal{ND} \rho_l, \rho_m \rangle = \int\limits_\Omega [\nabla \bar{v}_l \nabla v_m + q \bar{v}_l \, v_m - \lambda \bar{v}_l \, v_m] \, d\Omega. \tag{26}$$

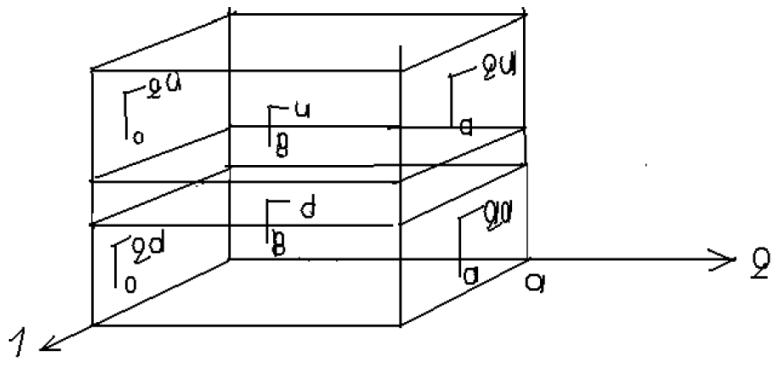

FIG. 5. Two-storied period of the periodic quasi-2D sandwich lattice

Consider the quasi-2D periodic lattice with a cubic period and the Schrödinger operator:

$$Lu = -\triangle u + q(x)u, \tag{27}$$

on the lattice, with periodic potential $q(x^1, x^2) = q(x^1 + ma, x^2 + na)$, $m, n = \pm 1, \pm 2, \ldots$, zero boundary conditions on the lower and the upper lids $\Gamma_0^3 : x^3 = 0$, $\Gamma_h^3 : x^3 = h$ of the lattice (see Fig. 5).

In this way, the whole spectral problem on the lattice is reduced to the spectral problem on the period, with the same boundary conditions on the lids $\Gamma^3_{0,h}$, and the quasi-periodic conditions on the vertical walls $\Gamma^{1,2}_{0,a}$. The positive normal on $\Gamma^{1,2}_a$ is defined by e_1, e_2, and the positive normals on the walls $\Gamma^{1,2}_0$ are $-e_1, -e_2$. The quasi-periodic boundary conditions permit us to eliminate the boundary data $u\big|_{\Gamma^{1,2}_0}$, $\frac{\partial u}{\partial n}\big|_{\Gamma^{1,2}_0}$ on the walls $\Gamma^{1,2}_0$:

$$u\Big|_{\Gamma^{1,2}_0} = e^{-ip_{1,2}a}u\Big|_{\Gamma^{1,2}_a}, \qquad \frac{\partial u}{\partial n}\Big|_{\Gamma^{1,2}_0} = -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^{1,2}_a}.$$

Then, the quasi-periodic boundary conditions on the walls $\Gamma^{1,2}_{0,a}$ are reduced to a linear system with respect to the "independent variables" $\vec{u} = \left(u^1_a, u^2_a; \frac{\partial u}{\partial n}\Big|_{\Gamma^1_a}, \frac{\partial u}{\partial n}\Big|_{\Gamma^2_a}\right)$, with a matrix composed of the components of the $\mathcal{DN}$ on the walls:

$$\begin{pmatrix} \frac{\partial u}{\partial n}\Big|_{\Gamma^1_0} \\ \frac{\partial u}{\partial n}\Big|_{\Gamma^2_0} \\ -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^1_a} \\ -e^{-ip_{1,2}a}\frac{\partial u}{\partial n}\Big|_{\Gamma^2_a} \end{pmatrix} \equiv \begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ -\mu^{-1}\frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \mathcal{DN}\begin{pmatrix} u\Big|_{\Gamma^1_a} \\ u\Big|_{\Gamma^2_a} \\ e^{-ip_1 a}u\Big|_{\Gamma^1_a} \\ e^{-ip_2 a}u\Big|_{\Gamma^2_a} \end{pmatrix}, \tag{28}$$

$$\mathcal{DN}\begin{pmatrix} u\Big|_{\Gamma^1_a} \\ u\Big|_{\Gamma^2_a} \\ e^{-ip_1 a}u\Big|_{\Gamma^1_a} \\ e^{-ip_2 a}u\Big|_{\Gamma^2_a} \end{pmatrix} \equiv \mathcal{DN}\begin{pmatrix} \vec{u}_a \\ \mu^{-1}\vec{u}_a \end{pmatrix}. \tag{29}$$

Here, $\mu = [\mu_1, \mu_2] = [e^{ip_i a}, e^{1p_2 a}]$ is a diagonal matrix. The DN-map $\mathcal{DN}$ can be represented in matrix form with 2×2 blocks $\mathcal{DN}^{ik}_{\alpha\beta}$ connecting the Dirichlet data on Γ^k_β to the Neumann data on Γ^i_α.

Matrix elements of the DN map connect the Dirichlet data on Γ^{ik}_α with Neumann data on $\Gamma^{jl}_{\alpha'}$, $\alpha, \alpha' = o, a$:

$$\begin{pmatrix} \mathcal{DN}^{11}_{aa} & \mathcal{DN}^{12}_{aa} \\ \mathcal{DN}^{21}_{aa} & \mathcal{DN}^{22}_{aa} \end{pmatrix} \equiv \mathcal{DN}_{aa}, \begin{pmatrix} \mathcal{DN}^{11}_{a0} & \mathcal{DN}^{12}_{a0} \\ \mathcal{DN}^{21}_{a0} & \mathcal{DN}^{22}_{a0} \end{pmatrix} \equiv \mathcal{DN}_{a0}.$$

$$\begin{pmatrix} \mathcal{DN}^{11}_{0a} & \mathcal{DN}^{12}_{0a} \\ \mathcal{DN}^{21}_{0a} & \mathcal{DN}^{22}_{0a} \end{pmatrix} \equiv \mathcal{DN}_{0a}, \begin{pmatrix} \mathcal{DN}^{11}_{00} & \mathcal{DN}^{12}_{00} \\ \mathcal{DN}^{21}_{00} & \mathcal{DN}^{22}_{00} \end{pmatrix} \equiv \mathcal{DN}_{00}.$$

Then the DN-map is represented by the block-matrix:

$$\mathcal{DN} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix}.$$

with blocks mapping the data $\vec{u}_a$, $\vec{u}_0$ onto the positive normal derivatives $\frac{\partial \vec{u}_a}{\partial n}$, $\frac{\partial \vec{u}_0}{\partial n}$.

In particular, the 0-components of the Bloch function can be eliminated based on $\vec{u}_0 = \mu^{-1}\vec{u}_a$, $\frac{\partial \vec{u}_0}{\partial n} = -\mu^{-1}\frac{\partial \vec{u}_a}{\partial n}$, which implies the following linear homogeneous system for the data $\left(\vec{u}_a, \frac{\partial \vec{u}_a}{\partial n}\right)$ of the Bloch-function:

$$\begin{pmatrix} \frac{\partial \vec{u}_a}{\partial n} \\ -\mu^{-1}\frac{\partial \vec{u}_a}{\partial n} \end{pmatrix} = \begin{pmatrix} \mathcal{DN}_{aa} & \mathcal{DN}_{a0} \\ \mathcal{DN}_{0a} & \mathcal{DN}_{00} \end{pmatrix}\begin{pmatrix} \vec{u}_a \\ \mu^{-1}\vec{u}_a \end{pmatrix}. \tag{30}$$

Eliminating $\dfrac{\partial \vec{u}_a}{\partial n}$ we conclude that a nontrivial solution of the equation (30) exists if and only if zero is an eigenvalue of the operator:

$$\left[\mu\mathcal{DN}_{00}\mu^{-1} + \mu\mathcal{DN}_{0a} + \mathcal{DN}_{aa} + \mathcal{DN}_{a0}\mu^{-1}\right]\vec{u}_a = 0. \tag{31}$$

Then, the Bloch function is obtained as a solution of the boundary problem for the Schrödinger equation:

$$-\triangle\chi + q\chi = \lambda\chi, \quad \chi\Big|_{\Delta_a^{1,2}} = u_a^{1,2}, \quad \chi\Big|_{\Delta_0^{1,2}} = e^{-ip_{1,2}a}\ u_a^{1,2}.$$

Equation (31) is an analog of the quadratic equation (23), however questions on the existence of the corresponding solution of it in the general case is not trivial, because we can't use the classical determinant condition of existence of non-trivial solutions of the homogeneous equation (31).

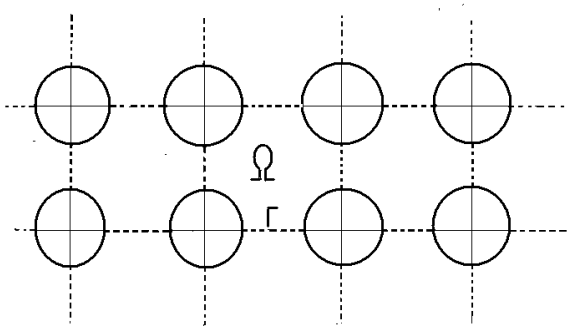

FIG. 6. 2D periodic lattice with romboidal periods

5. Examples of iso-energetic surfaces associated with solvable models of periodic lattices

Consider a typical example of a 2D lattice generated by a non-dimensional Schrödinger operator with real periodic potential obtained via restriction of Yukawa potential on the romboidal period (see Fig. 6) framed by the arcs of circles radius 0.05 centered on the corners of the square 1.1×1.1 and by the central intervals Γ_α^i length δ on the sides of the period. We choose the contacts Γ_α^i in form of intervals $0 < \gamma < \delta^i$ centered at the mid-points 0_α^i of the corresponding sides of the square period and span the contact spaces by $\sqrt{2/\delta^i}\sin l\pi\gamma/\delta^i$ and use the basic equation (31). The direction of vector ν is defined by the angle $\varphi = 0, 15^0, 30^0, 45^0$ between the orth e_1 and ν.

For strong Yukawa potential the dispersion function $\lambda(|p|)$ with 3D contact spaces $l = 1, 2, 3$ on the on the contacts is calculated for selected angles and is represented based on straightforward computing for the corresponding DN-map.

Our numerical experiments showed that beginning from dim $N = 3$ the shape of the dispersion function in the domain of low energy reveals clear features of stability, which gives a good reason to assume that the finite dimension of the contact subspace already allows to construct a realistic soluble model of the Schrödinger operator with Yukawa potential on the above square lattice (see Fig. 7, Fig. 8, Fig. 9).

Interesting resonance properties are revealed by Heine-Abarenkov potential constructed on a period as a potential well surrounded by the thick wall. The Dirichlet problem on the "romboidal" period for the corresponding Schrödinger operator has a single simple eigenvalue represented by an isolated pole of the DN-map plus a regular correcting term.

The rational approximation of the corresponding DN-map bordered by the projections on the corresponding 1D contact spaces N_1, N_2 , spanned by $\sqrt{2/\delta^i}\sin l\pi\gamma/\delta^i,\ l = 1$, for low temperature on the corresponding small temperature interval centered at the lowest resonance eigenvalue λ_1 has the form:

$$A\frac{Q}{\lambda - \lambda_1} + B = A_1\frac{\begin{pmatrix} Q_{aa} & Q_{a0} \\ Q_{0a} & Q_{00} \end{pmatrix}}{\lambda - \lambda_1} + \begin{pmatrix} B_{aa} & B_{a0} \\ B_{0a} & B_{00} \end{pmatrix},$$

with an one-dimensional orthogonal projection Q and a constant Hermitian matrix.

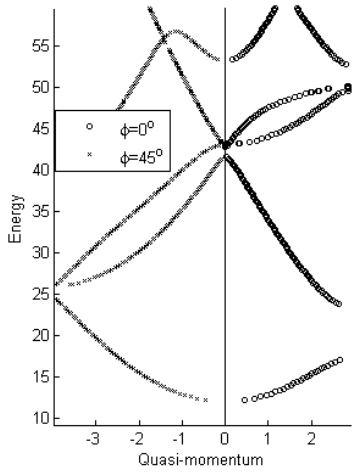

FIG. 7. Sections of the dispersion surface of the Yukawa lattice.

We select:

$$Q_{aa} = \frac{1}{2}\begin{pmatrix} \nu_1\rangle\langle\nu_1 & 0 \\ 0 & 0 \end{pmatrix}; \quad Q_{a0} = \frac{1}{2}\begin{pmatrix} 0 & \nu_1\rangle\langle\nu_2 \\ 0 & 0 \end{pmatrix}; \tag{32}$$

$$Q_{0a} = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ \nu_2\rangle\langle\nu_1 & 0 \end{pmatrix}; \quad Q_{00} = e_0\rangle\langle e_0 = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & \nu_2\rangle\langle\nu_2 \end{pmatrix}, \tag{33}$$

see Fig. 8. The regular term B depends on the upper eigenvalues and eigenfunctions.

We consider an example selecting the regular term as:

$$B = \begin{pmatrix} B_{aa} & B_{a0} \\ B_{0a} & 0 \end{pmatrix},$$

where:

$$B_{00} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \; B_{aa} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$B_{a0} = b_{a0}\begin{pmatrix} 0 & \nu_1\rangle\langle\nu_2 \\ \nu_2\rangle\langle\nu_1 & 0 \end{pmatrix}, \; B_{0a} = b_{0a}\begin{pmatrix} 0 & \nu_2\rangle\langle\nu_1 \\ \nu_1\rangle\langle\nu_2 & 0 \end{pmatrix}.$$

Elimination of the variables u_0', u_a', u_0 gives an equation for the 2-vector u_a:

$$\begin{aligned} &\frac{A}{\lambda - \lambda_1^D}\left[\mu Q_{0a}^N + \mu Q_{00}^N \mu^{-1} + Q_{aa}^N + Q_{a0}^N \mu^{-1}\right]\vec{u}_a + \\ &\left[\mu B_{0a}^N + \mu B_{00}^N \mu^{-1} + B_{aa}^N + B_{a0}^N \mu^{-1}\right]\vec{u}_a \equiv \\ &\left[\frac{A\mathcal{D}_Q(\lambda,p)}{\lambda - \lambda_1^D} + \mathcal{D}_B(\lambda,p)\right]\vec{u}_a = 0. \end{aligned} \tag{34}$$

The corresponding equation (34) has a nontrivial solution $\vec{u}_a$ if the determinant of the corresponding 2×2 matrix:

$$A\mathcal{D}_Q + (\lambda - \lambda_1^D)\mathcal{D}_B(\lambda, p),$$

vanishes. This condition yields the dispersion equation $\lambda = \lambda(\vec{p})$, with the quasi-momentum $\vec{p}$ defined by the quasi-momentum exponentials $\mu = \text{diag}\,(\mu_1, \mu_2) = \text{diag}\left(e^{ip_1}, e^{ip_2}\right)$.

In the case when the Heine-Abarenkov potential well is deep enough, there may be several eigenvalues with eigenfunctions localized in the well.

In particular, there is an eigenfunction symmetric with respect to reflection in the line connecting the mid points of Γ_0^1, Γ_a^1 and antisymmetric with respect to reflection in the line connecting the mid-points of Γ_0^2, Γ_a^2, or vice versa. The corresponding eigenvalue is non-degenerated if the potential is not symmetric with respect to the

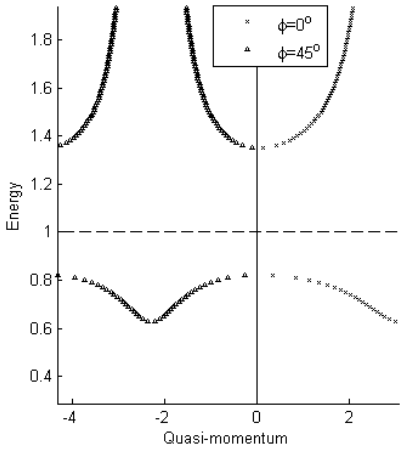

FIG. 8. Sections of the dispersion surface of an abstract model emulating Heine-Abarenkov potential with the lower resonance eigenvalue $\lambda_1 = 1$ (punctured line)

change of the variables $1 \to 2, 2 \to 1$. The corresponding DN-map is characterized by the polar term AQ with the projection:

$$Q = \frac{1}{2}\begin{pmatrix} \nu_1\rangle\langle\nu_1 & 0 & -\nu_1\rangle\langle\nu_1 & 0 \\ 0 & 0 & 0 & -\nu_1\rangle\langle\nu_1 \\ -\nu_1\rangle\langle\nu_1 & 0 & 0 & 0 \\ 0 & -\nu_1\rangle\langle\nu_1 & 0 & \nu_1\rangle\langle\nu_1 \end{pmatrix}.$$

If the correcting term is selected as above, we obtain the dispersion curves in various direction as shown one Fig. 5:

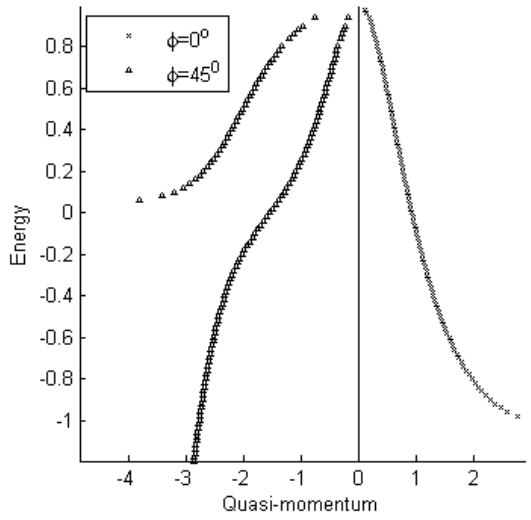

FIG. 9. Sections of the dispersion surface of the abstract model emulating Heine–Abarenkov potential with resonance eigenvalue $\lambda_2 > \lambda_1$

In fact, our proposal has a softer nature (in the sense of V. Arnold), due to the freedom of selection of the rational approximation (probably a multi-pole- approximation) for the real material lattice or sandwich on the resonance domain:

$$\mathcal{DN} \approx \sum_{s \le m} A_s \frac{Q_s}{\lambda - \lambda_s} + P_m(\lambda), \tag{35}$$

the choice of the contacts/contact subspaces and temperature (interval of admissible values of energy). We speculate that this problem, although it appears to be a mathematical one, lies outside of mathematics, on the interface with quantum chemistry, with its specific system of notions (covalent bonds, etc...) and methods.

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Appendix 1: Lagrangian version of the operator extension algorithm

John von Neumann – nearly 90 years ago – tried to attract attention of physicists to the basic difference between symmetric and self-adjoint operators, see [18], and proposed a geometrical solution to the most important problem of construction of a self-adjoint extension of a symmetric operator. Unfortunately, this solution was not, at that time, properly recognized by physicists. A few years later, E. Fermi, attempting to describe scattering of neutrons by nuclei, considered the Laplacian on a domain of smooth $L_2(R_3)$ functions with typical singularity at the origin $u = \dfrac{A^u}{4\pi|x|} + B^u + O(|x|)$ and discovered that the boundary form of the Laplacian:

$$J(u,v) = \lim_{\delta\to 0} \int\limits_{|x|>\delta} \left[-\Delta\bar{u}v + \bar{u}\Delta v\right] d^3x = \bar{A}^u B^v - \bar{B}^u A^v \tag{36}$$

vanishes under the boundary condition $B = \gamma A$ with real γ. Later probably used another approach to the problem of extending of a symmetric operator to the corresponding self-adjoint, which yields a convenient formula for the scattered waves, see [19]. Though the conventional proof of self-adjointness of the Laplacian under the above boundary conditions was proposed 25 years later, see [20], the approach to operator extension based on the boundary form proved to be extremely efficient, see for instance [12, 13, 21] [1]In 1970's, it was modified by introducing the inner structure into zero-range potential, see [12, 13], that allowed consideration of resonance interaction, which allows admission of fitting based on asymptotics Dirichlet-to-Neumann map of the corresponding unperturbed problem, see [22]. This approach allows one to develop an analytic perturbation technique for embedded eigenvalues, based on two step analytic perturbation procedure - a quantum Jump-Start analog of the corresponding classical techniques developed by Poincare [23] and, in particular, to propose a convenient solvable model for Quantum Networks, supplied with inner structure on the nodes, see [24] [2].

Hereafter, we produce a brief review of the Lagrangian operator extension techniques for an abstract operator, presenting the corresponding symplectic boundary form in terms of appropriate analog of boundary values, and imposing the corresponding boundary conditions, to select a domain of the relevant self-adjoint extension as a Lagrangian plane of the symplectic boundary form.

Consider a finite Hermitian matrix A in a finite-dimensional Hilbert space $A : K \to K$, dim $K = k$. Select a deficiency subspace $N_i \in K$, dim $N_i < k/2$, such that does not overlap with $N_{-i} = \dfrac{A+iI}{A-iI}N_i$ and consider the restriction $A_0 = A\Big|_{D_0}$ onto the subspace $D_0 \equiv (A-iI)^{-1}\left[K \ominus N_i\right]$. The restricted operator is not densely defined, but its formal adjoint can be defined by J. von Neumann formulae on the defect $N = N_i + N_{-i}$ as $A^+n_i + in_i = 0$, $n_i \in N_i$, $A^+n_{-i} - in_{-i} = 0$, $n_{-i} \in N_{-i}$, see [25], where the operator extension procedure is developed for A_0. In [12, 13], see also references therein, a simplectic version of the operator extension procedure was proposed for A_0, which is convenient for manufacturing zero-range perturbations with inner structure for differential operators, see for instance [12, 13, 24]. In particular, a quantum dot attached to the star-graph $\Gamma = \cup\gamma_l$ is modeled in [24] based on zero-range potential with inner structure while reducing $L \to L_0$ the Schrödinger operator by the condition of vanishing elements of the domain $D(L_0)$ near the knot $x = 0$ of the star, such that the adjoint opeartor L_0^+ has the boundary form represented as a sum over all branches γ_l of the star graph Γ, meeting at the node $x = 0$:

$$J^{ext}(u,v) = \sum_l \int\limits_{\gamma_l} \left[-\bar{u}_l^{"} v_l + \bar{u}_l v_l^{"}\right] dx = \sum_l \left[-\bar{u}_l' v_l + \bar{u}_l v_l'\right]\Big|_0, \tag{37}$$

[1]I. M. Gelfand attracted attention of mathematicians to importance of development a Lagrangian approach to operator extensions, based on selecting a Lagrangian plane in the domain of the adjoint operator, which would serve an alternative to the J. von Neumann geometrical construction, [26].

[2]Notice, that I. Prigogine in 1973 formulated the hypothesis on the validity of the Poincare two-step algorithm of analytic perturbation procedure for quantum problems, see [27], but could not prove it, because selected an incorrect anzsatz was selected for the corresponding Intermediate operator. The hypothesis was later proved for Quantum Networks based on the correct ansatz, [22], for the intermediate operator, presented in the form of zero-range model with an inner structure, constructed with use of Lagrangian technique of operator extension procedure [23]

with differentiation in an outgoing direction at the node. The boundary form of the inner Hamiltonian A is calculated in a special representation of the boundary form $J^{int}(u,v)$, constructed based on an orthogonal basis $\{e_l\} \subset N_i$:

$$\{W_+^l\} = \left\{\frac{1}{2}\left[e_l + \frac{A+iI}{A-iI}e_l\right]\right\} = \left\{\frac{A}{A-iI}e_l\right\} \text{ and } \{W_-^l\} = \left\{\frac{1}{2}\left[e_l - \frac{A+iI}{A-iI}e_l\right]\right\} = \left\{-\frac{1}{A-iI}e_l\right\}. \quad (38)$$

$$J^{ext}(u,v) = \sum_l \int\limits_{\gamma_l} \left[-\bar{u}_l^{"} v_l + \bar{u}_l v_l^{"}\right] dx = \sum_l \left[-\bar{u}_l' v_l + \bar{u}_l v_l'\right]\Big|_0, \quad (39)$$

with differentiation in an outgoing direction at the node. The boundary form of the inner Hamiltonian A is calculated in a special representation of the boundary form $J^{int}(u,v)$, constructed based on an orthogonal basis $\{e_l\} \subset N_i$:

$$\{W_+^l\} = \left\{\frac{1}{2}\left[e_l + \frac{A+iI}{A-iI}e_l\right]\right\} = \left\{\frac{A}{A-iI}e_l\right\} \text{ and } \{W_-^l\} = \left\{\frac{1}{2}\left[e_l - \frac{A+iI}{A-iI}e_l\right]\right\} = \left\{-\frac{1}{A-iI}e_l\right\}. \quad (40)$$

Then, each element from the defect $N = N_i + N_{-i}$ can be represented as $u = \sum_l \frac{A}{A-iI}\xi_+^l - \frac{1}{A-iI}\xi_-^l \equiv \frac{A}{A-iI}\vec{\xi}_+^u - \frac{1}{A-iI}\vec{\xi}_-^u$, and the vectors $\vec{\xi}_\pm^u \in N_i$ play roles of the boundary data. The boundary form of the formal adjoint operator A_0^+ is calculated on elements $u, v \in N$ from the defect as:

$$J^{int}(u,v) = \langle A^+u, v\rangle - \langle u, A^+v\rangle = \langle \vec{\xi}_+^u, \vec{\xi}_-^v\rangle - \langle \vec{\xi}_-^u, \vec{\xi}_+^v\rangle. \quad (41)$$

The ultimate formula is valid tot only on the defect, but on the whole space $K = D_0 + N$ with A_0^+ extended from N onto D_0 as A_0, that is , for $u = u_0 + u_N$:

$$A^+(u_0 + u_N) = A_0u_0 + A_0^+u_N,$$

so that the addendum A_0u_0 does not contribute to the boundary form $J^{ext}(u,v)$, and $J^{ext}(u,v) = \langle A^+u_N, v_N\rangle - \langle u_N, A^+v_N\rangle$. In particular, the boundary data $\xi_\pm^u$ for a solution of the homogeneous adjoint equation:

$$A^+(u_0 + u_N) - \lambda(u_0 + u_N) = 0$$

are connected by the Krein function $M(\lambda) = P_{N_i}\frac{I+\lambda A}{A-\lambda I}\Big|_{N_i}$ as:

$$\xi_-^u + P_{N_i}\frac{I+\lambda A}{A-\lambda I}\Big|_{N_i}\xi_+^u = 0. \quad (42)$$

A self-adjoint extension of the restricted operator A_0 on the defect is constructed as a part of the extended adjoint operator onto the Lagrangian plane N^B in the defect, submitted to the boundary condition:

$$\vec{\xi}_-^u + B\vec{\xi}_+^u = 0, \quad (43)$$

with an Hermitian operator $B : N_i \to N_i$ The boundary form (41) vanishes on the plane. Then, the corresponding self-adjoint extension of an original restricted operator A_0 is defined as a sum $A_0 + A^B$ acting according to the von Neumann formulae respectively in D_0 and in $N^B \subset N$ on elements:

$$u = u_0 + \frac{A}{A-iI}\vec{\xi}_+^u - \frac{I}{A-iI}\vec{\xi}_-^u$$

with the boundary values connected by the above boundary conditions .

The spectrum of the extension is defined by the Krein function:

$$P_{N_i}\frac{I+\lambda A}{A-\lambda I}P_{N_i} \equiv \mathcal{M}(\lambda), \quad (44)$$

which connects the boundary values $\vec{\xi}_\pm^u$ of the solution u of the homogeneous adjoint equation $A^+u - \lambda u = 0$:

$$\vec{\xi}_-^u + \mathcal{M}(\lambda)\vec{\xi}_+^u = 0. \quad (45)$$

and the spectrum of the extension A^B is defined by the singularities of the corresponding ratio

$$\frac{I}{B - \mathcal{M}(\lambda)}, \quad (46)$$

which serves the inner factor in the Krein formula for the resolvent of the extension:

$$\frac{I}{A^B-\lambda I}=\frac{I}{A-\lambda I}+\frac{A+iI}{A-\lambda I}P_{N_i}\frac{I}{B-\mathcal{M}(\lambda)}P_{N_i}\frac{A-iI}{A-\lambda I}. \tag{47}$$

Appendix 2: Solvable models of selected one-body spectral problems

In this section we construct a one-body model of a quantum dot Ω attached to the node of a 1D quantum star-graph $\Gamma=\Gamma_1\cup\Gamma_2\cup\Gamma_3\dots\Gamma_n$ and a one-body model of 1D periodic chain. Despite selection of simplest algebraic parameters for the corresponding solvable models, they have rich spectral propeties which can be easily monitored due to the algebraic nature of the parameters selected. Both models are constructed via Lagrangian version of the operator extension procedure, with regard of the symplectic boundary forms J balancing to zero on Lagrangian planes, selected based on the corresponding boundary conditions.

Quantum dot attached to the node of a quantum graph

On a star-graph $\Gamma=\Gamma_1\cup\Gamma_2\cup\Gamma_3\dots\Gamma_n$ of straight shoulders Γ_s attached to a compact domain Ω with a smooth boundary, we consider a spectral problem for a the 1D Schrödinger equation $L^\Gamma=-\vec{u}_\Gamma''$ in $L_2(\Gamma,E^\Gamma)$ with $E^\Gamma=C_n$, with regard of appropriate boundary condition connecting it with the Schrödinger operator $L_\Omega u_\Omega=-\Delta u_\Omega+Vu_\Omega$ on the domain Ω supplied with the zero boundary condition $L_2(\partial\Omega)\ominus E^\Omega$. A bond B is imposed on the contact $E^\Omega\times E^\Gamma$ with the projection $P^\Omega\equiv P_{E^\Omega}$. This was done with the consideration of the boundary forms calculated on both sides of the contact $\Gamma\cap\partial\Omega$ in the corresponding contact subspaces $C_n=E^\Gamma,E^\Omega$, with $P^\Omega\equiv P_{_{E^\Omega}}$:

$$J_\Gamma(u_\Gamma,v_\Gamma)\equiv\langle\vec{u}_\Gamma',\vec{v}_\Gamma\rangle-\langle\vec{u}_\Gamma,\vec{v}_\Gamma'\rangle,\;\; J_\Omega(u_\Omega,v_\Omega)\equiv-\langle\frac{\partial u_\Omega}{\partial n},P^\Omega v_\Omega\rangle+\langle P^\Omega u_\Omega,\frac{\partial v_\Omega}{\partial n}\rangle, \tag{48}$$

and a boundary condition imposed with an Hermitian matrix:

$$B=\begin{pmatrix}0 & b_{ei}\\ b_{ie} & a_{ii}\end{pmatrix},\;\begin{pmatrix}\vec{u}_\Gamma'\\ -P^\Omega\frac{\partial u_\Omega}{\partial n}\end{pmatrix}+B\begin{pmatrix}\vec{u}_\Gamma\\ P^\Omega u_\Omega\end{pmatrix}=0, \tag{49}$$

with an Hermitian operator $a_{ii}:E^\Omega\to E^\Omega$ and $b_{ei}:E^\Omega\to E^\Gamma$, $b_{ie}=b_{ei}^+$. We denote by $\mathcal{M}\equiv-P^\Omega\mathcal{D}\mathcal{N}P^\Omega=\sum_l\frac{P^\Omega\frac{\partial\varphi_l}{\partial n}\rangle\langle\frac{\partial\varphi_l}{\partial n}P^\Omega}{\lambda_l-\lambda}$ the framed DN-map [3] of the quantum dot:

$$-\Delta u_\Omega+Vu_\Omega=\lambda u_\Omega,\;\mathcal{D}\mathcal{N}:u_\Omega\to\left.\frac{\partial u_\Omega}{\partial n}\right|_{\partial\Omega},$$

and rewrite equation (49), for the scattering Ansatz $e^{ipx}\vec{e}+e^{-ipx}S\vec{e}=\vec{u},\;p^2=\lambda$:

$$\begin{array}{rr}ip(I-S)e+ & b_{ei}P^\Omega u_\Omega=\;\;0\\ \left[\mathcal{M}+a_{ii}\right]P^\Omega u_\Omega+ & b_{ie}(I+S)e=\;\;0.\end{array} \tag{50}$$

Eliminating $P^\Omega u_\Omega$ and introducing $b_{ei}\frac{1}{\mathcal{M}+a_{ii}}b_{ie}\equiv\mathcal{N}^b(\lambda)$, we obtain an expression for the scattering matrix:

$$S(p)=\frac{ip-\mathcal{N}^b}{ip+\mathcal{N}^b},\;\text{ with }\;\Im\mathcal{N}^b\,\Im\lambda>0, \tag{51}$$

in terms of the framed Neumann-to-Dirichlet map $\mathcal{N}^b$.

Though the Dirichlet-to-Neumann map of the 3D domain Ω can be computed with standard programs, see for instance [28], yet it is also convenient to substitute it by perturbation analysis [] using finite-dimensional approximation, taking into account only a finite number of eigenvalues λ_l or substituting the quantum dot by zero-range potential with inner structure, see [12, 13]. In particular, for a 1D framed DN map, the framed ND-map $\mathcal{N}^b\equiv b_{ei}\frac{1}{\mathcal{M}+a_{ii}}b_{ie}$ has generally has asymptotes at infinity $\lambda\to\infty$:

$$\mathcal{N}^b(\lambda)=\hat{A}\lambda+\hat{A}_0+\sum_{l=1}^{k}\frac{A_l}{\lambda_l-\lambda}, \tag{52}$$

with $\hat{A}\geq0$, $A_0=\bar{A}_0$, $A_l\geq0$. It is possible to select a finite-dimensional self-adjoint operator $A:K\to K$ and an interaction B, with non-overlapping deficiency subspaces N_i,N_{-i} such that, being attached to node of the

[3] The above formal series is actually divergent, but may be properly regularized, see for instance [29].

above star-graph Γ, plays a role of an inner Hamiltonian of a quantum dot with the scattering matrix (51) on the star-graph, with the boundary conditions .

A solvable model of a discrete lattice

Consider a 1D periodic lattice (a chain) of equivalent quantum dots $\Omega \equiv \Omega_l$ arising of equivalent finite-dimensional operators $A_l \equiv A : K_l \to K_l$, with equivalent non-overlapping 1D deficiency subspaces N_i^l, N_{-i}^l. Each quantum dot is substituted by the zero-range potential with an inner structure as described in Appendix 1:

$$\xi_+ \sim P_E u^\Omega\Big|_\Gamma, \ \xi_- \sim -P_E \frac{\partial u^\Omega}{\partial n}\Big|_\Gamma, \ \xi_- + \mathcal{M}\xi_+ = 0, \tag{53}$$

and a pair of infinite-dimensional vectors $\vec{\xi}_+ = \sum_l \xi_-^l$, $\vec{\xi}_- = \sum_l \xi_+^l$, which play a role of the boundary values for the whole chain. We choose the simplest translation - invariant boundary conditions, connecting the nearest neighbors in the chain as:

$$\xi_-^l + b^+ \xi_+^{l-1} + b_0 + b\ \xi_+^{l+1} = 0, \text{ or, alternatively} \xi_+^l + c^- \xi_-^{l-1} + c_0 + c\ \xi_-^{l+1} = 0. \tag{54}$$

Denoting the sequence ξ^l shifted one step to the left as $T^+\vec{\xi} = \left\{\xi^{l+1}\right\}$ and, similarly the sequence shifted one step to the right $T\vec{\xi} = \left\{\xi^{l-1}\right\}$, we represent the above boundary conditions respectively as:

$$\begin{aligned} \vec{\xi}_- + \left[b^+T^+ + b_0 + bT\right]\vec{\xi}_+ = 0 \equiv \vec{\xi}_- + B\vec{\xi}_+, \\ \vec{\xi}_+ + \left[c^+T^+ + c_0 + cT\right]\vec{\xi}_+ = 0 \equiv \vec{\xi}_+ + C\vec{\xi}_-, \end{aligned} \tag{55}$$

Regarding the periodicity of the chain of quantum dots, the corresponding sequences of their Weyl-Titchmatsh or Krein finctions diag $\mathcal{M} \equiv \oplus \sum \mathcal{M}_l$ are also periodics:

$$T^+ \text{diag}\mathcal{M}T = T\text{diag}\mathcal{M}T^+ = \text{diag}\mathcal{M}.$$

With 1D contact subspaces $E_l \equiv E$ and the interaction B or C between the boundary data on the chain, the boundary values of the relevant Bloch functions $\vec{\Xi}$ are quasi-periodic $\Xi_\pm^l = e^{ipl}\ \Xi_\pm^0$, with regard to the quasimomentum p:

$$\begin{aligned} \mathcal{M}\Xi_+^0 - \left[b^+e^{-ip} + b_0 + be^{ip}\right]\Xi_+^0 = 0, \text{ for the boundary codition } B, \text{ and} \\ \Xi_+^0 - \mathcal{M}\left[c^+e^{-ip} + c_0 + ce^{ip}\right]\Xi_+^0 = 0 \end{aligned} \tag{56}$$

for the boundary condition C. In the case of the quantum dot substituted by the zero-range boundary condition with an inner structure, as in Appendix 1:

$$\mathcal{M} = P_E\frac{I+\lambda A}{A-\lambda I}P_E = -P_EAP_E + P_E\frac{I+A^2}{A-\lambda I}P_E \approx -P_EAP_E - \frac{P_E(I+A^2)P_E}{\lambda} + O(1/\lambda)^2 \tag{57}$$

For a special choice of the boundary parameters $-P_EAP_E = b_0$ with regards to $\mathcal{M} + b_0 \to 0$ or, correspondingly, $c_0P_EAP_E = 1$ with regards to $I + \mathcal{M}c_0 \to 0$ while $\lambda \to \infty$, we get for the special choice of the boundary parameters:

$$P_A\frac{I+A^2}{A-\lambda}P_E\Xi_+^0 + 2|b|\cos(p+\varphi_b)\Xi_+^0 = 0, \tag{58}$$

and correspondingly:

$$\left(I + c_0P_EAP_E\right)\Xi_+^0 - P_E\frac{(I+A^2)}{A-\lambda I}P_E 2|c|\cos(p+\varphi_c)\Xi_+^0 = 0. \tag{59}$$

The Nevanlinna function $P_A\frac{(I+A^2)}{A-\lambda}P_E$ is invertible on real axis, and the innverse is also a Nevanlinna function arising from a pair E, G with a finite-dimensional operator $G : K \to K$ with selected deficiency subspace $N_i = E$ [4]

$$-\left[P_E\frac{(I+A^2)}{A-\lambda}P_E\right]^{-1} = \lambda\left[P_E(I+A^2)P_E\right]^{-1} - P_EGP_E + P_E\frac{I+G^2}{G-\lambda I}P_E, \tag{60}$$

hence first addendum in (59) multiplied by $\left[P_E\frac{(I+A^2)}{A-\lambda}P_E\right]^{-1}$ yields:

$$\left(I + c_0P_EAP_E\right)\left[\lambda\left[P_A(I+A^2)P_E\right]^{-1}\Xi_+^0 - P_EGP_E + P_E\frac{I+G^2}{G-\lambda I}P_E\right]\Xi_+^0. \tag{61}$$

[4]The operators A and G are connected similarly to Laplacean with Dirichlet and Neumann boundary conditions on a domain with a smooth boundary.

This allows one to rewrite the dispersion equation (59) as:

$$(I + c_0 P_E A P_E)\left[\lambda\left[P_A(I+A^2)P_E\right]^{-1}\Xi_+^0 - P_E G P_E + P_E\frac{I+G^2}{G-\lambda I}P_E\right]\Xi_+^0 + 2|c|\cos(p+\varphi_c)\Xi_+^0 = 0. \quad (62)$$

The equations (58, 62) show typical dispersion functions of 1D periodic lattices.

The most important characteristics of periodic lattices are the quasimomentum and the effective mass, which are calculated from the dispersion function as the inverse of the derivative of energy with respect to the quasimomentum $\left[\frac{\partial\lambda}{\partial p_s \partial_t}\right]^{-1} \equiv m_{st}$. For a 1D discrete periodic chain of "quantum dots", we calculate the effective mass in terms of the relevant Krein function (abstract analog of the Weyl-Titchmarsh function) and the boundary parameter β.

