

Threshold resonances and discrete spectrum of a two-boson hamiltonian with a molecular channel on the one-dimensional lattice

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ABSTRACT We study a two-channel lattice Hamiltonian in a fixed particle-number sector on the one-dimensional lattice $\mathbb{Z}$. The model consists of a molecular channel coupled to a bosonic two-particle channel with on-site interaction. In the momentum representation, translation invariance yields a family of reduced Hamiltonians $H_{\gamma,\lambda}(K)$ parametrized by total quasi-momentum $K \in \mathbb{T}$, each acting in $\mathbb{C} \oplus L^{2,e}(\mathbb{T})$.

For contact interactions, each reduced Hamiltonian is a rank-two perturbation of the free diagonal operator. By means of the Lippmann–Schwinger method, the eigenvalue problem for energies outside the essential spectrum $[\mathcal{E}_K^-, \mathcal{E}_K^+]$ is reduced to a 2×2 linear system and, equivalently, to the vanishing of an explicit scalar Fredholm determinant involving the one-dimensional lattice Green function. The square-root singularities of this Green function at the band edges $\mathcal{E}_K^\pm$ determine the threshold asymptotics of the determinant and lead to explicit criteria for the existence of eigenvalues below the lower threshold and above the upper threshold.

We obtain a complete classification of the discrete spectrum of $H_{\gamma,\lambda}(K)$ for all quasi-momenta in terms of the parameters γ , λ , and E_0 . We also analyze the threshold configurations $E_0 = \mathcal{E}_K^\pm$, the exceptional flat-band fiber $K = \pi$, where the essential spectrum collapses to a single point, and the threshold states of the auxiliary rank-one operator $\mathbf{h}_\lambda(K)$. For the latter, we provide a weighted-space description of threshold resonances, clarifying how an eigenvalue emerges from a threshold resonance of $\mathbf{h}_\lambda(K)$ and approaches a band edge when the interchannel coupling is switched on.

KEYWORDS Lattice Hamiltonian, two-channel model, fixed particle-number sector, Fredholm determinant, Lippmann–Schwinger equation, discrete spectrum, threshold asymptotics, threshold resonance.

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1. Introduction

1.1. Background and motivation

The spectral theory of lattice hamiltonians for interacting quantum particles has been studied intensively for several decades, beginning with the works [1, 2]; see also [3–5] and the monographs [6, 7]. The works of Mogilner [2, 5] established the basic spectral properties of multiparticle discrete Schrödinger operators on lattices, including the structure of the essential spectrum and the existence of bound states for systems of three identical bosons. His review [2] systematically formulated the N -particle lattice problem as a theory of bounded operators and outlined a number of open problems that have subsequently stimulated intensive research. Unlike continuum Schrödinger operators, lattice hamiltonians have bounded dispersion relations and are naturally formulated on the Brillouin zone $\mathbb{T}^d$. Consequently, their essential spectra are compact, and their threshold behavior differs substantially from that of continuum models. Important examples arise from few-particle sectors of Bose–Hubbard models, which lead to discrete Schrödinger operators with short-range interactions; see, for example, [8–11]. In one dimension, the corresponding Green functions exhibit square-root singularities at the band edges, making this setting especially suitable for the explicit analysis of threshold resonances, virtual levels, and bound states.

Lattice models are widely used in mathematical physics. One such model is the lattice N -body hamiltonian [1] that represents a minimalist version of the corresponding Bose– or Fermi–Hubbard models involving just N particles of a certain type. The lattice N -body hamiltonians are of great interest even for $1 \leq N \leq 3$ and the respective lattice N -particle problems have been intensively studied over the past several decades [8, 12, 13]. An additional reason to study such hamiltonians is that, in fact, they serve as a natural discrete approximation of the continuous N -body Schrödinger operators. Setting down the N -body problem on a lattice allows one to study it in the context of the theory of bounded

operators. Notice that the one-particle 1D lattice case is essentially covered by the general perturbation theory for infinite Jacobi matrices (see, e.g., [14, 15]).

The lattice N -body Schrödinger operators also serve as a model for systems formed by N particles traveling through periodic structures, e.g. for ultracold atoms injected into optical crystals [16]. In the last decades, the study of ultracold few-atom systems in optical lattices has become of particular interest due to the availability of controllable parameters such as temperature, particle masses, and interaction potentials (see e.g. [16] and references therein).

Such models provide natural testbeds for finite-rank perturbation methods, Fredholm determinant techniques, and threshold singularity analysis, which are central themes in mathematical physics. The present paper fits into this circle of ideas. We study a two-channel lattice model for two identical bosons coupled to an internal molecular mode. The model is considered as a coupled two-channel hamiltonian in a fixed particle-number sector. Our main goal is to give a complete description of the discrete spectrum of the associated reduced hamiltonians, to analyze their threshold behavior, and to identify the mechanisms of bound-state formation.