Assuming that the dispersion equation for the chain is $\mathcal{M} - b\cos p = 0$, we differentiate the dispersion equation twice with respect to quazimomentum:

$$\mathcal{M}(\lambda) - \beta\cos p = 0 \longrightarrow \frac{d\mathcal{M}}{d\lambda}\ \frac{d\lambda}{dp} + \beta\sin\ p = 0 \longrightarrow$$

$$\longrightarrow \frac{d^2\mathcal{M}}{d\lambda^2}\ \left[\frac{d\lambda}{dp}\right]^2 + \frac{d\mathcal{M}}{+}d\lambda\ \frac{d^2\lambda}{dp^2} + \beta\cos\ p = 0,$$

and use the 1D the 1D formula for the effective mass $m = \left[\frac{d^2\lambda}{dp^2}\right]^{-1}$. This implies:

$$m = -\frac{\frac{d\mathcal{M}}{d\lambda}}{\beta\cos p + \frac{d^2\mathcal{M}}{d\lambda^2}\left(\frac{d\lambda}{dp}\right)^2}.$$

In experiment, the effective mass is usually measured at the ends of the spectral bands $\sin p = 0$, where $\frac{d\lambda}{dp} = 0$. Then the second term in the denominator vanishes and we get at the ends of spectral bands:

$$m = -\frac{\frac{d\mathcal{M}}{d\lambda}}{\beta\cos p} = -\frac{\frac{d\mathcal{M}}{d\lambda}}{\mathcal{M}(\lambda)}.$$

Spectral structure of a 1D superlattice via analytic perturbation procedure

We consider a couple of two non-enteracting 1D discrete periodic lattices with typical dispersion equations similar to above (58,62) and the corresponding weakly perturbed pair:

$$-\frac{A_1}{\lambda}e_1 + B_1\lambda e_1 + C_1 e_1 - \beta_1\cos p,\quad e_1 = 0,\quad \frac{2A_2\lambda}{1-\lambda^2}\,e_2 - \beta_2\cos p\ e_2 = 0$$

$$-\frac{A_1}{\lambda}\,e_1 + B_1\,\lambda\,e_1 + C_1\,e_1 - \cos p\,[\beta_1\,e_1 + \delta\,e_2] = 0,\ \frac{2A_2\lambda}{1-\lambda^2}e_2 - \cos p\,[\beta_2\,e_2 + \delta\,e_1] = 0. \quad (63)$$

Hereafter we assume, with regard of the diagram (10) that $B_1 > 0$, $A_{1,2} > 0$ are small, and $\delta_{1,2} > 0$ are much smaller and $\beta_{1,2} > 0$. The perturbed dispersion equation is reduced to the determinant condition for the above linear system:

$$\det\begin{pmatrix} -\frac{A_1}{\lambda} + B_1\,\lambda + C_1 - \cos p\,\beta_1 & \delta\,\cos p \\ \delta\,\cos p & \frac{2A_2\lambda}{1-\lambda^2} - \cos\,p\,\beta_2 \end{pmatrix} = 0. \quad (64)$$

The perturbed spectral bands are found from the determinant condition with regard of real quasimomentum $p : -1 < \cos p < 1$. The determinant condition is presented as:

$$\left[-\frac{2A_1A_2}{1-\lambda^2} - \frac{2A_2B_1\lambda^2}{1-r\lambda^2}\right] + \cos p\left[(\frac{A_1}{\lambda} - B_1\lambda)\beta_2 - \beta_1\frac{2A_2\lambda}{1-\lambda^2}\right] +$$

$$+(\beta_1\,\beta_2 - \delta^2)\cos^2 p \equiv -K_0 - \cos pK_1 + K_2\cos^2 p = 0, \quad (65)$$

which implies:

$$|K_0 \pm \sqrt{K_1^2 + 4K_0\,K_2}| \le 2K_0. \quad (66)$$

The ultimate condition corresponds, depending on the choice of parameter, to various physical conditions and the corresponding different physical properties of the perturbed superlattice.

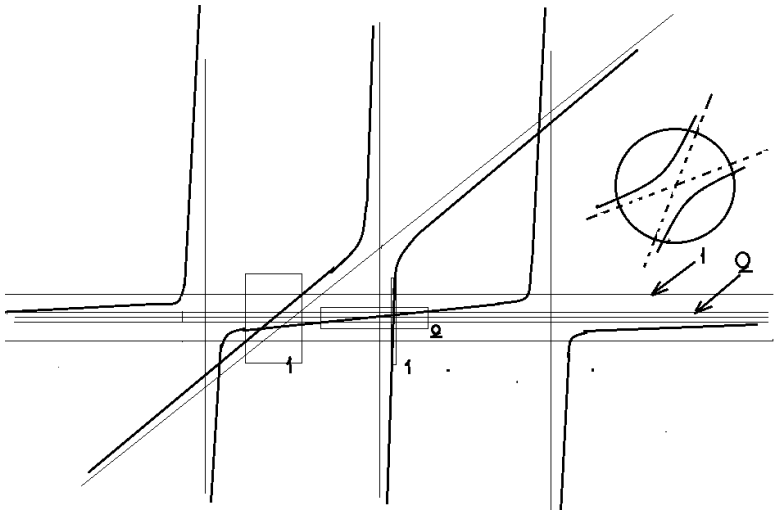

FIG. 10. The spectral structure of the perturbed superlattice with regards to quasi-crossings of terms of the underlying unperturbed lattices. The typical quasi-crossing for terms of the Nevanlinna-class dispersion equations. The unperturbed spetral bands are shown as thin rectangles marked by numbers 1, 2

Acnowledgements

The autors are grateful to V. B. Bogevolnov for providing extremely interesting and inspiring material – the carbon flakes obtained by detonation – which served main object of our experimental and the theoretical study. We are also grateful to Prof. G. Fursey, Prof. P. Konorov, Prof. P. Schwerdtfegger and Dr. Krista Steenbergen for an inspirating discussion of the mathematical analog of the shaky concept of chemical bound with respect to the problem of selection appropriate contact subspaces for fitted solvable models of periodic lattices.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 835–841

Control and inverse problems for networks of vibrating strings with attached masses

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DOI 10.17586/2220-8054-2016-7-5-835-841

We consider the control and inverse problems for serially connected and tree-like networks of strings with point masses loaded at the internal vertices. We prove boundary controllability of the systems and the identifiability of varying coefficients of the string equations along with the complete information on the graph, i.e. the loaded masses, the lengths of the edges and the topology (connectivity) of the graph. The results are achieved using the Titchmarch-Weyl function for the spectral problem and the Steklov-Poincaré operator for the dynamic wave equation on the tree. The general result is obtained by the leaf peeling method which reduces the inverse problem layer-by-layer from the leaves to the fixed root of the tree.

Keywords: wave equation on graphs, inverse problem, boundary control.

Received: 12 September 2016

1. Introduction

This paper concerns the control and inverse problems for differential equations on quantum graphs. By quantum graphs, we understand differential operators on geometric graphs coupled by certain vertex matching conditions. B. S. Pavlov and his former student N. I. Gerasimenko were among the first researchers to develop a mathematically rigorous approach to differential operators on metric graphs in the 1980's [1, 2].

Network-like structures play a fundamental role in many scientific and engineering problems. The classical problem here that aries from applications is the problem of oscillations of the flexible structures made of strings, beams, cables, and struts. These models describe bridges, space-structures, antennas, transmission-line posts, steel-grid reinforcements and other typical objects of civil engineering. More recently, the applications on a much smaller scale have come into focus. In particular, hierarchical materials like ceramic or metallic foams, percolation networks and carbon and graphene nano-tubes, and graphene ribbons have attracted much attention.

Papers discussing differential and difference equations on graphs have been appearing in various areas of science and mathematics since the 1930's, but in the last two decades, their numbers have grown enormously. Quantum graphs arise as natural models of various phenomena in chemistry (free-electron theory of conjugated molecules), biology (genetic networks, dendritic trees), geophysics, environmental science, disease control, and even in the internet (internet or network tomography). In physics, interest in quantum graphs arose, in particular, from applications to nano-electronics and quantum waveguides. On the other hand, quantum graph theory gives rise to numerous challenging problems related to many areas of mathematics from combinatorics to PDEs and spectral theory. Work on quantum graph theory and its applications have truly interdisciplinary character, and a series of meetings on this topic has stimulated collaboration of researchers from different areas of science, engineering and mathematics. A number of surveys and collections of papers on quantum graphs have appeared recently, and the first book on this topic by Berkolaiko and Kuchment [3] contains an excellent list of references.

Control and inverse theories constitute important parts of this rapidly developing area of applied mathematics — analysis on graphs. It is tremendously important for all aforementioned applications. However, these theories have not been sufficiently developed. Control and inverse problems for DEs on graphs appear to be much more complicated than similar problems on an interval (see, e.g. [4, 5] and references therein).

A new effective leaf-peeling method for solving inverse problems for differential equations on graphs without cycles has been proposed in [5] and developed further in [6, 7]. The main goal of the present paper is to extend this method to DEs on graphs with attached point masses.

Let $\Gamma = E \cup V$ be a finite compact metric graph without cycles, where $E = \{e_j\}_{j=1}^N$ is a set of edges and $V = \{\nu_j\}_{j=1}^{N+1}$ is a set of vertices. We recall that a graph is called a *metric graph* if every edge $e_j \in E$ is identified with an interval (a_{2j-1}, a_{2j}) of the real line with a positive length $l_j = |a_{2j-1} - a_{2j}|$, and a graph is a tree if it

has no cycles. The edges are connected at the vertices v_j which can be considered as equivalence classes of the edge end points $\{a_j\}$.

Let $\{\gamma_1, \dots, \gamma_m\} = \partial\Gamma \subset V$ be the boundary vertices, i.e. if the index (or multiplicity) of a vertex, $id(\nu)$, is the number of edges incident to it, then $\partial\Gamma = \{\nu \in V | id(\nu) = 1\}$. A nonnegative mass M_ν is attached to each vertex $\nu \in V \setminus \partial\Gamma$.

In Fig. 1 we give an example of a star graph (a graph with one internal vertex). Such graphs play an important role in the leaf peeling method described below in Sec. 3. A tree with $m = 9$ and $N = 12$ is presented in Fig. 2.

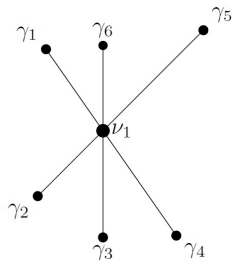

FIG. 1. A star graph

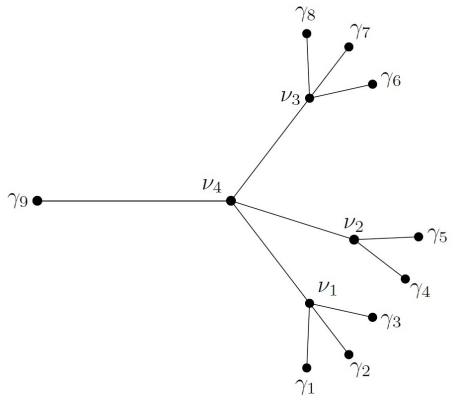

FIG. 2. A metric tree

Let q be a continuous function on Γ. Our initial boundary value problem is:

$$u_{tt} - u_{xx} + q(x)u = 0 \text{ in } \{\Gamma \setminus V\} \times (0, T) \tag{1.1}$$

$$\begin{array}{l} \sum_{e_j \sim \nu} \partial u_j(\nu, t) = M_\nu u_{tt}(\nu, t) \text{ at each vertex } \nu \in V \setminus \partial\Gamma, \text{ and } t \in [0, T] \\ u(\cdot, t) \text{ is continuous at each vertex, for } t \in [0, T] \end{array} \tag{1.2}$$

$$u = f \text{ on } \partial\Gamma \times [0, T] \tag{1.3}$$

$$u|_{t=0} = 0 \text{ in } \Gamma. \tag{1.4}$$

In (1.2) (and below), $\partial u_j(\nu)$ denotes the derivative of u at the vertex ν taken along the edge e_j in the direction outwards from the vertex. Also, $e_j \sim \nu$ means edge e_j is incident to the vertex ν, and the sum is taken over all edges incident to ν. Since $\partial\Gamma$ consists of m vertices, f can be naturally identified with a function acting from $[0, T]$ to $\mathbb{R}^m$.

The metric graph Γ determines naturally the Hilbert space of square integrable functions $\mathcal{H} = L^2(\Gamma)$. We define the space $\mathcal{H}^1$ of continuous functions v on Γ such that $v_{|_e} \in H^1(e)$ for every $e \in E$.

The f appearing in (1.3) is the (boundary) control for the problem (1.1)-(1.4), and a solution to (1.1)-(1.4) will be denoted u^f. One can prove that for $f \in \mathcal{F}^T := L^2([0, T]; \mathbb{R}^m)$, the generalized solution v^f of (1.1)-(1.4) belongs to $C([0, T]; \mathcal{H})$ (see Theorem 1 below), and the *control operator* $W^T : \mathcal{F}^T \to \mathcal{H}$, given by $W^T f := u^f(\cdot, T)$ is bounded.

The *response operator* (Steklov-Poincaré operator) for the system, $R^T = \{R^T_{ij}\}^m_{i,j=1}$, defined on $\mathcal{F}^T$ is defined by:

$$(R^T f)(t) = \partial u^f(\cdot, t)|_{\partial\Gamma}\,, \qquad 0 < t < T\,. \tag{1.5}$$

Our *dynamic* inverse problem is to recover the unknown coefficient $q(x)$ on each edge of the graph from the response operator R^T. We can also recover the graph topology, all $M_\nu, \nu \in V \setminus \partial\Gamma$, and the lengths of all the edges. We can actually do this with the reduced operator $\{R^T_{ij}\}^{m-1}_{i,j=1}$. That is, the method has the flexibility of not needing the control and observation at one of the boundary vertices. We prove the dynamic inverse problem has a unique solution for sufficiently large T (see Theorem 2 below) and give a constructive method for finding it.

Applying formally the Fourier–Laplace transform

$$g \mapsto \int_0^\infty g(t) e^{i\omega t} dt$$

to equations (1.1)–(1.3), we obtain the following boundary value problem depending on a complex parameter $\lambda = \omega^2$:

$$-\phi_{xx}(x,\lambda) + q(x)\,\phi(x,\lambda) = \lambda\,\phi(x,\lambda) \text{ on } \{\Gamma \setminus V\}, \tag{1.6}$$

$$\begin{array}{l} \sum_{e_j \sim \nu} \partial\phi_j(\nu,\lambda) = -\lambda\, M_\nu \phi(\nu,\lambda) \text{ at each vertex } \nu \in V \setminus \partial\Gamma, \\ \phi(\cdot,\lambda) \text{ is continuous at each vertex,} \end{array} \tag{1.7}$$

The system of differential equations (1.6), (1.7) with zero Dirichlet boundary condition has only a trivial solution for $\lambda \notin \mathbb{R}$. Therefore, for any $\alpha \in \mathbb{C}^m$, this system of equations has a unique solution, $\phi^\alpha(x,\lambda)$, satisfying non-zero boundary conditions:

$$\phi^\alpha(\gamma_j,\lambda) = \alpha_j, \;\; j = 1,2,...,m, \;\; \alpha = \; \mathrm{col}\,\{\alpha_1,\ldots,\alpha_m\}, \tag{1.8}$$

The $m \times m$ matrix $\mathcal{M}(\lambda)$ defined by $\mathcal{M}(\lambda)\,\alpha = \partial\phi^\alpha|_{\partial\Gamma}$ is called the Titchmarsh–Weyl matrix function, or the TW-function. The TW-function is also known as the (spectral) Dirichlet-to-Neumann map. The TW-function $\mathcal{M}(\lambda)$ known for $\Im\lambda > 0$ will play the role of the spectral data for solving boundary inverse problems on graphs.

2. Main results

In the case of a string with loaded masses it was noticed [8, 9] that the wave transmitted through a mass is more regular than the incoming wave. A similar effect also occurs for networks of strings. To formulate the result, we need the following definition. Among all paths from edge e_i to the boundary vertex γ_j, let the degree, d_i, of the edge e_i be the minimal (with respect to j) number of nonzero loaded masses on the path. For the following theorem we assume that $q|_{\overline{e_j}} \in C^{d_j}(\overline{e_j})$.

Theorem 1. *Assume $M_\nu > 0$ for all ν. If $f \in \mathcal{F}^T$, then for any $t \in [0,T]$, $u^f(\cdot,t) \in \mathcal{H}$ and $u^f \in C([0,T];\mathcal{H})$. Furthermore, for each $e_j \in E$, $u^f|_{e_j} \in C([0,T];H^{d_j}(e_j))$.*

The proof of the theorem is based on the analysis of the waves incoming to, transmitted through and reflected from an inner vertex, taking into account the conditions (1.2). For the simplest graph of serially connected strings with attached masses such a result was obtained in [8].

The next theorem describes the solution of the dynamic inverse problem.

Theorem 2. *Let $T_* = 2\max_{j\neq m} dist\{\gamma_j,\gamma_m\}$. The operator $\{R^T_{ij}\}_{i,j=1}^{m-1}$ known for $T > T_*$ uniquely determines q on Γ, $\{M_\nu : \nu \in V \setminus \partial\Gamma\}$, $\{l_j : j = 1,\ldots,N\}$ and the graph topology. If the topology is known, all other parameters can be found from the main diagonal $\{R^T_{ii}\}_{i=1}^{m-1}$ of the reduced response operator.*

We also extend to our networks the leaf peeling method proposed in [5] (and generalized for strings with attached masses in [10]) and develop a constructive algorithm solving the inverse problem.

A spectral analog of Theorem 2 reads as follows.

Theorem 3. *The reduced TW matrix function $\{\mathcal{M}_{ij}(\lambda)\}_{i,j=1}^{m-1}$ known for $\Im\lambda > 0$ uniquely determines q on Γ, $\{M_\nu : \nu \in V \setminus \partial\Gamma\}$, $\{l_j : j = 1,\ldots,N\}$ and the graph topology. If the topology is known, all other parameters can be found from the main diagonal $\{\mathcal{M}_{ii}(\lambda)\}_{i=1}^{m-1}$ of the reduced TW matrix function.*

3. Proof of Theorem 3

The response operator R^T and TW-function $\mathcal{M}(\lambda)$ are connected with each other by the Fourier–Laplace transform (see, e.g. [5]). Therefore, knowledge of $\mathcal{M}(\lambda)$ allows one to find R^T for all $T > 0$, and knowledge of R^T for all $T > 0$ allows one to find $\mathcal{M}(\lambda)$.

In this section, we prove Theorem 3. We will give a brief description of an algorithm which allows us to recalculate the TW matrix function from the original graph to a smaller graph by "pruning" boundary edges. Ultimately, doing so allows us to reduce the original inverse problem on the graph to the inverse problem on a single interval.

Our reduction algorithm combines both spectral and dynamical approaches, i.e. uses $\mathcal{M}(\lambda)$ and R^T. As we mentioned above, the TW matrix function determines the response operator for the system (1.1)-(1.4). Therefore, under the conditions of Theorem 3 the entries $R^T_{ij}, i,j = 1,\ldots,m-1$ are known for $T > 0$.

Step 1. Knowledge of R^T_{jj} for sufficiently large T allows one to recover the length of the edge $e \in E$ incident to γ_j, the potential q on e and the mass M_ν, where $\nu \in V \setminus \partial\Gamma$ is an inner vertex to which e is incident. We can also recover $id(\nu)$, the total number of edges incident to ν. The proof of these statements is based on the analysis

of the waves incoming to, transmitted through and reflected from vertex ν. Similar analysis was presented in [5] without the loaded masses; this was based on the boundary control method in inverse theory.

Step 2. We determine the boundary edges which have a common end point using the non-diagonal entries R^T_{ij} of the response operator. Since the speed of wave propagation in the system (1.1)-(1.4) equals one, two boundary edges, say, e_i and e_j, incident to the boundary edges γ_i and γ_j with the lengths l_i and l_j have a common end point if and only if:

$$R^T_{ij} = \begin{cases} 0 & \text{for } T < l_i + l_j \\ \neq 0, & \text{for } T > l_i + l_j. \end{cases} \tag{3.1}$$

Definition of a sheaf. We consider a subgraph of Γ which is a star graph consisting of *all* edges incident to an internal vertex v. This star graph is called a sheaf if all but one its edges are the boundary edges of Γ. It is known that any tree has at least two sheaves.

Step 3. Leaf peeling. We consider now a sheaf consisting, say, of several boundary edges $e_1, \dots, e_p,\ p < m$, incident to boundary vertices $\gamma_1, \dots, \gamma_p$ are connected at the vertex ν_s (see, e.g. vertices $\gamma_1, \gamma_2, \gamma_3, \nu_1$ on Fig. 2). From Step 1, we know the potential on these edges, their lengths and the index of the vertex ν_s.

The index of the vertex ν_s is $p+1$ and there is exactly one internal edge incident to ν_s. We denote by $\widetilde{\mathcal{M}}(\lambda)$ the TW matrix function associated with the reduced graph $\widetilde{\Gamma}$, i.e. the original graph Γ without the boundary edges $e_1, \dots, e_p$ and vertices $\gamma_1, \dots, \gamma_p$.

We denote by $\widetilde{\mathcal{M}}_{0i}(\lambda)$, $\widetilde{\mathcal{M}}_{i0}(\lambda)$ and $\widetilde{\mathcal{M}}_{00}(\lambda)$ the entries of $\widetilde{\mathcal{M}}(\lambda)$ related to the "new" boundary point ν_{s_0} of the graph $\widetilde{\Gamma}$. The other entries of $\widetilde{\mathcal{M}}(\lambda)$ are denoted by $\widetilde{\mathcal{M}}_{ij}$, $i, j = p+1, \dots, m$. We demonstrate now how to find the entries of $\widetilde{\mathcal{M}}(\lambda)$.

First, we recalculate the entries $\widetilde{\mathcal{M}}_{00}(\lambda)$ and $\widetilde{\mathcal{M}}_{0i}(\lambda)$, $i = p+1, \dots, m-1$. we choose a boundary point, say γ_1, of the star-subgraph. Let $\phi(x, \lambda)$ be the solution to the problem (1.6), (1.7) subject to the boundary conditions:

$$\phi(\gamma_1, \lambda) = 1, \quad \phi(\gamma_j, \lambda) = 0, \quad j = 2, \dots, m-1, m. \tag{3.2}$$

We notice that on the boundary edge e_1 the function ϕ solves the Cauchy problem:

$$-\phi'' + q(x)\phi = \lambda\phi, \quad x \in e_1, \tag{3.3}$$

$$\phi(\gamma_1, \lambda) = 1,\ \phi'(\gamma_1, \lambda) = \mathcal{M}_{11}(\lambda). \tag{3.4}$$

On the other edges of the star subgraph it solves

$$-\phi'' + q(x)\phi = \lambda\phi, \quad x \in e_i, \quad i = 2, \dots, p, \tag{3.5}$$

$$\phi(\gamma_i, \lambda) = 0,\ \phi'(\gamma_i, \lambda) = \mathcal{M}_{1i}(\lambda), \quad i = 2, \dots, p. \tag{3.6}$$

Since the potential on the edges $e_1, \dots, e_p$ is known, we can solve the Cauchy problems (3.3), (3.4) and (3.5), (3.6) and use the matching conditions (1.7) at the internal vertex ν_s to recover the values $\phi(\nu_s, \lambda)$ and $\phi'(\nu_s, \lambda)$ on the "new" boundary edge at the "new" boundary point ν_s. Thus we obtain:

$$\begin{aligned} \widetilde{\mathcal{M}}_{00}(\lambda) &= \tfrac{\phi'(\nu_s,\lambda)}{\phi(\nu_s,\lambda)}, \\ \widetilde{\mathcal{M}}_{0i}(\lambda) &= \tfrac{\mathcal{M}_{1i}(\lambda)}{\phi(\nu_s,\lambda)}, \quad i = p+1, \dots, m. \end{aligned} \tag{3.7}$$

We recall that here $\Im\lambda \neq 0$, and so, $\phi(\nu_s, \lambda) \neq 0$. Otherwise, λ would be an eigenvalue of a selfadjoint operator.

To find $\widetilde{\mathcal{M}}_{i0}(\lambda)$ and $\widetilde{\mathcal{M}}_{ij}(\lambda)$, $i = p+1, \dots, m-1$ we fix γ_i $(i > p)$ and consider the solution $\psi(x, \lambda)$ to (1.6), (1.7) with boundary conditions

$$\psi(\gamma_i, \lambda) = 1, \quad \psi(\gamma_j, \lambda) = 0, \quad j \neq i. \tag{3.8}$$

The function ψ then solves the following Cauchy problems on the edges $e_1, \dots, e_p$:

$$-\psi'' + q(x)\psi = \lambda\psi, \quad x \in e_j, \quad j = 1, \dots, p, \tag{3.9}$$

$$\psi(\gamma_j, \lambda) = 0,\ \psi'(\gamma_j, \lambda) = \mathcal{M}_{ij}(\lambda). \tag{3.10}$$

Since we know the potential on the edges $e_1, \dots, e_p$, we can solve the Cauchy problems (3.9), (3.10) and use the conditions at the internal vertex ν_s to recover the values $\psi(\nu_s, \lambda)$ and $\psi'(\nu_s, \lambda)$ at the "new" boundary edge with the "new" boundary point ν_s.

Now, we consider the following linear combination of the solutions ϕ and ψ:

$$\varphi(x, \lambda) = \psi(x, \lambda) - \frac{\psi(\nu_s, \lambda)}{\phi(\nu_s, \lambda)}\phi(x, \lambda)\,. \tag{3.11}$$

It is easy to verify that on the subgraph $\widetilde{\Gamma}$ the function φ satisfies the boundary conditions:

$$\varphi(\gamma_i, \lambda) = 1,\ \varphi(\gamma_j, \lambda) = 0,\ j \neq i\,. \tag{3.12}$$

Thus, from (3.11), we obtain that:

$$\begin{aligned} \widetilde{\mathcal{M}}_{i0}(\lambda) &= \psi'(\nu_s, \lambda) - \psi(\nu_s, \lambda)\widetilde{\mathcal{M}}_{00}(\lambda), \\ \widetilde{\mathcal{M}}_{ij}(\lambda) &= \mathcal{M}_{ij}(\lambda) - \psi(\nu_s, \lambda)\widetilde{\mathcal{M}}_{0j}(\lambda). \end{aligned} \tag{3.13}$$

To recover all elements of the reduced TW matrix function, we need to use this procedure for all $i, j = p+1, \dots, m-1$.

We conclude that the (reduced) TW-function for the graph Γ determines the (reduced) TW-function for the graph $\widetilde{\Gamma}$. The inverse problem is reduced to the inverse problem for a smaller graph. Since the graph $\widetilde{\Gamma}$ is finite, this procedure may be continued, but it ends after a finite number of steps.

The proofs of Theorems 1 and 2 for arbitrary tree will be presented in a forthcoming paper. The quantum graph with the simplest topology — a network of serially connected strings — is considered in the next section.

4. Network of serially connected strings

We consider the wave equation on the interval $[0, \ell]$ with N masses $M_j > 0$ attached at the points $a_j,\ j = 1, \dots, N$, where $0 = a_0 < a_1 < ... < a_N < a_{N+1} = \ell$. This is modeled by:

$$\rho(x)\,\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0,\ t \in (0,T),\ x \in \Omega := (0, a_1) \cup (a_1, a_2) \cup \ldots \cup (a_N, \ell),$$

$$u(a_j^-, t) = u(a_j^+, t), \quad M_j\, u_{tt}(a_j, t) = u_x(a_j^+, t) - u_x(a_j^-, t),$$

$$u(x, 0) = u_t(x, 0) = 0,$$

$$u(0, t) = f(t),\ f \in \mathcal{F}^T := L^2(0, T), \quad u(\ell, t) = 0.$$

Here ρ is a positive function on $[0, \ell]$ and $\rho|_{[a_j, a_{j+1}]} \in C^{j+2}[a_j, a_{j+1}],\ j = 0, \dots, N$.

We show that the wave transmitted through a mass is more regular than the incoming wave. We define the spaces W, W^T :

$$W = \big\{\phi \in L^2(0, a_1) \times H^1(a_1, a_2) \times ...H^N(a_N, \ell) :$$

$$\phi(a_j^-) = \phi(a_j^+),\ \phi'(a_j^-) = \phi'(a_j^+) - M_j\,\phi''(a_j^+)/\rho(a_j^+),\ \phi(\ell) = 0\big\}\,,$$

$$W^T = \{\phi \in W : \phi(x) = 0 \ \text{ for } \ x \geq X(T)\}\,,$$

where

$$T = \int_0^{X(T)} \sqrt{\rho(x)}\,dx\,, \quad L = \int_0^{l} \sqrt{\rho(x)}\,dx\,.$$

The following result on the regularity of the solution of the initial boundary value problem stated above and on the controllability of this dynamical system has been proved in [8].

Theorem 4. *Suppose* $T \leq L := \int_0^l \sqrt{\rho(x)}\,dx$. *For any* $f \in \mathcal{F}^T,\ u^f \in C(0, T; W^T)$ *and for any* $\phi \in W^T$, *there exists a unique* $f \in W^T$ *such that* $u^f(x, T) = \phi(x)$. *Furthermore,*

$$\|u^f(\cdot, T)\|_W \asymp \|f\|_{\mathcal{F}^T}.$$

For $T > L$,

$$\{u^f(\cdot, T) :\ f \in L^2(0, T)\} = W.$$

Our dynamical inverse problem is to recover unknown parameters of the system from the *response operator*

$$R^T : \mathcal{F}^T \mapsto \mathcal{F}^T, \quad Dom(R^T) = \{f \in H^1(0, T),\ f(0) = 0\},$$

$$(R^T f)(t) = u_x^f(0, t),\ t \in (0, T).$$

The main result is this section is:

Theorem 5. *Let* $T > 2L$. *Given* R^T, *one can find* $\rho(x),\ l,\ a_j$, *and* $M_j,\ j = 1, \dots, N$.

We prove this theorem in several steps. First, we consider the spectral boundary value problem corresponding our dynamical system:

$$-\varphi''(x,\lambda) = \lambda^2\rho(x)\varphi(x,\lambda), \quad x \in \Omega,$$
$$\varphi(0,\lambda) = \varphi(\ell,\lambda) = 0, \quad \varphi(a_j^-,\lambda) = \varphi(a_j^+,\lambda),$$
$$-M_j\,\lambda^2\varphi(a_j,\lambda) = \varphi'(a_j^+,\lambda) - \varphi'(a_j^-,\lambda) \quad \forall j.$$

The eigenvalues λ_n^2 of this problem are simple and the eigenfunctions φ_n form the orthonormal basis in the space $\mathcal{H} := L^2_\rho(0,l) \oplus \mathcal{R}^N$ with the inner product:

$$\langle \phi, \psi \rangle_{\mathcal{H}} = \int_0^l \phi(x)\psi(x)\rho(x)dx + \sum_{j=1}^N M_j\phi(a_j)\psi(a_j)\,.$$

We set

$$\mathcal{H}^T = \{\phi \in \mathcal{H} : \phi(x) = 0 \ \text{ for } \ x \geq X(T)\}\,.$$

The *connecting operator* is defined as:

$$C^T : \mathcal{F}^T \mapsto \mathcal{F}^T, \quad (C^T f, g)_{\mathcal{F}^T} := \left\langle u^f(\cdot,T), u^g(\cdot,T)\right\rangle_{\mathcal{H}}\,.$$

The connecting operator can be written in the form $C^T = (U^T)^*(U^T)$ where

$$U^T : \mathcal{F}^T \mapsto W^T, \ U^T f = u^f(\cdot,T).$$

The exact controllability (see Theorem 4) implies that C^T is bounded and boundedly invertible.

Our second step is:

Theorem 6. *Operator C^T can be explicitly expressed through the response operator on the double interval: $C^T = -\frac{1}{2}(S^T)^* I^{2T} R^{2T} S^T$, where:*

$$(S^T f)(t) = \begin{cases} f(t) & \text{if} \quad t \in [0,T], \\ -f(2T-t) & \text{if} \quad t \in (T,2T], \end{cases} \quad (I^{2T} f)(t) = \int_0^t f(s)ds.$$

Sketch of the proof of Theorem 6. Set $w(s,t) := \left\langle u^f(\cdot,s), u^g(\cdot,t)\right\rangle_{\mathcal{H}}$.

We notice that $(C^T f, g)_{\mathcal{F}^T} = w(T,T$ and

$$w_{tt}(s,t) - w_{ss}(s,t) = \int_0^l [u^f(x,s)u^g_{tt}(x,t) - u^f_{ss}(x,s)u^g(x,t)]\rho(x)dx$$

$$+ \sum_j M_j[u^f(a_j,s)u^g_{tt}(a_j,t) - u^f_{ss}(a_j,s)u^g(a_j,t)] = (\text{using } \rho u_{tt} = u_{xx})$$

$$= \left[u^f(x,s)u^g_x(x,t) - u^f_x(x,s)u^g(x,t)\right]_{x=0}^{l} = (Rf)(s)g(t) - f(s)(Rg)(t).$$

We use $w(s,0) = w_t(s,0) = w(0,t) = 0$ to find $w(T,T)$ by D'Alembert's formula.

The next step is the construction of special bases in spaces $\mathcal{F}^T$ and $\mathcal{H}^T$. Let $T \leq L$ and $\{f_n\}$, $n \in \mathbb{N}$, be a basis in $\mathcal{F}^T$ such that:

$$f \in C^2[0,T], \ f(0) = f'(0) = 0, \quad \left(C^T f_k, f_n\right)_{\mathcal{F}^T} = \delta_{kn}.$$

Due to controllability, $\{u^{f_n}(\cdot,T)\}$ is an orthonormal basis in $\mathcal{H}^T$.

Next, we introduce two functions: $\phi^0(x) = 1$, $\phi^1(x) = x$, $x \in [0,l]$ and let ϕ^0_T and ϕ^1_T be their restrictions to the interval $[0, X(t)]$.

Theorem 7. *The coefficients in the series representations of the functions ϕ^0_T, ϕ^1_T with respect to the basis $\{u^{f_j}(\cdot,T)\}$ have the form*

$$c^0_n := \langle \phi^0, u^{f_n}(\cdot,T)\rangle_{\mathcal{H}} = -\int_0^T (T-t)(R^T f_n)(t)\,dt\,,$$

$$c^1_n := \langle \phi^1, u^{f_n}(\cdot,T)\rangle_{\mathcal{H}} = \int_0^T (T-t)\,f_n(t)\,dt\,.$$

Sketch of the proof of Theorem 7. By the definition of the connection operator, we have:

$$\langle \phi^0, u^{f_n}(\cdot,T)\rangle_{\mathcal{H}} = \int_0^l u^{f_n}(x,T)\rho(x)dx + \sum_j M_j\, u^{f_n}(a_j,T)$$

$$= \int_0^T (T-t)\left[\int_0^{X(T)} u_{tt}^{f_n}(x,t)\rho(x)dx + \sum_j M_j\, u_{tt}^{f_n}(a_j,t)\right] dt$$

$$= \int_0^T (T-t)\left[\int_0^{X(T)} u_{xx}^{f_n}(x,t)dx + \sum_j M_j\, u_{tt}^{f_n}(a_j,t)\right] dt$$

$$= -\int_0^T (T-t)u_x^{f_n}(0,t)\,dt = -\int_0^T (T-t)(R^T f_n)(t)\,dt.$$

This proves the first statement of Theorem 7. The second one can be proved in a similar way.

Now, we are ready to complete the solution of the dynamical inverse problem. We introduce two functions:

$$\mu(T) = \int_0^{X(T)} \rho(x)dx + \sum_{j:\, a_j<X(T)} M_j\,,$$

$$\nu(T) = \int_0^{X(T)} x\rho(x)dx + \sum_{j:\, a_j<X(T)} M_j\, a_j\,.$$

They can be found using the theorem:

$$\mu(T) = \langle \phi_T^0, \phi_T^0\rangle_{\mathcal{H}} = \sum_n |c_n^0|^2, \quad \nu(T) = \langle \phi_T^0, \phi_T^1\rangle_{\mathcal{H}} = \sum_n c_n^0\, c_n^1\,.$$

Separating the singular and regular (integral) parts, we find M_j and a_j from the singular parts. From the regular parts, we have:

$$\dot{\mu_r}(T) = \rho(X(T))\,\dot{X}(T), \quad \dot{\nu_r}(T) = X(T)\rho(X(T))\,\dot{X}(T)\,.$$

From these relations, we find $X(T)$ and, finally, $\rho(x)$.

Acknowledgments

The research of S. Avdonin was supported in part by the National Science Foundation, grant DMS 1411564 and by the Ministry of Education and Science of Republic of Kazakhstan under the grant No. 4290/GF4.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 842–853

Dynamical inverse problem for the discrete Schrödinger operator

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DOI 10.17586/2220-8054-2016-7-5-842-853

We consider the inverse problem for the dynamical system with discrete Schrödinger operator and discrete time. As inverse data, we take a *response operator*, the natural analog of the dynamical Dirichlet-to-Neumann map. We derive two types of equations of inverse problem and answer a question on the characterization of the inverse data, i.e. we describe the set of operators, which are *response operators* of the dynamical system governed by the discrete Schrödinger operator.

Keywords: inverse problem, discrete Schrödinger operator, Boundary Control method, characterization of inverse data.

Received: 19 July 2016

Revised: 21 August 2016

Dedicated to the memory of B. S. Pavlov

1. Introduction

The theory of dynamical inverse problems is a wide area of modern mathematics, by now for all or almost all linear nonstationary equations of mathematical physics there exist an inverse theory more or less developed. Theories mostly covers the case of continuous problems, at the same time just a few attention is paid to discrete ones. The primary goal of the paper is to improve this situation.

Let $\mathbb{N}$ be the set of positive natural numbers, $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. We fix the infinite sequence of real numbers $(b_1, b_2, \ldots)$, which we call the potential and consider the dynamical system with discrete time which is a natural analog of dynamical systems governed by the wave equation with potential on a semi-axis:

$$\begin{cases} u_{n,t+1} + u_{n,t-1} - u_{n+1,t} - u_{n-1,t} + b_n u_{n,t} = 0, \quad n, t \in \mathbb{N}_0, \\ u_{n,-1} = u_{n,0} = 0, \quad n \in \mathbb{N}, \\ u_{0,t} = f_t, \quad t \in \mathbb{N}_0. \end{cases} \tag{1.1}$$

By analogy with continuous problems [1], we treat the real sequence $f = (f_0, f_1, \ldots)$ as a *boundary control*. The solution to (1.1) we denote by $u^f_{n,t}$.

Having fixed $\tau \in \mathbb{N}$, with (1.1) we associate the *response operators*, which maps the control $f = (f_0, \ldots f_{\tau-1})$ to $u^f_{1,t}$:

$$(R^\tau f)_t := u^f_{1,t}, \quad t = 1, \ldots, \tau. \tag{1.2}$$

The inverse problem we will be dealing with is to recover from R^τ (part of the) potential $(b_1, b_2, \ldots, b_n)$ for some n. This problems is a natural discrete analog of the inverse problem for the wave equation where the inverse data is the dynamical Dirichlet-to-Neumann map, see [1].

We will be using the Boundary Control method [1] which was initially developed to treat multidimensional dynamical inverse problems, but since then was applied to multi- and one- dimensional inverse dynamical, spectral and scattering problems, problems of signal processing and identification problems [2, 3].