1.2. The model

We consider two identical spinless bosons on $\mathbb{Z}$ with on-site interaction strength $\lambda \in \mathbb{R}$, coupled to a molecular channel of internal energy $E_0 \in \mathbb{R}$. The interchannel coupling is governed by $\gamma \in \mathbb{R}$. After the Fourier transform and the Floquet–Bloch decomposition, translation invariance yields a direct-integral decomposition with respect to the total quasi-momentum $K \in \mathbb{T}$. The corresponding reduced hamiltonians are denoted by $H_{\gamma,\lambda}(K)$, $K \in \mathbb{T}$, and act in the fiber Hilbert spaces $\mathcal{H}_K = \mathbb{C} \oplus L^{2,e}(\mathbb{T})$, where $\mathbb{C}$ represents the molecular channel in the fiber and $L^{2,e}(\mathbb{T})$ denotes the subspace of even functions in the two-boson channel.

For contact interactions, the perturbation of the free reduced hamiltonian has rank at most two: one rank-one term is generated by the on-site interaction, and the other by the molecular coupling. Thus the analysis reduces to the fiber operators $H_{\gamma,\lambda}(K)$. The eigenvalue problem outside the essential spectrum reduces, by the Lippmann–Schwinger method [17], to a 2×2 linear system and, equivalently, to a scalar Fredholm determinant. Alongside $H_{\gamma,\lambda}(K)$, the auxiliary rank-one fiber operator $\mathbf{h}_\lambda(K)$, acting in the bosonic channel alone, provides useful information on how isolated eigenvalues approach the band edges.

1.3. Main results

- (i) **Reduced hamiltonians and essential spectrum.** For fixed $K \in \mathbb{T}$, the essential spectrum of $H_{\gamma,\lambda}(K)$ equals the range of the free two-particle dispersion

$$\varepsilon_K(p) = 4 \left(1 - \cos \frac{K}{2} \cos p \right),$$

namely,

$$\sigma_{\text{ess}}(H_{\gamma,\lambda}(K)) = [\mathcal{E}_K^-, \mathcal{E}_K^+], \quad \mathcal{E}_K^\pm = 4 \left(1 \pm \left| \cos \frac{K}{2} \right| \right). \quad (1)$$

The fiber $K = \pi$ is exceptional: the dispersion is flat, and the essential spectrum collapses to the singleton $\{4\}$.

- (ii) **Lippmann–Schwinger reduction.** For

$$z \notin [\mathcal{E}_K^-, \mathcal{E}_K^+],$$

the eigenvalue problem reduces to a scalar equation

$$\Delta_{\gamma,\lambda}(K; z) = 0, \quad (2)$$

where $\Delta_{\gamma,\lambda}(K; z)$ is an explicit Fredholm determinant involving the one-dimensional lattice Green function

$$a_K(z) = \frac{1}{2\pi} \int_0^{2\pi} \frac{dp}{\varepsilon_K(p) - z}. \quad (3)$$

Thus the discrete spectrum outside the essential band is completely determined by zeros of a single scalar function.

- (iii) **Threshold analysis and bound-state classification.** The square-root singularities of $a_K(z)$ at the band edges $\mathcal{E}_K^\pm$ give asymptotic expansions of $\Delta_{\gamma,\lambda}(K; z)$ near the thresholds. The leading coefficients provide criteria for the existence of eigenvalues below the lower threshold and above the upper threshold. This yields a complete classification of the discrete spectrum in terms of γ , λ , E_0 , and the position of E_0 relative to $[\mathcal{E}_K^-, \mathcal{E}_K^+]$.
- (iv) **Decoupled case, threshold configurations, and flat band.** The decoupled case $\gamma = 0$ serves as a reference case. It shows how new spectral phenomena, such as the creation, displacement, or disappearance of eigenvalues near the band edges, emerge when γ is switched on. This is especially relevant for the threshold configurations

$$E_0 = \mathcal{E}_K^- \quad \text{or} \quad E_0 = \mathcal{E}_K^+,$$

where virtual-level behavior may occur. For the flat fiber $K = \pi$, the spectral problem reduces to an explicit quadratic equation, giving a closed-form description of the discrete spectrum.

- (v) **Threshold states of the auxiliary rank-one operator.** For $\mathbf{h}_\lambda(K)$, we introduce weighted threshold spaces adapted to the singular behavior at the band edges and classify its threshold states. This yields a weighted-space description of threshold resonances and clarifies how threshold profiles transform into genuine eigenvalues outside the essential spectrum when γ is perturbed away from zero. In this way, the analysis of $\mathbf{h}_\lambda(K)$ complements the decoupled case and explains the emergence of new spectral effects in the coupled model.