In the second section, we study the forward problem: for (1.1) we prove the analog of d'Alembert integral representation formula. Prescribing the Dirichlet condition at $n = N+1$, we consider the second dynamical system with boundary control at $n = 0$ (which will be an analog of the problem on the finite interval) and develop the solution of this system in Fourier series. We analyze the dependence of two solutions on the potential, which lead us to the natural set up of the inverse problem. In the third section, we introduce and prove the representation formulae for the main operators of the BC method: response operator, control and connecting operators. In the fourth section, we derive two types of equations for the inverse problem and give a characterization of the inverse data. In the last section, we highlight the connections between the different types of inverse data.

The case of the Jacobi matrices of general type as well as the studying of the inverse spectral problem, i.e. recovering the semi-infinite matrix from the spectral measure, will be the subject of forthcoming publications.

2. Forward problems

We fix some positive integer T. By $\mathcal{F}^T$ we denote the space of controls: $\mathcal{F}^T := \mathbb{R}^T$, $f \in \mathcal{F}^T$, $f = (f_0, \dots, f_{T-1})$.

First, we derive the representation formulas for the solution to (1.1) which could be considered as analogs of known formulas for the wave equation [4].

Lemma 1. *The solution to (1.1) admits the representation:*

$$u_{n,t} = f_{t-n} + \sum_{s=n}^{t-1} w_{n,s} f_{t-s-1}, \quad n, t \in \mathbb{N}_0. \tag{2.1}$$

where $w_{n,s}$ satisfies the Goursat problem:

$$\begin{cases} w_{n,t+1} + w_{n,t-1} - w_{n+1,t} - w_{n-1,t} + b_n w_{n,t} = 0, \quad n, s \in \mathbb{N}_0,\ s > n, \\ w_{n,n} = -\sum_{k=1}^{n} b_k, \quad n \in \mathbb{N}, \\ w_{0,t} = 0, \quad t \in \mathbb{N}_0. \end{cases} \tag{2.2}$$

Proof. We assume that $u^f_{n,t}$ has a form (2.1) with unknown $w_{n,s}$ and plug it to equation in (1.1):

$$0 = b_n f_{t-n} + \sum_{s=n}^{t-1} b_n w_{n,s} f_{t-s-1} + \sum_{s=n}^{t} w_{n,s} f_{t-s} + \sum_{s=n}^{t-2} w_{n,s} f_{t-s-2} - \sum_{s=n+1}^{t-1} w_{n,s} f_{t-s-1} - \sum_{s=n-1}^{t-1} w_{n-1,s} f_{t-s-1}.$$

Changing the order of summation, we get:

$$\begin{aligned} 0 = \quad & b_n f_{t-n} + w_{n+1,n} f_{t-n-1} - w_{n-1,n-1} f_{t-n} + \sum_{s=n}^{t-1} f_{t-s-1} \left(b_n w_{n,s} - w_{n+1,s} - w_{n-1,s} \right) \\ + \quad & \sum_{s=n-1}^{t-1} w_{n,s+1} f_{t-s-1} + \sum_{s=n+1}^{t-1} w_{n,s-1} f_{t-s-1} = f_{t-n-1}(w_{n+1,n} - w_{n,n-1}) + b_n f_{t-n} \\ + \quad & \sum_{s=n}^{t-1} f_{t-s-1} \left(w_{n,s+1} + w_{n.s-1} - w_{n+1,s} - w_{n-1,s} + b_n w_{n,s} \right) + f_{t-n}(w_{n,n} - w_{n-1,n-1}). \end{aligned}$$

Counting that $w_{n,s} = 0$ when $n > s$ and arbitrariness of $f \in \mathcal{F}^T$, we arrive at (2.1). □

We fix $N \in \mathbb{N}$. Along with (1.1) we consider the analog of the wave equation with the potential on the interval: we assume that (b_n) is finite: $n = 1, \dots, N$ and impose the Dirichlet condition at $n = N + 1$. Then for a control $f = (f_0, f_1, \dots)$ we consider:

$$\begin{cases} v_{n,t+1} + v_{n,t-1} - v_{n+1,t} - v_{n-1,t} + b_n v_{n,t} = 0, \quad t \in \mathbb{N}_0,\ n \in 0, \dots, N+1 \\ v_{n,-1} = v_{n,0} = 0, \quad n = 1, 2, \dots, N+1 \\ v_{0,t} = f_t, \quad v_{N+1,t} = 0, \quad t \in \mathbb{N}_0. \end{cases} \tag{2.3}$$

We denote the solution to (2.3) by v^f.

Let $\phi_n(\lambda)$ be the solution to:

$$\begin{cases} \phi_{i+1} + \phi_{i-1} - b_n \phi_i = \lambda \phi_i, \\ \phi_0 = 0,\ \phi_1 = 1. \end{cases} \tag{2.4}$$

We introduce the Hamiltonian:

$$H_N := \begin{pmatrix} -b_1 & 1 & 0 & \dots & 0 \\ 1 & -b_2 & 1 & \dots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & 0 & 1 & -b_N \end{pmatrix}$$

Let $\{\varphi^k, \lambda_k\}_{k=1}^N$ be eigenvectors chosen such that $\varphi^k_1 = 1$ and eigenvalues of H_N. Introduce the numbers ρ_k by:

$$(\varphi^k, \varphi^l) = \delta_{kl} \rho_k, \tag{2.5}$$

where $(\cdot, \cdot)$– is a scalar product in $\mathbb{R}^N$.

Definition 1. *The set*

$$\{\lambda_k, \rho_k\}_{k=1}^N \tag{2.6}$$

is called the spectral data.

On introducing vectors $\phi^n \in \mathbb{R}^N$ by the rule $\phi_i^n := \phi_i(\lambda_n)$, $n, i = 1, \ldots, N$, we have

Proposition 1. *The solutions of $\phi_{N+1}(\lambda) = 0$ are λ_n, $n = 1, \ldots, N$; and $\phi_i^n = \varphi_i^n$, $n, i = 1, \ldots, N$.*

Proof. Take eigenvector φ^n corresponding to eigenvalue λ_n and compare it with ϕ^n. By the definition of φ^n and condition in (2.4): $\varphi_1^n = \phi_1^n = 1$. On the other hand, comparing the first line in the equation on eigenvalues $H_N\varphi^n = \lambda^n\varphi^n$ and (2.4) for $i = 1$ we have:

$$-\varphi_1^n b_1 + \varphi_2^n = \lambda_n \varphi_1^n,$$
$$\phi_2^n - b_1\phi_1^n = \lambda_n \phi_1^n,$$

which implies $\varphi_2^n = \phi_2^n$, for $k < N$ comparing $k-$th line in $H_N\varphi^n = \lambda^n\varphi^n$ and (2.4) for $i = k$, we arrive at $\varphi_{k+1}^n = \phi_{k+1}^n$. And for $k = N$:

$$-\varphi_N^n b_N + \varphi_{N-1}^n = \lambda_n \varphi_N^n,$$
$$\phi_{N+1}^n + \phi_{N-1}^n - b_N\phi_N^n = \lambda_n \phi_N^n,$$

which holds if and only if $\phi_{N+1}^n(\lambda_n) = 0$. □

We take $y \in \mathbb{R}^N$, $y = (y_1, \ldots, y_N)$, for each n we multiply the equation in (2.3) by y_n, sum up and evaluate the following expression, changing the order of summation:

$$0 = \sum_{n=1}^N \left(v_{n,t+1}y_n + v_{n,t-1}y_n - v_{n+1,t}y_n - v_{n-1,t}y_n + b_n v_{n,t}y_n\right) =$$

$$\sum_{n=1}^N \left(v_{n,t+1}y_n + v_{n,t-1}y_n - v_{n,t}(y_{n-1} + y_{n+1}) + b_n v_{n,t}y_n\right) - v_{N+1,t}y_N - v_{0,t}y_1 + v_{1,t}y_0 + v_{N,t}y_{N+1}. \tag{2.7}$$

Now, we choose $y = \varphi^l$, $l = 1 \ldots, N$. On counting that $\varphi_0^l = \varphi_{N+1}^l = 0$, $\varphi_1^l = 1$, $v_{0,t} = f_t$, $v_{N+1,t} = 0$ we evaluate (2.7) arriving at:

$$0 = \sum_{n=1}^N \left(v_{n,t+1}\varphi_n^l + v_{n,t-1}\varphi_n^l - v_{n,t}\left(\varphi_{n-1}^l + \varphi_{n+1}^l - b_n\varphi_n^l\right)\right) - f_t = 0. \tag{2.8}$$

Definition 2. *For $a, b \in l^\infty$, we define the convolution $c = a * b \in l^\infty$ by the formula:*

$$c_t = \sum_{s=0}^t a_s b_{t-s}, \quad t \in \mathbb{N}.$$

We assume that the solution to (2.3) has the form:

$$v_{n,t}^f = \begin{cases} \displaystyle\sum_{k=1}^N c_t^k \varphi_n^k, & n = 1, \ldots, N \\ f_t, & n = 0. \end{cases} \tag{2.9}$$

Proposition 2. *The coefficients c^k admits the representation:*

$$c^k = \frac{1}{\rho_k} T\left(\lambda_k\right) * f, \tag{2.10}$$

where $T(2\lambda) = (T_1(2\lambda), T_2(2\lambda), T_3(2\lambda), \ldots)$ are Chebyshev polynomials of the second kind.

Proof. We plug (2.9) into (2.8) and evaluate, counting that $\varphi_{n-1}^l + \varphi_{n+1}^l - b_n\varphi_n^l = \lambda_l\varphi_n^l$:

$$\sum_{n=1}^N \left(v_{n,t+1} + v_{n,t-1} - \lambda_l v_{n,t}\right)\varphi_n^l = f_t,$$

$$\sum_{n=1}^N \sum_{k=1}^N \left(c_{t+1}^k\varphi_n^k + c_{t-1}^k\varphi_n^k - \lambda_l c_t^k\varphi_n^k\right)\varphi_n^l = f_t.$$

Changing the order of summation and using (2.5), we finally arrive at the following equation on c_t^k, $k = 1, \dots, N$:

$$\begin{cases} c_{t+1}^k + c_{t-1}^k - \lambda_k c_t^k = \dfrac{1}{\rho_k} f_t, \\ c_{-1}^k = c_0^k = 0. \end{cases} \tag{2.11}$$

We assume that the solution to (2.11) has the form: $c^k = \dfrac{1}{\rho_k} T * f$, or

$$c_t^k = \frac{1}{\rho_k} \sum_{l=0}^{t} T_l f_{t-l}. \tag{2.12}$$

Plugging it into (2.11), we get:

$$\frac{1}{\rho_k} \left(\sum_{l=0}^{t+1} f_l T_{t+1-l} + \sum_{l=0}^{t-1} f_l T_{t-1-l} - \lambda_k \sum_{l=0}^{t} f_l T_{t-l} \right) = \frac{1}{\rho_k} f_t,$$

$$\sum_{l=0}^{t} f_l \left(T_{t+1-l} + T_{t-1-l} - \lambda_k T_{t-l} \right) + f_t T_1 - f_{t-1} T_0 = f_t.$$

We see that (2.12) holds if T solves:

$$\begin{cases} T_{t+1} + T_{t-1} - \lambda_k T_t = 0, \\ T_0 = 0, \;\; T_1 = 1. \end{cases}$$

Thus $T_k(2\lambda)$ are Chebyshev polynomials of the second kind.

□

3. Operators of the the BC method

As inverse data for (1.1), we use the analog of the dynamical response operator (dynamical Dirichlet-to-Neumann map) [1].

Definition 3. *For (1.1), the* response operator $R^T : \mathcal{F}^T \mapsto \mathbb{R}^T$ *is defined by the rule*

$$\left(R^T f\right)_t = u_{1,t}^f, \quad t = 1, \dots, T.$$

Introduce the notation: the *response vector* is the convolution kernel of the response operator, $r = (r_0, r_1, \dots, r_{T-1}) = (1, w_{1,1}, w_{1,2}, \dots w_{1,T-1})$. Then, in accordance with (2.1):

$$\left(R^T f\right)_t = u_{1,t}^f = f_{t-1} + \sum_{s=1}^{t-1} w_{1,s} f_{t-1-s}, \quad t = 1, \dots, T; \tag{3.1}$$

$$\left(R^T f\right) = r * f_{\cdot -1}, \quad \text{where } r_0 = 1.$$

For system (2.3), we introduce the response operator by:

Definition 4. *For the system in (2.3) the* response operator $R_i^T : \mathcal{F}^T \mapsto \mathbb{R}^T$ *is defined by the rule:*

$$\left(R_i^T f\right)_t = v_{1,t}^f, \quad t = 1, \dots, T. \tag{3.2}$$

The corresponding *response vector* we denote by $(r_1^i, r_2^i, \dots)$. More information on this operator and on the inverse spectral problem one can find in the last section.

We introduce the inner space of dynamical system (1.1) $\mathcal{H}^T := \mathbb{R}^T$, $h \in H^T$, $h = (h_1, \dots, h_T)$. For (1.1) The *control operator* $W^T : \mathcal{F}^T \mapsto \mathcal{H}^T$ is defined by the rule:

$$W^T f := u_{n,T}^f, \quad n = 1, \dots, T.$$

Directly from (2.1), we deduce that:

$$\left(W^T f\right)_n = u_{n,T}^f = f_{T-n} + \sum_{s=n}^{T-1} w_{n,s} f_{T-s-1}, \quad n = 1, \dots, T. \tag{3.3}$$

The following statement imply the controllability of the dynamical system (1.1).

Theorem 1. *The operator W^T is an isomorphism between $\mathcal{F}^T$ and $\mathcal{H}^T$.*

Proof. We fix some $a \in \mathcal{H}^T$ and look for a control $f \in \mathcal{F}^T$ such that $W^T f = a$. To this aim we write down the operator as:

$$W^T f = \begin{pmatrix} u_{1,T} \\ u_{2,T} \\ \cdot \\ u_{k,T} \\ \cdot \\ u_{T,T} \end{pmatrix} = \begin{pmatrix} 1 & w_{1,1} & w_{1,2} & \dots & \dots & w_{1,T-1} \\ 0 & 1 & w_{2,2} & \dots & \dots & w_{2,T-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & 1 & w_{k,k} & \dots & w_{k,T-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} f_{T-1} \\ f_{T-2} \\ \cdot \\ f_{T-k-1} \\ \cdot \\ f_0 \end{pmatrix} \tag{3.4}$$

We introduce the notations:

$$J_T : \mathcal{F}^T \mapsto \mathcal{F}^T, \quad (J_T f)_n = f_{T-1-n}, \quad n = 0, \dots, T-1,$$
$$K \in \mathbb{R}^{T \times T}, \quad k_{ij} = 0, \quad i > j, \quad k_{ii} = 1, \quad k_{ij} = w_{ij-1}, \quad i < j.$$

Then, $W^T = (I + K) J^T$. Obviously, this operator is invertible, which proves the statement of the theorem. □

For the system (2.3) the *control operator* $W_i^T : \mathcal{F}^T \mapsto \mathcal{H}^N$ is defined by the rule:

$$W_i^T f := v^f_{n,T}, \quad n = 1, \dots, N.$$

The representation for this operator immediately follows from (2.9), (2.10).

For the system (1.1) we introduce the *connecting operator* $C^T : \mathcal{F}^T \mapsto \mathcal{F}^T$ by the quadratic form: for arbitrary $f, g \in \mathcal{F}^T$ we define

$$\left(C^T f, g\right)_{\mathcal{F}^T} = \left(u^f_{\cdot,T}, u^g_{\cdot,T}\right)_{\mathcal{H}^T} = \left(W^T f, W^T g\right)_{\mathcal{H}^T}. \tag{3.5}$$

We observe that $C^T = \left(W^T\right)^* W^T$, so C^T is an isomorphism in $\mathcal{F}^T$. The fact that C^T can be expressed in terms of response R^{2T} is crucial in BC-method.

Theorem 2. *Connecting operator admits the representation in terms of inverse data:*

$$C^T = C^T_{ij}, \quad C^T_{ij} = \sum_{k=0}^{T-\max i,j} r_{|i-j|+2k}, \quad r_0 = 1. \tag{3.6}$$

$$C^T = \begin{pmatrix} 1 + r_2 + \ldots + r_{2T-2} & r_1 + r_3 + \ldots + r_{2T-3} & \dots & r_T + r_{T-2} & r_{T-1} \\ r_1 + r_3 + \ldots + r_{2T-3} & 1 + r_2 + \ldots + r_{2T-4} & \dots & \dots & r_{T-2} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ r_{T-3} + r_{T-1} + r_{T+1} & \dots & 1 + r_2 + r_4 & r_1 + r_3 & r_2 \\ r_T + r_{T-2} & \dots & r_1 + r_3 & 1 + r_2 & r_1 \\ r_{T-1} & r_{T-2} & \dots & r_1 & 1 \end{pmatrix}$$

Proof. For fixed $f, g \in \mathcal{F}^T$, we introduce the *Blagoveshchensky function* by:

$$\psi_{n,t} := \left(u^f_{\cdot,n}, u^g_{\cdot,t}\right)_{\mathcal{H}^T} = \sum_{k=1}^{T} u^f_{k,n} u^g_{k,t}.$$

Then, we show that $\psi_{n,t}$ satisfies some difference equation. Indeed, we can evaluate:

$$\psi_{n,t+1} + \psi_{n,t-1} - \psi_{n+1,t} - \psi_{n-1,t} =$$
$$\sum_{k=1}^{T} u^f_{k,n} \left(u^g_{k,t+1} + u^g_{k,t-1}\right) - \sum_{k=1}^{T} \left(u^f_{k,n+1} + u^f_{k,n-1}\right) u^g_{k,t} =$$
$$\sum_{k=1}^{T} u^f_{k,n} \left(u^g_{k+1,t} + u^g_{k-1,t}\right) - \sum_{k=1}^{T} \left(u^f_{k+1,n} + u^f_{k-1,n}\right) u^g_{k,t} =$$
$$\sum_{k=1}^{T} u^g_{k,t} \left(u^f_{k+1,n} + u^f_{k-1,n}\right) + u^g_{0,t} u^f_{1,n} - u^f_{0,n} u^g_{1,t} + u^g_{T+1,t} u^f_{T,n} - u^f_{T+1,n} u^g_{T,t} - \sum_{k=1}^{T} u^g_{k,t} \left(u^f_{k+1,n} + u^f_{k-1,n}\right) =$$
$$g_t (Rf)_n - f_n (Rg)_t.$$

So, we arrive at the following boundary problem for $\psi_{n,t}$:

$$\begin{cases} \psi_{n,t+1} + \psi_{n,t-1} - \psi_{n+1,t} - \psi_{n-1,t} = h_{n,t}, \quad n,t \in \mathbb{N}_0, \\ \psi_{0,t} = 0,\ \psi_{n,0} = 0, \\ h_{n,t} = g_t(Rf)_n - f_n(Rg)_t. \end{cases} \tag{3.7}$$

We introduce the set:

$$K(n,t) := \Big\{(n,t) \cup \{(n-1,t-1),(n+1,t-1)\} \cup \{(n-2,t-2),(n,t-2),(n+2,t-2)\} \cup \dots$$
$$\cup \{(n-t,0),(n-t+2,0),\dots,(n+t-2,0),(n+t,0)\}\Big\} = \bigcup_{\tau=0}^{t} \bigcup_{k=0}^{\tau} (n-\tau+2k, t-\tau).$$

The solution to (3.7) is given by:

$$\psi_{n,t} = \sum_{k,\tau \in K(n,t-1)} h(k,\tau).$$

We observe that $\psi_{T,T} = \left(C^T f, g\right)$, so:

$$\left(C^T f, g\right) = \sum_{k,\tau \in K(T,T-1)} h(k,\tau). \tag{3.8}$$

Notice that in the r.h.s. of (3.8) the argument k runs from 1 to $2T-1$. We extend $f \in \mathcal{F}^T$, $f = (f_0,\dots,f_{T-1})$ to $f \in \mathcal{F}^{2T}$ by:

$$f_T = 0, \quad f_{T+k} = -f_{T-k}, \quad k = 1,2,\dots,T-1.$$

Due to this odd extension, $\sum_{k,\tau \in K(T,T-1)} f_k (R^T g)_\tau = 0$, so (3.8) gives:

$$\left(C^T f, g\right) = \sum_{k,\tau \in K(T,T-1)} g_\tau \left(R^{2T} f\right)_k = g_0 \left[\left(R^{2T} f\right)_1 + \left(R^{2T} f\right)_3 + \dots + \left(R^{2T} f\right)_{2T-1}\right]$$
$$+ g_1 \left[\left(R^{2T} f\right)_2 + \left(R^{2T} f\right)_4 + \dots + \left(R^{2T} f\right)_{2T-2}\right] + \dots + g_{T-1} \left(R^{2T} f\right)_T.$$

Finally, we infer that:

$$C^T f = \left(\left(R^{2T} f\right)_1 + \dots + \left(R^{2T} f\right)_{2T-1}, \left(R^{2T} f\right)_2 + \dots + \left(R^{2T} f\right)_{2T-2}, \dots, \left(R^{2T} f\right)_T\right)$$

from where the statement of the theorem follows. □

One can observe that C^T_{ij} satisfies the difference boundary problem.

Corollary 1. *The kernel of C^T satisfy:*

$$\begin{cases} C^T_{i,j+1} + C^T_{i,j-1} - C^T_{i+1,j} - C^T_{i-1,j} = 0, \\ C^T_{i,T} = r_{T-i},\ C^T_{T,j} = r_{T-j},\ r_0 = 1. \end{cases}$$

For the system (2.3) the *connecting operator* $C^T_i : \mathcal{F}^T \mapsto \mathcal{F}^T$ is introduced in the similar way: for arbitrary $f, g \in \mathcal{F}^T$ we define:

$$\left(C^T_i f, g\right)_{\mathcal{F}^T} = \left(v^f_{\cdot,T}, v^g_{\cdot,T}\right)_{\mathcal{H}^N} = \left(W^T_i f, W^T_i g\right)_{\mathcal{H}^N}. \tag{3.9}$$

More information on C^T_i one can find in the final section.

4. Inverse problem

The dependence of the solution (1.1) u^f on the potential $(b_1, b_2, \dots)$ resembles one of the wave equation with the potential: take some $M \in \mathbb{N}$. From the very equation, one can see that the term $u^f_{n,t}$ with smallest $\{n,t\}$, which depends on b_M is $u^f_{M,M+1}$. Thus, $u^f_{1,t}$ becomes dependent upon b_M starting from $t = 2M$. This is an analog of the finite wave propagation speed effect in the wave equation. Consider (2.3) with $N = M$. We see that the solution to (2.3) $v^f_{1,t}$ does not 'feel' the boundary condition at $n = M+1$: $u^f_{1,t} = v^f_{1,t}$ for $t = 1,\dots,2M$. Or in other words, that means that $R^{2M} = R^{2M}_i$. This leads to the following natural set up of the inverse problem: By the given operator R^{2M} to recover the (part) of the potential $(b_1,\dots,b_M)$. In what follows, we will be dealing with the IP for the system (1.1), only in the last section we comment on the system (2.3).

4.1. Krein equations

Let $\alpha, \beta \in \mathbb{R}$ and y be solution to:

$$\begin{cases} y_{k+1} + y_{k-1} - b_k y_k = 0, \\ y_0 = \alpha, \ y_1 = \beta. \end{cases} \tag{4.1}$$

We set up the following control problem: to find a control $f^T \in \mathcal{F}^T$ such that:

$$\left(W^T f^T\right)_k = y_k, \quad k = 1, \ldots, T. \tag{4.2}$$

Due to Theorem 1, this problem has unique solution. Let $\varkappa^T$ be a solution to

$$\begin{cases} \varkappa^T_{t+1} + \varkappa^T_{t-1} = 0, \quad t = 0, \ldots, T, \\ \varkappa^T_T = 0, \ \varkappa^T_{T-1} = 1. \end{cases} \tag{4.3}$$

We show that the control f^T satisfies the Krein equation:

Theorem 3. *The control f^T, defined by (4.2) satisfies the following equation in $\mathcal{F}^T$:*

$$C^T f^T = \beta \varkappa^T - \alpha \left(R^T\right)^* \varkappa^T. \tag{4.4}$$

Proof. Let us take f^T solving (4.2). We observe that for any fixed $g \in \mathcal{F}^T$:

$$u^g_{k,T} = \sum_{t=1}^{T-1} \left(u^g_{k,t+1} + u^g_{k,t-1}\right) \varkappa^T_t. \tag{4.5}$$

Indeed, changing the order of summation in the r.h.s. of (4.5), we get:

$$\sum_{t=1}^{T-1} \left(u^g_{k,t+1} + u^g_{k,t-1}\right) \varkappa^T_t = \sum_{t=1}^{T-1} \left(\varkappa^T_{t+1} + \varkappa^T_{t-1}\right) u^g_{k,t} + u^g_{k,0} \varkappa^T_1 - u^g_{k,T} \varkappa^T_{T-1}.$$

which gives (4.5) due to (4.3). Using this observation, we can evaluate:

$$\begin{aligned} \left(C^T f^T, g\right) = \sum_{k=1}^{T} y_k u^g_{k,T} &= \sum_{k=1}^{T} \sum_{t=0}^{T-1} \left(u^g_{k,t+1} + u^g_{k,t-1}\right) \varkappa^T_t y_k \\ &= \sum_{t=0}^{T-1} \varkappa^T_t \left(\sum_{k=1}^{T} \left(u^g_{k+1,t} y_k + u^g_{k-1,t} y_k - b_k u^g_{k,t} y_k\right)\right) \\ = \sum_{t=0}^{T-1} \varkappa^T_t \left(\sum_{k=1}^{T} \left(u^g_{k,t}(y_{k+1} + y_{k-1} - b_k y_k\right) + u^g_{0,t} y_1 + u^g_{T+1,t} y_T - u^g_{1,t} y_0 - u^g_{T,t} y_{T+1}\right) \\ = \sum_{t=0}^{T-1} \varkappa^T_t \left(\beta g_t - \alpha \left(R^T g\right)_t\right) = \left(\varkappa^T, \beta g - \alpha \left(R^T g\right)\right) = \left(\beta \varkappa^T - \alpha \left(\left(R^T\right)^* \varkappa^T\right), g\right). \end{aligned}$$

From where (4.4) follows. □

Having found f^τ for $\tau = 1, \ldots, T$, we can recover the potential b_n, $n = 1, \ldots, T-1$. Indeed: by the constructions of f^τ we have $\left(W^\tau f^\tau\right)_\tau = y_\tau$, on the other hand, from (3.3) we can infer that $\left(W^\tau f^\tau\right)_\tau = f^\tau_0$, thus y (4.1) can be recovered by:

$$y_\tau = f^\tau_0, \quad \tau = 1, \ldots, T. \tag{4.6}$$

And the potential can be found by:

$$b_n = \frac{y_{n+1} + y_{n-1}}{y_n}, \quad n = 1, \ldots, T-1. \tag{4.7}$$

4.2. Factorization method

We make use the fact that matrix C^T has a special structure – it is a product of triangular matrix and its conjugate. We rewrite the operator $W^T = \overline{W}^T J$ as:

$$W^T f = \begin{pmatrix} 1 & w_{1,1} & w_{1,2} & \dots & w_{1,T-1} \\ 0 & 1 & w_{2,2} & \dots & w_{2,T-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & 1 & \dots & w_{k,T-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & 1 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} f_0 \\ f_2 \\ \cdot \\ f_{T-k-1} \\ \cdot \\ f_{T-1} \end{pmatrix}.$$

Using the definition (3.5) and the invertibility of W^T (cf. Theorem 1), we have:

$$C^T = \left(W^T\right)^* W^T, \quad \text{or} \quad \left(\left(W^T\right)^{-1}\right)^* C^T \left(W^T\right)^{-1} = I.$$

We can rewrite the latter equation as:

$$\left(\left(\overline{W}^T\right)^{-1}\right)^* \overline{C}^T \left(\overline{W}^T\right)^{-1} = I, \quad \overline{C}^T = JC^T J. \tag{4.8}$$

Here the matrix $\overline{C}^T$ has the entries:

$$\overline{C}_{ij} = C_{T+1-j,T+1-i}, \quad \overline{C}^T = \begin{pmatrix} 1 & r_1 & r_2 & \dots & r_{T-1} \\ r_1 & 1+r_2 & r_1+r_3 & \dots & .. \\ r_3 & r_1+r_3 & 1+r_2+r_4 & \dots & .. \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \tag{4.9}$$

and operator $\left(\overline{W}^T\right)^{-1}$ has the form:

$$\left(\overline{W}^T\right)^{-1} = \begin{pmatrix} 1 & \widetilde{k}_{11} & \widetilde{k}_{12} & \dots & \widetilde{k}_{1,T-1} \\ 0 & 1 & \widetilde{k}_{22} & \dots & .. \\ \cdot & \cdot & \cdot & \cdot & \widetilde{k}_{T-1,T-1} \\ 0 & \dots & \dots & 0 & 1 \end{pmatrix}, \tag{4.10}$$

where $\widetilde{k}_{\alpha,\alpha} = -w_{\alpha,\alpha}$, $\alpha = 1, \dots, T-1$. So we can rewrite (4.8) as:

$$\begin{pmatrix} 1 & 0 & . & 0 \\ k_{11} & 1 & 0 & . \\ \cdot & \cdot & \cdot & \cdot \\ k_{T-1,1} & . & . & 1 \end{pmatrix} \begin{pmatrix} \overline{c}_{11} & .. & .. & \overline{c}_{1T} \\ .. & .. & .. & .. \\ \cdot & \cdot & \cdot & \cdot \\ \overline{c}_{T1} & .. & & \overline{c}_{TT} \end{pmatrix} \begin{pmatrix} 1 & k_{11} & k_{21} & .. \\ 0 & 1 & k_{22} & .. \\ \cdot & \cdot & \cdot & \cdot \\ 0 & \dots & \dots & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & .. & 0 \\ 0 & 1 & .. & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & . & 1 \end{pmatrix}.$$

In the above equation $\overline{C}_{ij}$ are given (see (4.9)), the entries k_{ij} of $\left(\left(\overline{W}^T\right)^{-1}\right)^*$ are unknown. We denote by $K_i := (k_{i1}, k_{i2}, \dots, k_{ii}, 1, 0, \dots, 0)$ the $(i+1)-$th row ($i = 0, \dots, T-1$) in $\left(\left(\overline{W}^T\right)^{-1}\right)^*$, then we have

$$K_i \overline{C}^T K_j^* = \delta_{i,j}.$$

We use this equality in the form:

$$K_i \overline{C}^T K_j^* = 0, \quad i < j. \tag{4.11}$$

Notice that $K_0 = (1, 0, \dots, 0)$. The second row K_1 can be recovered from $K_0 \overline{C}^T K_1^* = 0$, which is equivalent to:

$$\overline{c}_{11} k_{11} + \overline{c}_{21} = 0, \text{ or } k_{11} = -\frac{\overline{c}_{21}}{\overline{c}_{11}} = -\overline{c}_{21}. \tag{4.12}$$

The third row K_2 we recover from the pair of equations $K_0 \overline{C}^T K_2^* = 0$, $K_1 \overline{C}^T K_2^* = 0$, which are equivalent to:

$$\begin{pmatrix} 1 & 0 \\ k_{11} & 1 \end{pmatrix} \begin{pmatrix} \overline{c}_{11} & \overline{c}_{12} & \overline{c}_{13} \\ \overline{c}_{21} & \overline{c}_{22} & \overline{c}_{23} \end{pmatrix} \begin{pmatrix} k_{21} \\ k_{22} \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Due to the invertibility of $\begin{pmatrix} 1 & 0 \\ k_{1,1} & 1 \end{pmatrix}$, we can rewrite the latter equation as:

$$\begin{pmatrix} \overline{c}_{11} & \overline{c}_{12} \\ \overline{c}_{21} & \overline{c}_{22} \end{pmatrix} \begin{pmatrix} k_{21} \\ k_{22} \end{pmatrix} = - \begin{pmatrix} \overline{c}_{13} \\ \overline{c}_{23} \end{pmatrix}. \tag{4.13}$$

We introduce the notation, by c_i^k we denote the i-th column in the matrix $\overline{C}^T$ truncated by first k elements:

$$\overline{c}_i^k := \begin{pmatrix} \overline{c}_{1i} & \overline{c}_{2i} & \dots & \overline{c}_{ki} \end{pmatrix}^*.$$

Since C^T is invertible, (4.13) has a unique solution, moreover, we can infer that:

$$k_{22} = - \frac{\det \begin{pmatrix} \overline{c}_{11} & \overline{c}_{13} \\ \overline{c}_{21} & \overline{c}_{23} \end{pmatrix}}{\det \begin{pmatrix} \overline{c}_{11} & \overline{c}_{12} \\ \overline{c}_{21} & \overline{c}_{22} \end{pmatrix}} = - \det(\overline{c}_1^2, \overline{c}_3^2).$$

Assume that we have already recovered $K_0, K_1, \dots, K_l$, to recover K_{l+1} we need to consider the equations $K_0 \overline{C}^T K_{l+1}^* = 0$, $K_1 \overline{C}^T K_{l+1}^* = 0, \dots,$ $K_l \overline{C}^T K_{l+1}^* = 0$, which are equivalent to:

$$\begin{pmatrix} 1 & 0 & .. & 0 \\ k_{11} & 1 & 0 & .. \\ . & . & . & . \\ k_{l1} & k_{l2} & . & 1 \end{pmatrix} \begin{pmatrix} \overline{c}_{11} & .. & .. & \overline{c}_{1,l+2} \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ \overline{c}_{l+1,1} & .. & .. & \overline{c}_{l+1,l+2} \end{pmatrix} \begin{pmatrix} k_{l+1,1} \\ k_{l+1,2} \\ .. \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ .. \\ .. \\ 0 \end{pmatrix}.$$

We can rewrite the latter equation as:

$$\begin{pmatrix} \overline{c}_{1,1} & .. & .. & \overline{c}_{1,l+1} \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ \overline{c}_{l+1,1} & .. & .. & \overline{c}_{l+1,l+1} \end{pmatrix} \begin{pmatrix} k_{l+1,1} \\ k_{l+1,2} \\ .. \\ k_{l+1,l+1} \end{pmatrix} + \begin{pmatrix} \overline{c}_{1,l+2} \\ \overline{c}_{2,l+2} \\ .. \\ \overline{c}_{l+1,l+2} \end{pmatrix} = 0. \tag{4.14}$$

Due to the invertibility of C^T the latter equation has unique solution, moreover

$$k_{l+1,l+1} = - \det(\overline{c}_1^{l+1}, \overline{c}_2^{l+1}, \dots \overline{c}_l^{l+1}, \overline{c}_{l+2}^{l+1}), \quad l = 0, \dots, T-2. \tag{4.15}$$

Having recovered $k_{\alpha,\alpha} = -w_{\alpha,\alpha}$, we recover the potential by (see (2.2)):

$$b_n = w_{n-1,n-1} - w_{n,n} = k_{n,n} - k_{n-1,n-1}, \quad n = 1, \dots, T-1. \tag{4.16}$$

4.3. Gelfand–Levitan equations

If we introduce $\widetilde{C}^T$ by

$$\overline{C}^T = I + \widetilde{C}^T, \tag{4.17}$$

(see (3.6),(4.9)), then we can rewrite (4.14) for $l = T-2$ as:

$$\left(I + \widetilde{C}^T\right) K_T + \widetilde{C}_T = 0, \text{ where } K_T = \begin{pmatrix} k_{T-1,1} \\ k_{T-1,2} \\ . \\ k_{T-1,T-1} \end{pmatrix}, \ \widetilde{C}_T = \begin{pmatrix} \widetilde{C}_{1,T}^T \\ \widetilde{C}_{2,T}^T \\ . \\ \widetilde{C}_{T-1,T}^T \end{pmatrix}$$

or as a system:

$$k_{T-1,\beta} + \sum_{j=1}^{T-1} \widetilde{C}_{\beta,j}^T k_{T-1,j} + \widetilde{C}_{\beta,T}^T = 0, \quad \beta = 1, \dots, T-1. \tag{4.18}$$

If we pass to (more standard) entries of $\left(\overline{W}^T\right)^{-1}$

$$\widetilde{k}_{\alpha,\beta} = k_{\beta,\alpha}, \tag{4.19}$$

then (4.18) can be rewritten as:

$$\widetilde{k}_{\beta,T-1} + \sum_{j=1}^{T-1} \widetilde{C}^T_{\beta,j} \widetilde{k}_{j,T-1} + \widetilde{C}^T_{\beta,T} = 0, \quad \beta = 1, \dots, T-1. \tag{4.20}$$

The last equation is an analog of Gelfand-Levatan equation for continuous problem [4,5]. We conclude this section with

Theorem 4. *The kernel of the operator* $\left(\overline{W}^T\right)^{-1}$ *(see (4.10)) satisfies equation (4.20), where the entries* $\widetilde{C}^T_{i,j}$ *are defined in (4.17), (3.6).*

The equation in (4.18) has a unique solution due to the invertibility of C^T. The potential can be recovered by (4.16).

Now, we make some remarks on the dependence of the connecting operator C^T and the solution of the inverse problem equations (i.e. the potential) on the inverse data. As a direct consequence of (3.6) we can formulate the following:

Remark 1. *The operator* C^T *depends on* R^{2T-2}*, i.e. it depends on the potential* $(b_1, \dots, b_{T-1})$*, so the results obtained from* C^T *via Krein-type equations (4.4), (4.6),(4.7), factorization method (4.15), (4.16) and Gelfand-Levitan type equations (4.20), (4.16) are the best possible.*

In the subsection on the factorization method, we used the fact that $\det C^\tau = 1$, $\tau = 2, \dots, T$. More precisely, we used it in the form $\det(\overline{c}^\tau_1, \overline{c}^\tau_2, \dots \overline{c}^\tau_\tau) = 1$. That fact actually says that not all elements in the response vector are independent. Indeed: the element k_{11} we recovered (see (4.12)) from $\overline{c}_{21}$, i.e. from r_1. The element k_{22} we recovered from $\overline{c}_{11}$, $\overline{c}_{13}$, $\overline{c}_{21}$, $\overline{c}_{23}$, that is from r_1, r_2, r_3. But since $\det(\overline{c}^2_1, \overline{c}^2_2) = 1$, we have that $r_2 = r_1^2$, so in fact k_{22} was recovered from r_1 and r_3. Arguing in the same fashion, we see that r_{2k} depends on r_{2l+1}, $l = 0, \dots, k-1$. So we recovered $(k_{11}, \dots, k_{T-1,T-1})$ from the response vector $(r_0, r_1, \dots, r_{2t-2})$, $r_0 = 1$, whose components with even numbers depend in explicit form on the components with odd numbers. That observation plays an important role in the next subsection.

4.4. Characterization of the inverse data

In the second section, we considered the forward problem (1.1), for the potential $(b_1, \dots, b_{T-1})$ we constructed the matrix W^T (2.1), (2.2), the response vector $(1, r_1, \dots, r_{2T-2})$ (see (3.1)) and the connecting operator C^T by formula (3.6). It will be more convenient for us to deal with the rotated matrix $\overline{C}^T$ defined in (4.9). From the representation $\overline{C}^T = (\overline{W}^T)^* \overline{W}^T$ and triangularity of $\overline{W}^T$ we know that

$$\det \overline{C}^l = 1 \quad \forall l = 1, \dots, T.$$

Also, we have proven that if coefficients $r_1, \dots, r_{2T-2}$ correspond to some potential $(b_1, \dots, b_{T-1})$, then we can recover the potential using (4.15)–(4.16).

Now, we set up a question: can one determine whether a vector $(1, r_1, r_2, \dots, r_{2T-2})$ is a response vector for the dynamical system (1.1) with a potential $(b_1, \dots, b_{T-1})$ or not? The answer is the following theorem.

Theorem 5. *The vector* $(1, r_1, r_2, \dots, r_{2T-2})$ *is a response vector for the dynamical system (1.1) if and only if the matrix* C^T *(3.6) is positively definite and* $\det C^l = 1$, $l = 1, \dots, T$.