Taken together, these results provide a complete explicit spectral analysis of the reduced hamiltonians $H_{\gamma,\lambda}(K)$ in the one-dimensional contact-interaction regime, together with a detailed description of threshold behaviour for the associated rank-one fiber operators.

1.4. Relation to previous works

We begin by recalling the well-known connection between one-dimensional lattice operators, Jacobi matrices, and the theory of orthogonal polynomials. Comprehensive treatments appear in the monographs by Simon [18–20]. Related results for discrete one-dimensional Schrödinger and Jacobi operators, including spectral and perturbative aspects, can be found in, e.g., the work of Damanik, Hundertmark, Killip, and Simon [21].

Another relevant direction concerns one-dimensional lattice models whose spectral problem admits explicit or semi-explicit analysis. In this context, the approach developed in [22, 23] provides a useful point of comparison for the study of bound states in one-dimensional lattice hamiltonians. The present paper is also conceptually related to the theory of threshold states and virtual levels. We particularly refer to Yafaev’s foundational work on virtual levels for the three-dimensional continuous Schrödinger equation [24]. Although Yafaev’s setting is continuous and three-dimensional, whereas our model is discrete and one-dimensional, the functional-analytic idea of describing a virtual level as a non-square-integrable threshold solution in a suitable weighted space is relevant for our threshold analysis below.

Our work is most directly connected to the spectral theory of two-particle lattice hamiltonians and Bose–Hubbard type models, especially results concerning threshold effects, discrete spectra, and resonant phenomena on lattices [8, 10–13, 25, 26]. Recent studies of lattice Schrödinger operators with short-range and nearest-neighbor interactions have revealed a rich spectral structure, notably the appearance of isolated eigenvalues and threshold phenomena [27, 28]. These results provide further motivation for investigating the coupled-channel lattice hamiltonians considered in the present work. In contrast to these works, the novel feature of the present model is the inclusion of an additional molecular channel with purely on-site interactions in one dimension, together with a systematic analysis of resonances on such lattices. This structure yields a transparent block-operator formulation and reduces the spectral problem to a scalar Birman–Schwinger equation, or equivalently, to a Fredholm determinant equation.

The methods employed here are also related to rank-one and finite-rank perturbation techniques for solvable quantum models [6, 7]. In our setting, the effective finite-rank structure makes it possible to combine the Lippmann–Schwinger reduction with explicit one-dimensional lattice Green functions. This yields a complete characterization of the discrete spectrum, threshold configurations, and resonant phenomena for all values of the model parameters.

1.5. Organization

Section 2 introduces the model in the quasi-momentum representation, performs the fiber decomposition, and defines the reduced hamiltonians $H_{\gamma,\lambda}(K)$. Section 3 presents the Lippmann–Schwinger reduction and the scalar Fredholm determinant. Section 4 classifies the discrete spectrum of $H_{\gamma,\lambda}(K)$, including threshold configurations and the flat-band fiber. Section 5 studies threshold states of the auxiliary rank-one fiber operator $\mathbf{h}_\lambda(K)$.

2. The reduced hamiltonian at fixed total quasi-momentum

In this section, we study the reduced hamiltonians $H_{\gamma,\lambda}(K)$ corresponding to fixed total quasi-momentum $K \in \mathbb{T}$. In the constant-profile case $\alpha \equiv 1$, both the contact interaction in the two-particle channel and the interchannel coupling are generated by the constant mode

$$\varphi_0(p) = 1, \quad \forall p \in \mathbb{T}.$$

We will only need this definition; from now on we work directly with the constant function 1 and do not refer to φ_0 again. As a consequence, the perturbation of the free reduced hamiltonian is of rank at most two. In particular, the eigenvalue problem outside the essential spectrum can be reduced to a 2×2 linear system and, equivalently, to the vanishing of a scalar Fredholm determinant.

For each fixed $K \in \mathbb{T}$, the reduced hamiltonian is defined by

$$H_{\gamma,\lambda}(K) = \begin{pmatrix} E_0 & C_\gamma^* \\ C_\gamma & H_0(K) + \lambda P_0 \end{pmatrix} \quad (4)$$

in the Hilbert space

$$\mathcal{H}_K := \mathbb{C} \oplus L^{2,e}(\mathbb{T}).$$

Here $E_0 \in \mathbb{R}$ is the molecular-channel energy,

$$(H_0(K)g)(p) = \varepsilon_K(p) g(p), \quad g \in L^{2,e}(\mathbb{T}), \quad (5)$$

and the fiber dispersion relation is given by

$$\varepsilon_K(p) = \varepsilon\left(\frac{K}{2} - p\right) + \varepsilon\left(\frac{K}{2} + p\right) = 4\left(1 - \cos \frac{K}{2} \cos p\right). \quad (6)$$

Furthermore, P_0 denotes the orthogonal projection onto the one-dimensional subspace spanned by the constant function 1, that is,

$$P_0 g = (g, 1) 1, \quad (g, 1) = \int_{\mathbb{T}} g(p) d\nu(p), \quad (7)$$

where the Haar measure on $\mathbb{T}$ is normalized, so $\|1\|_{L^2} = 1$.

Because the coupling profile is constant, the interchannel coupling operator does not depend on K . More precisely,

$$(C_\gamma c)(p) = \gamma c, \quad c \in \mathbb{C}, \quad (8)$$

i.e. $C_\gamma c$ is the constant function equal to γc . Its adjoint is given by

$$C_\gamma^* g = \gamma \int_{\mathbb{T}} g(p) d\nu(p) = \gamma (g, 1), \quad g \in L^{2,e}(\mathbb{T}). \quad (9)$$

Hence $H_{\gamma,\lambda}(K)$ is a bounded self-adjoint operator on $\mathcal{H}_K$.

We next determine its essential spectrum.

Proposition 1. *For every $K \in \mathbb{T}$, $\sigma_{\text{ess}}(H_{\gamma,\lambda}(K)) = \text{Ran } \varepsilon_K$.*

Proof. By (4), the operator $H_{\gamma,\lambda}(K)$ differs from

$$H_{\text{free}}(K) := \begin{pmatrix} E_0 & 0 \\ 0 & H_0(K) \end{pmatrix}$$

by the finite-rank perturbation

$$\begin{pmatrix} 0 & C_\gamma^* \\ C_\gamma & \lambda P_0 \end{pmatrix}.$$

Since the scalar part E_0 acts in a one-dimensional subspace, it can contribute only an isolated eigenvalue of finite multiplicity and therefore does not affect the essential spectrum. Hence, by Weyl's theorem, $\sigma_{\text{ess}}(H_{\gamma,\lambda}(K)) = \sigma_{\text{ess}}(H_0(K)) = \text{Ran } \varepsilon_K$. $\square$

2.1. The free resolvent and the finite-rank perturbation

Let

$$H_{\text{free}}(K) := \begin{pmatrix} E_0 & 0 \\ 0 & H_0(K) \end{pmatrix}, \quad V_{\gamma,\lambda} := H_{\gamma,\lambda}(K) - H_{\text{free}}(K). \quad (10)$$

Then

$$V_{\gamma,\lambda}(K) = \begin{pmatrix} 0 & C_\gamma^* \\ C_\gamma & \lambda P_0 \end{pmatrix}. \quad (11)$$

For

$$z \in \mathbb{C} \setminus (\text{Ran } \varepsilon_K \cup \{E_0\}), \quad (12)$$

the free resolvent is

$$R_{\text{free}}(K; z) := (H_{\text{free}}(K) - zI)^{-1} = \begin{pmatrix} (E_0 - z)^{-1} & 0 \\ 0 & r_K(z) \end{pmatrix}, \quad (13)$$

where

$$r_K(z) := (H_0(K) - z)^{-1}, \quad (r_K(z)g)(p) = \frac{g(p)}{\varepsilon_K(p) - z}. \quad (14)$$

We also introduce the Lippmann–Schwinger operator

$$B_{\gamma,\lambda}(K; z) := -V_{\gamma,\lambda} R_{\text{free}}(K; z). \quad (15)$$

Proposition 2. *Let*

$$e_0 := (1, 0) \in \mathcal{H}_K, \quad e_c := (0, 1) \in \mathcal{H}_K,$$

where the second component is the constant function 1. Then

$$\text{Ran } V_{\gamma, \lambda} \subset \text{span}\{e_0, e_c\}.$$

In particular,

$$\text{rank } V_{\gamma, \lambda} \leq 2,$$

and therefore $B_{\gamma, \lambda}(K; z)$ is a finite-rank, hence compact, operator.

Proof. Let $(c, g) \in \mathcal{H}_K$. By (11), (8), (9), and (7),

$$V_{\gamma, \lambda} \begin{pmatrix} c \\ g \end{pmatrix} = \begin{pmatrix} \gamma(g, 1) \\ (\gamma c + \lambda(g, 1)) 1 \end{pmatrix},$$

which belongs to $\text{span}\{e_0, e_c\}$. This proves the claim. $\square$

3. Lippmann–Schwinger Reduction for the fiber hamiltonian

In this section we analyze the reduced hamiltonians $H_{\gamma, \lambda}(K)$ corresponding to fixed total quasi-momentum $K \in \mathbb{T}$. Since both the contact interaction and the interchannel coupling act through the constant function 1 (the constant mode), the perturbation of the free fiber operator is of rank at most two. As a consequence, the eigenvalue problem outside the essential spectrum reduces to a 2×2 linear system and, equivalently, to the vanishing of a scalar Fredholm determinant.