Proof. First we observe that in the conditions of the theorem we can substitute C^T by $\overline{C}^T$ (4.9). The necessary part of the theorem is proved in the preceding sections. We are left to prove the sufficiency of these conditions.

Let there be a vector $(1, r_1, \dots, r_{2T-2})$ such that the matrix $\overline{C}^T$ constructed from it using (4.9) satisfies conditions of the theorem. Then we can construct the potential $(b_1, \dots, b_{T-1})$ using (4.15)–(4.16) and consider the dynamical system (1.1) with this potential. For this system, we construct the connecting operator C^T_{new} and its rotated $\overline{C}^T_{new}$ using (2.2), (3.1), (3.6) and (4.9). We will show that the matrices $\overline{C}^T$ and $\overline{C}^T_{new}$ coincide.

First, we note that we have two matrices constructed by (4.9), one comes from the vector $(1, r_1, \dots, r_{2T-2})$ and the other comes from $(1, r_1^{new}, \dots, r_{2T-2}^{new})$. Also they have a common property that $\det \overline{C}^l = \det \overline{C}^l_{new} = 1$ for all $l = 1, \dots, T$ (one by theorem's condition and the other by representation $\overline{C}^T_{new} = (\overline{W}^T_{new})^* \overline{W}^T_{new}$).

Secondly, we note that if we calculate the potential $(b_1, \dots, b_{T-1})$ using (4.15)–(4.16) from any of $\overline{C}^T$ and $\overline{C}^T_{new}$ matrices, we obtain the same answer.

Therefore we have two matrices of the type (4.9) with the unit principal minors and the property

$$\det(\overline{c}_1^{l+1}, \dots \overline{c}_l^{l+1}, \overline{c}_{l+2}^{l+1}) = \det(\overline{c_{new}}_1^{l+1}, \dots \overline{c_{new}}_l^{l+1}, \overline{c_{new}}_{l+2}^{l+1}) \quad \forall l = 0, \dots, T-2. \tag{4.21}$$

If we look at (4.21) for $l = 0$, we see that $r_1 = r_1^{new}$. From the fact that for both matrices $\overline{C}^T$, $\overline{C}_{new}^T$ the principal minors of the second order are equal to one, we infer that $r_2 = r_2^{new}$. We continue this procedure, and from (4.21) with $l = n$, we infer that $r_{2n+1} = r_{2n+1}^{new}$ and from equality to one of principal minor of the order $n+2$ of $\overline{C}^T$, $\overline{C}_{new}^T$, we can infer that $r_{2n+2} = r_{2n+2}^{new}$ for all $n = 2, \dots, T-2$ by induction. This finishes the proof. □

5. Spectral representation of $\mathbf{C^T}$ and $\mathbf{r}_t$

In this section, we consider the inverse spectral problem and show the connection of the spectral (2.5), (2.6) and dynamical (3.1), (3.2) inverse data. If we introduce the special control $\delta = (1, 0, 0, \dots)$, then the kernel of response operator (3.2) is:

$$r_t^i = (R_i\delta)_t = v_{1,t}^{\delta}, \tag{5.1}$$

on the other hand, we can use (2.9), (2.10) to obtain:

$$v_{1,t}^{\delta} = \sum_{k=1}^{N} \frac{1}{\rho_k} T_t(\lambda_k). \tag{5.2}$$

So on introducing the spectral function:

$$\rho^N(\lambda) = \sum_{\{k \,|\, \lambda_k < \lambda\}} \frac{1}{\rho_k}, \tag{5.3}$$

from (5.1), (5.2) we deduce that:

$$r_t^i = \int_{-\infty}^{\infty} T_t(\lambda)\, d\rho^N(\lambda), \quad t \in \mathbb{N}.$$

Let us evaluate $(C_i^T f, g)$ for $f, g \in \mathcal{F}^T$, using the expansion (2.9):

$$\begin{aligned}(C_i^T f, g) = \sum_{n=1}^{N} v_{n,T}^f v_{n,T}^g &= \sum_{n=1}^{N}\sum_{k=1}^{N} \frac{1}{\rho_k} T_T(\lambda_k) * f\varphi_n^k \sum_{l=1}^{N} \frac{1}{\rho_l} T_T(\lambda_l) * g\varphi_n^l \\ &= \sum_{k=1}^{N} \frac{1}{\rho_k} T_T(\lambda_k) * f T_T(\lambda_k) * g = \int_{-\infty}^{\infty} \sum_{l=0}^{T-1} T_{T-l}(\lambda) f_l \sum_{m=0}^{T-1} T_{T-m}(\lambda) g_m \, d\rho^N(\lambda).\end{aligned}$$

From the equality above, it is evident that (cf. (3.6)):

$$\{C_i^T\}_{l+1,m+1} = \int_{-\infty}^{\infty} T_{T-l}(\lambda) T_{T-m}(\lambda)\, d\rho^N(\lambda), \quad l, m = 0, \dots, T-1. \tag{5.4}$$

Let us consider the spectral problem:

$$\begin{cases} \phi_{i+1} + \phi_{i-1} - b_n\phi_i = \lambda\phi_i, \quad n = 0, \dots, N+1, \\ \phi_0 = 0, \ \phi_{N+1} = 0. \end{cases} \tag{5.5}$$

In the second section, we construct the spectral data for this problem – eigenvalues of the corresponding Hamiltonian and norming coefficients (2.5), (2.6). Now we answer the question how to recover the potential $(b_1, \dots, b_N)$ from this data.

Our strategy will be to use the dynamical approach from the fourth section to treat this IP. First, we observe that to know (2.6) is the same as to know the spectral function (5.3). Consider the system (1.1) with the same potential b_n for $n = 1, \dots, N$. We notice that as explained in the beginning of section four, $R^{2N} = R_i^{2N}$ and correspondingly, $r_t = r_t^i$, $t = 1, \dots, 2N$. Due to this, we deduce that $C^T = C_i^T$ for $T = N+1$. Thus, the inverse

problem can be solved in the following way: from the spectral data (2.6), we construct the spectral function by (5.3). Then, we construct:

$$r_t = r_t^i = \int\limits_{-\infty}^{\infty} T_t(\lambda)\, d\rho^N(\lambda), \quad t = 1, \dots, 2N,$$

$$C_{lm}^T = \{C_i^T\}_{l+1,m+1} = \int\limits_{-\infty}^{\infty} T_{T-l}(\lambda) T_{T-m}(\lambda)\, d\rho^N(\lambda), \quad l, m = 0, \dots, N-1.$$

After we have in hands the connecting operator, we can use the methods of section four to find $(b_1, \dots, b_N)$.

Acknowledgements

The research of Victor Mikhaylov was supported in part by NIR SPbGU 11.38.263.2014 and RFBR 14-01-00535. Alexandr Mikhaylov was supported by RFBR 14-01-00306; A. S. Mikhaylov and V. S. Mikhaylov were partly supported by VW Foundation program 'Modeling, Analysis, and Approximation Theory toward application in tomography and inverse problems'.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 854–864

On direct and inverse spectral problems for sloshing of a two-layer fluid in an open container

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PACS 02.30.Jr, 47.35.Bb **DOI 10.17586/2220-8054-2016-7-5-854-864**

We study the direct and inverse eigenvalue problems for a pair of harmonic functions with a spectral parameter in boundary and coupling conditions. The direct problem is relevant to sloshing frequencies of free oscillations of a two-layer fluid in a container. The upper fluid occupies a layer bounded above by a free surface and below by a layer of fluid of greater density. Both fluids are assumed to be inviscid, incompressible, and heavy, whereas the free surface and the interface between fluids are considered bounded.

Keywords: Laplace equation, sloshing problem, two-layer fluid, eigenvalue, eigenfunction, inverse spectral problem.

Received: 19 August 2016

Revised: 5 September 2016

In memory of B. S. Pavlov (1936–2016)

1. Introduction

Linear water wave theory is a widely used approach for describing the behavior of surface waves in the presence of rigid boundaries. In particular, this theory is a common tool for determining sloshing frequencies and modes in containers occupied by a homogeneous fluid, that is, having constant density. The corresponding boundary spectral problem, usually referred to as the sloshing problem, has been the subject of a great number of studies over more than two centuries (a historical review can be found, for example, in [1]). In the comprehensive book [2], an advanced technique based on spectral theory of operators in a Hilbert space was presented for studying this problem.

In the framework of the mathematical theory of linear water waves, substantial work has been done in the past two decades for understanding the difference between the results valid for homogeneous and two-layer fluids (in the latter case the upper fluid occupies a layer bounded above by a free surface and below by a layer of fluid whose density is greater than that in the upper one). These results concern wave/structure interactions and trapping of waves by immersed bodies (see, for example, [3–5] and references cited therein), but much less is known about the difference between sloshing in containers occupied by homogeneous and two-layer fluids. To the author's knowledge, there is only one related paper [6] with rigorous results for multilayered fluids, but it deals only with the spectral asymptotics in a closed container. Thus, the first aim of the present paper is to fill in this gap at least partially.

Another aim is to consider the so-called inverse sloshing problem; that is, the problem of recovering some physical parameters from known spectral data. The parameters to be recovered are the depth of the interface between the two layers and the density ratio that characterizes stratification. It is demonstrated that for determining these two characteristics for fluids occupying a vertical-walled container with a horizontal bottom, one has to measure not only the two smallest sloshing eigenfrequencies, which must satisfy certain inequalities, but also to analyze the corresponding free surface elevations.

1.1. Statement of the direct problem

Let two immiscible, inviscid, incompressible, heavy fluids occupy an open container whose walls and bottom are rigid surfaces. We choose rectangular Cartesian coordinates (x_1, x_2, y) so that their origin lies in the mean free surface of the upper fluid and the y-axis is directed upwards. Then, the whole fluid domain W is a subdomain of the lower half-space $\{-\infty < x_1, x_2 < +\infty,\ y < 0\}$. The boundary ∂W is assumed to be piece-wise smooth and such that every two adjacent smooth pieces of ∂W are not tangent along their common edge. We also suppose that each horizontal cross-section of W is a bounded two-dimensional domain; that is, a connected, open set in the corresponding plane. (The latter assumption is made for the sake of simplicity because it excludes the possibility of two or more interfaces between fluids at different levels.) The free surface F bounding above the

upper fluid of density $\rho_1 > 0$ is the non-empty interior of $\partial W \cap \{y = 0\}$. The interface $I = W \cap \{y = -h\}$, where $0 < h < \max\{|y| : (x_1, x_2, y) \in \partial W\}$, separates the upper fluid from the lower one of density $\rho_2 > \rho_1$. We denote by W_1 and W_2 the domains $W \cap \{y > -h\}$ and $W \cap \{y < -h\}$ respectively; they are occupied by the upper and lower fluids respectively. The surface tension is neglected and we suppose the fluid motion to be irrotational and of small amplitude. Therefore, the boundary conditions on F and I may be linearized. With a time-harmonic factor, say $\cos \omega t$, removed, the velocity potentials $u^{(1)}(x_1, x_2, y)$ and $u^{(2)}(x_1, x_2, y)$ (they may be taken to be real functions) for the flow in W_1 and W_2 respectively must satisfy the following coupled boundary value problem:

$$u^{(j)}_{x_1x_1} + u^{(j)}_{x_2x_2} + u^{(j)}_{yy} = 0 \quad \text{in } W_j, \quad j = 1, 2, \tag{1}$$

$$u^{(1)}_y = \nu u^{(1)} \quad \text{on } F, \tag{2}$$

$$\rho\left(u^{(2)}_y - \nu u^{(2)}\right) = u^{(1)}_y - \nu u^{(1)} \quad \text{on } I, \tag{3}$$

$$u^{(2)}_y = u^{(1)}_y \quad \text{on } I, \tag{4}$$

$$\partial u^{(j)}/\partial n = 0 \quad \text{on } B_j \quad j = 1, 2. \tag{5}$$

Here, $\rho = \rho_2/\rho_1 > 1$ is the non-dimensional measure of stratification, the spectral parameter ν is equal to ω^2/g, where ω is the radian frequency of the water oscillations and g is the acceleration due to gravity; $B_j = \partial W_j \backslash (\bar{F} \cup \bar{I})$ is the rigid boundary of W_j. By combining (3) and (4), we get another form of the spectral coupling condition (3):

$$(\rho - 1)u^{(2)}_y = \nu\left(\rho u^{(2)} - u^{(1)}\right) \quad \text{on } I. \tag{6}$$

We also suppose that the orthogonality conditions

$$\int_F u^{(1)}\,\mathrm{d}x = 0 \quad \text{and} \quad \int_I \left(\rho u^{(2)} - u^{(1)}\right)\mathrm{d}x = 0, \quad \mathrm{d}x = \mathrm{d}x_1\mathrm{d}x_2, \tag{7}$$

hold, thus excluding the zero eigenvalue of (1)–(5).

When $\rho = 1$, conditions (3) and (4) mean that the functions $u^{(1)}$ and $u^{(2)}$ are harmonic continuations of each other across the interface I. Then, problem (1)–(5) complemented by the first orthogonality condition (7) (the second condition (7) is trivial), becomes the usual sloshing problem for a homogeneous fluid. It is well-known since the 1950s that the latter problem has a positive discrete spectrum. This means that there exists a sequence of positive eigenvalues $\{\nu^W_n\}^\infty_1$ of finite multiplicity (the superscript W is used here and below for distinguishing the sloshing eigenvalues that correspond to the case, when a homogeneous fluid occupies the whole domain W, from those corresponding to a two-layer fluid which will be denoted simply by ν_n). In this sequence the eigenvalues are written in increasing order and repeated according to their multiplicity; moreover, $\nu^W_n \to \infty$ as $n \to \infty$. The corresponding eigenfunctions $\{u_n\}^\infty_1 \subset H^1(W)$ form a complete system in an appropriate Hilbert space. These results can be found in many sources, for example, in the book [2].

2. Variational principle

Let W be bounded. It is well known that the sloshing problem in W for homogeneous fluid can be cast into the form of a variational problem and the corresponding Rayleigh quotient is as follows:

$$R_W(u) = \frac{\int\limits_W |\nabla u|^2\,\mathrm{d}xy}{\int\limits_F u^2\,\mathrm{d}x}. \tag{8}$$

In order to obtain the fundamental eigenvalue ν^W_1 one has to minimize $R_W(u)$ over the subspace of the Sobolev space $H^1(W)$ consisting of functions that satisfy the first orthogonality condition (7). To find ν^W_n for $n > 1$, one has to minimize (8) over the subspace of $H^1(W)$ such that each of its element u satisfies the first condition (7) along with the following equalities $\int\limits_F u\,u_j\,\mathrm{d}x = 0$, where u_j is either of the eigenfunctions $u_1, \ldots, u_{n-1}$ corresponding to the eigenvalues $\nu^W_1, \ldots, \nu^W_{n-1}$.

In the case of a two-layer fluid, we assume that the usual embedding theorems hold for both subdomains W_j, $j = 1, 2$ (the theorem about traces on smooth pieces of the boundary for elements of H^1 included). This imposes some restrictions on ∂W, in particular, on the character of the intersections of F and I with $\partial W \cap \{y < 0\}$. Then

using (6), it is easy to verify that the Rayleigh quotient for the two-layer sloshing problem has the following form:

$$R(u^{(1)}, u^{(2)}) = \frac{\int\limits_{W_1} \left|\nabla u^{(1)}\right|^2 \mathrm{d}x\mathrm{d}y + \rho \int\limits_{W_2} \left|\nabla u^{(2)}\right|^2 \mathrm{d}x\mathrm{d}y}{\int\limits_F \left[u^{(1)}\right]^2 \mathrm{d}x + (\rho-1)^{-1} \int\limits_I \left[\rho u^{(2)} - u^{(1)}\right]^2 \mathrm{d}x}. \tag{9}$$

To determine the fundamental sloshing eigenvalue ν_1 one has to minimize $R(u^{(1)}, u^{(2)})$ over the subspace of $H^1(W_1) \oplus H^1(W_2)$ defined by both orthogonality conditions (7). In order to find ν_n for $n > 1$, one has to minimize (9) over the subspace of $H^1(W_1) \oplus H^1(W_2)$ such that every element $\left(u^{(1)}, u^{(2)}\right)$ of this subspace satisfies the equalities:

$$\int\limits_F u^{(1)}\, u_j^{(1)}\, \mathrm{d}x = 0 \quad \text{and} \quad \int\limits_I \left[\rho u^{(2)} - u^{(1)}\right] \left[\rho u_j^{(2)} - u_j^{(1)}\right] \mathrm{d}x = 0, \quad j = 1, \ldots, n-1,$$

along with both conditions (7). Here, $\left(u_j^{(1)}, u_j^{(2)}\right)$ is either of the eigensolutions corresponding to $\nu_1, \ldots, \nu_{n-1}$.

Now we are in a position to prove the following assertion.

Proposition 1. *Let ν_1^W and ν_1 be the fundamental eigenvalues of the sloshing problem in the bounded domain W for homogeneous and two-layer fluids respectively. Then the inequality $\nu_1 < \nu_1^W$ holds.*

The restriction that W is bounded is essential as the example considered in Proposition 4 below demonstrates.

Proof. If u_1 is an eigenfunction corresponding to ν_1^W, then

$$\nu_1^W = \frac{\int\limits_W |\nabla u_1|^2 \,\mathrm{d}x\mathrm{d}y}{\int\limits_F u_1^2 \,\mathrm{d}x}\,.$$

Let $u^{(1)}$ and $u^{(2)}$ be equal to the restrictions of ρu_1 and u_1 to W_1 and W_2, respectively. Then the pair $\left(u^{(1)}, u^{(2)}\right)$ is an admissible element for the Rayleigh quotient (9). Substituting it into (9), we obtain that:

$$R(\rho u_1, u_1) = \frac{\int\limits_{W_1} |\nabla u_1|^2 \,\mathrm{d}x\mathrm{d}y + \rho^{-1} \int\limits_{W_2} |\nabla u_1|^2 \,\mathrm{d}x\mathrm{d}y}{\int\limits_F u_1^2 \,\mathrm{d}x}.$$

Comparing this equality with the previous one and taking into account that $\rho > 1$, one finds that $R(\rho u_1, u_1) < \nu_1^W$. Since ν_1 is the minimum of (9), we conclude that $\nu_1 < \nu_1^W$. □

3. Containers with vertical walls and horizontal bottoms

Let us consider the fluid domain $W = \{x = (x_1, x_2) \in D,\, y \in (-d, 0)\}$, where D is a piece-wise smooth two-dimensional domain (the container's horizontal cross-section) and $d \in (0, \infty]$ is the container's constant depth. Thus, the container's side wall $\partial D \times (-d, 0)$ is vertical, the bottom $\{x \in D,\, y = -d\}$ is horizontal, whereas the free surface and the interface are $F = \{x \in D,\, y = 0\}$ and $I = \{x \in D,\, y = -h\}$ respectively, $0 < h < d$.

For a homogeneous fluid occupying such a container, the sloshing problem is equivalent to the free membrane problem. Indeed, putting

$$u(x, y) = v(x) \cosh k(y + d) \quad \left(\, u(x, y) = v(x)\, \mathrm{e}^{ky} \text{ when } d = \infty \,\right),$$

one reduces problem (1)–(5) with $\rho = 1$, complemented by the first orthogonality condition (7) to the following spectral problem:

$$\nabla_x^2 v + k^2 v = 0 \ \text{ in } \ D, \quad \partial v/\partial n_x = 0 \ \text{ on } \ \partial D, \quad \int\limits_D v \,\mathrm{d}x = 0, \tag{10}$$

where $\nabla_x = (\partial/\partial x_1, \partial/\partial x_2)$ and n_x is a unit normal to ∂D in $\mathbb{R}^2$. It is clear that ν^W is an eigenvalue of the former problem if and only if k^2 is an eigenvalue of (10) and

$$\nu^W = k \tanh kd \quad \text{when } d < \infty \quad \left(\, \nu^W = k \quad \text{when } d = \infty \,\right), \quad k > 0. \tag{11}$$

It is well-known that problem (10) has a sequence of positive eigenvalues $\{k_n^2\}_1^\infty$ written in increasing order and repeated according to their finite multiplicity, and such that $k_n^2 \to \infty$ as $n \to \infty$. The corresponding eigenfunctions form a complete system in $H^1(D)$.

Let us describe the same reduction procedure in the case when W is occupied by a two-layer fluid and $d < \infty$. Putting

$$u^{(1)}(x,y) = v(x)\,[A\cosh k(y+h) + B\sinh k(y+h)], \tag{12}$$

$$u^{(2)}(x,y) = v(x)\,C\cosh k(y+d), \tag{13}$$

where A, B and C are constants, one reduces problem (1)–(5) and (7), $\rho > 1$, to problem (10) combined with the following quadratic equation:

$$\nu^2\cosh kd - \nu k\,[\sinh kd + (\rho-1)\cosh kh\,\sinh k(d-h)] + k^2(\rho-1)\sinh kh\,\sinh k(d-h) = 0, \quad k > 0. \tag{14}$$

Thus ν is an eigenvalue of the former problem if and only if ν satisfies (14), where k^2 is an eigenvalue of (10).

Indeed, the quadratic polynomial in ν on the left-hand side of (14) is the determinant of the following linear algebraic system for A, B and C:

$$A = C\,\left[\cosh k(d-h) - \nu^{-1}(\rho-1)\,k\,\sinh k(d-h)\right], \quad B = C\,\sinh k(d-h), \tag{15}$$

$$A\,(k\,\sinh kh - \nu\,\cosh kh) + C\,\sinh k(d-h)\,(k\,\cosh kh - \nu\,\sinh kh) = 0. \tag{16}$$

The latter arises when one substitutes expressions (12) and (13) into the boundary condition (2) and the coupling conditions (3) and (4). This homogeneous system defines eigensolutions of the sloshing problem provided there exists a non-trivial solution, and so the determinant must vanish which is expressed by (14).

Let us show that the roots $\nu^{(+)}$ and $\nu^{(-)}$ of (14) are real in which case

$$\nu^{(\pm)} = k\,\frac{b \pm \sqrt{\mathcal{D}}}{2\,\cosh kd} > 0\,, \tag{17}$$

where the inequality is a consequence of the formulae:

$$b = \sinh kd + (\rho-1)\,\cosh kh\,\sinh k(d-h), \tag{18}$$

$$\mathcal{D} = b^2 - 4\,(\rho-1)\,\cosh kd\,\sinh kh\,\sinh k(d-h). \tag{19}$$

Since $\mathcal{D}$ is a quadratic polynomial of $\rho - 1$, it is a simple application of calculus to demonstrate that it attains the minimum at

$$\rho - 1 = \frac{2\,\cosh kd\,\sinh kh - \sinh kd\,\cosh kh}{\cosh^2 kh\,\sinh k(d-h)}\,,$$

and after some algebra one finds that this minimum is equal to

$$\frac{4\,\cosh kd\,\sinh kh\,\sinh k(d-h)}{\cosh^2 kh} > 0,$$

which proves the assertion. Thus we arrive at the following.

Proposition 2. *If W is a vertical cylinder with horizontal bottom, then the sloshing problem for a two-layer fluid occupying W has two sequences of eigenvalues*

$$\left\{\nu_n^{(+)}\right\}_1^\infty \quad \textit{and} \quad \left\{\nu_n^{(-)}\right\}_1^\infty$$

defined by (17) *with $k = k_n > 0$, where k_n^2 is an eigenvalue of problem* (10).

The same eigensolution $(u^{(1)}, u^{(2)})$ corresponds to both $\nu_n^{(+)}$ and $\nu_n^{(-)}$, where $u^{(1)}$ and $u^{(2)}$ (sloshing modes in W_1 and W_2 respectively) are defined by formulae (12) *and* (13) *with v belonging to the set of eigenfunctions of problem* (10) *that correspond to k_n^2; furthermore, C is an arbitrary non-zero real constant, whereas A and B depend on C through* (15).

Next, we analyze the behavior of $\nu_n^{(\pm)}$ as a function of ρ.

Proposition 3. *For every $n = 1, 2, \ldots$ the functions $\nu_n^{(-)}$ and $\nu_n^{(+)}$ are monotonically increasing as ρ goes from* 1 *to infinity. Their ranges are:*

$$(0,\, k_n \tanh k_n h) \quad \textit{and} \quad (k_n \tanh k_n d,\, \infty)$$

respectively.

Proof. In order to prove the proposition, it is sufficient to show that:

$$\frac{\partial(b \pm \sqrt{\mathcal{D}}\,)}{\partial\rho} = \sinh k(d-h)\Big\{ \cosh kh \pm \mathcal{D}^{-1/2}\big[\cosh kh\, \sinh kd + (\rho-1)\cosh^2 kh\, \sinh k(d-h) - 2\cosh kd\, \sinh kh\big]\Big\} > 0\,. \tag{20}$$

Since

$$\left.\frac{\partial(b+\sqrt{\mathcal{D}}\,)}{\partial\rho}\right|_{\rho=1} = \frac{2\sinh^2 k(d-h)}{\sinh kd} > 0 \quad \text{and} \quad \left.\frac{\partial(b-\sqrt{\mathcal{D}}\,)}{\partial\rho}\right|_{\rho\to\infty} = 0\,,$$

inequality (20) is a consequence of the following one:

$$\pm\frac{\partial^2(b \pm \sqrt{\mathcal{D}}\,)}{\partial\rho^2} = \frac{4\,\cosh kd\, \sinh kh\, \sinh^3 k(d-h)}{\mathcal{D}^{3/2}} > 0 \quad \text{for all } \rho > 1.$$

The second assertion immediately follows from the first one and formulae (17)–(19). □

Combining Proposition 3 and formula (11), we arrive at the following assertion.

Corollary 1. *The inequalities* $\nu_n^{(-)} < \nu_n^W < \nu_n^{(+)}$ *hold for each* $n = 1, 2, \ldots$ *and every* $\rho > 1$.

Dividing (17) by k and letting $k = k_n$ to infinity, it is straightforward to obtain the following.

Lemma 1. *For every* $\rho > 1$*, the asymptotic formula:*

$$\nu_n^{(\pm)} \sim \frac{\rho + 1 \pm |\rho - 3|}{4}\, k_n \quad as\ n \to \infty,$$

holds with the exponentially small remainder term; here k_n^2 *is an eigenvalue of* (10).

In other words, there are three cases:

(i) if $\rho = 3$, then $\nu_n^{(\pm)} \sim k_n$ as $n \to \infty$;
(ii) if $\rho > 3$, then $\nu_n^{(-)} \sim k_n$ and $\nu_n^{(+)} \sim (\rho-1)\,k_n/2$ as $n \to \infty$;
(iii) if $\rho \in (1,3)$, then $\nu_n^{(-)} \sim (\rho-1)\,k_n/2$ and $\nu_n^{(+)} \sim k_n$ as $n \to \infty$.

Combining these relations and the asymptotic formula $\nu_n^W \sim k_n$ as $n \to \infty$ (it is a consequence of formula (11) defining ν_n^W when a homogeneous fluid occupies W), we obtain the following.

Corollary 2. *As* $n \to \infty$*, we have that* $\nu_n^{(-)} \sim \nu_n^W$ *when* $\rho \geq 3$*, whereas* $\nu_n^{(+)} \sim \nu_n^W$ *provided* $\rho \in (1, 3]$.

Another corollary of Lemma 1 concerns the distribution function $\mathcal{N}(\nu)$ for the spectrum of problem (1)–(5) and (7). This function is equal to the total number of eigenvalues ν_n that do not exceed ν. An asymptotic formula for $\mathcal{N}(\nu)$ immediately follows from Lemma 1 and the asymptotic formula for the distribution of the spectrum for the Neumann Laplacian (see [7], Chapter 6).

Corollary 3. *The distribution function* $\mathcal{N}(\nu)$ *of the spectrum for the sloshing of a two-layer fluid in a vertical cylinder of cross-section* D *has the following asymptotics:*

$$\mathcal{N}(\nu) \sim \left[\frac{4}{(\rho-1)^2} + 1\right] \frac{|D|\,\nu^2}{4\pi} \quad as\ \nu \to \infty.$$

Here, $|D|$ *stands for the area of* D.

It should be also mentioned that in [6] the asymptotics for $\mathcal{N}(\nu)$ was obtained for a multi-layer fluid occupying a bounded closed container.

It follows from Lemma 1 and Corollary 2 that the asymptotic formula for the distribution function of the spectrum $\{\nu_n^W\}_1^\infty$ is similar to the above one, but the first term in the square brackets must be deleted. Moreover, in the case of homogeneous fluid the same asymptotic formula (up to the remainder term) holds for arbitrarily shaped fluid domains (see [2], Section 3.3). Since the first term in the square brackets tends to infinity as $\rho \to 1$, the transition from the two-layer fluid to the homogeneous one in the asymptotic formula for $\mathcal{N}(\nu)$ is a singular limit in the sense described in [8]. A similar effect occurs for modes trapped by submerged bodies in two-layer and homogeneous fluids as was noted in [4].

In conclusion of this section, it should be noted that in the case of an infinitely deep vertical cylinder it is easy to verify that $\nu = k$ is an eigenvalue of the sloshing problem for a two-layer fluid if and only if k^2 is an eigenvalue of problem (10). Comparing this assertion with that at the beginning of this section, we obtain the following.

Proposition 4. *In an infinitely deep vertical-walled container, the sloshing problem for a two-layer fluid has the same set of eigenvalues and the same eigenfunctions of the form* $v(x)\,\mathrm{e}^{ky}$, $k>0$, *as the sloshing problem for a homogeneous fluid in the same container; here,* k^2 *is an eigenvalue and* v *is the corresponding eigenfunction of problem* (10).

4. Inverse problem

Let a given container W be occupied by a two-layer fluid, but now we assume that the position of the interface between layers and the density of the lower layer are unknown. The density of the upper layer is known because one can measure it directly. The sequence of eigenvalues $\{\nu_n^W\}_1^\infty$ corresponding to the homogeneous fluid is also known because it depends only on the domain W. The inverse problem we are going to consider is to recover the ratio of densities ρ and the depth of the interface h from measuring some sloshing frequencies on the free surface. Thus, we let the fundamental eigenvalue ν_1 be known along with the second-largest one.

The formulated inverse problem is not always solvable. Indeed, according to Proposition 4, *it has no solution when* W *is an infinitely deep container with vertical walls*. Moreover, the inverse problem is trivial for all domains when $\nu_1=\nu_1^W$. In this case, Proposition 1 implies that the fluid is homogeneous, that is, $\rho=1$ and $h=d$. Therefore, we restrict ourselves to the case of vertically-walled containers having a finite depth d in what follows.

4.1. Reduction to transcendental equations

In view of what was said above, the inverse problem for $W=D\times(-d,0)$ can be stated as follows. Find conditions that allow us to determine $\rho>1$ and $h\in(0,d)$ when the following two eigenvalues are known: the fundamental one ν_1 and the smallest eigenvalue ν_N that is greater than ν_1. Thus, N is such that $k_n^2=k_1^2$ for all $n=1,\dots,N-1$, which means that the fundamental eigenvalue k_1^2 of problem (10) is of multiplicity $N-1$ (of course, ν_1 has the same multiplicity). For example, if D is a disc, then the multiplicity of k_1^2 is two (see [9], Section 3.1), and so $\nu_N=\nu_3$ in this case.

According to formula (17), we have that $\nu_1=\nu_1^{(-)}$. Hence the first equation for ρ and h is as follows:

$$b_1-\sqrt{\mathcal{D}_1}=\frac{2\,\nu_1}{k_1}\cosh k_1 d. \tag{21}$$

Here, b_1 and $\mathcal{D}_1$ are given by formulae (18) and (19) respectively with $k=k_1$.

To write down the second equation for ρ and h, we have the dilemma whether

$$\nu_N=\nu_N^{(-)}\quad\text{or}\quad\nu_N=\nu_1^{(+)}\,? \tag{22}$$

Let us show that either of these options is possible. Indeed, Proposition 3 implies that $\nu_N=\nu_N^{(-)}$ provided $\rho-1$ is sufficiently small. On the other hand, let us demonstrate that there exists a triple (ρ,d,h) for which $\nu_N=\nu_1^{(+)}$. For this purpose we have to demonstrate that the inequality

$$\nu_N^{(-)}=k_N\frac{b_N-\sqrt{\mathcal{D}_N}}{2\cosh k_N d}\ge k_1\frac{b_1+\sqrt{\mathcal{D}_1}}{2\cosh k_1 d}=\nu_1^{(+)}$$

holds for some ρ, d and h. As above b_j and $\mathcal{D}_j$, $j=1,N$, are given by formulae (18) and (19), respectively, with $k=k_j$.

Let $h=d/2$, then we have:

$$4\,\nu_j^{(\pm)}=k_j\left\{(\rho+1)\,\tanh k_j d\pm\left[(\rho+1)^2\,\tanh^2 k_j d+8\,(\rho-1)\frac{1-\cosh k_j d}{\cosh k_j d}\right]^{1/2}\right\},$$

and so

$$4\left[\nu_N^{(-)}-\nu_1^{(+)}\right]\to k_N\,(\rho+1-|\rho-3|)-k_1\,(\rho+1+|\rho-3|)\quad\text{as } d\to\infty.$$

The limit is piecewise linear function of ρ, attains its maximum value $4(k_N-k_1)$ at $\rho=3$ and is positive for $\rho\in(1+2\,(k_1/k_N),\,1+2\,(k_N/k_1))$.

Summarizing, we arrive at the following.

Proposition 5. *Let* k_N^2 *be the smallest eigenvalue of problem* (10) *other than* k_1^2, *and let* $\nu_N^{(-)}$ *be the sloshing eigenvalue defined by* (17)–(19) *with* $k=k_N$. *Then*

(i) $\nu_N^{(-)}<\nu_1^{(+)}$ *when* $\rho-1>0$ *is sufficiently small* (*of course, its value depends on* d, h *and the domain* D);

(ii) $\nu_N^{(-)}>\nu_1^{(+)}$ *when* $\rho\in(1+2\,(k_1/k_N),\,1+2\,(k_N/k_1))$, $h=d/2$ *and* d *is sufficiently large* (*of course, its value depends on* ρ *and* D).

Obviously, assertion (ii) can be extended to values of h that are sufficiently close to $d/2$.

4.2. Options for the second equation

Let us develop a procedure for determining which of the two equalities (22) can be chosen to complement equation (21) in order to find ρ and h. Our procedure is based on an analysis of the free surface elevations corresponding to the measured values ν_1 and ν_N. Indeed, when a two-layer fluid oscillates at the frequency defined by some ν_j, the free surface elevation is proportional to the trace $u_j^{(1)}(x,0)$ (see, for example, [10], Section 227).

According to formula (12), the trace $u_1^{(1)}(x,0)$ is a linear combination of linearly independent eigenfunctions $v_1(x),\dots,v_{N-1}(x)$ corresponding to the fundamental eigenvalue k_1^2 of problem (10); of course, its multiplicity is taken into account. By Proposition 2 the free surface elevation associated with $\nu_1^{(+)}$ is also proportional to a linear combination of $v_1,\dots,v_{N-1}$. Since these functions are known, one has to determine whether the measured free-surface elevation corresponding to ν_N can be represented in the form of such a combination and only in such a form. If this is the case, then $\nu_N=\nu_1^{(+)}<\nu_N^{(-)}$ and the following equation:

$$b_1+\sqrt{\mathcal{D}_1}=\frac{2\,\nu_N}{k_1}\cosh k_1 d \tag{23}$$

forms the system for ρ and h together with (21).

Besides, it can occur that the measured free-surface elevation corresponding to ν_N is representable in two forms, one of which is a linear combination of $v_1,\dots,v_{N-1}$, whereas the other one involves the function v_N as well as other eigenfunctions corresponding to the eigenvalue k_N^2 of problem (10) along with $v_1,\dots,v_{N-1}$. It is clear that this happens when $\nu_N=\nu_1^{(+)}=\nu_N^{(-)}$. Indeed, if all coefficients at the eigenfunctions of k_N^2 vanish, then the profile is represented by $v_1,\dots,v_{N-1}$, otherwise not. In this case, equation (21) can be complemented by either equation (23) or the following one:

$$b_N-\sqrt{\mathcal{D}_N}=\frac{2\,\nu_N}{k_N}\cosh k_N d. \tag{24}$$

Of course, it is better to use the system that comprises equations (21) and (23) because the right-hand side terms in these equations are proportional.

If the measured free-surface elevation corresponding to ν_N cannot be represented as a linear combination of $v_1,\dots,v_{N-1}$, then $\nu_N=\nu_N^{(-)}<\nu_1^{(+)}$, in which case the elevation is a linear combination of eigenfunctions that correspond to the eigenvalue k_N^2 of problem (10) the second largest after k_1^2. In this case, equation (21) must be complemented by (24).

Thus, we arrive at the following procedure for reducing the inverse sloshing problem to a system of two equations.

Procedure. *Let $v_1,\dots,v_{N-1}$ be the set of linearly independent eigenfunctions of problem* (10) *corresponding to k_1^2. If the observed elevation of the free surface that corresponds to the measured value ν_N has a representation as a linear combination of $v_1,\dots,v_{N-1}$, then ρ and d must be determined from equations* (21) *and* (23)*. Otherwise, equations* (21) *and* (24) *must be used.*

The simplest case is when the fundamental eigenvalue of problem (10) is simple, that is, $N=2$. Then the above procedure reduces to examining whether the free surface elevations corresponding to ν_1 and ν_2 are proportional or not. In the case of proportionality, equations (21) and (23) must be used. Equations (21) and (24) are applicable when there is no proportionality.

5. Solution of the transcendental systems

In this section, we consider the question how to solve systems (21) and (24), and (21) and (23) for finding ρ and h.

5.1. System (21) and (23)

Equations (21) and (23) can be easily simplified. Indeed, the sum and difference of these equations are as follows:

$$b_1=\frac{\nu_N+\nu_1}{k_1}\cosh k_1 d \quad\text{and}\quad \mathcal{D}_1=\left(\frac{\nu_N-\nu_1}{k_1}\right)^2\cosh^2 k_1 d\,.$$

Substituting the first expression into the second equation (see formulae (18) and (19)), we obtain:

$$(\rho-1)\,\sinh k_1 h\,\sinh k_1(d-h)=\frac{\nu_N\,\nu_1}{k_1^2}\,\cosh k_1 d\,, \tag{25}$$

whereas the first equation itself has the following form:

$$(\rho-1)\,\cosh k_1 h\,\sinh k_1(d-h)=\frac{\nu_N+\nu_1}{k_1}\,\cosh k_1 d-\sinh k_1 d\,. \tag{26}$$

The last two equations immediately yield:

$$\tanh k_1 h=\frac{\nu_N\,\nu_1}{k_1\,(\nu_N+\nu_1-\nu_1^W)}\,,$$

where formula (11) is applied. Thus we are in a position to formulate the following.

Proposition 6. *Let ν_1 and $\nu_N\neq\nu_1$ be the smallest two sloshing eigenvalues measured for a two-layer fluid occupying $W=D\times(-d,0)$. Let also:*

$$0<\frac{\nu_N\,\nu_1}{k_1\,(\nu_N+\nu_1-\nu_1^W)}<\tanh k_1 d\,,$$

where k_1^2 is the fundamental eigenvalue of problem (10) *in D and ν_1^W is defined by formula* (11) *with $k=k_1$. If Procedure guarantees that ρ and h satisfy equations* (21) *and* (23)*, then:*

$$h=\frac{1}{k_1}\tanh^{-1}\,\frac{\nu_N\,\nu_1}{k_1\,(\nu_N+\nu_1-\nu_1^W)}\,,$$

whereas ρ is determined either by (25) *or by* (26) *with this h.*

We recall that $\tanh^{-1} z=\frac{1}{2}\ln\frac{1+z}{1-z}$ (see [11], Section 4.6).