3.1. Finite-dimensional reduction and the reduced determinant

For

$$z \in \mathbb{C} \setminus \text{Ran } \varepsilon_K, \quad a_K(z) := (r_K(z)\varphi_0, \varphi_0) = \int_{\mathbb{T}} \frac{d\nu(p)}{\varepsilon_K(p) - z},$$

where $d\nu$ is the normalized Haar measure on $\mathbb{T}$. The function a_K is holomorphic on $\mathbb{C} \setminus \text{Ran } \varepsilon_K$, and for real $z \notin \text{Ran } \varepsilon_K$ it is real-valued.

Theorem 1 (Finite-dimensional reduction). *Let*

$$z \in \mathbb{R} \setminus \text{Ran } \varepsilon_K.$$

Then the following statements are equivalent:

- (i) *z is an eigenvalue of $H_{\gamma, \lambda}(K)$;*
- (ii) *there exists a nonzero vector $(c_0, c_1) \in \mathbb{C}^2$ such that*

$$\begin{pmatrix} E_0 - z & \gamma \\ \gamma a_K(z) & 1 + \lambda a_K(z) \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = 0; \quad (16)$$

- (iii) *the reduced determinant*

$$\Delta_{\gamma, \lambda}(K; z) := (E_0 - z)(1 + \lambda a_K(z)) - \gamma^2 a_K(z) \quad (17)$$

vanishes at z .

Proof. Let

$$\psi = (c_0, g) \in \mathcal{H}_K \setminus \{0\}.$$

The eigenvalue equation

$$H_{\gamma, \lambda}(K)\psi = z\psi$$

is equivalent to the system

$$(E_0 - z)c_0 + \gamma(g, \varphi_0) = 0, \quad (18)$$

$$(\varepsilon_K(p) - z)g(p) + \gamma c_0 \varphi_0(p) + \lambda(g, \varphi_0)\varphi_0(p) = 0. \quad (19)$$

Since $\varphi_0 \equiv 1$, the term $\gamma c_0 \varphi_0(p)$ may be identified with γc_0 .

Set

$$c_1 := (g, \varphi_0).$$

Then the first equation in the eigenvalue system becomes

$$(E_0 - z)c_0 + \gamma c_1 = 0.$$

Since $z \notin \text{Ran } \varepsilon_K$, the resolvent

$$r_K(z) := (H_0(K) - z)^{-1}$$

is bounded. Hence the second equation in the eigenvalue system can be written as

$$(H_0(K) - z)g = -(\gamma c_0 + \lambda c_1)\varphi_0.$$

Therefore

$$g = -(\gamma c_0 + \lambda c_1)r_K(z)\varphi_0. \quad (20)$$

Taking the scalar product of (20) with φ_0 , and using

$$a_K(z) := (r_K(z)\varphi_0, \varphi_0),$$

we obtain

$$c_1 = -(\gamma c_0 + \lambda c_1)a_K(z),$$

Equivalently,

$$\gamma a_K(z)c_0 + (1 + \lambda a_K(z))c_1 = 0.$$

Thus c_0 and c_1 satisfy the reduced finite-dimensional system

$$\begin{cases} (E_0 - z)c_0 + \gamma c_1 = 0, \\ \gamma a_K(z)c_0 + (1 + \lambda a_K(z))c_1 = 0. \end{cases} \quad (21)$$

This system is exactly the matrix equation (16).

Moreover, the vector (c_0, c_1) is nonzero. Indeed, if

$$c_0 = 0 \quad \text{and} \quad c_1 = 0,$$

then (20) implies $g = 0$, which contradicts $\psi \neq 0$. Hence $(i) \Rightarrow (ii)$.

Conversely, suppose that a nonzero vector

$$(c_0, c_1) \in \mathbb{C}^2$$

satisfies (16). Define

$$g = -(\gamma c_0 + \lambda c_1)r_K(z)\varphi_0.$$

Then

$$(g, \varphi_0) = -(\gamma c_0 + \lambda c_1)a_K(z).$$

By the second equation of (16), we have

$$\gamma a_K(z)c_0 + (1 + \lambda a_K(z))c_1 = 0.$$

Hence

$$-(\gamma c_0 + \lambda c_1)a_K(z) = c_1,$$

and therefore

$$(g, \varphi_0) = c_1.$$

Using the first equation of (16), we obtain

$$(E_0 - z)c_0 + \gamma(g, \varphi_0) = 0.$$

Thus (18) holds.

Furthermore, by the definition of g ,

$$(H_0(K) - z)g = -(\gamma c_0 + \lambda c_1)\varphi_0.$$

Since $c_1 = (g, \varphi_0)$, this is equivalent to

$$(H_0(K) - z)g + \gamma c_0\varphi_0 + \lambda(g, \varphi_0)\varphi_0 = 0.$$

Therefore (19) also holds.