5.2. System (21) and (24)

Since equations (21) and (24) have the same form, we treat them simultaneously. Eliminating square roots, we get:

$$(\rho-1)\,\sinh k_j(d-h)\,(\nu_j\cosh k_j h-k_j\sinh k_j h)=\frac{\nu_j}{k_j}\,(\nu_j\cosh k_j d-k_j\sinh k_j d)\,,\quad j=1,N,$$

which is linear with respect to $\rho-1$. Taking into account formula (11), we write this system in the form:

$$(\rho-1)\,\sinh k_j(d-h)\,(k_j\sinh k_j h-\nu_j\cosh k_j h)=\frac{\nu_j}{k_j}\left(\nu_j^W-\nu_j\right)\cosh k_j d,\quad j=1,N, \tag{27}$$

where the right-hand side term is positive in view of Corollary 1. We eliminate $\rho-1$ from system (27), thus obtaining the following equation for h:

$$\begin{aligned}&\frac{\nu_1}{k_1}\left(\nu_1^W-\nu_1\right)\cosh k_1 d\,\sinh k_N(d-h)\,(k_N\sinh k_N h-\nu_N\cosh k_N h)\\&\quad-\frac{\nu_N}{k_N}\left(\nu_N^W-\nu_N\right)\cosh k_N d\,\sinh k_1(d-h)\,(k_1\sinh k_1 h-\nu_1\cosh k_1 h)=0.\end{aligned} \tag{28}$$

Let us denote by $U(h)$ the expression on the left-hand side and investigate its behaviour for $h\geq 0$, because solving equation (28) is equivalent to finding zeroes of $U(h)$ that belong to $(0,d)$.

It is obvious that $U(d)=0$, and we have that:

$$U(0)=-\nu_N\,\nu_1\left(\frac{\nu_1^W-\nu_1}{k_1}\,\cosh k_1 d\,\sinh k_N d-\frac{\nu_N^W-\nu_N}{k_N}\,\cosh k_N d\,\sinh k_1 d\right).$$

After applying formula (11), this takes the form:

$$U(0)=\left(\nu_N^W\,\nu_1-\nu_N\,\nu_1^W\right)\frac{\nu_N\,\nu_1}{k_N\,k_1}\cosh k_N d\,\cosh k_1 d\,, \tag{29}$$

and so $U(0)$ is positive, negative or zero simultaneously with $\nu_N^W\,\nu_1-\nu_N\,\nu_1^W$.

We have that

$$U'(h) = \frac{\nu_1\, k_N\, \cosh k_1 d}{k_1}\,(\nu_1^W - \nu_1)\,[k_N\, \sinh k_N(d-2h) + \nu_N\, \cosh k_N(d-2h)]$$
$$-\frac{\nu_N\, k_1\, \cosh k_N d}{k_N}\,(\nu_N^W - \nu_N)\,[k_1\, \sinh k_1(d-2h) + \nu_1\, \cosh k_1(d-2h)]\,,$$
$$\frac{U''(h)}{2} = \frac{\nu_N\, k_1^2\, \cosh k_N d}{k_N}\,(\nu_N^W - \nu_N)\,[k_1\, \cosh k_1(d-2h) + \nu_1\, \sinh k_1(d-2h)]$$
$$-\frac{\nu_1\, k_N^2\, \cosh k_1 d}{k_1}\,(\nu_1^W - \nu_1)\,[k_N\, \cosh k_N(d-2h) + \nu_N\, \sinh k_N(d-2h)]\,.$$

Then, formula (11) yields the following asymptotic formula:

$$U(h) \sim (d-h)\,(\nu_N^W - \nu_N)\,(\nu_1^W - \nu_1)\left[\frac{\nu_1\, k_N}{k_1} - \frac{\nu_N\, k_1}{k_N}\right]\cosh k_N d\, \cosh k_1 d \quad \text{as } d-h \to +0. \tag{30}$$

Since equation (28) is obtained under the assumption that $\nu_N = \nu_N^{(-)}$ and $\nu_1 = \nu_1^{(-)}$, Corollary 1 yields that each factor in the asymptotic formula is positive except for the difference in the square brackets.

The next lemma gives a condition providing a relationship between the value $U(0)$ and the behavior of $U(h)$ for $h < d$ and sufficiently close to d.

Lemma 2. *If the following inequality holds:*

$$\frac{\nu_1\, k_N}{k_1} - \frac{\nu_N\, k_1}{k_N} \le 0, \tag{31}$$

then $U(0) < 0$ and $U(h) < 0$ when $h < d$ and sufficiently close to d.

Proof. Let us prove the inequality $U(0) < 0$ first. Since

$$\nu_N^W\, \nu_1 - \nu_N\, \nu_1^W = \nu_1\, k_N\, \tanh k_N d - \nu_N\, k_1\, \tanh k_1 d,$$

according to formula (11). Furthermore, it follows from (31) that:

$$\nu_N^W\, \nu_1 - \nu_N\, \nu_1^W \le \nu_N\, k_1^2\, d\left[\frac{\tanh k_N d}{k_N d} - \frac{\tanh k_1 d}{k_1 d}\right] < 0, \tag{32}$$

because $z^{-1}\tanh z$ is a monotonically decreasing function on $(0, +\infty)$ and $k_1 < k_N$. Then (29) implies that $U(0) < 0$.

If inequality (31) is strict, then the second assertion immediately follows from the asymptotic formula (30).

In the case of equality in (31), the asymptotic formula (30) must be extended to include the second-order term with respect to $d-h$ (see the second derivative above). Thus we obtain that:

$$U(h) \sim (d-h)^2 \left\{ \frac{\nu_N\, k_1^2\, \cosh k_N d}{k_N}\,(\nu_N^W - \nu_N)\,[k_1\, \cosh k_1 d - \nu_1\, \sinh k_1 d] \right.$$
$$\left. -\frac{\nu_1\, k_N^2\, \cosh k_1 d}{k_1}\,(\nu_1^W - \nu_1)\,[k_N\, \cosh k_N d - \nu_N\, \sinh k_N d] \right\} \quad \text{as } d-h \to +0.$$

Applying the equality $\nu_N = \nu_1\,(k_N/k_1)^2$ along with formula (11), we write the expression in braces as follows:

$$\nu_1\, k_N\, k_1^{-1} \cosh k_N d\, \cosh k_1 d\,\left[(\nu_N^W - \nu_N)\,(k_1^2 - \nu_1 \nu_1^W) - (\nu_1^W - \nu_1)\,(k_N^2 - \nu_N \nu_N^W)\right]\,,$$

and we have in the square brackets:

$$k_1^2\, \nu_N^W - k_N^2\, \nu_1^W + \nu_N^W\, \nu_1^W\, \nu_N - \nu_N^W\, \nu_1^W\, \nu_1 + \nu_1^W\, \nu_N\, \nu_1 - \nu_N^W\, \nu_N\, \nu_1\,.$$

Substituting $\nu_N = \nu_1\,(k_N/k_1)^2$, we see that this expression is the following quadratic polynomial in ν_1:

$$\left(\nu_1^W - \nu_N^W\right)(k_N/k_1)^2\, \nu_1^2 + \nu_N^W\, \nu_1^W\left[(k_N/k_1)^2 - 1\right]\nu_1 + \nu_N^W\, k_1^2 - \nu_1^W\, k_N^2\,.$$

Its first and third coefficients are negative (for the latter one this follows from formula (32) because it is equal to the expression in the square brackets multiplied by a positive coefficient). On the other hand, the second coefficient is positive. Therefore, the last expression is negative when $\nu_1 > 0$, which implies that the right-hand side of the last asymptotic formula is negative. This completes the proof of the second assertion. □

The immediate consequences of Lemma 2 are the following two corollaries.

Corollary 4. *If inequality* (31) *holds, then equation* (28) *for* h (*and the inverse sloshing problem for a two-layer fluid occupying* W) *either has no solution or have more than one solution.*

Proof. Inequality (31) implies that $U(0) < 0$ and $U(h) < 0$ for $h < d$, but sufficiently close to d. Hence $U(h)$ either has no zeroes on $(0, d)$, or has more than one zero. □

Corollary 5. *Let* ν_1 *and* $\nu_N \in (\nu_1, \nu_N^W)$ *be the smallest two measured sloshing eigenvalues for a two-layer fluid occupying* $W = D \times (-d, 0)$. *Then a necessary condition that equation* (28) *has a unique solution* h *is the simultaneous validity of the following two inequalities:*

$$\frac{\nu_1\, k_N}{k_1} - \frac{\nu_N\, k_1}{k_N} > 0 \quad \textit{and} \quad \nu_N^W\, \nu_1 - \nu_N\, \nu_1^W < 0. \tag{33}$$

Proof. Let equation (28) have a unique solution on $(0, d)$. According to Corollary 4, inequality (31) contradicts to this assumption, and so the first inequality (33) must hold. Then the asymptotic formula (30) implies that $U(h) > 0$ when $h < d$ and is sufficiently close to d. Hence, the assumption that equation (28) has a unique solution on $(0, d)$ implies that either the second inequality (33) is true or $\nu_N^W\, \nu_1 = \nu_N\, \nu_1^W$. Let us show that this equality is impossible which completes the proof.

Indeed, according to formula (29), the latter equality means that $U(0) = 0$, and so

$$U(h) \sim h\left(\nu_N^W\, \nu_1^W - \nu_N\, \nu_1\right)\left(\frac{\nu_1\, k_N}{k_1} - \frac{\nu_N\, k_1}{k_N}\right)\cosh k_N d\, \cosh k_1 d \quad \text{as } h \to +0.$$

Here, the formula for U' is used along with (11) and the fact that $\nu_N^W\, \nu_1 = \nu_N\, \nu_1^W$. Since the first inequality (33) is already shown to be true, we have that $U(h) > 0$ when $h \neq 0$, but is sufficiently close to $+0$. Since we also have that $U(h) > 0$ when $h < d$ and is sufficiently close to d, we arrive at a contradiction to the assumption that equation (28) has a unique solution on $(0, d)$. □

Now we are in a position to formulate the following

Proposition 7. *Let* ν_1 *and* $\nu_N \in (\nu_1, \nu_N^W)$ *be the smallest two sloshing eigenvalues measured for a two-layer fluid occupying* $W = D \times (-d, 0)$. *If inequalities* (33) *hold for* ν_1 *and* ν_N, *then either of the following two conditions is sufficient for equation* (28) *to have a unique solution* $h \in (0, d)$:

(i) $U'(h)$ *vanishes only once for* $h \in (0, d)$;

(ii) $U''(h) < 0$ *on* $(0, d)$.

Proof. Inequalities (33) and formulae (29) and (30) imply that $U(0) < 0$ and $U(h) > 0$ for $h < d$ and sufficiently close to d. Then, either of the formulated conditions is sufficient to guarantee that equation (28) has a unique solution on $(0, d)$. □

It is an open question whether equation (28) can have more than one solution (consequently, at least three solutions), when inequalities (33) are fulfilled.

6. Conclusions

We have considered the direct and inverse sloshing problems for a two-layer fluid occupying an open container. Several results obtained for the direct problem include:

(i) variational principle and its corollary concerning inequality between the fundamental sloshing eigenvalues for homogeneous and two-layer fluids occupying the same bounded domain.

(ii) Analysis of the behavior of eigenvalues for containers with vertical walls and horizontal bottoms. It demonstrates that there are two sequences of eigenvalues with the same eigenfunctions corresponding to eigenvalues having the same number in each of these sequences. The elements of these sequences are expressed in terms of eigenvalues for the Neumann Laplacian in the two-dimensional domain which is a horizontal cross-section of the container.

(iii) In the particular case of infinitely deep container with vertical boundary, eigenvalues and eigenfunctions for homogeneous and two-layer fluids are the same for any depth of the interface. This makes senseless the inverse sloshing problem in a two-layer fluid occupying such a container.

Inverse sloshing problem for a two-layer fluid, that occupies a container of finite constant depth with vertical walls, is formulated as the problem of finding the depth of the interface and the ratio of fluid densities from the smallest two eigenvalues measured by observing them at the free surface. This problem is reduced to two transcendental equations depending on the measured eigenvalues. There are two systems of such equations and to obtain these systems one has to take into account the behavior of the observed free surface elevation. Sufficient conditions for solubility of both systems have been found.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 865–868

Computer simulation of periodic nanostructures

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DOI 10.17586/2220-8054-2016-7-5-865-868

An algorithm and code for spectrum calculation for periodic nanostructures in homogeneous magnetic field are developed. The approach is based on the zero-range potentials model. The mathematical background of the model is based on the theory of self-adjoint extensions of symmetric operators.

Keywords: Periodic nanostructure, MPI, parallel computing.

Received: 11 September 2016

Revised: 18 September 2016

In memory of B. S. Pavlov (1936–2016)

1. Introduction

Rapid development of research in the field of nanostructures and complex molecules is not possible without computer modeling and simulations. Over the last two decades, a few algorithms and codes have appeared for computer modeling of such systems. These approaches allow researchers to predict properties of nanosystems and to construct nanostructures and molecules with predetermined properties without expensive experimentation. Some of the most popular programs of such type are HyperChem [1], Gamess [2], Gasussian and Molden.

In most cases, codes for nanostructure calculations do not use the direct solution to the Schrödinger equation due to difficulties (or even impossibility) of obtaining explicit formulas and numerical approach complications. Even the use of the Hartree-Fock-Roothaan method in many cases cannot give results in a timely fashion. The complexity of calculations growths exponentially if the number of atoms in the basic cell increases. One faces this problem when calculating the spectrum of periodic arrays of quantum dots or nanotubes, graphene, etc.

This paper is devoted to describing the algorithm and code for the spectrum calculations of periodic nanostructures in an homogeneous magnetic field [3], based on the operator extensions theory [4, 5]. This approach leads to an explicitly solvable model.

2. Model construction

Let us construct a model of spinless charged particle of mass m and charge e in a $2D$-periodic nanostructure with the Bravais lattice Λ in a homogeneous magnetic field $\mathbf{B}$. Let K be a set of atoms in the basic cell of Λ. The whole structure is described by the set:

$$\Gamma = \Lambda + K = \{\kappa + \lambda : \ \kappa \in \mathrm{K}, \ \lambda \in \mathbf{\Lambda}\}.$$

Consider the free particle magnetic Hamiltonian (Landau operator),

$$H_0 = \frac{\hbar}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2, \tag{1}$$

where $\mathbf{p} = i\hbar\nabla$ is the momentum operator in $\mathbf{R}^3$, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ is the vector potential of the field $\mathbf{B}$ in symmetric gauge. The Hamiltonian of the particle in $2D$-periodic lattice is constructed as a perturbation of operator (1) by zero-range potentials posed at nodes of lattice Γ. This can formally be written as:

$$H = H_0 + \sum_{\lambda \in \mathbf{\Lambda}} \sum_{\mathbf{k} \in \mathbf{K}} \hat{\alpha}_k \delta(\mathbf{r} - \lambda - \mathbf{k}), \tag{2}$$

where $\hat{\alpha}_k$ related to the interaction of the particle with the atom posed at $\mathbf{k} \in K$. If the structure is homogeneous, then $\hat{\alpha}_{\mathbf{k}} = \hat{\alpha}$ for any $\mathbf{k} \in K$. Examples of such structures include graphene and carbon nanotubes.

We use "restriction-extension" procedure (see, e.g., [6–8]). Consider symmetric operator S, being a restriction of H on the space of functions from $D(H_0)$ are vanishing at $\gamma \in \Gamma$. We seek the model Hamiltonian as a self-adjoint extension of the operator S. Resolvents of such operators are described by Krein's formula:

$$R_A(\zeta) = R^0(\zeta) - \Gamma(\zeta)[Q(\zeta) - A]^{-1}\Gamma^*(\overline{\zeta}), \tag{3}$$

where $\Gamma(\zeta)$ is Krein Γ-function, $Q(\zeta)$ is the Q-function, correspondingly. Self-adjoint operator A, defined in the space of boundary values (the dimension of the space coincides with the deficiency index of S), parameterize self-adjoint extension H_A of S. We choose a diagonal A Relation [9] leads to an expression of the Green function G_A of H_A:

$$G_A(\mathbf{r}, \mathbf{r}'; \zeta) = G_0(\mathbf{r}, \mathbf{r}'; \zeta) - \sum_{\gamma,\gamma' \in \mathbf{\Gamma}} [Q(\zeta) - A]^{-1}_{\gamma,\gamma'}\, G_0(\mathbf{r}, \gamma; \zeta) G_0(\gamma', \mathbf{r}'; \zeta)\,. \tag{4}$$

Here:

$$G_0(\mathbf{r}, \mathbf{r}\,'; \zeta) = \Phi(\mathbf{r}, \mathbf{r}\,') F_1(\mathbf{r} - \mathbf{r}\,'; \zeta) = \Phi(\mathbf{r}, \mathbf{r}\,') F_2(\mathbf{r} - \mathbf{r}\,'; \zeta);$$

$$\Phi(\mathbf{r}, \mathbf{r}\,') = \frac{m}{2\hbar^2}\sqrt{\frac{\xi}{\pi}} \exp\left[-\pi i \xi(\mathbf{r} \times \mathbf{r}\,') - \pi\xi(\mathbf{r}_\perp - \mathbf{r}_\perp{}')^{\mathbf{2}}/\mathbf{2}\right], \tag{5}$$

$$F_1(\mathbf{r}; \zeta) = \sum_{\ell=0}^{\infty} \frac{\exp\left[-\sqrt{4\pi\xi(\ell + 1/2) - \zeta}|\mathbf{r}_{||}|\right]}{\sqrt{\ell + 1/2 - \zeta/4\pi\xi}} L_\ell(\pi\xi\mathbf{r}_\perp^2), \tag{6}$$

$$F_2(\mathbf{r}; \zeta) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\exp\left[-\pi\xi\left(\mathbf{r}_\perp^2/(e^t - 1) + \mathbf{r}_{||}^2/t\right)\right]}{(1 - e^{-t}) \exp\left[(1/2 - \zeta/4\pi\xi)t\right]} \frac{dt}{\sqrt{t}}. \tag{7}$$

In (5–7), $\mathbf{r}_\perp$ is a projection of $\mathbf{r}$ on the plane of lattice Λ, $\mathbf{r}_{||} = \mathbf{r} - \mathbf{r}_\perp$, $L_\ell(x)$ is the Laguerre polynomial, ξ is the density of the magnetic field $\mathbf{B}$ flux in units of flux quanta $\Phi_0 = 2\pi\hbar c/|e|$. The Q-function in (4) has the form of matrix $Q(\zeta) = (Q(\gamma, \gamma'))_{\gamma,\gamma' \in \mathbf{\Gamma}}$ with entries:

$$Q(\gamma, \gamma'; \zeta) = \begin{cases} G_0(\gamma, \gamma'; \zeta), & \gamma \neq \gamma'; \\ \dfrac{m}{2\hbar^2}\sqrt{\dfrac{\xi}{\pi}} Z\left(\dfrac{1}{2}, \dfrac{1}{2} - \dfrac{\zeta}{4\pi\xi}\right), & \gamma = \gamma', \end{cases} \tag{8}$$

where $Z(s, v)$ Hurvitz ζ [10].

The spectrum of H_A consists of two parts: the spectrum of H_0 (well-known) and points in which the operator $Q(\zeta) - A$ is not invertible or its inverse operator is bounded.

It is known ([11]) that for rational number of the magnetic flux $\eta = N/M$ values that ($N \in \mathbf{Z},\ M \in \mathbf{N}$) does not change Λ when seeking of the spectrum for H_A. The spectrum is determined by:

$$\det\left[\widetilde{Q}(\mathbf{p}; \zeta) - \widetilde{A}(\mathbf{p})\right] = 0, \tag{9}$$

for each $\mathbf{p} \in \mathbf{T}^2_\eta = [0, 1/M) \times [0, 1)$. Matrices $\widetilde{Q}(\mathbf{p}; \zeta)$ is known and:

$$\widetilde{Q}(\mathbf{p}; m, \kappa; m', \kappa'; \zeta) = \exp[\pi i(m - m')\xi(\kappa \times \mathbf{a}_2)] \times$$

$$\sum_{\lambda_1, \lambda_2 = -\infty}^{\infty} Q\left(\lambda_1\mathbf{a}_1 + (\lambda_2 M + m - m')\mathbf{a}_2 + \kappa, \kappa'; \zeta\right) \times \tag{10}$$

$$\exp\left\{\pi i\xi\left[\kappa \times (\lambda_1\mathbf{a}_1 + \lambda_2 M\mathbf{a}_2)\right] - 2\pi i\left(\lambda\mathbf{p} + \frac{\eta}{2}\lambda_1(\lambda_2 M + m + m')\right)\right\},$$

$\kappa, \kappa' \in$ K и $m, m' = 0, \ldots M - 1$.Matrix $\widetilde{A}(\mathbf{p})$ is block-diagonal with identical $|K| \times |K|$ blocks. The diagonal block is in turn diagonal with constants characterizing the point-like interactions as the diagonal entries.

For each $\mathbf{p} \in \mathbf{T}^2_\eta$, equation (9) has $|K|M$ solutions. The continuous branches of equation (9) solutions $z_l(\mathbf{p})$ ($l = 1, \ldots, |K|M$) give one the bands of the operator spectrum. The dispersion equation can be solved numerically.

3. Code description

The most interesting problem in the field is construction of "flux-energy" diagrams, i.e. to find the spectrum for each magnetic flux value η. The most remarkable diagram of such type is "Hofstadter butterfly" [12]. To construct the diagram, it is necessary to solve equation (9) for different η values. For each η, we should find $|K|M$ bands. Calculations for different η and different bands are independent, and can be performed simultaneously, i.e., it is natural to use parallel computation methods. Independence of computing with respect to the data allows one to use interface MPI [13]. Testing showed that organization of the following parallelization using of OpenMP is not useful and leads to decreased calculation performance due to increase processor cores cache-misses.

The initial data for the code are:

- basic vectors of the Bravais lattice Λ,
- coordinates of atoms from K, belonging to basic cell of the lattice Λ,
- "interaction constants" for each atom from K,
- vector $\mathbf{B}$ of the applied magnetic field.

The following instruments were used: compiler Free Pascal, libraries AlgLib and MPI Chamelion. Such a choice allows one to use clusters of various architecture, controlled by operational systems such as Microsoft Windows HPC Server, Linux, FreeBSD.

After initiation, the code, using MPI, creates one control and a few calculating processes. The control process reads (from an input file) values of $\eta = N/M$ and the bands numbers, distributes those among calculating processes and then collects the results. The calculating processes receive tasks from the control and send results to the control. For data exchange, the blocking functions MPI_Send and MPI_Recv are used. Due to the small amount of data transfer, the speed of calculations is, really, independent on the interconnection and grows linearly with respect to the number of cores used.

The code was used for for computing the spectrum of multi-layered graphene in a magnetic field [14] and periodic arrays of nanotubes.The results are in agreement with other models [15]. In the case of nanotube array calculations, the code works with $|K| = 224$ carbon atoms in a basic cell. Using of codes analogous to HyperChem, leads to operation with hundreds of basic cells (correspondingly,tens of thousands atoms), and it gives one only small part of the periodic array. Our approach gives an essential acceleration but, of course, cannot simulate edges of the real nanostructure.

Acknowledgements

This work was partially financially supported by the Government of the Russian Federation (grant 074-U01), by Ministry of Science and Education of the Russian Federation (GOSZADANIE 2014/190, Projects No 14.Z50.31.0031 and No. 1.754.2014/K), by DFG Grant NE 1439/3-1, by grant 16-11-10330 of Russian Science Foundation. The authors thanks National Research Ogarev Mordovia State University for the possibility to carry out calculations.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 869–879

Cauchy problem for some fourth-order nonstrictly hyperbolic equations

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DOI 10.17586/2220-8054-2016-7-5-869-879

We describe the analytic solution of the Cauchy problem for some fourth-order linear hyperbolic equations with constant coefficients in a half-plane in the case of two independent variables, assuming certain conditions for the coefficients. Suitable conditions are assumed for the coefficients, and the equation operator is composed of first-order linear operators.

Keywords: Cauchy problem, analytic solution, fourth-order hyperbolic equations, nonstrictly hyperbolic equations.

Received: 18 April 2016

Revised: 5 May 2016

1. Introduction

This work is devoted to considering the Cauchy problem on a half-plane for some fourth-order nonstrictly hyperbolic linear equation with constant coefficients. The operator appearing in the equation involves a composition of first-order differential operators. The Cauchy problem for such an equation was previously considered in [1, 2] in the case of a strictly hyperbolic equation (a Petrovskii hyperbolic equation [3, 4]). The general solution for both strictly and nonstrictly hyperbolic equations of arbitrary order was constructed there as well. The case of a nonstrictly hyperbolic equation with the coincidence of all characteristics was considered in [5], and the solutions of the Cauchy problem in all cases of a nonstrictly hyperbolic third-order equation of such a form were obtained in [6].

Unique solvability of the problem and the construction of solution for the Cauchy problem is one of the classical problems in the theory of differential equations. Differential equations arise in the modelling of several natural phenomena, and the Cauchy problem is one of the first and most important.

The Cauchy problem for hyperbolic partial differential equations was studied by many mathematicians for a long time, mostly by methods of functional analysis. In this paper, we suggest the following analytical methods for solving the Cauchy problem. First, we find the general solutions using the characteristics of the equation. Next, from the general solution, we determine the solution which satisfies the Cauchy conditions. The latter step is the main difficulty for the determination of the required analytical solution. The general solution of the homogeneous equation depends on a number of arbitrary functions. To determine them, we use Cauchy differential conditions. This leads to the corresponding system of differential equations. In each particular case, solving this system requires a different method and approach. In addition, the solutions depend on a number of arbitrary constants. In order to prove the uniqueness of the solution for a given Cauchy problem, it is necessary to prove that all these arbitrary constants are cross-eliminated after substitution into the general solution.

Partial differential equations of fourth order are encountered when studying mathematical models for certain natural and physical processes. An example of such type of equations, is the fourth-order governing differential equation for nanorod based on nonlocal second-order strain gradient model [see [7, 8]]:

$$EA(\epsilon_0 a)^2 \frac{\partial^4 u(t,x)}{\partial x^4} + EA\frac{\partial^2 u(t,x)}{\partial x^2} - \rho A \frac{\partial^2 u(t,x)}{\partial t^2} = 0, \tag{1}$$

and the flexural wave equation for an Euler-Bernoulli beam has a fourth order derivative in space and is given as [see [9, 10]]:

$$EI\frac{\partial^4 u(t,x)}{\partial x^4} + \eta A \frac{\partial u(t,x)}{\partial t} + \rho A \frac{\partial^2 u(t,x)}{\partial t^2} = 0. \tag{2}$$

On the plane $\mathbb{R}^2$ of two independent variables t and x, we introduce the half-plane $Q = [0, +\infty) \times \mathbb{R}$ on which we consider the following partial differential equation of fourth-order, for a function $u : \mathbb{R}^2 \ni Q \supset (t,x) \to u(t,x) \in \mathbb{R}$:

$$\mathcal{L}^{(4)} u\,(t,x) = \prod_{k=1}^{4} \left(\partial_t - a^{(k)}\partial_x + b^{(k)}\right) u\,(t,x) = f(t,x), \qquad (t,x) \in Q, \tag{3}$$

together with the initial conditions:

$$u|_{t=0} = \varphi_0(x), \quad \left.\frac{\partial u}{\partial t}\right|_{t=0} = \varphi_1(x), \quad \left.\frac{\partial^2 u}{\partial t^2}\right|_{t=0} = \varphi_2(x), \quad \left.\frac{\partial^3 u}{\partial t^3}\right|_{t=0} = \varphi_3(x), \tag{4}$$

where $\partial_t = \dfrac{\partial}{\partial t}$, $\partial_x = \dfrac{\partial}{\partial x}$ – are the first derivatives with respect to t, x and $a^{(k)}$, $b^{(k)}$ are given real numbers, $f : \overline{Q} \to \mathbb{R}$ with $\overline{Q} = [0, +\infty) \times \mathbb{R}$, the closure of Q.

Consider the fourth-order homogeneous equation:

$$\mathcal{L}^{(4)} u(t,x) = 0, \qquad (t,x) \in Q, \tag{5}$$

with

$$\mathcal{L}^{(4)} = \prod_{k=1}^{p} \left(\partial_t - a^{(k)}\partial_x + b^{(k)}\right)^{r(k)}, \tag{6}$$

where p and $r^{(k)}$ are positive integers such that $p \le 4$ and $r^{(1)} + r^{(2)} + ... + r^{(p)} = 4$. By [2], the general solution of Eq. (5) has the form:

$$u(t,x) = \sum_{k=1}^{p} e^{-b^{(k)}t} \sum_{s=1}^{r(k)} t^{s-1} f^{(ks)}\left(x + a^{(k)}t\right). \tag{7}$$

In this paper, we study five cases of fourth-order non-strictly hyperbolic equations, in particular:

Case 1: $r^{(1)} = 4$ and $r^{(j)} = 0$, $j = \overline{2,4}$.
Case 2: $r^{(1)} = 3$,$r^{(2)} = 1$ and $r^{(m)} = 0$ with $m = 3, 4$.
Case 3: $r^{(1)} = 2$,$r^{(2)} = 2$ and $r(m) = 0$ with $m = 3, 4$.
Case 4: $r^{(1)} = 2$,$r^{(2)} = 1$,$r^{(3)} = 1$ and $r^{(4)} = 0$.
Case 5: $r^{(i)} = 1$ $\forall i = \overline{1,4}$.

2. Main results

In this section, we consider the some cases for fourth-order non-strictly hyperbolic equations of the form (5).

Case 1: $r^{(1)} = 4$ and $r^{(j)} = 0$, $j = \overline{2,4}$. Assume that the coefficients of (5) satisfy $a^{(k)} = a$, $b^{(k)} = b$, $\forall k = \overline{1,4}$. Then, according to (7), the general solution of (5) can be written in the following form:

$$u(t,x) = e^{-bt}\left(f_1(x+at) + tf_2(x+at) + t^2 f_3(x+at) + t^3 f_4(x+at)\right). \tag{8}$$

By plugging (8) into (4), after simplifying, we obtain:

$$\begin{aligned}
f_1(x) &= \varphi_0(x);\\
-bf_1(x) + f_2(x) + af_1'(x) &= \varphi_1(x);\\
b^2 f_1(x) + 2f_3(x) - 2b(f_2(x) + af_1'(x)) + 2af_2'(x) + a^2 f_1''(x) &= \varphi_2(x);\\
-b^3 f_1(x) + 6f_4(x) + 3b^2(f_2(x) + af_1'(x)) + 6af_3'(x)&\\
-3b\left(2f_3(x) + 2af_2'(x) + a^2 f_1''(x)\right) + 3a^2 f_2''(x) + a^3 f_1'''(x) &= \varphi_3(x);
\end{aligned}$$

or equivalently:

$$\begin{aligned}
f_1(x) &= \varphi_0(x);\\
f_2(x) &= \varphi_1(x) + b\varphi_0(x) - a\varphi_0'(x);\\
f_3(x) &= \frac{1}{2}\left(\varphi_2(x) + b^2\varphi_0(x) + 2b\varphi_1(x) - 2a\varphi_1'(x) - 2ab\varphi_0'(x) + a^2\varphi_0''(x)\right);\\
f_4(x) &= \frac{1}{6}\Big(\varphi_3(x) + b^3\varphi_0(x) - 3b^2(\varphi_1(x) + b\varphi_0(x))\\
&\quad - 3a\big(\varphi_2'(x) + 2b\varphi_1'(x) + b^2\varphi_0'(x) - 2a\varphi_1''(x) - 2ab\varphi_0''(x) + a^2\varphi_0'''(x)\big)\\
&\quad + 3b\big(\varphi_2(x) + b^2\varphi_0(x) + 2b\varphi_1(x)\big) - 3a^2\big(\varphi_1''(x) + b\varphi_0''(x) - a\varphi_0'''(x)\big) - a^3\varphi_0'''(x)\Big).
\end{aligned}$$

Substituting $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ into (8), finally we have:

$$\begin{aligned}u(t,x) = \frac{1}{6}e^{-bt}((6+6bt+3b^2t^2+b^3t^3)\varphi_0(x+at) + t(3(2+2bt+b^2t^2)\varphi_1(x+at)\\ + 3t(1+bt)\varphi_2(x+at) + t^2\varphi_3(x+at) - 6a\varphi_0'(x+at) - 6abt\varphi_0'(x+at) - 3ab^2t^2\varphi_0'(x+at)\\ - 6at\varphi_1'(x+at) - 6abt^2\varphi_1'(x+at) - 3at^2\varphi_2'(x+at) + 3a^2t\varphi_0''(x+at)\\ + 3a^2bt^2\varphi_0''(x+at) + 3a^2t^2\varphi_1''(x+at) - a^3t^2\varphi_0'''(x+at)).\end{aligned}$$

Case 2: The coefficients of (5) satisfy $a^{(k)} = a$, $b^{(k)} = b$ with $k = 1, 2, 3$ and $a^{(4)} \neq a$, $b^{(k)}$ – arbitrary constants. According to (7), the general solution of equation (5) has the form:

$$u\,(t,x) = e^{-bt}\left(f_1(x+at) + tf_2(x+at) + t^2f_3(x+at)\right) + e^{-b^{(4)}t}f_4(x+a^{(4)}t). \tag{9}$$

Similarly, due to (4), we get the following system of differential equations for the functions $f_k(x)$ with $k = 1, 2, 3, 4$:

$$\begin{aligned}f_1(x) + f_4(x) &= \varphi_0(x);\\ -bf_1(x) + f_2(x) - b^{(4)}f_4(x) + af_1'(x) + a^{(4)}f_4'(x) &= \varphi_1(x);\\ b^2f_1(x) + 2f_3(x) + (b^{(4)})^2f_4(x) - 2b(f_2(x) + af_1'(x)) + 2af_2'(x) - 2a^{(4)}b^{(4)}f_4'(x)&\\ +a^2f_1''(x) + (a^{(4)})^2f_4''(x) &= \varphi_2(x);\\ -b^3f_1(x) - (b^{(4)})^3f_4(x) + 3b^2(f_2(x) + af_1'(x)) + 6af_3'(x) + 3a^{(4)}(b^{(4)})^2f_4'(x) + 3a^2f_2''(x)&\\ -3b(2f_3(x)) + 2af_2'(x) + a^2f_1''(x)) - 3b^{(4)}(a^{(4)})^2f_4''(x) + a^3f_1'''(x) + (a^{(4)})^3f_4'''(x) &= \varphi_3(x).\end{aligned}$$

For the sake of convenience, we introduce the following notations of differential operators: $d_1 = ad/dx - b$, $d_4 = a^{(4)}d/dx - b^{(4)}$ and $d_1^j = (ad/dx - b)^j$, $d_4^j = \left(a^{(4)}d/dx - b^{(4)}\right)^j$. The system of differential equations for the unknown function $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ becomes:

$$\begin{aligned}f_1(x) + f_4(x) &= \varphi_0(x);\\ d_1f_1(x) + f_2(x) + d_4f_4(x) &= \varphi_1(x);\\ d_1^2f_1(x) + 2d_1f_2(x) + 2f_3(x) + d_4^2f_4(x) &= \varphi_2(x);\\ d_1^3f_1(x) + 3d_1^2f_2(x) + 6d_1f_3(x) + d_4^3f_4(x) &= \varphi_3(x).\end{aligned}$$

Observe that the preceding system can be reduced to the one of differential equations with diagonal matrix. To this end, we apply the operator d_4 to the first three equations in the system and subtract every other equation of the resulting system from the preceding one. As a result, we obtain:

$$\begin{aligned}f_1(x) + f_4(x) &= \varphi_0(x);\\ (d_1 - d_4)f_1(x) + f_2(x) &= \varphi_1(x) - d_4\varphi_0(x);\\ (d_1^2 - d_1d_4)f_1(x) + (2d_1 - d_4)f_2(x) + 2f_3(x) &= \varphi_2(x) - d_4\varphi_1(x);\\ (d_1^3 - d_1^2d_4)f_1(x) + (3d_1^2 - 2d_1d_4)f_2(x) + (6d_1 - 2d_4)f_3(x) &= \varphi_3(x) - d_4\varphi_2(x).\end{aligned}$$

By continuing transformations in a similar way, we receive:

$$\begin{aligned}f_1(x) + f_4(x) &= \varphi_0(x);\\ (d_1 - d_4)f_1(x) + f_2(x) &= \varphi_1(x) - d_4\varphi_0(x);\\ (d_1^2 - d_1d_4)f_1(x) + (2d_1 - d_4)f_2(x) + 2f_3(x) &= \varphi_2(x) - d_4\varphi_1(x);\\ (d_1^3 - d_1^2d_4 - (d_1^2 - d_1d_4)(3d_1 - d_4))f_1(x) + (3d_1^2 - 2d_1d_4 - (2d_1 - d_4)(3d_1 - d_4))f_2(x) &=\\ \varphi_3(x) - d_4\varphi_2(x) - (3d_1 - d_4)(\varphi_2(x) - d_4\varphi_1(x)),&\end{aligned}$$

instead of $f_2(x)$ by $f_1(x)$, we obtain third-order ODE for $f_1(x)$

$$\begin{aligned}\left(3d_1^2 - 2d_1d_4 - (2d_1 - d_4)(3d_1 - d_4)\right)(\varphi_1(x) - d_4\varphi_0(x) - (d_1 - d_4)f_1(x))&\\ + \left(d_1^3 - d_1^2d_4 - (d_1^2 - d_1d_4)(3d_1 - d_4)\right)f_1(x) = \varphi_3(x) - d_4\varphi_2(x) - (3d_1 - d_4)\,(\varphi_2(x) - d_4\varphi_1(x))&\end{aligned}$$

or

$$(d_1 - d_4)^3f_1(x) = \Phi(x), \tag{10}$$

where

$$\Phi(x) = \varphi_3(x) - 3d_1\varphi_2(x) + 3d_1^2\varphi_1(x) - d_4\left(3d_1^2 - 3d_1d_4 + d_4^2\right)\varphi_0(x).$$

After solving (10), we have:

$$f_1(x) = e^{\frac{b-b^{(4)}}{a-a^{(4)}}x}(C_1 + xC_2 + x^2C_3) + \Psi(x), \tag{11}$$

with $\Psi(x) = \dfrac{1}{2(a-a^{(4)})^3}\displaystyle\int_0^x \Phi(z)e^{\frac{b-b^{(4)}}{a-a^{(4)}}(x-z)}(x-z)^2dz,$

where C_1, C_2 and C_3 are arbitrary integration constants. Then, using (11) and the first three equations of system of differential equations, it is easy to find three other functions for the solution of (9):

$$\begin{aligned}
f_4(x) &= \varphi_0(x) - e^{\frac{b-b^{(4)}}{a-a^{(4)}}x}(C_1 + xC_2 + x^2C_3) - \Psi(x),\\
f_2(x) &= \varphi_1(x) - (d_1 - d_4)\Psi(x) - d_4\varphi_0(x) - (a-a^{(4)})e^{\frac{b-b^{(4)}}{a-a^{(4)}}x}(C_2 + 2xC_3),\\
f_3(x) &= \frac{1}{2}\left(\varphi_2(x) - d_1^2f_1(x) - 2d_1f_2(x) - d_4^2f_4(x)\right)\\
&= \frac{1}{2}\varphi_2(x) - \frac{1}{2}(d_1^2 - d_4^2)\Psi(x) - \frac{1}{2}d_4^2\varphi_0(x) - d_1\varphi_1(x) + d_1(d_1-d_4)\Psi(x) + d_1d_4\varphi_0(x)\\
&+ e^{\frac{b-b^{(4)}}{a-a^{(4)}}x}\left((a^{(4)})^2C_3 - ba^{(4)}C_2 - 2ba^{(4)}C_3x - a^2C_3 + ab^{(4)}C_2 + 2ab^{(4)}C_3x\right)\\
&+ e^{\frac{b-b^{(4)}}{a-a^{(4)}}x}\left(-2aa^{(4)}C_3 + ba^{(4)}C_2 + 2ba^{(4)}C_3x + 2a^2C_3 - ab^{(4)}C_2 - 2ab^{(4)}C_3x\right).
\end{aligned}$$

Now, substituting $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ into 9, we get the solution:

$$\begin{aligned}
u(t,x) = e^{-bt}&\left(\Psi(x+at) + t(\varphi_1(x+at) - (d_1-d_4)\Psi(x+at) - d_4\varphi_0(x+at))\right)\\
&+ e^{-bt}t^2\left(\frac{1}{2}\varphi_2(x+at) - \frac{1}{2}(d_1^2-d_4^2)\Psi(x+at) - \frac{1}{2}d_4^2\varphi_0(x+at)\right)\\
&+ e^{-bt}t^2\Big(-d_1\varphi_1(x+at) + d_1(d_1-d_4)\Psi(x+at) + d_1d_4\varphi_0(x+at)\Big)\\
&+ e^{-b^{(4)}t}\left(\varphi_0(x+a^{(4)}t) - \Psi(x+a^{(4)}t)\right).
\end{aligned}$$

Case 3: We have coefficients of equation (5) satisfy $a^{(k)} = a$, $b^{(k)} = b$ with $k = 1, 2$, $a^{(k)} = c$, $b^{(k)} = d$ with $k = 3, 4$, $c \neq a$ and b, d – arbitrary constants. According to equation (7), the general solution of equation (5) in this case has the form:

$$u(t,x) = e^{-bt}\left(f_1(x+at) + tf_2(x+at)\right) + e^{-dt}\left(f_3(x+ct) + tf_4(x+ct)\right), \tag{12}$$

we compute partial derivatives of first,second and third order in t and substitute them into the initial conditions (4), we get the following system of differential equations on the functions $f_k(x)$ with $k = 1, 2, 3, 4$:

$$\begin{aligned}
f_1(x) + f_3(x) &= \varphi_0(x);\\
-bf_1(x) + f_2(x) - df_3(x) + f_4(x) + af_1'(x) + cf_3'(x) &= \varphi_1(x);\\
b^2f_1(x) + d^2f_3(x) - 2bf_2(x) - 2abf_1'(x) + 2af_2'(x) - 2df_4(x) - 2cdf_3'(x) + 2cf_4'(x)&\\
+a^2f_1''(x) + c^2f_3''(x) &= \varphi_2(x);\\
-b^3f_1(x) - d^3f_3(x) + 3b^2f_2(x) + 3b^2af_1'(x) + 3d^2f_4(x) + 3d^2cf_3'(x) - 6abf_2'(x)&\\
3ba^2f_1''(x) + 3a^2f_2''(x) - 6cdf_4'(x) - 3dc^2f_3''(x) + 3c^2f_4''(x) + a^3f_1'''(x) + c^3f_3'''(x) &= \varphi_3(x).
\end{aligned}$$

We introduce the following notation for differential operators: $d_1 = ad/dx - b$, $d_2 = cd/dx - d$ and $d_1^j = (ad/dx - b)^j$, $d_2^j = (cd/dx - d)^j$. In this notation, we rewrite system of differential equations for the

unknown function $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ in the form:

$$\begin{aligned} f_1(x) + f_3(x) &= \varphi_0(x);\\ d_1 f_1(x) + f_2(x) + d_2 f_3(x) + f_4(x) &= \varphi_1(x);\\ d_1^2 f_1(x) + 2d_1 f_2(x) + d_2^2 f_3(x) + 2d_2 f_4(x) &= \varphi_2(x);\\ d_1^3 f_1(x) + 3d_1^2 f_2(x) + d_2^3 f_3(x) + 3d_2^2 f_4(x) &= \varphi_3(x), \end{aligned}$$

instead of $f_2(x)$, $f_3(x)$, $f_4(x)$ by $f_1(x)$, we obtain third-order ODE for $f_1(x)$:

$$\left(\frac{-1}{2}d_1^3 + \frac{3}{2}d_2 d_1^2 + \frac{1}{2}d_2^3 - \frac{3}{2}d_1 d_2^2\right) f_1(x) = \\ \varphi_3(x) - \frac{3}{2}d_2\varphi_2(x) - \frac{3}{2}d_1\varphi_2(x) + 3d_1 d_2\varphi_1(x) + \frac{1}{2}d_2^3\varphi_0(x) - \frac{3}{2}d_1 d_2^2\varphi_0(x),$$

or

$$\left(d_1^3 - 3d_2 d_1^2 + 3d_1 d_2^2 - d_2^3\right) f_1(x) = \Phi(x), \tag{13}$$

where $\Phi(x) = -2\varphi_3(x) + 3d_2\varphi_2(x) + 3d_1\varphi_2(x) - 6d_1 d_2\varphi_1(x) - d_2^3\varphi_0(x) + 3d_1 d_2^2\varphi_0(x)$.

Solving the third-order differential equation from (13), we get:

$$f_1(x) = e^{\frac{b-d}{a-c}x}\left(C_1 + xC_2 + x^2 C_3\right) + \frac{1}{2(a-c)^3}\int\limits_0^x \Phi(z)e^{\frac{b-d}{a-c}(x-z)}(x-z)^2 dz,$$

with $\Psi(x) = \dfrac{1}{2(a-c)^3}\displaystyle\int\limits_0^x \Phi(z)e^{\frac{b-d}{a-c}(x-z)}(x-z)^2 dz$, we obtain:

$$f_1(x) = e^{\frac{b-d}{a-c}x}\left(C_1 + xC_2 + x^2 C_3\right) + \Psi(x), \tag{14}$$

where C_1, C_2 and C_3 are arbitrary integration constants. Then, using function 14 and the first three equations of system of differential equations it is easy to find three other functions for the solution of (12):

$$\begin{aligned} f_3(x) &= \varphi_0(x) - e^{\frac{b-d}{a-c}x}(C_1 + xC_2 + x^2 C_3) - \Psi(x),\\ f_2(x) &= C_4 e^{\frac{b-d}{a-c}x} - (a-c)C_3 e^{\frac{b-d}{a-c}x}x\\ &\quad + \int\limits_0^x \frac{\left(\varphi_2(z) - 2d_2\varphi_1(z) - (d_1^2 - 2d_2 d_1)\Psi(z) + d_2^2\varphi_0(z) - d_2^2\Psi(z)\right)e^{\frac{b-d}{a-c}(x-z)}}{2(a-c)}dz,\\ f_4(x) &= \varphi_1(x) - d_1\Psi(x) - d_2\varphi_0(x) + d_2\Psi(x) - C_4 e^{\frac{b-d}{a-c}x} + (a-c)C_3 e^{\frac{b-d}{a-c}x}x\\ &\quad - \int\limits_0^x \frac{\left(\varphi_2(z) - 2d_2\varphi_1(z) - (d_1^2 - 2d_2 d_1)\Psi(z) + d_2^2\varphi_0(z) - d_2^2\Psi(z)\right)e^{\frac{b-d}{a-c}(x-z)}}{2(a-c)}dz\\ &\quad - (a-c)e^{\frac{b-d}{a-c}x}\left(C_2 + 2C_3 x\right). \end{aligned}$$

Now, substitute $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ into (12), we get the solution:

$$\begin{aligned} u(t,x) = e^{-bt}\Psi(x+at) + te^{-bt}\Omega(x+at) + e^{-dt}\varphi_0(x+ct) - e^{-dt}\Psi(x+ct)\\ + te^{-dt}\left(-\Omega(x+ct) + \varphi_1(x+ct) - d_1\Psi(x+ct) - d_2\varphi_0(x+ct) + d_2\Psi(x+ct)\right), \end{aligned}$$

where

$$\Omega(x) = \int\limits_0^x \frac{\left(\varphi_2(z) - 2d_2\varphi_1(z) - (d_1^2 - 2d_2 d_1)\Psi(z) + d_2^2\varphi_0(z) - d_2^2\Psi(z)\right)e^{\frac{b-d}{a-c}(x-z)}}{2(a-c)}dz.$$

Case 4: We have coefficients of equation (5) satisfy $a^{(k)} = a$, $b^{(k)} = b$ with $k = 1, 2$, $a^{(3)} = c$, $b^{(3)} = d$, $a^{(4)} = e$, $b^{(4)} = f$, $c \neq a \neq e$ and $(b-d)(a-e) \neq (b-f)(a-c)$. According to equation (7), the general solution of equation (5) in this case has the form:

$$u(t,x) = e^{-bt}\left(f_1(x+at) + tf_2(x+at)\right) + e^{-dt}f_3(x+ct) + e^{-ft}f_4(x+et), \tag{15}$$

we compute partial derivatives of first,second and third order in t and substitute them into the initial conditions (4), we get the following system of differential equations on the functions $f_k(x)$ with $k = 1, 2, 3, 4$:

$$\begin{aligned}
f_1(x) + f_3(x) + f_4(x) &= \varphi_0(x);\\
-bf_1(x) + f_2(x) - df_3(x) - ff_4(x) + af_1'(x) + cf_3'(x) + ef_4'(x) &= \varphi_1(x);\\
b^2f_1(x) + d^2f_3(x) + f^2f_4(x) - 2bf_2(x) - 2abf_1'(x) + 2af_2'(x)&\\
-2cdf_3'(x) - 2eff_4'(x) + a^2f_1''(x) + c^2f_3''(x) + e^2f_4''(x) &= \varphi_2(x);\\
-b^3f_1(x) - d^3f_3(x) - f^3f_4(x) + 3b^2f_2(x) + 3b^2af_1'(x) + 3cd^2f_3'(x) + 3ef^2f_4'(x) - 6abf_2'(x)&\\
-3ba^2f_1''(x) + 3a^2f_2''(x) - 3c^2df_3''(x) - 3e^2ff_4''(x) + a^3f_1'''(x) + c^3f_3'''(x) + e^3f_4'''(x) &= \varphi_3(x).
\end{aligned}$$

We introduce the following notation of differential operators: $d_1 = ad/dx - b$, $d_3 = cd/dx - d$, $d_4 = ed/dx - f$ and $d_1^j = (ad/dx - b)^j$, $d_3^j = (cd/dx - d)^j$, $d_4^j = (ed/dx - f)^j$. In this notation, we rewrite system of differential equations for the unknown function $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ in the form:

$$\begin{aligned}
f_1(x) + f_3(x) + f_4(x) &= \varphi_0(x),\\
d_1f_1(x) + f_2(x) + d_3f_3(x) + d_4f_4(x) &= \varphi_1(x),\\
d_1^2f_1(x) + 2d_1f_2(x) + d_3^2f_3(x) + d_4^2f_4(x) &= \varphi_2(x),\\
d_1^3f_1(x) + 3d_1^2f_2(x) + d_3^3f_3(x) + d_4^3f_4(x) &= \varphi_3(x),
\end{aligned}$$

or

$$\begin{aligned}
f_1(x) + f_3(x) + f_4(x) &= \varphi_0(x),\\
(d_1 - d_4)f_1(x) + f_2(x) + (d_3 - d_4)f_3(x) &= \varphi_1(x) - d_4\varphi_0(x),\\
(d_1^2 - d_4d_1)f_1(x) + (2d_1 - d_4)f_2(x) + (d_3^2 - d_3d_4)f_3(x) &= \varphi_2(x) - d_4\varphi_1(x),\\
(d_1^3 - d_4d_1^2)f_1(x) + (3d_1^2 - 2d_4d_1)f_2(x) + (d_3^3 - d_4d_3^2)f_3(x) &= \varphi_3(x) - d_4\varphi_2(x),
\end{aligned}$$

or

$$\begin{aligned}
f_1(x) + f_3(x) + f_4(x) &= \varphi_0(x),\\
(d_1 - d_4)f_1(x) + f_2(x) + (d_3 - d_4)f_3(x) &= \varphi_1(x) - d_4\varphi_0(x),\\
(d_1^2 - d_4d_1 - d_3d_1 + d_3d_4)f_1(x) + (2d_1 - d_4 - d_3)f_2(x) &= \varphi_2(x) - d_4\varphi_1(x) - d_3\varphi_1(x) + d_3d_4\varphi_0(x),\\
(d_1^3 - d_4d_1^2 - d_3d_1^2 + d_3d_4d_1)f_1(x) + (3d_1^2 - 2d_4d_1 - 2d_3d_1 + d_3d_4)f_2(x) &= \varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x),
\end{aligned}$$

instead of $f_1(x)$ by $f_2(x)$, we obtain second-order ODE for $f_2(x)$:

$$\begin{aligned}
&(d_1^2 - d_4d_1 - d_3d_1 + d_3d_4)f_2(x) =\\
&\quad\varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x) - d_1\varphi_2(x) + d_1d_4\varphi_1(x) + d_1d_3\varphi_1(x) - d_1d_3d_4\varphi_0(x),
\end{aligned}$$

or

$$(d_1^2 - d_4d_1 - d_3d_1 + d_3d_4)f_2(x) = \Phi(x), \tag{16}$$

where

$$\Phi(x) = \varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x) - d_1\varphi_2(x) + d_1d_4\varphi_1(x) + d_1d_3\varphi_1(x) - d_1d_3d_4\varphi_0(x).$$

Solving the second-order differential equation from (16), we get:

$$f_2(x) = C_1e^{\frac{b-d}{a-c}x} + C_2e^{\frac{b-f}{a-e}x} + \int\limits_0^x \frac{\Phi(z)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz,$$

with $\Omega(x) = \displaystyle\int\limits_0^x \frac{\Phi(z)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz$, we obtain:

$$f_2(x) = C_1e^{\frac{b-d}{a-c}x} + C_2e^{\frac{b-f}{a-e}x} + \Omega(x), \tag{17}$$

Then, using function (17), we find three other functions for the solution of (15):

$$
\begin{aligned}
f_1(x) &= C_3 e^{\frac{b-d}{a-c}x} + C_4 e^{\frac{b-f}{a-e}x} - \int_0^x \frac{(2d_1 - d_4 - d_3)\Omega(z)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz \\
&\quad + \int_0^x \frac{(\varphi_2(z) - d_4\varphi_1(z) - d_3\varphi_1(z) + d_3d_4\varphi_0(z))\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz \\
&\quad - \int_0^x \frac{\left((a-e)C_1 e^{\frac{b-d}{a-c}z} - (a-c)C_2 e^{\frac{b-f}{a-e}z}\right)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{(a-c)(a-e)}dz \\
&= \Theta(x) + C_3 e^{\frac{b-d}{a-c}x} + C_4 e^{\frac{b-f}{a-e}x} - \int_0^x \frac{\left((a-e)C_1 e^{\frac{b-d}{a-c}z} - (a-c)C_2 e^{\frac{b-f}{a-e}z}\right)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{(a-c)(a-e)}dz
\end{aligned}
$$

with

$$
\begin{aligned}
\Theta(x) &= -\int_0^x \frac{(2d_1 - d_4 - d_3)\Omega(z)\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz \\
&\quad + \int_0^x \frac{(\varphi_2(z) - d_4\varphi_1(z) - d_3\varphi_1(z) + d_3d_4\varphi_0(z))\left(e^{\frac{b-d}{a-c}(x-z)} - e^{\frac{b-f}{a-e}(x-z)}\right)}{b(c-e) + d(e-a) + f(a-c)}dz,
\end{aligned}
$$

and

$$
\begin{aligned}
f_3(x) &= C_5 e^{\frac{d-f}{c-e}x} + \int_0^x \frac{(\varphi_1(z) - d_4\varphi_0(z) - (d_1 - d_4)f_1(z) - f_2(z))\, e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz \\
&= C_5 e^{\frac{d-f}{c-e}x} + \int_0^x \frac{(\varphi_1(z) - d_4\varphi_0(z) - (d_1 - d_4)\Theta(z) - \Omega(z))\, e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz \\
&\quad - \int_0^x \frac{\left(C_1 e^{\frac{b-d}{a-c}z} + C_2 e^{\frac{b-f}{a-e}z} - (b-f)(C_3 e^{\frac{b-d}{a-c}z} + C_4 e^{\frac{b-f}{a-e}z}\right) e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz \\
&\quad - \int_0^x \int_0^z \frac{(b-f)\left((a-e)C_1 e^{\frac{b-d}{a-c}t} - (a-c)C_2 e^{\frac{b-f}{a-e}t}\right)\left(e^{\frac{b-d}{a-c}(z-t)} - e^{\frac{b-f}{a-e}(z-t)}\right) e^{\frac{d-f}{c-e}(x-z)}}{(a-c)(a-e)(c-e)}dtdz \\
&\quad - \int_0^x \frac{\left((a-e)\left(\frac{b-d}{a-c}C_3 e^{\frac{b-d}{a-c}z} + \frac{b-f}{a-e}C_4 e^{\frac{b-f}{a-e}z}\right)\right) e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz \\
&\quad + \int_0^x \int_0^z \frac{\left((a-e)C_1 e^{\frac{b-d}{a-c}t} - (a-c)C_2 e^{\frac{b-f}{a-e}t}\right)\left(\frac{b-d}{a-c}e^{\frac{b-d}{a-c}(z-t)} - \frac{b-f}{a-e}e^{\frac{b-f}{a-e}(z-t)}\right) e^{\frac{d-f}{c-e}(x-z)}}{(a-c)(c-e)}dtdz,
\end{aligned}
$$

$$f_4(x)=\varphi_0(x)-\Theta(x)-\int\limits_0^x\frac{(\varphi_1(z)-d_4\varphi_0(z)-(d_1-d_4)\Theta(z)-\Omega(z))\,e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz$$
$$+\int\limits_0^x\frac{\left((a-e)C_1e^{\frac{b-d}{a-c}z}-(a-c)C_2e^{\frac{b-f}{a-e}z}\right)\left(e^{\frac{b-d}{a-c}(x-z)}-e^{\frac{b-f}{a-e}(x-z)}\right)}{(a-c)(a-e)}dz$$
$$+\int\limits_0^x\frac{\left(C_1e^{\frac{b-d}{a-c}z}+C_2e^{\frac{b-f}{a-e}z}-(b-f)(C_3e^{\frac{b-d}{a-c}z}+C_4e^{\frac{b-f}{a-e}z}\right)e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz$$
$$+\int\limits_0^x\int\limits_0^z\frac{(b-f)\left((a-e)C_1e^{\frac{b-d}{a-c}t}-(a-c)C_2e^{\frac{b-f}{a-e}t}\right)\left(e^{\frac{b-d}{a-c}(z-t)}-e^{\frac{b-f}{a-e}(z-t)}\right)e^{\frac{d-f}{c-e}(x-z)}}{(a-c)(a-e)(c-e)}dtdz$$
$$+\int\limits_0^x\frac{\left((a-e)\left(\frac{b-d}{a-c}C_3e^{\frac{b-d}{a-c}z}+\frac{b-f}{a-e}C_4e^{\frac{b-f}{a-e}z}\right)\right)e^{\frac{d-f}{c-e}(x-z)}}{(c-e)}dz$$
$$-\int\limits_0^x\int\limits_0^z\frac{\left((a-e)C_1e^{\frac{b-d}{a-c}t}-(a-c)C_2e^{\frac{b-f}{a-e}t}\right)\left(\frac{b-d}{a-c}e^{\frac{b-d}{a-c}(z-t)}-\frac{b-f}{a-e}e^{\frac{b-f}{a-e}(z-t)}\right)e^{\frac{d-f}{c-e}(x-z)}}{(a-c)(c-e)}dtdz$$
$$-C_3e^{\frac{b-d}{a-c}x}-C_4e^{\frac{b-f}{a-e}x}-C_5e^{\frac{d-f}{c-e}x}.$$

After substitution of $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ into equation (15), we get a solution of the Cauchy problem in this case :

$$u(t,x)=e^{-bt}\Theta(x+at)+te^{-bt}\Omega(x+at)+e^{-ft}\varphi_0(x+et)-e^{-ft}\Theta(x+et)$$
$$+e^{-dt}\int\limits_0^{x+ct}\frac{(\varphi_1(z)-d_4\varphi_0(z)-(d_1-d_4)\Theta(z)-\Omega(z))\,e^{\frac{d-f}{c-e}(x+ct-z)}}{(c-e)}dz$$
$$-e^{-ft}\int\limits_0^{x+et}\frac{(\varphi_1(z)-d_4\varphi_0(z)-(d_1-d_4)\Theta(z)-\Omega(z))\,e^{\frac{d-f}{c-e}(x+et-z)}}{(c-e)}dz.$$

Case 5: We have coefficients of equation (5) satisfy $a^{(i)}\neq a^{(j)}$ with $\forall i,j=\overline{1,4}$ and $(b^{(1)}-b^{(2)})(a^{(1)}-a^{(3)})\neq(b^{(1)}-b^{(3)})(a^{(1)}-a^{(2)})$, $(b^{(1)}-b^{(2)})(a^{(1)}-a^{(4)})\neq(b^{(1)}-b^{(4)})(a^{(1)}-a^{(2)})$. According to equation (7), the general solution of equation (5) in this case has the form:

$$u\,(t,x)=e^{-b^{(1)}t}f_1(x+a^{(1)}t)+e^{-b^{(2)}t}f_2(x+a^{(2)}t)+e^{-b^{(3)}t}f_3(x+a^{(3)}t)+e^{-b^{(4)}t}f_4(x+a^{(4)}t),\qquad(18)$$

we compute partial derivatives of first,second and third order in t and substitute them into the initial conditions (4), we get the following system of differential equations on the functions $f_k(x)$ with $k=1,2,3,4$ and we introduce the following notation for differential operators: $d_i=a^{(i)}d/dx-b^{(i)}$, and $d_i^j=\left(a^{(i)}d/dx-b^{(i)}\right)$ with $i=\overline{1,4}$ and $j=\overline{1,3}$. In this notation, we rewrite the system of differential equations for the unknown function $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ in the form:

$$f_1(x)+f_2(x)+f_3(x)+f_4(x)=\varphi_0(x);$$
$$d_1f_1(x)+d_2f_2(x)+d_3f_3(x)+d_4f_4(x)=\varphi_1(x);$$
$$d_1^2f_1(x)+d_2^2f_2(x)+d_3^2f_3(x)+d_4^2f_4(x)=\varphi_2(x);$$
$$d_1^3f_1(x)+d_2^3f_2(x)+d_3^3f_3(x)+d_4^3f_4(x)=\varphi_3(x);$$

or

$$f_1(x)+f_2(x)+f_3(x)+f_4(x)=\varphi_0(x);$$
$$(d_1-d_4)f_1(x)+(d_2-d_4)f_2(x)+(d_3-d_4)f_3(x)=\varphi_1(x)-d_4\varphi_0(x);$$
$$(d_1^2-d_1d_4-d_3d_1+d_3d_4)f_1(x)+(d_2^2-d_2d_4-d_3d_2+d_3d_4)f_2(x)=\varphi_2(x)-d_4\varphi_1(x)-d_3\varphi_1(x)+d_3d_4\varphi_0(x),$$

instead of $f_2(x)$ by $f_1(x)$, we obtain third-order ODE for $f_1(x)$

$$(d_1^3 - d_4d_1^2 - d_3d_1^2 + d_3d_1d_4)f_1(x) + (d_2^3 - d_4d_2^3 - d_3d_2^2 + d_3d_2d_4)f_2(x) = \varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x);$$

$$(d_1^3 - d_4d_1^2 - d_3d_1^2 + d_3d_1d_4 - d_2d_1^2 + d_2d_1d_4 + d_2d_3d_1 - d_2d_3d_4)f_1(x) = \varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x) - d_2\varphi_2(x) + d_2d_4\varphi_1(x) + d_2d_3\varphi_1(x) - d_2d_3d_4\varphi_0(x);$$

where

$$\Phi(x) = \varphi_3(x) - d_4\varphi_2(x) - d_3\varphi_2(x) + d_3d_4\varphi_1(x) - d_2\varphi_2(x) + d_2d_4\varphi_1(x) + d_2d_3\varphi_1(x) - d_2d_3d_4\varphi_0(x).$$

After solving this equation, we receive

$$f_1(x) = C_1e^{\frac{b^{(1)}-b^{(2)}}{a^{(1)}-a^{(2)}}x} + C_2e^{\frac{b^{(1)}-b^{(3)}}{a^{(1)}-a^{(3)}}x} + C_3e^{\frac{b^{(1)}-b^{(4)}}{a^{(1)}-a^{(4)}}x} + \sum_{k=2}^{4}\int_0^x \frac{\Phi(z)e^{\frac{b^{(1)}-b^{(k)}}{a^{(1)}-a^{(k)}}(x-z)}}{P'\left(\frac{b^{(1)}-b^{(k)}}{a^{(1)}-a^{(k)}}\right)(a^{(1)}-a^{(2)})(a^{(1)}-a^{(3)})(a^{(1)}-a^{(4)})}dz = C_1e^{\frac{b^{(1)}-b^{(2)}}{a^{(1)}-a^{(2)}}x} + C_2e^{\frac{b^{(1)}-b^{(3)}}{a^{(1)}-a^{(3)}}x} + C_3e^{\frac{b^{(1)}-b^{(4)}}{a^{(1)}-a^{(4)}}x} + \Omega(x),$$

where $P(\lambda) = \left(\lambda - \dfrac{b^{(1)}-b^{(2)}}{a^{(1)}-a^{(2)}}\right)\left(\lambda - \dfrac{b^{(1)}-b^{(3)}}{a^{(1)}-a^{(3)}}\right)\left(\lambda - \dfrac{b^{(1)}-b^{(4)}}{a^{(1)}-a^{(4)}}\right)$ and

$$\Omega(x) = \sum_{k=2}^{4}\int_0^x \frac{\Phi(z)e^{\frac{b^{(1)}-b^{(k)}}{a^{(1)}-a^{(k)}}(x-z)}}{P'\left(\frac{b^{(1)}-b^{(k)}}{a^{(1)}-a^{(k)}}\right)(a^{(1)}-a^{(2)})(a^{(1)}-a^{(3)})(a^{(1)}-a^{(4)})}dz.$$

Then, using function $f_1(x)$, we find three other functions for the solution of (18):

$$\begin{aligned} f_2(x) = {} & \Psi(x) + C_4e^{\frac{b^{(2)}-b^{(3)}}{a^{(2)}-a^{(3)}}x} + C_5e^{\frac{b^{(2)}-b^{(4)}}{a^{(2)}-a^{(4)}}x} \\ & - \sum_{k=2}^{4}\int_0^x \frac{(a^{(1)}-a^{(3)})(a^{(1)}-a^{(4)})C_{k-1}(b^{(1)}-b^{(k)})^2\Pi(x,z)}{(a^{(1)}-a^{(k)})^2(a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)}))}dz \\ & + \sum_{k=2}^{4}\int_0^x \frac{(b^{(1)}-b^{(3)})(a^{(1)}-a^{(4)})C_{k-1}(b^{(1)}-b^{(k)})\Pi(x,z)}{(a^{(1)}-a^{(k)})(a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)}))}dz \\ & + \sum_{k=2}^{4}\int_0^x \frac{(b^{(1)}-b^{(4)})(a^{(1)}-a^{(3)})C_{k-1}(b^{(1)}-b^{(k)})\Pi(x,z)}{(a^{(1)}-a^{(k)})(a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)}))}dz \\ & - \sum_{k=2}^{4}\int_0^x \frac{(b^{(1)}-b^{(4)})(b^{(1)}-b^{(3)})C_{k-1}\Pi(x,z)}{(a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)}))}dz, \end{aligned}$$

$$f_3(x) = \int_0^x \frac{(\varphi_1(z) - d_4\varphi_0(z) - (d_1-d_4)f_1(z) - (d_2-d_4)f_2(z))e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}(x-z)}}{a^{(3)}-a^{(4)}}dz + C_6e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}x},$$

$$f_4(x) = \varphi_0(x) - f_0(x) - f_1(x) - f_2(x) - f_3(x),$$

where

$$\begin{aligned} \Psi(x) = {} & -\int_0^x \frac{((d_1^2 - d_1d_4 - d_3d_1 + d_3d_4)\Omega(z))\left(e^{\frac{b^{(2)}-b^{(4)}}{a^{(2)}-a^{(4)}}(x-z)} - e^{\frac{b^{(2)}-b^{(3)}}{a^{(2)}-a^{(3)}}(x-z)}\right)}{a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)})}dz \\ & + \int_0^x \frac{(\varphi_2(z) - d_4\varphi_1(z) - d_3\varphi_1(z) + d_3d_4\varphi_0(z))\left(e^{\frac{b^{(2)}-b^{(4)}}{a^{(2)}-a^{(4)}}(x-z)} - e^{\frac{b^{(2)}-b^{(3)}}{a^{(2)}-a^{(3)}}(x-z)}\right)}{a^{(4)}(b^{(2)}-b^{(3)}) + a^{(2)}(b^{(3)}-b^{(4)}) + a^{(3)}(b^{(4)}-b^{(2)})}dz, \end{aligned}$$

$$\Pi(x,z)=e^{\frac{b^{(1)}-b^{(k)}}{a^{(1)}-a^{(k)}}z}\left(e^{\frac{b^{(2)}-b^{(4)}}{a^{(2)}-a^{(4)}}(x-z)}-e^{\frac{b^{(2)}-b^{(3)}}{a^{(2)}-a^{(3)}}(x-z)}\right).$$

After substitution of $f_1(x)$, $f_2(x)$, $f_3(x)$, $f_4(x)$ into equation (18), we get a solution of the Cauchy problem in this case:

$$\begin{aligned}u(t,x)&=e^{-b^{(1)}t}\Omega(x+a^{(1)}t)+e^{-b^{(2)}t}\Psi(x+a^{(2)}t)\\&\quad+e^{-b^{(3)}t}\int\limits_0^{x+a^{(3)}t}\frac{(\varphi_1(z)-d_4\varphi_0(z))e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}(x+a^{(3)}t-z)}}{a^{(3)}-a^{(4)}}dz\\&\quad-e^{-b^{(3)}t}\int\limits_0^{x+a^{(3)}t}\frac{((d_1-d_4)\Omega(z)+(d_2-d_4)\Psi(z))e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}(x+a^{(3)}t-z)}}{a^{(3)}-a^{(4)}}dz\\&\quad+e^{-b^{(4)}t}\left(\varphi_0(x+a^{(4)}t)-\Omega(x+a^{(4)}t)-\Psi(x+a^{(4)}t)\right)\\&\quad-e^{-b^{(4)}t}\int\limits_0^{x+a^{(4)}t}\frac{(\varphi_1(z)-d_4\varphi_0(z))e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}(x+a^{(4)}t-z)}}{a^{(3)}-a^{(4)}}dz\\&\quad+e^{-b^{(4)}t}\int\limits_0^{x+a^{(4)}t}\frac{((d_1-d_4)\Omega(z)+(d_2-d_4)\Psi(z))e^{\frac{b^{(3)}-b^{(4)}}{a^{(3)}-a^{(4)}}(x+a^{(4)}t-z)}}{a^{(3)}-a^{(4)}}dz.\end{aligned}$$

We obtain the following theorem:

Theorem 2.1. *The Cauchy problem* (4) – (5) *has a unique classical solution in* $C^4(\overline{Q})$ *for arbitrary functions* $\varphi_j(j=\overline{0,3})$ *in the class* $C^{3-j}(\mathbb{R})$, $j=\overline{0,3}$.

Now, consider the Cauchy problem for the inhomogeneous equation. Since the considered problem is linear, it follows that its solution u can be represented as the sum of two functions $u=\overline{u}+v$, where $\overline{u}$ is a solution of problem (4) – (5), and v is a solution of following equations:

$$\mathcal{L}^{(4)}v\,(t,x)=f(t,x),\qquad (t,x)\in Q, \tag{19}$$

with the homogeneous Cauchy conditions:

$$v|_{t=0}=0,\quad \left.\frac{\partial v}{\partial t}\right|_{t=0}=0,\quad \left.\frac{\partial^2 v}{\partial t^2}\right|_{t=0}=0,\quad \left.\frac{\partial^3 v}{\partial t^3}\right|_{t=0}=0. \tag{20}$$

We define the function $v(t,x)$ via the function $w(t,\tau,x)$ with a parameter $\tau\in[0,\infty)$ by the relation:

$$v\,(t,x)=\int\limits_0^t\omega\,(t-\tau,\tau,x)d\tau.$$

The function w treated as a function of the independent variables t and x is a solution of the homogeneous equation (5) with the Cauchy conditions:

$$\omega|_{t=\tau}=0,\quad \left.\frac{\partial\omega}{\partial t}\right|_{t=\tau}=0,\quad \left.\frac{\partial^2\omega}{\partial t^2}\right|_{t=\tau}=0,\quad \left.\frac{\partial^3\omega}{\partial t^3}\right|_{t=\tau}=f\,(\tau,x)\,.$$

Indeed, we have:

$$v|_{t=0}=\int\limits_0^0\omega\,(-\tau,\tau,x)d\tau=0,$$

$$\left.\frac{\partial v}{\partial t}\right|_{t=0}=\omega(0,0,x)+\int\limits_0^0\frac{\partial\omega\,(t-\tau,\tau,x)}{\partial t}d\tau=0,$$

$$\left.\frac{\partial^2 v}{\partial t^2}\right|_{t=0}=\frac{\partial\omega(0,0,x)}{\partial t}+\int\limits_0^0\frac{\partial^2\omega\,(t-\tau,\tau,x)}{\partial t^2}d\tau=0,$$

$$\left.\frac{\partial^3 v}{\partial t^3}\right|_{t=0} = \frac{\partial^2 \omega(0,0,x)}{\partial t^2} + \int\limits_0^0 \frac{\partial^3 \omega\left(t-\tau,\tau,x\right)}{\partial t^3} d\tau = 0,$$

$$\mathcal{L}^{(4)} v\left(t,x\right) = \prod_{k=1}^{4} \left(\partial_t - a^{(k)}\partial_x + b^{(k)}\right) v\left(t,x\right) = f(t,x) + \int\limits_0^t \left(\mathcal{L}^{(4)} \omega\left(t-\tau,\tau,x\right)\right) d\tau = f(t,x).$$

Theorem 2.2. *If the right-hand side of Eq.* (3) *belongs to the set* $C^{0,4}(\overline{Q})$ *and the functions* $\varphi_j (j = \overline{0,3})$ *occurring in condition* (4) *belong to the class* $C^{3-j}(\mathbb{R})$*, then for such arbitrary functions, there exists a unique classical solution* $u = \overline{u} + v$ *of problem* (3), (4) *in the class* $C^4(Q)$*, where* $\overline{u}$ *is the classical solution for problem* (4), (5) *and* v *is the solution for problem* (19), (20).

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 880–887

Spectral properties of a two–particle hamiltonian on a *d*-dimensional lattice

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DOI 10.17586/2220-8054-2016-7-5-880-887

A system of two arbitrary quantum particles moving on d-dimensional lattice interacting via some attractive potential is considered. The number of eigenvalues of the family $h(k)$ is studied depending on the interaction energy of particles and the total quasi-momentum $k \in \mathbb{T}^d$ ($\mathbb{T}^d$ – d-dimensional torus). Depending on the interaction energy, the conditions for $h(\mathbf{0})$ that has simple or multifold virtual level at 0 are found.

Keywords: two-particle hamiltonian, virtual level, multiplicity of virtual level.

Received: 17 May 2016

Revised: 6 June 2016

1. Introduction

Lattice two-particle Hamiltonians have been investigated in [1–3]. In [1], the problem of the two-particle bound states for the transfer-matrix in a wide class of Gibbs fields on the lattices in the high temperature domains of ($t \gg 1$), as well in [2] the appearance of bound state levels standing in a definite distance from the essential spectrum has been shown for some quasi-momenta values. The spectral properties of the two-particle operator depending on total quasi-momentum have been studied in [3].

In [4], it was proven that if the operator $h(\mathbf{0})$ has a virtual level at the lower edge of essential spectrum, then the discrete spectrum of $h(k)$ lying below the essential spectrum is always nonempty for any $k \in \mathbb{T}^d \setminus \{\mathbf{0}\}$. In [5], assuming that dispersion relations $\varepsilon_1(\cdot)$ and $\varepsilon_2(\cdot)$ are linearly dependent, it was proven that the positivity of $h(\mathbf{0})$ implies the positivity of $h(k)$ for all k.

In recent work [6], conditions were obtained for the discrete two-particle Schrödinger operator with zero-range attractive potential to have an embedded eigenvalue in the essential spectrum depending on the dimension of the lattice. In [7], the discrete spectra of one-dimensional discrete Laplacian with short range attractive perturbation were studied.

In [8], a system of two arbitrary particles in a three-dimensional lattice with some dispersion relation was considered. Particles interact via an attractive potential only on the neighboring knots of lattice. The existence and absence of eigenvalues of the family $h(k)$ depending on the energy of interaction and quasi-momentum $k \in \mathbb{T}^3$ ($\mathbb{T}^3$ – three dimensional torus) have been investigated. Moreover, depending on the interaction energy, the conditions were found for $h(\mathbf{0})$ to have a simple, two-fold, or three-fold virtual level at 0. In [9], the two-particle Schrödinger operator $h(k)$, $k \in \mathbb{T}^3$, associated with a system of two particles on the three-dimensional lattice, was considered. Here, some $6N$-dimensional integral operator is taken as the potential and the dispersion relation is chosen depending on N. In this work, the existence or absence of eigenvalues has also been studied for the family $h(k)$ depending on the interaction energy and total quasi-momentum k. Moreover, dependending on the interaction energy, conditions were found for the operator $h(\mathbf{0})$ that has $3N$-fold eigenvalue and a $3N$-fold virtual level.

The current work is a generalization of [8]. In this work, we consider the system of two arbitrary quantum particles moving on the d-dimensional lattice and interacting via an attractive potential. For all values of $k \in \mathbb{T}^d$ ($\mathbb{T}^d$ – d-dimensional torus) the dependence of the number of eigenvalues of the family $h(k)$ on the interaction energy is studied. The conditions for that $h(\mathbf{0})$ has simple or multifold virtual level (eigenvalue) at 0 are found for $d = 3, 4$ ($d \geq 5$).

2. Statement of the Main Result

Let $L_2(\mathbb{T}^d)$ be the Hilbert space of square-integrable functions defined on d-dimensional lattice $\mathbb{T}^d$.

Consider the two-particle Schrödinger operator $h(k)$, $k \in \mathbb{T}^d$, associated with the direct integral expansion of Hamiltonian of the system of two arbitrary particles, interacting via short-range pair potential [8], acting in $L_2(\mathbb{T}^d)$ as

$$h(k) = h_0(k) - \mathbf{v},$$

here $h_0(k)$ – multiplication operator by a function:

$$\mathcal{E}_k(p) = \varepsilon_1(p) + \varepsilon_2(k-p)$$

and $\mathbf{v}$ is an integral operator with kernel

$$v(p-s) = \mu_0 + \sum_{\alpha=1}^{d} \mu_\alpha \cos(p_\alpha - s_\alpha), \quad \mu_\alpha > 0.$$

Assumption 1. *Additionally, we assume that ε_l, $l = 1, 2$ are real-valued, continuous, even and periodic functions with period π in every variable.*

Please note that the Weyl theorem on the essential spectrum [10] implies that the essential spectrum $\sigma_{ess}(h(k))$ of the operator $h(k)$ coincides with the spectrum of the unperturbed operator $h_0(k)$:

$$\sigma_{ess}(h(k)) = \sigma(h_0(k)) = [m(k), M(k)],$$

where $m(k) = \min\limits_{p\in\mathbb{T}^d} \mathcal{E}_k(p)$, $M(k) = \max\limits_{p\in\mathbb{T}^d} \mathcal{E}_k(p)$.