It remains to check that $(c_0, g) \neq 0$. Suppose, on the contrary, that

$$c_0 = 0 \quad \text{and} \quad g = 0.$$

Then

$$0 = g = -\lambda c_1 r_K(z)\varphi_0.$$

Since $r_K(z)\varphi_0 \neq 0$, it follows that $\lambda c_1 = 0$. If $\lambda \neq 0$, then $c_1 = 0$. If $\lambda = 0$, then the second equation of (16) gives $c_1 = 0$. In both cases,

$$(c_0, c_1) = (0, 0),$$

which contradicts the assumption that $(c_0, c_1) \neq 0$. Therefore $(c_0, g) \neq 0$, and hence (c_0, g) is an eigenvector of $H_{\gamma, \lambda}(K)$ corresponding to z . Thus $(ii) \Rightarrow (i)$.

Finally, the homogeneous system (16) has a nontrivial solution if and only if its determinant is equal to zero. Since

$$\det \begin{pmatrix} E_0 - z & \gamma \\ \gamma a_K(z) & 1 + \lambda a_K(z) \end{pmatrix} = (E_0 - z)(1 + \lambda a_K(z)) - \gamma^2 a_K(z),$$

this condition is precisely

$$\Delta_{\gamma,\lambda}(K; z) = 0.$$

Hence (ii) $\Leftrightarrow$ (iii). The theorem is proved. $\square$

Corollary 1 (Fredholm determinant). *For*

$$z \in \mathbb{C} \setminus (\text{Ran } \varepsilon_K \cup \{E_0\}),$$

the Fredholm determinant of $I - B_{\gamma,\lambda}(K; z)$ is given by

$$D_{\gamma,\lambda}(K; z) := \det(I - B_{\gamma,\lambda}(K; z)) = \frac{\Delta_{\gamma,\lambda}(K; z)}{E_0 - z} = 1 + \lambda a_K(z) - \frac{\gamma^2 a_K(z)}{E_0 - z}. \quad (22)$$

In particular, for $z \in \mathbb{R} \setminus \text{Ran } \varepsilon_K$,

$$z \in \sigma_{\text{disc}}(H_{\gamma,\lambda}(K)) \iff \Delta_{\gamma,\lambda}(K; z) = 0.$$

Moreover, if $z \neq E_0$, then

$$z \in \sigma_{\text{disc}}(H_{\gamma,\lambda}(K)) \iff D_{\gamma,\lambda}(K; z) = 0.$$

Proof. By Proposition 2,

$$\text{Ran } B_{\gamma,\lambda}(K; z) \subset \text{span}\{e_0, e_c\}.$$

where $e_0 := (1, 0)$ and $e_c := (0, 1)$ (the second component is the constant function 1). Hence the Fredholm determinant reduces to the determinant of the restriction of $I - B_{\gamma,\lambda}(K; z)$ to this two-dimensional subspace.

Using (13) and (15), one computes

$$B_{\gamma,\lambda}(K; z)e_0 = -\frac{\gamma}{E_0 - z} e_c, \quad B_{\gamma,\lambda}(K; z)e_c = -\gamma a_K(z)e_0 - \lambda a_K(z)e_c.$$

Therefore the matrix of $I - B_{\gamma,\lambda}(K; z)$ in the basis $\{e_0, e_c\}$ is

$$\begin{pmatrix} 1 & \gamma a_K(z) \\ \frac{\gamma}{E_0 - z} & 1 + \lambda a_K(z) \end{pmatrix},$$

whose determinant equals the right hand side of (22). $\square$

3.2. The one-dimensional lattice Green function

We next compute explicitly the scalar Green function associated with the one-dimensional lattice dispersion. This computation is one of the key technical ingredients of the spectral analysis below, since it gives the explicit form of the perturbation determinant and describes its behavior near the spectral thresholds.

We emphasize that formulas of this type are standard in the spectral theory of one-dimensional discrete Schrödinger and Jacobi operators. In particular, the Green function of the discrete Schrödinger operator with a point interaction was studied in detail by Yafaev [15], where closely related computations are expressed in terms of generalized Chebyshev polynomials. More generally, Green functions and Weyl-type functions for broad classes of Jacobi operators are systematically discussed in Teschl's monograph [14]. The calculation below is included for completeness and to make the dependence on the total quasi-momentum K explicit in the present model.

Assume first that

$$K \in \mathbb{T} \setminus \{\pi\},$$

and set

$$\kappa_K := |\cos(K/2)| \in (0, 1]. \quad (23)$$

Then the band edges of the multiplication operator with dispersion ε_K are

$$\mathcal{E}_K^- := 4(1 - \kappa_K), \quad \mathcal{E}_K^+ := 4(1 + \kappa_K), \quad (24)$$

and therefore

$$\text{Ran } \varepsilon_K = [\mathcal{E}_K^-, \mathcal{E}_K^+].$$

For

$$z \in \mathbb{R} \setminus [\mathcal{E}_K^-, \mathcal{E}_K^+],$$

we define

$$a_K(z) := \frac{1}{2\pi} \int_0^{2\pi} \frac{dp}{\varepsilon_K(p) - z}. \quad (25)$$

Equivalently,

$$a_K(z) = (r_K(z)\varphi_0, \varphi_0), \quad r_K(z) := (H_0(K) - z)^{-1}, \quad \varphi_0 \equiv 1.$$

Lemma 1. *Let $K \in \mathbb{T} \setminus \{\pi\}$. Then, for*

$$z \in \mathbb{R} \setminus [\mathcal{E}_K^-, \mathcal{E}_K^+],$$

one has

$$a_K(z) = \begin{cases} \frac{1}{\sqrt{(z - \mathcal{E}_K^-)(z - \mathcal{E}_K^+)}} , & z < \mathcal{E}_K^-, \\ -\frac{1}{\sqrt{(z - \mathcal{E}_K^-)(z - \mathcal{E}_K^+)}} , & z > \mathcal{E}_K^+. \end{cases} \quad (26)$$

Here the square root denotes the positive branch.

In particular,

$$a_K(z) > 0 \quad \text{for } z < \mathcal{E}_K^-, \quad a_K(z) < 0 \quad \text{for } z > \mathcal{E}_K^+.$$

Moreover, a_K is strictly increasing on both intervals

$$(-\infty, \mathcal{E}_K^-) \quad \text{and} \quad (\mathcal{E}_K^+, \infty),$$

and

$$\lim_{z \rightarrow -\infty} a_K(z) = 0^+, \quad \lim_{z \rightarrow +\infty} a_K(z) = 0^-. \quad (27)$$

Finally, as $z \uparrow \mathcal{E}_K^-$,

$$a_K(z) = \frac{1}{2\sqrt{2\kappa_K}} (\mathcal{E}_K^- - z)^{-1/2} + O(1), \quad (28)$$

and as $z \downarrow \mathcal{E}_K^+$,

$$a_K(z) = -\frac{1}{2\sqrt{2\kappa_K}} (z - \mathcal{E}_K^+)^{-1/2} + O(1). \quad (29)$$

Proof. By the explicit form of the one-dimensional two-particle dispersion, one has

$$\varepsilon_K(p) = 4 - 4\kappa_K \cos p.$$

Therefore

$$a_K(z) = \frac{1}{2\pi} \int_0^{2\pi} \frac{dp}{4 - z - 4\kappa_K \cos p}.$$

This is the standard diagonal Green function of a one-dimensional Jacobi operator. Using the classical integral identity

$$\frac{1}{2\pi} \int_0^{2\pi} \frac{dp}{a - b \cos p} = \frac{\operatorname{sgn}(a)}{\sqrt{a^2 - b^2}}, \quad |a| > |b|,$$

with

$$a = 4 - z, \quad b = 4\kappa_K,$$

we obtain

$$a_K(z) = \frac{\operatorname{sgn}(4 - z)}{\sqrt{(4 - z)^2 - 16\kappa_K^2}}.$$

Since

$$(4 - z)^2 - 16\kappa_K^2 = (z - \mathcal{E}_K^-)(z - \mathcal{E}_K^+),$$

formula (26) follows.

The sign properties are immediate from (26). The limits

$$\lim_{z \rightarrow -\infty} a_K(z) = 0^+, \quad \lim_{z \rightarrow +\infty} a_K(z) = 0^-$$

also follow directly from the same formula.

To prove monotonicity, it is enough to differentiate under the integral sign:

$$a'_K(z) = \frac{1}{2\pi} \int_0^{2\pi} \frac{dp}{(\varepsilon_K(p) - z)^2} > 0.$$

Hence a_K is strictly increasing on each connected component of

$$\mathbb{R} \setminus [\mathcal{E}_K^-, \mathcal{E}_K^+].$$

It remains to derive the threshold asymptotics. As $z \uparrow \mathcal{E}_K^-$, one has

$$(z - \mathcal{E}_K^-)(z - \mathcal{E}_K^+) = (\mathcal{E}_K^- - z)(\mathcal{E}_K^+ - z),$$

and

$$\mathcal{E}_K^+ - z = \mathcal{E}_K^+ - \mathcal{E}_K^- + \mathcal{E}_K^- - z = 8\kappa_K + \mathcal{E}_K^- - z.$$

Therefore

$$a_K(z) = \frac{1}{\sqrt{(\mathcal{E}_K^- - z)(8\kappa_K + \mathcal{E}_K^- - z)}} = \frac{1}{2\sqrt{2\kappa_K}} (\mathcal{E}_K^- - z)^{-1/2} + O(1),$$

which proves (28).