Since $\mathbf{v} \geq 0$, one has:

$$\sup(h(k)f, f) \leq \sup(h_0(k)f, f) = M(k)(f, f), \quad f \in L_2(\mathbb{T}^d),$$

and, thus, $h(k)$ does not have eigenvalues lying above the essential spectrum:

$$\sigma(h(k)) \cap (M(k), +\infty) = \emptyset.$$

We set:

$$\mu_i^{\pm}(k;z) = \frac{c_i(k;z) + s_i(k;z) \pm \sqrt{(c_i(k;z) - s_i(k;z))^2 + 4\xi_i^2(k;z)}}{2[c_i(k;z)s_i(k;z) - \xi_i^2(k;z)]},$$

where

$$c_i(k;z) = \int\limits_{T^d} \frac{\cos^2 s_i\, ds}{\mathcal{E}_k(s) - z}, \quad s_i(k;z) = \int\limits_{T^d} \frac{\sin^2 s_i\, ds}{\mathcal{E}_k(s) - z},$$

$$\xi_i(k;z) = \int\limits_{T^d} \frac{\sin s_i\, \cos s_i\, ds}{\mathcal{E}_k(s) - z}, \quad z \leq m(k).$$

Recall that $c_i(k;z)s_i(k;z) - \xi_i^2(k;z) \geq 0$.

There exist (finite or infinite) limits:

$$\lim_{z\to m(k)-0} b(k;z), \ \lim_{z\to m(k)-0} c_i(k;z), \ \lim_{z\to m(k)-0} s_i(k;z), \ \lim_{z\to m(k)-0} \xi_i^2(k;z),$$

where

$$b(k;z) = \int\limits_{\mathbb{T}^d} \frac{ds}{\mathcal{E}_k(s) - z}.$$

Lemma 1. *For any $k \in \mathbb{T}^d$ there exists finite limits:*

$$\mu^0(k) = \lim_{z\to m(k)-0} \frac{1}{b(k;z)}, \tag{2.1}$$

$$\mu_i^{\pm}(k) = \lim_{z\to m(k)-0} \mu_i^{\pm}(k;z), \quad i = 1, \ldots, d. \tag{2.2}$$

Moreover,

$$\mu_i^-(k) \leq \mu_i^+(k) \quad \textit{for all} \quad k \in \mathbb{T}^d, \quad i = 1, \ldots, d.$$

Let us define the functions:

$$\alpha(\mu;k) = \begin{cases} 0 & \text{if } \ \mu_0 \in (0; \mu^0(k)], \\ 1 & \text{if } \ \mu_0 \in (\mu^0(k); \infty), \end{cases} \tag{2.3}$$

$$\beta_i(\mu;k) = \begin{cases} 0 & \text{if } \ \mu_i \in (0; \mu_i^-(k)], \\ 1 & \text{if } \ \mu_i \in (\mu_i^-(k); \mu_i^+(k)], \\ 2 & \text{if } \ \mu_i \in (\mu_i^+(k); \infty) \end{cases} \tag{2.4}$$

for all $i = 1, \ldots, d$.

Theorem 1. *Let $\mu=(\mu_0,\cdots,\mu_d)\in\mathbb{R}_+^{d+1}$. Then, counting multiplicity, $h(k)$ has exactly:*

$$\alpha(\mu;k)+\sum_{i=1}^{d}\beta_i(\mu;k)$$

eigenvalues below the essential spectrum.

Assumption 2. *Assume that $m(\mathbf{0})=\min\limits_{p\in\mathbb{T}^d}\mathcal{E}_{\mathbf{0}}(p)=0$ and*

$$\mathcal{M}=\{p\in\mathbb{T}^d:\ m(\mathbf{0})=0\}=\{p_1,\cdots,p_n\},\quad n<\infty.$$

Moreover, assume that around points of $\mathcal{M}$ $\mathcal{E}_{\mathbf{0}}(p)$ is of order $\rho>0$:

$$c|p-p_l|^{\rho}\le\mathcal{E}_{\mathbf{0}}(p)\le c_1|p-p_l|^{\rho}\qquad as\quad p\to p_l,\quad l=1,\dots,n.$$

Let $C(\mathbb{T}^d)$ be a Banach space of continuous periodic functions on $\mathbb{T}^d$ and $G(k;z)$ denote the (Birman-Schwinger) integral operator in $L_2(\mathbb{T}^d)$ with the kernel:

$$G(k;z;p,q)=v(p-q)(\mathcal{E}_k(q))^{-1},\ p,q\in\mathbb{T}^d.$$

Definition 1. *We say that the operator $h(\mathbf{0})$ has a virtual level at 0 (lower edge of essential spectrum) if 1 is an eigenvalue of $G(\mathbf{0};0)$ with some associated eigenfunction $\psi\in L_2(\mathbb{T}^d)$ satisfying:*

$$\frac{\psi(\cdot)}{\mathcal{E}_{\mathbf{0}}(\cdot)}\in L_1(\mathbb{T}^d)\setminus L_2(\mathbb{T}^d).$$

The number of such linearly independent vectors ψ is called the multiplicity of virtual level of $h(\mathbf{0})$.

We set:

$$\mu_\alpha^0=\min\left\{\frac{1}{c_\alpha(\mathbf{0};0)},\frac{1}{s_\alpha(\mathbf{0};0)}\right\},\ \alpha=1,\dots,d.$$

We define the following sets depending on $c_\alpha(\mathbf{0};0)$ and $s_\alpha(\mathbf{0};0)$:

$$L_{\alpha1}=\left\{\mu_\alpha^0:\ \frac{1}{c_\alpha(\mathbf{0};0)}>\mu_\alpha^0\right\},$$

$$L_{\alpha2}=\left\{\mu_\alpha^0:\ \frac{1}{c_\alpha(\mathbf{0};0)}=\mu_\alpha^0,\ p_i^\alpha=\frac{\pi}{2}\ \text{or}\ p_i^\alpha=-\frac{\pi}{2}\quad\text{for all}\quad i=1,\cdots,n\right\},$$

$$L_{\alpha3}=\left\{\mu_\alpha^0:\ \frac{1}{c_\alpha(\mathbf{0};0)}=\mu_\alpha^0,\ p_i^\alpha\ne\frac{\pi}{2}\ \text{or}\ p_i^\alpha\ne-\frac{\pi}{2}\quad\text{at least one}\quad i=1,\dots,n\right\},$$

$$M_{\alpha1}=\left\{\mu_\alpha^0:\ \frac{1}{s_\alpha(\mathbf{0};0)}>\mu_\alpha^0\right\},$$

$$M_{\alpha2}=\left\{\mu_\alpha^0:\ \frac{1}{s_\alpha(\mathbf{0};0)}=\mu_\alpha^0,\ p_i^\alpha=0\ \text{or}\ p_i^\alpha=\pi\quad\text{for all}\quad i=1,\dots,n\right\},$$

$$M_{\alpha3}=\left\{\mu_\alpha^0:\ \frac{1}{s_\alpha(\mathbf{0};0)}=\mu_\alpha^0,\ p_i^\alpha\ne0\ \text{or}\ p_i^\alpha\ne\pi\quad\text{at least one}\quad i=1,\dots,n\right\},$$

where p_i^α – α-th coordinate of minimum point p_i of $\mathcal{E}_{\mathbf{0}}(\cdot)$.

Let us define the following functions:

$$\beta(\mu_0)=\begin{cases}0 & \text{if}\quad \mu_0\in(0;\mu^0(\mathbf{0})),\\ 1 & \text{if}\quad \mu_0=\mu^0(\mathbf{0}),\end{cases}$$

$$\gamma(\alpha)=\begin{cases}0 & \text{if}\quad \mu_\alpha\in(0;\mu_\alpha^0)\quad\text{or}\,\mu_\alpha\in L_{\alpha1}\cup L_{\alpha2},\\ 1 & \text{if}\quad \mu_\alpha\in L_{\alpha3},\end{cases}$$

$$\overline{\gamma}(\alpha)=\begin{cases}0 & \text{if}\quad \mu_\alpha\in(0;\mu_\alpha^0)\quad\text{or}\quad\mu_\alpha\in L_{\alpha1}\cup L_{\alpha3},\\ 1 & \text{if}\quad \mu_\alpha\in L_{\alpha2},\end{cases}$$

$$\eta(\alpha)=\begin{cases}0 & \text{if}\quad \mu_\alpha\in(0;\mu_\alpha^0)\quad\text{or}\quad\mu_\alpha\in M_{\alpha1}\cup M_{\alpha2},\\ 1 & \text{if}\quad \mu_\alpha\in M_{\alpha3},\end{cases}$$

$$\overline{\eta}(\alpha)=\begin{cases}0 & \text{if}\quad \mu_\alpha\in(0;\mu_\alpha^0)\quad\text{or}\quad\mu_\alpha\in M_{\alpha1}\cup M_{\alpha3},\\ 1 & \text{if}\quad \mu_\alpha\in M_{\alpha2}.\end{cases}$$

Theorem 2. *(i) Let* $\rho = 2$, $\mu_0 \in (0; \mu^0(\mathbf{0})]$, $\mu_\alpha \in (0, \mu_\alpha^0]$, $\alpha = 1, \dots, d$. *Then*

1) if $d = 3, 4$, *then* 0 *is*

$$\beta(\mu_0) + \sum_{\alpha=1}^{d} [\gamma(\alpha) + \eta(\alpha)]$$

– fold virtual level of $h(\mathbf{0})$. *In addition, if* $\bigcup_{\alpha=1}^{d} L_{\alpha 2} \cap M_{\alpha 2} \neq \emptyset$, *then* 0 *is simultaneously*

$$\sum_{\alpha=1}^{d} [\bar{\gamma}(\alpha) + \bar{\eta}(\alpha)]$$

– fold eigenvalue of $h(\mathbf{0})$.

2) if $d \geq 5$, *then* 0 *is*

$$\beta(\mu_0) + \sum_{\alpha=1}^{d} [\gamma(\alpha) + \eta(\alpha)]$$

– fold eigenvalue of $h(\mathbf{0})$.

(ii) Let $\rho \in (\frac{d}{2}, d)$, $d > 3$, $\mu_0 \in (0; \mu^0(\mathbf{0})]$, $\mu_\alpha \in (0, \mu_\alpha^0]$, $\alpha = 1, \dots, d$. *Then* 0 *is at least*

$$\beta(\mu_0) + \sum_{\alpha=1}^{d} [\gamma(\alpha) + \eta(\alpha)]$$

-fold virtual level of $h(\mathbf{0})$.

Remark 1. *1) By definition of sets* $L_{\alpha 2}$ *and* $M_{\alpha 2}$ *for each* $\alpha = 1, \dots, d$ *one has* $L_{\alpha 3} \cup M_{\alpha 3} \neq \emptyset$. *Moreover, in this case, the multiplicity of the virtual level of* $h(\mathbf{0})$ *is always not less than* d *if* $\mu_\alpha = \mu_\alpha^0$, $\alpha = 1, \dots, d$.

2) For $\rho = 2$ *the function*

$$\mathcal{E}_{\mathbf{0}}(\cdot) = \mathcal{E}_{\mathbf{0}}(p) = \varepsilon_1(p) + \varepsilon_2(p), \quad \varepsilon_1(p) = \varepsilon_2(p) = \cos^2 p_1 + \sum_{i=1}^{d} (1 + \cos 2p_i)$$

satisfies the assumptions of Theorem 2 with $\bigcup_{\alpha=1}^{d} L_{\alpha 2} \cap M_{\alpha 2} \neq \emptyset$. *In addition,* $L_{12} \neq \emptyset$.

3) For $\rho \in \left(\frac{d}{2}, d\right)$ *the function:*

$$\mathcal{E}_{\mathbf{0}}(p) = \varepsilon_1(p) + \varepsilon_2(p), \quad \varepsilon_1(p) = \varepsilon_2(p) = \left(\sum_{i=1}^{d} (1 - \cos 2p_i) \right)^{\rho/2}$$

satisfies the assumptions of Theorem 2.

3. Eigenvalues of $h(k)$

Proof of Lemma 1. Note that proof of (2.1) is obvious.

By definition $\mu_\alpha^-(k; z) < \mu_\alpha^+(k; z)$ for any $z < m(k)$ and $k \in \mathbb{T}^d$. Notice that:

$$c_\alpha(k; z) s_\alpha(k; z) - \xi_\alpha^2(k; z) = \int_{\mathbb{T}^d} \frac{\cos^2 s_\alpha ds}{\mathcal{E}_k(s) - z} \int_{\mathbb{T}^d} \frac{\sin^2 t_\alpha dt}{\mathcal{E}_k(t) - z} - \int_{\mathbb{T}^d} \frac{\sin s_\alpha \cos s_\alpha ds}{\mathcal{E}_k(s) - z} \int_{\mathbb{T}^d} \frac{\sin t_\alpha \cos t_\alpha dt}{\mathcal{E}_k(t) - z}$$

$$= \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \frac{\frac{1}{2} \cos^2 s_\alpha \sin^2 t_\alpha ds dt}{(\mathcal{E}_k(s) - z)(\mathcal{E}_k(t) - z)} - \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \frac{\sin s_\alpha \cos s_\alpha \sin t_\alpha \cos t_\alpha ds dt}{(\mathcal{E}_k(s) - z)(\mathcal{E}_k(t) - z)} + \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \frac{\frac{1}{2} \cos^2 t_\alpha \sin^2 s_\alpha ds dt}{(\mathcal{E}_k(s) - z)(\mathcal{E}_k(t) - z)}$$

$$= \frac{1}{2} \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \frac{\sin^2(s_\alpha - t_\alpha) ds dt}{(\mathcal{E}_k(s) - z)(\mathcal{E}_k(t) - z)}. \quad (3.1)$$

Hence, $c_\alpha(k; z) s_\alpha(k; z) - \xi_\alpha^2(k; z) > 0$ for all $z < m(k)$ and $k \in \mathbb{T}^d$.

The function $\mu_\alpha^+(k;z)$ we estimate as follows:

$$\mu_\alpha^+(k;z) = \frac{c_\alpha(k;z)+s_\alpha(k;z)+\sqrt{(c_\alpha(k;z)-s_\alpha(k;z))^2+4\xi_\alpha^2(k;z)}}{2[c_\alpha(k;z)s_\alpha(k;z)-\xi_\alpha^2(k;z)]}$$
$$= \frac{c_\alpha(k;z)+s_\alpha(k;z)+\sqrt{(c_\alpha(k;z)+s_\alpha(k;z))^2-4[c_\alpha(k;z)s_\alpha(k;z)-\xi_\alpha^2(k;z)]}}{2[c_\alpha(k;z)s_\alpha(k;z)-\xi_\alpha^2(k;z)]}$$
$$< \frac{c_\alpha(k;z)+s_\alpha(k;z)}{c_\alpha(k;z)s_\alpha(k;z)-\xi_\alpha^2(k;z)}. \quad (3.2)$$

Since $\dfrac{\sin^2(s_\alpha-t_\alpha)}{\mathcal{E}_k(t)-z} > 0$ for any $z < m(k)$ and for a.e. $k,s,t \in \mathbb{T}^d$, there exists $\delta > 0$ such that:

$$\min_{k,z} \int\limits_{\mathbb{T}^d} \frac{\sin^2(s_\alpha-t_\alpha)dsdt}{\mathcal{E}_k(t)-z} \geq \delta.$$

From here and from (3.1) we get:

$$c_\alpha(k;z)s_\alpha(k;z)-\xi_\alpha^2(k;z) > \frac{\delta}{2}\int\limits_{\mathbb{T}^d}\frac{ds}{\mathcal{E}_k(s)-z}.$$

Since

$$c_\alpha(k;z)+s_\alpha(k;z) = \int\limits_{\mathbb{T}^d}\frac{ds}{\mathcal{E}_k(s)-z}$$

from (3.2) we get uniform upper estimate:

$$\mu_\alpha^+(k;z) < \frac{1}{2\delta}.$$

From here we get (2.2).

Lemma is proved.

Lemma 2. *$z < m(k)$ is an eigenvalue of $h(k)$ if and only if $\Delta(k;z) = 0$, where*

$$\Delta(k;z) = (1-\mu_0 b(k;z))\prod_{\alpha=1}^{d}\Big([1-\mu_\alpha c_\alpha(k;z)][1-\mu_\alpha s_\alpha(k;z)]-\mu_\alpha^2\xi_\alpha^2(k;z)\Big). \quad (3.3)$$

Proof. Let $z < m(k)$ be an eigenvalue of $h(k)$ with associated eigenfunction $f \neq 0$. Then $h(k)f = zf$ and so:

$$f = r_0(z)\mathbf{v}f, \quad (3.4)$$

where $r_0(z)$ is a resolvent of $h_0(k)$. Introduce the following notations:

$$\varphi_0 = \int\limits_{\mathbb{T}^d} f(s)ds, \quad (3.5)$$

$$\varphi_\alpha = \int\limits_{\mathbb{T}^d} \cos s_\alpha f(s)ds, \quad (3.6)$$

$$\psi_\alpha = \int\limits_{\mathbb{T}^d} \sin s_\alpha f(s)ds, \quad \alpha = 1,2,3,...d. \quad (3.7)$$

Then, (3.4) is rewritten as:

$$f(p) = \frac{\mu_0\varphi_0}{\mathcal{E}_k(p)-z} + \frac{1}{\mathcal{E}_k(p)-z}\sum_{\alpha=1}^{d}\mu_\alpha[\cos p_\alpha\varphi_\alpha + \sin p_\alpha\psi_\alpha]. \quad (3.8)$$

From the π-periodicity of $\mathcal{E}_k(\cdot)$ in each argument, it follows that:

$$\int\limits_{\mathbb{T}^d}\frac{\cos s_\alpha ds}{\mathcal{E}_k(s)-z} = \int\limits_{\mathbb{T}^d}\frac{\cos s_\alpha\cos s_\beta ds}{\mathcal{E}_k(s)-z} = \int\limits_{\mathbb{T}^d}\frac{\cos s_\alpha\sin s_\beta ds}{\mathcal{E}_k(s)-z} = \int\limits_{\mathbb{T}^d}\frac{\sin s_\alpha\sin s_\beta ds}{\mathcal{E}_k(s)-z} = 0, \ \alpha \neq \beta. \quad (3.9)$$

Putting (3.8) in the relations (3.5)–(3.7) and using (3.9), we get that $\varphi_0, \varphi_1, ..., \varphi_d$, $\psi_1, \psi_2, ..., \psi_d$ satisfy the system of $(2d+1)$-linear equations:

$$\begin{aligned} &\varphi_0 = \mu_0 b(k;z)\varphi_0, \\ &\varphi_\alpha = \mu_\alpha c_\alpha(k;z)\varphi_\alpha + \mu_\alpha \xi_\alpha(k;z)\psi_\alpha, \quad \alpha = 1, ..., d \\ &\psi_\alpha = \mu_\alpha \xi_\alpha(k;z)\varphi_\alpha + \mu_\alpha s_\alpha(k;z)\psi_\alpha, \quad \alpha = 1, ..., d. \end{aligned} \tag{3.10}$$

This system of equations has a nonzero solution $(\varphi_0, \dots, \varphi_d, \psi_1, \dots \psi_d)$ if and only if its determinant is zero, i.e. $\det D(k;z) = 0$. It is easy to see that $\det D(k;z) = \Delta(k;z)$.

Conversely, let $\Delta(k;z) = 0$, $z < m(k)$. Then, at least one of the equalities $1 - \mu_0 b(k;z) = 0$, $[1 - \mu_\alpha c_\alpha(k;z)][1 - \mu_\alpha s_\alpha(k;z)] - \mu_\alpha^2 \xi_\alpha^2(k;z) = 0$, $\alpha \in \{1, \dots, d\}$ holds. Thus, the vector $\mathbf{c} = (c_0, \cdots, c_{2d})$ where $c_0 = 1$, $c_\alpha = \varphi_\alpha$, $c_{d+\alpha} = \psi_\alpha$, is a solution of (3.10). Consequently, one of the functions:

$$\frac{1}{\mathcal{E}_k(p) - z}, \quad \frac{1}{\mathcal{E}_k(p) - z}\mu_\alpha[\varphi_\alpha \cos p_\alpha + \psi_\alpha \sin p_\alpha]$$

is an eigenfunction of $h(k)$ associated with eigenvelue $z < m(k)$.

Observe that $\Delta(k;\cdot)$ is the Fredholm determinant of the operator $I - r_0(z)\mathbf{v}$, i.e. $\Delta(k;z) = \det(I - r_0(z)\mathbf{v})$. Moreover, it is well-known [11] that geometric multiplicity of eigenvalue 1 of $r_0(z)\mathbf{v}$ coincides with the multiplicity of zero z of $\Delta(k;\cdot)$. Since the multiplicities of eigenvalues 1 and z of operators respectively $r_0(z)\mathbf{v}$ and $h(k)$ are the same, we get that multiplicity of zeros of $\Delta(k;\cdot)$ is equal to the multiplicity of eigenvalues of $h(k)$. The lemma is thus proved.

Proof of Theorem 1. Notice that the function:

$$\Delta_\alpha(k;z) = [1 - \mu_\alpha c_\alpha(k;z)][1 - \mu_\alpha s_\alpha(k;z)] - \mu_\alpha^2 \xi_\alpha^2(k;z),$$

is a Fredholm determinant associated with the operator $I - r_0(z)\mathbf{v}_\alpha$, where $\mathbf{v}_\alpha$ – is an integral operator with kernel $v_\alpha(p-s) = \mu_\alpha \cos(p_\alpha - s_\alpha)$.

Since $\mathbf{v}_\alpha$ is a two-dimensional operator, number of zeros $\beta_\alpha(\mu;k)$ with multiplicities of the function $\Delta_\alpha(k;\cdot)$, lying below $m(k)$, is not more than 2. Function $\Delta_\alpha(k;\cdot)$ can be represented as:

$$\Delta_\alpha(k;z) = [c_\alpha(k;z)s_\alpha(k;z) - \xi_\alpha^2(k;z)]\Big(\mu_\alpha - \mu_\alpha^-(k;z)\Big)\Big(\mu_\alpha - \mu_\alpha^+(k;z)\Big). \tag{3.11}$$

Since:

$$\lim_{z \to m(k) - 0} \mu_\alpha^\pm(k;z) = \mu_\alpha^\pm(k) < \infty,$$

one has:

$$\mu_\alpha - \mu_\alpha^\pm(k;m(k)) = \begin{cases} \geq 0 & \text{if} \quad \mu_\alpha \in (0, \mu_\alpha^\pm(k)], \\ < 0 & \text{if} \quad \mu_\alpha \in (\mu_\alpha^\pm(k), \infty). \end{cases}$$

Consequently, from (3.11) and (3.1) it can be deduced that:

$$\beta_\alpha(\mu;k) = \begin{cases} 0 & \text{if} \quad \mu_\alpha \in (0, \mu_\alpha^-(k)], \\ 1 & \text{if} \quad \mu_\alpha \in (\mu_\alpha^-(k), \mu_\alpha^+(k)], \\ 2 & \text{if} \quad \mu_\alpha \in (\mu_\alpha^+(k), \infty). \end{cases}$$

Observe that the function $1 - \mu_0 b(k;\cdot)$ is monotonously decreasing in $(\infty, m(k))$. Thus for the number of zeros $\alpha(\mu;k)$ of the function $\Delta_\alpha(k;\cdot)$ below $m(k)$ it holds:

$$\alpha(\mu;k) = \begin{cases} 0 & \text{if} \quad \mu_0 \in (0; \mu^0(k)], \\ 1 & \text{if} \quad \mu_0 \in (\mu^0(k); \infty). \end{cases}$$

If $\mu^0(k) = 0$, then $\lim\limits_{z \to m(k) - 0} b(k;z) = +\infty$. Obviously, in this case $\alpha(\mu;k) = 1$ for any $\mu_0 > 0$.

The aforementioned facts imply that if: $\mu = (\mu_0, \mu_1, \dots, \mu_d) \in R_+^{d+1}$, then the function $\Delta(k;\cdot)$ has exactly:

$$\alpha(\mu;k) + \sum_{i=1}^{d} \beta_i(\mu;k)$$

zeros (counting multiplicities) below $m(k)$.

Then, from Lemma 1, we get that for $\mu = (\mu_0, \mu_1, \dots, \mu_d) \in R_+^{d+1}$ the operator $h(k)$ exactly:

$$\alpha(\mu;k) + \sum_{i=1}^{d} \beta_i(\mu;k)$$

zeros (counting multiplicities) below $m(k)$.

This finishes the proof.

Proof of Theorem 2. We shall study the equation:

$$G(\mathbf{0};0)\varphi=\varphi.$$

Notice that the function $\Delta(k;z)$, defined as (3.3) is the Fredholm determinant of $I-G(k;z)$. From Hypothesis 2, the function $\Delta(k;z)$ is defined for $k=\mathbf{0}$, $m(\mathbf{0})=0$. Since $\mathcal{E}_{\mathbf{0}}(\cdot)$ is even, the function

$$\xi_i(\mathbf{0};z)=\int\limits_{\mathbb{T}^d}\frac{\sin s_i\cos s_i ds}{\mathcal{E}_{\mathbf{0}}(s)-z}=0,\quad z\leq 0.$$

Consequently, the function $\Delta(\mathbf{0};z)$ can be represented as:

$$\Delta(\mathbf{0};z)=(1-\mu_0 b(\mathbf{0};z))\prod_{\alpha=1}^{d}\Big([1-\mu_\alpha c_\alpha(\mathbf{0};z)][1-\mu_\alpha s_\alpha(\mathbf{0};z)]\Big).$$

The following lemma can be proved analogously to Lemma 2.

Lemma 3. *The number $\lambda=1$ is an eigenvlue of $G(\mathbf{0};0)$ if and only if $\Delta(\mu)=\Delta(\mathbf{0};0)=0$. In this case if $1-\mu_0 b(\mathbf{0};0)=0$ $\Big(1-\mu_\alpha c_\alpha(\mathbf{0};0)=0$ or $1-\mu_\alpha s_\alpha(\mathbf{0};0)=0\Big)$, then the function $\varphi_0=1$ $\Big(\varphi_\alpha(p)=\cos p_\alpha$ or $\psi_\alpha(p)=\sin p_\alpha\Big)$ is an eigenfucntion of the operator $G(\mathbf{0};0)$, associated with* 1.

Obviously, $\Delta(\mu)>0$ if $\mu_0\in(0;\mu^0(\mathbf{0}))$, $\mu_\alpha\in(0;\mu_\alpha^0)$, $\alpha=1,\dots,d$. By Lemma 3 $\lambda=1$ is not eigenvalue of $G(\mathbf{0};0)$. Hence 0 is not an eigenvalue of $h(\mathbf{0})$ for $\mu_0\in(0;\mu^0(\mathbf{0}))$, $\mu_\alpha\in(0;\mu_\alpha^0)$, $\alpha=1,\dots,d$.

Further, consider the equation $G(\mathbf{0};0)\varphi=\varphi$ for $\mu_0=\mu^0(\mathbf{0})$, $\mu_\alpha=\mu_\alpha^0$, $\alpha=1,\dots,d$.

(i) a) Let $\rho=2$, $\mu_0=\mu^0(\mathbf{0})$.

According to Lemma 3, $\lambda=1$ is an eigenvalue of $G(\mathbf{0};0)$, with associated eigenfunction $\varphi_0(p)=1$.

It is easy to check that if $d=3,4$, then:

$$F_0(\cdot)\in L_1(\mathbb{T}^d)\setminus L_2(\mathbb{T}^d),$$

and if $d\geq 5$, then:

$$F_0(\cdot)\in L_2(\mathbb{T}^d),$$

where

$$F_0(p)=\frac{1}{\mathcal{E}_{\mathbf{0}}(p)}.$$

It means that $z=0$ is virtual level of $h(\mathbf{0})$ for $d=3$, 4, and eigenvalue for $d\geq 5$.

b) Let $\mu_\alpha=\mu_\alpha^0$, $\alpha=1,\dots,d$. Then μ_α belongs one and only one of the sets $L_{\alpha1}$, $L_{\alpha2}$, $L_{\alpha3}$ $M_{\alpha1}$, $M_{\alpha2}$, $M_{\alpha3}$.

If $\mu_\alpha\in L_{\alpha1}\Big(\mu_\alpha\in M_{\alpha1}\Big)$, then $1-\mu_\alpha c_\alpha(\mathbf{0};0)>0$ $\Big(1-\mu_\alpha s_\alpha(\mathbf{0};0)>0\Big)$. If $\mu_\alpha\in L_{\alpha2}\Big(\mu_\alpha\in M_{\alpha2}\Big)$, then $\cos p_i^{(\alpha)}=0$ $\Big(\sin p_i^{(\alpha)}=0\Big)$ for all $i=1,\dots,d$. In this case

$$F_\alpha(\cdot)\in L_2(\mathbb{T}^d),\quad \Big(\Phi_\alpha(\cdot)\in L_2(\mathbb{T}^d)\Big),\quad d\geq 3,$$

where

$$F_\alpha(p)=\frac{\cos p_\alpha}{\mathcal{E}_{\mathbf{0}}(p)},\ \Phi_\alpha(p)=\frac{\sin p_\alpha}{\mathcal{E}_{\mathbf{0}}(p)},\ \alpha=1,...,d,$$

and, so, $z=0$ is not virtual level of $h(\mathbf{0})$ for $d\geq 3$, but is an eigenvalue of this operator.

If $\mu_\alpha\in L_{\alpha3}\Big(\mu_\alpha\in M_{\alpha3}\Big)$, then $\cos p_i^{(\alpha)}\neq 0$ $\Big(\sin p_i^{(\alpha)}\neq 0\Big)$ at least one of $i=\{1,\dots,d\}$. Consequently,

$$F_\alpha(\cdot)\in L_1(\mathbb{T}^d)\setminus L_2(\mathbb{T}^d),\quad \Big(\Phi_\alpha(\cdot)\in L_1(\mathbb{T}^d)\setminus L_2(\mathbb{T}^d)\Big)\quad \text{for}\quad d=3,4,$$

$$F_\alpha(\cdot)\in L_2(\mathbb{T}^d),\quad \Big(\Phi_\alpha(\cdot)\in L_2(\mathbb{T}^d)\Big)\quad \text{for}\quad d>4,$$

i.e. $z=0$ is a virtual level (eigenvalue) of the operator $h(\mathbf{0})$ for $d=3,4$ ($d>4$).

From a) and b) we deduce the following:

if $\mu_0=\mu^0(\mathbf{0})$, then $z=0$ is virtual level (eigenvalue) of $h(\mathbf{0})$ for $d=3,4$ ($d>4$);

if $\mu_\alpha\in L_{\alpha1}\cup L_{\alpha2}$, then $z=0$ is not virtual level of $h(\mathbf{0})$ for $d\geq 3$;

if $\mu_\alpha\in L_{\alpha3}$, then $z=0$ is virtual level (eigenvalue) of the operator $h(\mathbf{0})$ for $d=3,4$ ($d>4$);

if $\mu_\alpha \in L_{\alpha 2}$, then $z = 0$ is eigenvalue of the operator $h(\mathbf{0})$ for $d \geq 3$;
if $\mu_\alpha \in M_{\alpha 1} \cup M_{\alpha 2}$, then $z = 0$ is not virtual level of $h(\mathbf{0})$ for $d \geq 3$;
if $\mu_\alpha \in M_{\alpha 3}$, then $z = 0$ is a virtual level (eigenvalue) of $h(\mathbf{0})$ for $d = 3, 4$ $(d > 4)$;
if $\mu_\alpha \in M_{\alpha 2}$, then $z = 0$ is eigenvalue of $h(\mathbf{0})$ for $d \geq 3$.
Part (i) of Theorem 2 is proved.
Part (ii) of Theorem 2 is proved analogously.

Acknowledgements

This work was supported in part by the Malaysian Ministry of Education through the Research Management Centre (RMC), Universiti Teknologi Malaysia (PAS, Ref. No. PY/2014/04068, Vote: QJ130000.2726.01K82).

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 888–892

Characterization of the normal subgroups of finite index for the group representation of a Cayley tree

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DOI 10.17586/2220-8054-2016-7-5-888-892

In this paper we give a characterization of normal subgroups for the group representation of the Cayley tree.

Keywords: Cayley tree, G_k-group, normal subgroup, homomorphism, epimorphism.

Received: 4 August 2016

Revised: 29 August 2016

1. Introduction

The method used for the description of Gibbs measures on Cayley trees is the method of Markov random field theory and recurrent equations of this theory, however, the modern theory of Gibbs measures on trees uses new tools such as group theory, information flows on trees, node-weighted random walks, contour methods on trees, nonlinear analysis. A very recently published book [1] discusses all above-mentioned methods for describing Gibbs measures on trees. In the configuration of physical system is located on a lattice (in our case on the graph of a group), then the configuration can be considered as a function defined on the lattice. There are many works devoted to several kind of partitions of groups (lattices) (see e.g. [1–5, 7]).

One of the central problems in the theory of Gibbs measures is to study periodic Gibbs measures corresponding to a given Hamiltonian. For any normal subgroups H of the group G_k, we define H-periodic Gibbs measures.

In Chapter 1 of [1] several normal subgroups were constructed for the group representation of the Cayley tree. In [6], we found full description of normal subgroups of index four and six for the group. In this paper, we continue this investigation and construct all normal subgroups of index eight and ten for the group representation of the Cayley tree.

Cayley tree. A Cayley tree (Bethe lattice) Γ^k of order $k \geq 1$ is an infinite homogeneous tree, i.e., a graph without cycles, such that exactly $k+1$ edges originate from each vertex. Let $\Gamma^k = (V, L)$ where V is the set of vertices and L that of edges (arcs).

A group representation of the Cayley tree. Let G_k be a free product of $k+1$ cyclic groups of the second order with generators $a_1, a_2, ...a_{k+1}$, respectively.

A one to one correspondence is known to exist between the set of vertices V of the Cayley tree Γ^k and the group G_k(see [1]).

To obtain this correspondence, we fix an arbitrary element $x_0 \in V$ and let it correspond to the unit element e of the group G_k. Using $a_1, ..., a_{k+1}$, we numerate the nearest-neighbors of element e, moving by positive direction. Next, we give the numeration for the nearest-neighbors of each $a_i, i = 1, ..., k+1$ by $a_i a_j, j = 1, ..., k+1$. Since all a_i have the common neighbor e, we give to it $a_i a_i = a_i^2 = e$. Other neighbors are numerated starting from $a_i a_i$ by the positive direction. We numerate the set of all the nearest-neighbors of each $a_i a_j$ by words $a_i a_j a_q, q = 1, ..., k+1$, starting from $a_i a_j a_j = a_i$ by the positive direction. Iterating this argument, one gets a one-to-one correspondence between the set of vertices V of the Cayley tree Γ^k and the group G_k.

Any(minimally represented) element $x \in G_k$ has the following form: $x = a_{i_1} a_{i_2} ... a_{i_n}$, where $1 \leq i_m \leq k+1, m = 1, ..., n$. The number n is called the length of the word x and is denoted by $l(x)$. The number of letters $a_i, i = 1, ..., k+1$, that enter the non-contractible representation of the word x is denoted by $w_x(a_i)$.

Proposition 1. *[8] Let φ be homomorphism of the group G_k with the kernel H. Then H is a normal subgroup of the group G_k and $\varphi(G_k) \simeq G_k/H$, (where G_k/H is a quotient group) i.e., the index $|G_k : H|$ coincides with the order $|\varphi(G_k)|$ of the group $\varphi(G_k)$.*

Let H be a normal subgroup of a group G. The natural homomorphism g from G onto the quotient group G/H is given by the formula $g(a) = aH$ for all $a \in G$. Then, $\operatorname{Ker} \varphi = H$.

Definition 1. *Let $M_1, M_2, ..., M_m$ be some sets and $M_i \neq M_j$, for $i \neq j$. We call the intersection $\cap_{i=1}^{m} M_i$ contractible if there exists $i_0 (1 \leq i_0 \leq m)$ such that:*

$$\cap_{i=1}^{m} M_i = \left(\cap_{i=1}^{i_0-1} M_i\right) \cap \left(\cap_{i=i_0+1}^{m} M_i\right).$$

Let $N_k = \{1, ..., k+1\}$. The following Proposition describes several normal subgroups of G_k.
Put

$$H_A = \left\{ x \in G_k \mid \sum_{i \in A} \omega_x(a_i) \text{ is even} \right\}, \quad A \subset N_k. \tag{1.1}$$

Proposition 2. *[1] For any $\emptyset \neq A \subseteq N_k$, the set $H_A \subset G_k$ satisfies the following properties: (a) H_A is a normal subgroup and $|G_k : H_A| = 2$;*
(b) $H_A \neq H_B$, for all $A \neq B \subseteq N_k$;
(c) Let $A_1, A_2, ..., A_m \subseteq N_k$. If $\cap_{i=1}^{m} H_{A_i}$ is non-contractible, then it is a normal subgroup of index 2^m.

Theorem 1. *[6]*
1. The group G_k does not have normal subgroups of odd index $(\neq 1)$.
2. The group G_k has a normal subgroups of arbitrary even index.

2. New normal subgroups of finite index

2.1. The case of index eight

Definition 2. *A group G is called a **dihedral** group of degree 4 $(i.e., D_4)$ if G is generated by two elements a and b satisfying the relations:*

$$o(a) = 4, \ o(b) = 2, \ ba = a^3 b.$$

Definition 3. *A group G is called a **quaternion** group $(i.e., Q_8)$ if G is generated by two elements $a, \ b$ satisfying the relation:*

$$o(a) = 4, a^2 = b^2, ba = a^3 b.$$

Remark 1. [8] *D_4 is not isomorph to Q_8.*

Definition 4. *A commutative group G is called a **Klein 8-group** $(i.e., K_8)$ if G is generated by three elements a, b and c satisfying the relations: $o(a) = o(b) = o(c) = 2$.*

Proposition 3. [8] *There exist (up to isomorphism) only two noncommutative nonisomorphic groups of order 8*

Proposition 4. *Let φ be a homomorphism of the group G_k onto a group G of order 8. Then, $\varphi(G_k)$ is isomorph to either D_4 or K_8.*

Proof. `Case 1` Let $\varphi(G_k)$ be isomorph to any noncommutative group of order 8. By Proposition 1, $\varphi(G_k)$ is isomorph to either D_4 or Q_8. Let $\varphi(G_k) \simeq Q_8$ and e_q be an identity element of the group Q_8. Then, $e_q = \varphi(e) = \varphi(a_i^2) = (\varphi(a_i))^2$ where $a_i \in G_k, \ i \in N_k$. Hence, for the order of $\varphi(a_i)$, we have $o(\varphi(a_i)) \in \{1, 2\}$. It is easy to check there are only two elements of the group Q_8 which order of element less than two. This is contradict.

`Case 2` Let $\varphi(G_k, *)$ be isomorph to any commutative group $(G, *_1)$ of order 8. Then, there exist distinct elements $a, b \in G$ such that $o(a) = o(b) = 2$. Let $H = \{e, a, b, ab\}$. It's easy to check that $(H, *_1)$ is a normal subgroup of the group $(G, *_1)$. For $c \notin H$ we have $H \neq cH$ $(cH = c *_1 H)$. Hence $\varphi(G_k, *)$ is isomorph to only one commutative group $(cH \cup H, *_1)$. Clearly $(cH \cup H, *_1) \simeq K_8$. □

The group G has finit generators of the order two and r is the minimal number of such generators of the group G and without loss of generality, we can take these generators to be $b_1, b_2, ...b_r$. Let e_1 be an identity element of the group G. We define homomorphism from G_k onto G. Let $\Xi_n = \{A_1, \ A_2, ..., A_n\}$ be a partition of $N_k \backslash A_0, \ 0 \leq |A_0| \leq k + 1 - n$. Then, we consider homomorphism $u_n : \{a_1, a_2, ..., a_{k+1}\} \to \{e_1, b_1 ..., b_m\}$ as

$$u_n(x) = \begin{cases} e_1, & \text{if } x = a_i, i \in A_0 \\ b_j, & \text{if } x = a_i, i \in A_j, j = \overline{1, n}. \end{cases} \tag{2.1}$$

For $b \in G$, we denote that $R_b[b_1, b_2, ..., b_m]$ is a representation of the word b by generators $b_1, b_2, ..., b_r,\ r \leq m$. We define the homomorphism $\gamma_n : G \to G$ by the formula

$$\gamma_n(x) = \begin{cases} e_1, & \text{if } x = e_1 \\ b_i, & \text{if } x = b_i, i = \overline{1,r} \\ R_{b_i}[b_1, ..., b_r], & \text{if } x = b_i, i \neq \overline{1,r} \end{cases} \tag{2.2}$$

We set:

$$H^{(p)}_{\Xi_n}(G) = \{x \in G_k |\ l(\gamma_n(u_n(x))) \text{ is divisible by } 2p\},\ 2 \leq n \leq k-1. \tag{2.3}$$

Let $\gamma_n(u_n(x))) = \tilde{x}$. We introduce the following equivalence relation on the set $G_k : x \sim y$ if $\tilde{x} = \tilde{y}$. This relation is readily confirmed to be reflexive, symmetric and transitive.

Proposition 5. *Let $\Xi_n = \{A_1, A_2, ..., A_n\}$ be a partition of $N_k \backslash A_0,\ 0 \leq |A_0| \leq k+1-n$. Then $H^{(p)}_{\Xi_p}(G)$ is a normal subgroup of index $2p$ of the group G_k.*

Proof. For $x = a_{i_1}a_{i_2}...a_{i_n} \in G_k$ it's sufficient to show that $x^{-1}H^{(p)}_{\Xi_n}(G)\ x \subseteq H^{(p)}_{\Xi_n}(G)$. Suppose that there exist $y \in G_k$ such that $l(\tilde{y}) \geq 2p$. Let $\tilde{y} = b_{i_1}b_{i_2}...b_{i_q},\ q \geq 2p$ and $S = \{b_{i_1}, b_{i_1}b_{i_2}, ..., b_{i_1}b_{i_2}...b_{i_q}\}$. Since $S \subseteq G$ there exist $x_1, x_2 \in S$ such that $x_1 = x_2$. But this contradicts $\tilde{y}$, which is a non-contractible. Thus we have proved that $l(\tilde{y}) < 2p$. Hence, for any $x \in H^{(p)}_{\Xi_n}(G)$ we have $\tilde{x} = e_1$. Next, we take any element z from the set $x^{-1}H^{(p)}_{\Xi_n}(G)\ x$. Then, $z = x^{-1}h\ x$ for some $h \in H^{(p)}_{\Xi_n}(G)$. We have $\tilde{z} = \gamma_n(v_n(z)) = \gamma_n\left(v_n(x^{-1}h\ x)\right) = $ $= \gamma_n\left(v_n(x^{-1})v_n(h)v_n(x)\right) = \gamma_n\left(v_n(x^{-1})\right)\gamma_n\left(v_n(h)\right)\gamma_n\left(v_n(x)\right)$. From $\gamma_n\left(v_n(h)\right) = e_1$, we get $\tilde{z} = e_1$ i.e., $z \in H^{(p)}_{\Xi_n}(G)$. This completes the proof. □

Since $A_1, A_2, A_3 \subset N_k$ and $\cap_{i=1}^3 H_{A_i}$ is non-contractible we denote the following set:

$$\Re = \{\cap_{i=1}^3 H_{A_i} |\ A_1, A_2, A_3 \subset N_k\}.$$

Theorem 2. *For the group G_k, the following statement is hold:*

$$\{H |\ H \text{ is a normal subgroup of } G_k \text{ with } |G_k : H| = 8\} =$$

$$= \{H^{(4)}_{C_0C_1C_2}(D_4) |\ C_1, C_2 \text{ is a partition of } N_k \setminus C_0\} \cup \Re.$$

Proof. Let ϕ be a homomorphism with $|G_k : \operatorname{Ker}\phi| = 8$. Then by Proposition 2 we have $\phi(G_k) \simeq K_8$ and $\phi(G_k) \simeq D_4$.

Let $\phi : G_k \to K_8$ be an epimorphism. For any nonempty sets $A_1, A_2, A_3 \subset N_k$, we give a one to one correspondence between
$operatornameKer\phi |\ \phi(G_k) \simeq K_8\}$ and $\Re$. Let $a_i \in G_k, i \in N_k$. We define following homomorphism corresponding to the set A_1, A_2, A_3:

$$\phi_{A_1A_2A_3}(a_i) = \begin{cases} a, & \text{if } i \in A_1 \setminus (A_2 \cup A_3) \\ b, & \text{if } i \in A_2 \setminus (A_1 \cup A_3) \\ c, & \text{if } i \in A_3 \setminus (A_1 \cup A_2) \\ ab, & \text{if } i \in (A_1 \cap A_2) \setminus (A_1 \cap A_2 \cap A_3) \\ ac, & \text{if } i \in (A_1 \cap A_3) \setminus (A_1 \cap A_2 \cap A_3) \\ bc, & \text{if } i \in (A_2 \cap A_3) \setminus (A_1 \cap A_2 \cap A_3) \\ abc, & \text{if } i \in A_1 \cap A_2 \cap A_3 \\ e, & \text{if } i \in N_k \setminus (A_1 \cup A_2 \cup A_3). \end{cases}$$

If $i \in \emptyset$, then we'll accept that there is no index $i \in N_k$ for which that condition is not satisfied. It is easy to check $\operatorname{Ker}\phi_{A_1A_2A_3} = H_{A_1} \cap H_{A_2} \cap H_{A_3}$. Hence $\{\operatorname{Ker}\phi |\ \phi(G_k) \simeq K_8\} = \Re$.

Now, we'll consider the case $\phi(G_k) \simeq D_4$. Let $\phi : G_k \to D_4$ be epimorphisms. Put

$$C_0 = \{i |\ \phi(a_i) = e\},\ \ C_1 = \{i |\ \phi(a_i) = b\},\ C_2 = \{i |\ \phi(a_i) = ab\}.$$

One can construct following homomorphism (corresponding to C_0, C_1, C_2)

$$\phi_{C_0C_1C_2}(x) = \begin{cases} e, \text{ if } \tilde{x} = e \\ a, \text{ if } \tilde{x} = b_2b_1 \\ a^2, \text{ if } \tilde{x} = b_2b_1b_2b_1 \\ a^3, \text{ if } \tilde{x} = b_2b_1b_2b_1b_2b_1 \\ b, \text{ if } \tilde{x} = b_1 \\ ab, \text{ if } \tilde{x} = b_2 \\ a^2b, \text{ if } \tilde{x} = b_2b_1b_2 \\ a^3b, \text{ if } \tilde{x} = b_2b_1b_2b_1b_2. \end{cases}$$

Immediately, we conclude $\mathrm{Ker}(\phi_{C_0C_1C_2}) = H^{(4)}_{C_0C_1C_2}(D_4)$. We have constructed all homomorphisms ϕ on the group G_k which $|G_k : \mathrm{Ker}\,\phi| = 8$. Thus by Proposition 1, one gets:

$$\{H| \ |G_k : H| = 8\} \subseteq \{H^{(4)}_{C_0C_1C_2}(D_4)| \ C_1, C_2 \text{ is a partition of } N_k \setminus C_0\} \cup \Re.$$

By Proposition 2 and Proposition 5, we can easily see that:

$$\Re \cup \{H^{(4)}_{C_0C_1C_2}(D_4)| \ C_1, C_2 \text{ is a partition of } N_k \setminus C_0\} \subseteq \{H| \ |G_k : H| = 8\}.$$

The theorem is proved. □

Corollary 1. *The number of all normal subgroups of index* 8 *for the group* G_k *is equal to:* $8^{k+1} - 6 \cdot 4^{k+1} + 3^{k+1} + 9 \cdot 2^{k+1} - 5$.

Proof. Number of elements of the set $H_A \subset G_k, \emptyset \neq A \subset N_k$ is $2^{k+1} - 1$. Then $|\Re| = (2^{k+1})(2^{k+1} - 2)(2^{k+2} - 3)$. Let $C_0 \subset N_k$ be a fixed set and $|C_0| = p$. If C_1, C_2 is a partition of $N_k \setminus C_0$ then there are $2^{k-p+1} - 2$ ways to choose the sets C_1 and C_2. Hence the cardinality of $\{H^{(4)}_{C_0C_1C_2}(D_4)| \ C_1, C_2$ is a partition of $N_k \setminus C_0\}$ is equal to

$$(2^{k+1} - 2)C^0_{k+1} + (2^k - 2)C^1_{k+1} + ... + 2C^{k-1}_{k+1} = 3^{k+1} - 2^{k+2} + 1.$$

Since $\Re$ and $\{H^{(4)}_{C_0C_1C_2}(D_4)\}| \ C_1, C_2 \subset N_k$ are disjoint sets, the cardinality of the union of these sets is $8^{k+1} - 6 \cdot 4^{k+1} + 3^{k+1} + 9 \cdot 2^{k+1} - 5$. □

2.2. Case of index ten

Let the group R_{10} be generated by the permutations:

$$\pi_1 = (1, 2)(3, 4)(5, 6), \ \pi_2 = (2, 3)(4, 5).$$

Proposition 6. *Let* φ *be a homomorphism of the group* G_k *onto a group* G *of order 10. Then,* $\varphi(G_k)$ *is isomorph to* R_{10}.

Proof. Let $(G, *)$ be a group and $|G| = 10$. Suppose there exist an epimorphism from G_k onto G. It is easy to check that there are at least two elements $a, b \in G_k$ such that $o(a) = o(b) = 2$. If $a * b = b * a$, then $(H, *)$ is a subgroup of the group $(G, *)$, where $H = \{e, a, b, a*b\}$. Then, by Lagrange's theorem, $|G|$ is divided by $|H|$ but 10 is not divided by 4. Hence, $a*b \neq b*a$. We have $\{e, a, b, a*b, b*a\} \subset G$ If G is generated by three elements, then there exist an element c such that $c \notin \{e, a, b, a*b, b*a\}$. Then, the set $\{e, a, b, a*b, b*a, c, c*a, c*b, c*a*b, c*b*a\}$ must be equal to G. Since G is a group, we get $a * b * a = b$ but from $o(a) = 2$ the last equality is equivalent to $a * b = b * a$. This is a contradiction. Hence, by Lagrange's theorem it is easy to see:

$$G = \{e, a, b, a * b, b * a, a * b * a, b * a * b, a * b * a * b, b * a * b * a, a * b * a * b * a\},$$

where $o(a * b) = 5$. Namely $G \simeq R_{10}$. This completes the proof. □

Theorem 3. *For the group* G_k*, the following statement is holds:*

$$\{H| \ | \ H \text{ is a normal subgroup of } G_k \text{ with } |G_k : H| = 10\} =$$

$$= \{H^{(5)}_{B_0B_1B_2}(R_{10})| \ B_1, B_2 \text{ is a partition of the set } N_k \setminus B_0\}.$$

Proof. Let ϕ be a homomorphism with $|G_k : \operatorname{Ker}\phi| = 10$. By Proposition 6 $\phi(G_k) \simeq R_{10}$ and by Proposition 5 we can easily see:

$$\{H^{(5)}_{B_0B_1B_2}(R_{10})|\ B_1, B_2 \text{ is a partition of the set } N_k \setminus B_0\} \subset \{H|\ |G_k : H| = 10\}.$$

Let $\varphi : G_k \to R_{10}$ be epimorphisms. We denote:

$$B_0 = \{i|\ \varphi(a_i) = e\},\quad B_1 = \{i|\ \varphi(a_i) = a,\ B_2 = \{i|\ \varphi(a_i) = b\}.$$

Then, we can show this homomorphism (corresponding to $B_1,\ B_2,\ B_3$), i.e.,

$$\phi_{B_0B_1B_2}(x) = \begin{cases} e, \text{ if } \tilde{x} = e \\ a, \text{ if } \tilde{x} = b_1 \\ b, \text{ if } \tilde{x} = b_2 \\ a*b, \text{ if } \tilde{x} = b_1b_2 \\ b*a, \text{ if } \tilde{x} = b_2b_1 \\ a*b*a, \text{ if } \tilde{x} = b_1b_2b_1 \\ b*a*b, \text{ if } \tilde{x} = b_2b_1b_2 \\ a*b*a*b, \text{ if } \tilde{x} = b_1b_2b_1b_2 \\ b*a*b*a, \text{ if } \tilde{x} = b_2b_1b_2b_1 \\ a*b*a*b*a, \text{ if } \tilde{x} = b_1b_2b_1b_2b_1. \end{cases}$$

We have constructed all homomorphisms ϕ on the group G_k which $|G_k : \operatorname{Ker}\phi| = 10$. Hence:

$$\{\operatorname{Ker}\phi|\ |G_k : \operatorname{Ker}\phi| = 10\} \subset \{H^{(5)}_{B_0B_1B_2}(R_{10})|\ B_1, B_2 \text{ is a partition of the set } N_k \setminus B_0\}.$$

By Proposition 1:

$$\{H|\ |G_k : H| = 10\} = \{H^{(5)}_{B_0B_1B_2}(R_{10})|\ B_1, B_2 \text{ is a partition of the set } N_k \setminus B_0\}.$$

The theorem is proved. □

Corollary 2. *The number of all normal subgroups of index* 10 *for the group* G_k *is equal to* $3^{k+1} - 2^{k+2} + 1$.

Proof. The proof of this Corollary is similar to proof of Corollary 1. □

Acknowledgements

I am deeply grateful to Professor U. A. Rozikov for the attention to my work.

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NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2016, 7 (5), P. 893–899

Translation-invariant Gibbs measures for a model with logarithmic potential on a Cayley tree

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DOI 10.17586/2220-8054-2016-7-5-893-899

In this paper, we consider a model with logarithmical potential and with the set $[0,1]$ of spin values, on a Cayley tree Γ^k of the order k. In the case $k=2,3$, we shall prove that, there is a unique translation-invariant splitting Gibbs measure for this model. For the case $k=4$, we show that there are three translation-invariant Gibbs measures for this model.

Keywords: Cayley tree, configuration, translation-invariant Gibbs measure, fixed point, nonlinear operator.

Received: 15 April 2016. Revised: 25 May 2016.

1. Introduction

One of the central problems in the theory of Gibbs measures is to describe infinite-volume (or limiting) Gibbs measures corresponding to a Hamiltonian. The existence of such measures for a wide class of Hamiltonians was established in the ground-breaking work of Dobrushin. However, complete analysis of a set of limiting GMs for a specific Hamiltonian is quite often a difficult problem.

In [1,2,6,9–11,14–16] for several models on Cayley tree Γ^k with the order k, using the Markov random field theory, Gibbs measures are described. These papers are devoted to models with a *finite* set of spin values. In [8], the Potts model with a *countable* set of spin values on a Cayley tree Γ^k is considered and it was shown that the set of translation-invariant splitting Gibbs measures of the model contains at most one point, independently on parameters of the Potts model with countable set of spin values on the Cayley tree. This is a crucial difference from the models with a finite set of spin values, since those may have more than one translation-invariant Gibbs measure.

In [12], a Hamiltonian with an *uncountable* set (a set with continuum cardinality) of spin values (with the set $[0,1]$ of spin values) on a Cayley tree Γ^k is considered and it was shown that: the existence translation-invariant splitting Gibbs measure of the Hamiltonian is equivalent to the existence a positive fixed point of some nonlinear integral operator. For $k=1$, the model with the continuous potential function was shown to have a unique translation-invariant splitting Gibbs measure. In the case $k\geq 2$, some models which have the unique splitting Gibbs measure were constructed. In the paper [4], sufficient conditions were found for the potential function of the model on a Cayley tree Γ^k with an uncountable set of spin values under which the model had unique translation-invariant splitting Gibbs measure. In [3,5], several models were constructed, of which these models had at least two translational-invariant Gibbs measures, i.e the existence of phase transition for some models on a Cayley tree Γ^k $(k\geq 2)$ was proven.

This paper is a continuation of previous investigations [3–5,12]. We shall construct model with a logarithmic potential on a Cayley tree Γ^k. We reduced the studying of translation-invariant Gibbs measures to a description of the fixed points for some nonlinear operator on $\mathbb{R}^2$. In the case $k=2,3$, we shall prove that, for the Hamiltonian on a Cayley tree Γ^k with logarithmic potential, there is a unique translation-invariant splitting Gibbs measure. In the case $k=4$, we show that, for the model on Γ^4 with the logarithmic potential there are three translation-invariant Gibbs measures, i.e. there is a phase transition.

2. Preliminaries

A Cayley tree $\Gamma^k=(V,L)$ of order $k\in\mathbb{N}$ is an infinite homogeneous tree, i.e., a graph without cycles, with exactly $k+1$ edges incident to each vertex. Here, V is the set of vertices and L that of edges (arcs).

Consider models where the spin takes values in the set $[0,1]$, and is assigned to the vertices of the tree. For $A\subset V$, a configuration σ_A on A is an arbitrary function $\sigma_A: A\to[0,1]$. We denote $\Omega_A=[0,1]^A$ the set of all

configurations on A. A configuration σ on V is then defined as a function $x \in V \mapsto \sigma(x) \in [0,1]$; the set of all configurations is $[0,1]^V$. The Hamiltonian of the model is :

$$H(\sigma) = -J \sum_{\langle x,y\rangle \in L} \xi_{\sigma(x),\sigma(y)}, \quad \sigma \in \Omega_V, \tag{2.1}$$

where $J \in \mathbb{R} \setminus \{0\}$ and $\xi : (u,v) \in [0,1]^2 \to \xi_{uv} \in \mathbb{R}$ is a given bounded, measurable function. As usual, $\langle x,y\rangle$ represents the nearest neighbor vertices.

Let λ be the Lebesgue measure on $[0,1]$. On the set of all configurations on A, the *a priori* measure λ_A is introduced as the $|A|$ fold product of the measure λ. Here and subsequently, $|A|$ denotes the cardinality of A. Below, W_m represents a 'sphere' and V_m for a 'ball' on the tree, of radius $m = 1,2,\ldots$, centered at a fixed vertex x^0 (an origin):

$$W_m = \{x \in V : d(x,x^0) = m\}, \;\; V_m = \{x \in V : d(x,x^0) \le m\};$$

and

$$L_m = \{\langle x,y\rangle \in L : x,y \in V_m\}.$$

Here, distance $d(x,y)$, $x,y \in V$, is the length of (i.e. the number of edges in) the shortest path connecting x with y. Ω_{V_n} is the set of configurations in V_n (and Ω_{W_n} that in W_n; see below). Furthermore, $\sigma\big|_{V_n}$ and $\omega\big|_{W_{n+1}}$ denote the restrictions of configurations $\sigma,\omega \in \Omega$ to V_n and W_{n+1}, respectively. Next, $\sigma_n :\; x \in V_n \mapsto \sigma_n(x)$ is a configuration in V_n. For each $\sigma_n \in \Omega_{V_n}$, we define:

$$H(\sigma_n) = -J \sum_{\langle x,y\rangle \in L_n} \xi_{\sigma_n(x),\sigma_n(y)}.$$

We write $x < y$ if the path from x^0 to y goes through x. Call vertex y a direct successor of x if $y > x$ and x,y are nearest neighbors. We denote by $S(x)$ the set of direct successors of x. We observe that any vertex $x \ne x^0$ has k direct successors and x^0 has $k+1$.

Let $h :\; x \in V \mapsto h_x = (h_{t,x}, t \in [0,1]) \in R^{[0,1]}$ be mapping of $x \in V \setminus \{x^0\}$. Given $n = 1,2,\ldots$, consider the probability distribution $\mu^{(n)}$ on Ω_{V_n} defined by

$$\mu^{(n)}(\sigma_n) = Z_n^{-1} \exp\left(-\beta H(\sigma_n) + \sum_{x \in W_n} h_{\sigma(x),x}\right), \tag{2.2}$$

where $\beta = \dfrac{1}{T}$, $T > 0$ is temperature. Here, as before, $\sigma_n : x \in V_n \mapsto \sigma(x)$ and Z_n is the corresponding partition function:

$$Z_n = \int\limits_{\Omega_{V_n}} \exp\left(-\beta H(\widetilde{\sigma}_n) + \sum_{x \in W_n} h_{\widetilde{\sigma}(x),x}\right) \lambda_{V_n}(d\widetilde{\sigma}_n). \tag{2.3}$$

The probability distributions $\mu^{(n)}$ are compatible [12] if for any $n \ge 1$ and $\sigma_{n-1} \in \Omega_{V_{n-1}}$:

$$\int\limits_{\Omega_{W_n}} \mu^{(n)}(\sigma_{n-1} \vee \omega_n) \lambda_{W_n}(d(\omega_n)) = \mu^{(n-1)}(\sigma_{n-1}). \tag{2.4}$$

Here, $\sigma_{n-1} \vee \omega_n \in \Omega_{V_n}$ is the concatenation of σ_{n-1} and ω_n. In this case, there exists [12] a unique measure μ on Ω_V such that, for any n and $\sigma_n \in \Omega_{V_n}$, $\mu\left(\left\{\sigma\big|_{V_n} = \sigma_n\right\}\right) = \mu^{(n)}(\sigma_n)$.

The measure μ is called the *splitting Gibbs measure* corresponding to Hamiltonian (2.1) and function $x \mapsto h_x$, $x \ne x^0$.

Proposition 2.1. *[12] The probability distributions $\mu^{(n)}(\sigma_n)$, $n = 1,2,\ldots$, in (2.2) are compatible iff for any $x \in V \setminus \{x^0\}$ the following equality holds:*

$$f(t,x) = \prod_{y \in S(x)} \frac{\int_0^1 \exp(J\beta\xi_{tu}) f(u,y)du}{\int_0^1 \exp(J\beta\xi_{0u}) f(u,y)du}. \tag{2.5}$$

Here, and below $f(t,x) = \exp(h_{t,x} - h_{0,x})$, $t \in [0,1]$ and $du = \lambda(du)$ is the Lebesgue measure.

From Proposition 2.1, it follows that for any $h = \{h_x \in R^{[0,1]}, \ \ x \in V\}$ satisfying (2.5) there exists a unique Gibbs measure μ and vice versa. However, the analysis of solutions to (2.5) is not easy. Let ξ_{tu} be a continuous function. We put

$$C^+[0,1] = \{f \in C[0,1] : f(x) \geq 0\}, \quad C_0^+[0,1] = C^+[0,1] \setminus \{\theta \equiv 0\}.$$

We define the operator $R_k : C_0^+[0,1] \to C_0^+[0,1]$ by

$$(R_k f)(t) = \left(\frac{\int_0^1 K(t,u) f(u) du}{\int_0^1 K(0,u) f(u) du} \right)^k, \ \ k \in \mathbb{N},$$

where $K(t,u) = \exp(J\beta\xi_{tu})$, $f(t) > 0$, $t, u \in [0,1]$.

We will solve the equation (2.5) in the class of translational-invariant functions $f(t,x)$, i.e $f(t,x) = f(t)$ for any $x \in V$. For such functions, equation (2.5) can be written as:

$$R_k(f)(t) = f(t). \tag{2.6}$$

Note that equation (2.6) is not linear for any $k \in \mathbb{N}$. For every $k \in \mathbb{N}$ we consider Hammerstein's integral operator H_k acting in the cone $C^+[0,1]$ as

$$(H_k f)(t) = \int_0^1 K(t,u) f^k(u) du, \quad k \in \mathbb{N}.$$

We denote

$$\mathcal{M}_0 = \{f \in C^+[0,1] : \quad f(0) = 1\}.$$

Lemma 2.2. *[4] Let $k \geq 2$. The equation*

$$R_k f = f, \ \ f \in C_0^+[0,1] \tag{2.7}$$

has a nontrivial positive solution iff the Hammerstein's equation

$$H_k f = \lambda f, \ \ f \in C^+[0,1] \tag{2.8}$$

has a positive solution in $\mathcal{M}_0$ for some $\lambda > 0$.

Let $k \geq 2$. Then, we can easily verify that: if the number $\lambda_0 > 0$ is eigenvalue of the operator H_k, then an arbitrary positive number is an eigenvalue of the operator H_k (see [4]). Consequently, we obtain:

Lemma 2.3. *Let $k \geq 2$. The equation (2.7) has a nontrivial positive solution iff the Hammerstein's operator H_k has a nontrivial positive fixed point. Moreover, the number of nontrivial positive fixed points of the operator R_k is equal to the number of nontrivial positive fixed points of the Hammerstein's operator H_k.*

Note, that if there is more than one nontrivial positive fixed point for the the Hammerstein's operator, H_k, then there is more than one translation-invariant Gibbs measure for the model (2.1) corresponding to these fixed points. We say that a phase transition occurs for the model (2.1), if the Hammerstein's operator H_k has more than one nontrivial positive fixed point. The number of the fixed points depends on the parameters of the model (2.1) and the order of Cayley tree Γ^k.

3. A model on Cayley tree with logarithmic potential

We consider Hamiltonian H on the Cayley tree Γ^k by rule:

$$H(\sigma) = -\sum_{\langle x,y \rangle \in L} \frac{\ln\left(1 + 4\theta\left(\sigma(x) - \frac{1}{2}\right)\left(\sigma(y) - \frac{1}{2}\right)\right)}{\beta}, \ \ \sigma \in \Omega_V, \tag{3.1}$$

where θ is a coupling constant and $0 < \theta < 1$, i.e. in the (2.1) function of potential is defined by the formula:

$$\xi_{t,u} = \frac{\ln\left(1 + 4\theta\left(t - \frac{1}{2}\right)\left(u - \frac{1}{2}\right)\right)}{J\beta}.$$

The main aim of this paper is to study translation-invariant Gibbs measures for model (3.1) on the Cayley tree Γ^k. We define Hammerstein's operator H_k on $C[0,1]$ by the equality:

$$(H_k f)(t) = \int_0^1 \left(1 + 4\theta\left(t - \frac{1}{2}\right)\left(u - \frac{1}{2}\right)\right) f^k(u) du. \tag{3.2}$$

We set:

$$k_1 = \begin{cases} k, & \text{if } k \text{ is even,} \\ k-1, & \text{if } k \text{ is odd,} \end{cases}$$

and

$$k_2 = \begin{cases} k, & \text{if } k \text{ is odd,} \\ k-1, & \text{if } k \text{ is even.} \end{cases}$$

We define operator P on $\mathbb{R}^2$ by the rule:

$$P(x,y) \to (x',y'),$$

where

$$x' = \sum_{j=0}^{k_1/2} \frac{(2\theta)^{2j}}{2j+1} A_k^{2j} x^{k-2j} y^{2j},$$

$$y' = \sum_{j=1}^{(k_2+1)/2} \frac{(2\theta)^{2j-1}}{2(2j+1)} A_k^{2j-1} x^{k-2j+1} y^{2j-1}.$$

Here

$$A_n^m = \frac{n!}{m!(n-m)!}.$$

Lemma 3.1. *Let $k \geq 2$. The Hammerstein's operator H_k (3.2) has a nontrivial positive fixed point iff the operator P has a fixed point (x_0, y_0), such that $x_0 > 0$ and $f_0(t) = x_0 + 4\theta y_0 \left(t - \frac{1}{2}\right) > 0$ for all $t \in [0,1]$, moreover the function $f_0(t) = x_0 + 4\theta y_0 \left(t - \frac{1}{2}\right)$ is a positive fixed point of the Hammerstein's operator H_k.*

Proof. Necessity. We set:

$$c_1 = \int_0^1 f^k(u)du \tag{3.3}$$

and

$$c_2 = \int_0^1 \left(u - \frac{1}{2}\right) f^k(u)du. \tag{3.4}$$

It is clear, that $c_1 > 0$. Let the Hammerstein's operator H_k (3.2) has a positive fixed point $f(t)$. Then, for the function $f(t)$, the equality:

$$f(t) = c_1 + 4\theta c_2 \left(t - \frac{1}{2}\right) \tag{3.5}$$

is holds.

Consequently, for the parameter c_1, from the equality (3.3), we have:

$$c_1 = \int_0^1 \left(c_1 + 4\theta c_2 \left(u - \frac{1}{2}\right)\right)^k du = \sum_{j=0}^{k} A_k^j c_1^{k-j} (4\theta c_2)^j \int_0^1 \left(u - \frac{1}{2}\right)^j du =$$

$$= \sum_{j=0}^{k} A_k^j c_1^{k-j} (4\theta c_2)^j \int_{-1/2}^{1/2} u^j du = \sum_{j=0}^{k_1/2} \frac{(2\theta)^{2j}}{2j+1} A_k^{2j} c_1^{k-2j} c_2^{2j}.$$

Analogously, for the parameter c_2, by equality (3.4), we get:

$$c_2 = \int_0^1 \left(u - \frac{1}{2}\right)\left(c_1 + 4\theta c_2 \left(u - \frac{1}{2}\right)\right)^k du = \sum_{j=0}^{k} A_k^j c_1^{k-j} (4\theta c_2)^j \int_0^1 \left(u - \frac{1}{2}\right)^{j+1} du$$

$$= \sum_{j=0}^{k} A_k^j c_1^{k-j} (4\theta c_2)^j \int_{-1/2}^{1/2} u^{j+1} du = \sum_{j=1}^{(k_2+1)/2} \frac{(2\theta)^{2j-1}}{2j+1} A_k^{2j-1} c_1^{k-2j+1} c_2^{2j-1}.$$

Therefore, the point (c_1, c_2) is a fixed point of the operator P.

Sufficiency. We assume that $x_0 > 0$ and the point (x_0, y_0) is a fixed point of the operator P, i.e. the following equalities for numbers x_0 and y_0 numbers are satisfied:

$$\sum_{j=0}^{k_1/2} \frac{(2\theta)^{2j}}{2j+1} A_k^{2j} x_0^{k-2j} y_0^{2j} = x_0, \qquad \sum_{j=1}^{(k_2+1)/2} \frac{(2\theta)^{2j-1}}{2(2j+1)} A_k^{2j-1} x_0^{k-2j+1} y_0^{2j-1} = y_0.$$

We can simply prove that the function $f_0(t) = x_0 + 4\theta y_0 \left(t - \frac{1}{2}\right)$ is a fixed point of the Hammerstein's operator H_k, i.e. $H_k f_0 = f_0$. This completes the proof. □

Proposition 3.2. *For each $k \in \mathbb{N}$, the function $f_0(t) \equiv 1$ is a fixed point of the Hammerstein's operator H_k.*

Proof. One can clearly see that:

$$(H_k)f_0(t) = \int_0^1 \left(1 + 4\theta \left(t - \frac{1}{2}\right)\left(u - \frac{1}{2}\right)\right) du == \int_0^1 du + 4\theta \left(t - \frac{1}{2}\right) \int_{-1/2}^{1/2} u du = 1 = f_0(t).$$

□

4. Uniqueness of translation-invariant Gibbs measures for the model (3.1)

In [12], a Hamiltonian with an *uncountable* set of spin values (with the set $[0, 1]$ of spin values) on the Cayley tree Γ^k was considered for a continuous potential $\xi_{t,u}$. For $k = 1$, it was shown that the model (2.1) with the continuous potential function has a unique translation-invariant splitting Gibbs measure. This statement holds for the model (3.1). We study translation-invariant splitting Gibbs measure for the model (3.1) for the case $k \geq 2$.

Theorem 4.1. *The model H (3.1) on the Cayley tree of order two has a unique translation-invariant Gibbs measure.*

Proof. Let be $k = 2$. Then, the operator P assumes the following simple form:

$$P(x, y) = \left(x^2 + \frac{4}{3}y^2, \ \frac{2}{3}\theta xy\right).$$

For a fixed point (x, y) of the operator P, we have the following system of algebraic equations:

$$\begin{cases} x^2 + \frac{4}{3}y^2 = x, \\ \frac{2}{3}\theta xy = y. \end{cases}$$

It follows that, the operator P has a unique nontrivial fixed point $(1, 0)$, as $\theta \in (0, 1)$. By lemma 3.1, the Hammerstein's operator H_2 has a unique nontrivial positive fixed point $f_0(t) \equiv 1$. Therefore, by lemma 2.3, the model H (3.1) on the Cayley tree of order two has a unique translation-invariant Gibbs measure. □

Theorem 4.2. *The model H (3.1) on the Cayley tree of order three has the unique translation-invariant Gibbs measure.*

Proof. Let $k = 3$. Then, the operator P assumes the following form:

$$P(x, y) = \left(x^3 + 4\theta^2 xy^2, \ \theta x^2 y + \frac{4}{5}\theta^3 y^3\right).$$

For a fixed point (x, y) of the operator P, we have the following system of algebraic equations:

$$\begin{cases} x^3 + 4\theta^2 xy^2 = x, \\ \theta x^2 y + \frac{4}{5}\theta^3 y^3 = y. \end{cases}$$

It follows that, the point $(1, 0)$ is a fixed point of the operator P. Consequently, by lemma 3.1, the function $f_0(t) \equiv 1$ is a fixed point of the Hammerstein's operator H_3. Conversely, for the case $x > 0$, $y \neq 0$, the last system of algebraic equations is equivalent to the following system of algebraic equations:

$$\begin{cases} x^2 + 4\theta^2 y^2 = 1, \\ \theta x^2 + \frac{4}{5}\theta^3 y^2 = 1. \end{cases}$$

We find $x^2 = 1 - 4\theta^2 y^2$. Hence, for y, we have:

$$\left(1 - 4\theta^2 y^2\right)\theta + \frac{4}{5}\theta^3 y^2 = 1,$$

i.e.

$$y^2 = \frac{5(\theta - 1)}{16\theta^3}.$$

This is impossible, as $\theta \in (0, 1)$.

Thus, the operator P has a unique nontrivial fixed point $(1, 0)$. Therefore, by lemmas 3.1 and 2.3, the model H (3.1) on the Cayley tree of order three has a unique translation-invariant Gibbs measure. □

5. A phase transition for the model (3.1)

In this section, we consider the model (3.1) on the Cayley tree Γ^4. In the case $k = 4$, the operator P is acting on $\mathbb{R}^2$ by the rule:

$$P(x, y) = \left(x^4 + 8\theta^2 x^2 y^2 + \frac{16}{5}\theta^4 y^4,\ \ \frac{4}{3}\theta x^3 y + \frac{16}{5}\theta^3 x y^3\right).$$

Theorem 5.1. *Let $k = 4$. Then:*

(a) for all $\theta \in (0, 3/4]$ the model H (3.1) on the Cayley tree Γ^k has a unique translation-invariant Gibbs measure;

(b) for all $\theta \in (3/4, 1)$ the model H (3.1) on the Cayley tree Γ^k has three translation-invariant Gibbs measures.

Proof. Let $k = 4$. For a fixed point (x, y) of the operator P, we have the following system of algebraic equations:

$$\begin{cases} x^4 + 8\theta^2 x^2 y^2 + \dfrac{16}{5}\theta^4 y^4 = x, \\ \dfrac{4}{3}\theta x^3 y + \dfrac{16}{5}\theta^3 x y^3 = y. \end{cases}$$

In the case $x > 0$, $y = 0$, the above system of algebraic equations has the solution $(1, 0)$. We assume that $y \neq 0$. Then, we have $x \neq 0$ and from the second equation of the last system of equations, we obtain:

$$y^2 = \frac{5(3 - 4\theta x^3)}{48\theta^3 x}. \tag{5.1}$$

This means that:

$$0 < x < \sqrt[3]{\frac{3}{4\theta}}. \tag{5.2}$$

From the first equation of the system of equations, for a fixed point of the operator P, we obtain:

$$\frac{16}{9}x^6 + \frac{3\theta - 5}{3\theta}x^3 - \frac{5}{16\theta^2} = 0. \tag{5.3}$$

We set $z = x^3$. Then, $z > 0$ and for the unknown variable z, by the equality (5.3), we have the quadratic equation:

$$\frac{16}{9}z^2 + \frac{3\theta - 5}{3\theta}z - \frac{5}{16\theta^2} = 0. \tag{5.4}$$

One clearly sees that equation (5.4) has two roots:

$$z_1 = z_1(\theta) = \frac{-1 + \frac{5}{3\theta} - \sqrt{D}}{\frac{32}{9}} < 0, \quad z_2 = z_2(\theta) = \frac{-1 + \frac{5}{3\theta} + \sqrt{D}}{\frac{32}{9}} > 0,$$

where

$$D = D(\theta) = \left(1 - \frac{5}{3\theta}\right)^2 + \frac{20}{9\theta^2}.$$

Therefore, for x, by the lemma 3.1 and the inequality (5.2), we obtain $x = x_1 = x_1(\theta)$, where

$$x_1(\theta) = \sqrt[3]{z_2(\theta)} < \sqrt[3]{\frac{3}{4\theta}}.$$

The question then arises: does the inequality (5.2) hold for $x_1(\theta)$ for all values of the parameter $\theta \in (0,1)$? To this end, we consider the inequality $x_1(\theta) < \sqrt[3]{\frac{3}{4\theta}}$. This is equivalent to the inequality:

$$\frac{-1+\frac{5}{3\theta}+\sqrt{D}}{\frac{32}{9}} < \sqrt[3]{\frac{3}{4\theta}}. \tag{5.5}$$

Hence, it follows that $\sqrt{D} < 1+\frac{1}{\theta}$. It means

$$\left(1-\frac{5}{3\theta}\right)^2+\frac{20}{9\theta^2} < \left(1+\frac{1}{\theta}\right)^2.$$

From the last inequality, we get $\theta > \frac{3}{4}$. Thus, for the case $\frac{3}{4} < \theta < 1$, by equality (5.1), the operator P has three fixed points:

$$(1,0), \quad (x_1(\theta), y_1(\theta)), \quad (x_1(\theta), -y_1(\theta)),$$

where

$$y_1(\theta) = \frac{1}{4\theta}\sqrt{\frac{5(3-4\theta x_1^3(\theta))}{3\theta x_1(\theta)}} > 0.$$

We note that if $0 < \theta \le \frac{3}{4}$, then the operator P has a unique fixed point: $(1,0)$. Consequently, by lemmas 2.3 and 3.1, for all $\theta \in \left(0, \frac{3}{4}\right]$ the model H (3.1) on the Cayley tree Γ^4 has a unique translation-invariant Gibbs measure. In the case $\frac{3}{4} < \theta < 1$ by the lemma 3.1, the Hammerstein's operator H_4 has three positive fixed points:

$$f_0(t) \equiv 1, \quad f_1(t) = x_1(\theta) + 4\theta y_1(\theta)\left(t-\frac{1}{2}\right), \quad f_2(t) = x_1(\theta) - 4\theta y_1(\theta)\left(t-\frac{1}{2}\right).$$

Because $f_i(t) > 0$ for all $t \in [0,1]$, where $i = 1,2$. Therefore, By lemma 2.3 for all $\theta \in (3/4, 1)$ the model H (3.1) on the Cayley tree Γ^4 has three translation-invariant Gibbs measures. This completes the proof. □

Finally we note that in the case $\theta \in \left(\frac{3}{4}, 1\right)$ for the model H (3.1) on the Cayley tree Γ^4 there is a phase transition.

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(свидетельство ПИ № ФС 77 - 49048 от 22.03.2012 г.)
ISSN 2220-8054

Учредитель: федеральное государственное автономное образовательное учреждение высшего образования
«Санкт-Петербургский национальный исследовательский университет информационных технологий, механики и оптики»

Издатель: федеральное государственное автономное образовательное учреждение высшего образования
«Санкт-Петербургский национальный исследовательский университет информационных технологий, механики и оптики»

Отпечатано в Учреждении «Университетские телекоммуникации»
Адрес: 197101, Санкт-Петербург, Кронверкский пр., 49

Подписка на журнал НФХМ
На первое полугодие 2017 года подписка осуществляется через
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