Similarly, as $z \downarrow \mathcal{E}_K^+$,

$$(z - \mathcal{E}_K^-)(z - \mathcal{E}_K^+) = (8\kappa_K + z - \mathcal{E}_K^+)(z - \mathcal{E}_K^+).$$

Using the negative sign in the upper part of (26), we get

$$a_K(z) = -\frac{1}{\sqrt{(8\kappa_K + z - \mathcal{E}_K^+)(z - \mathcal{E}_K^+)}} = -\frac{1}{2\sqrt{2\kappa_K}} (z - \mathcal{E}_K^+)^{-1/2} + O(1).$$

This proves (29). □

3.3. A scalar Birman–Schwinger equation

For $z \in \mathbb{R} \setminus ([\mathcal{E}_K^-, \mathcal{E}_K^+] \cup \{E_0\})$, the equation $\Delta_{\gamma,\lambda}(K; z) = 0$ is equivalent to the scalar Birman–Schwinger equation

$$\Phi_K(z) = \Psi_{\gamma,\lambda}(z), \quad (30)$$

where

$$\Phi_K(z) := -\frac{1}{a_K(z)}, \quad \Psi_{\gamma,\lambda}(z) := \lambda - \frac{\gamma^2}{E_0 - z}. \quad (31)$$

Indeed, multiplying (30) by $-a_K(z)(E_0 - z)$ yields exactly $\Delta_{\gamma,\lambda}(K; z) = 0$.

Remark 1. By Lemma 1, the function Φ_K is strictly increasing on $(-\infty, \mathcal{E}_K^-)$ and on $(\mathcal{E}_K^+, \infty)$, and

$$\begin{aligned} \lim_{z \rightarrow -\infty} \Phi_K(z) &= -\infty, & \lim_{z \uparrow \mathcal{E}_K^-} \Phi_K(z) &= 0^-, \\ \lim_{z \downarrow \mathcal{E}_K^+} \Phi_K(z) &= 0^+, & \lim_{z \rightarrow +\infty} \Phi_K(z) &= +\infty. \end{aligned}$$

On the other hand,

$$\Psi'_{\gamma,\lambda}(z) = -\frac{\gamma^2}{(E_0 - z)^2} < 0 \quad (z \neq E_0),$$

so $\Psi_{\gamma,\lambda}$ is strictly decreasing on every interval not containing the pole E_0 .

3.4. The flat-band case $K = \pi$

If $K = \pi$, then $\cos(K/2) = 0$, and therefore

$$\varepsilon_\pi(p) \equiv 4. \quad (32)$$

Hence $\sigma_{\text{ess}}(H_{\gamma,\lambda}(\pi)) = \{4\}$, and

$$a_\pi(z) = \frac{1}{4 - z}, \quad z \neq 4. \quad (33)$$

Substituting (33) into (17), we obtain

$$\Delta_{\gamma,\lambda}(\pi; z) = (E_0 - z) \left(1 + \frac{\lambda}{4 - z} \right) - \frac{\gamma^2}{4 - z} = \frac{(E_0 - z)(4 + \lambda - z) - \gamma^2}{4 - z}. \quad (34)$$

Thus, in the flat-band case $K = \pi$, the spectral problem reduces to the explicit quadratic equation

$$(E_0 - z)(4 + \lambda - z) = \gamma^2. \quad (35)$$

4. Discrete spectrum of the reduced hamiltonian $H_{\gamma,\lambda}(K)$

In this section we classify the discrete spectrum of the reduced hamiltonians $H_{\gamma,\lambda}(K)$ in the constant-profile case $\alpha \equiv 1$. The analysis is based on the scalar Birman–Schwinger equation derived in Section 3.

Recall from Section 3 that the location of the molecular energy E_0 relative to the essential band $[\mathcal{E}_K^-, \mathcal{E}_K^+]$ determines three generic regimes: E_0 inside the band ($\mathcal{E}_K^- < E_0 < \mathcal{E}_K^+$), E_0 below the band ($E_0 < \mathcal{E}_K^-$), and E_0 above the band ($E_0 > \mathcal{E}_K^+$). The discrete spectrum of $H_{\gamma,\lambda}(K)$ is classified separately for each of these cases, with the threshold configurations $E_0 = \mathcal{E}_K^\pm$ treated as limiting situations.

Throughout this section, unless stated otherwise, we assume that $K \in \mathbb{T} \setminus \{\pi\}$. Recall that the essential spectrum of $H_{\gamma,\lambda}(K)$ is the interval

$$\sigma_{\text{ess}}(H_{\gamma,\lambda}(K)) = [\mathcal{E}_K^-, \mathcal{E}_K^+], \quad (36)$$

with $\mathcal{E}_K^\pm$ defined in (24).

We write

$$n_-(H_{\gamma,\lambda}(K)) := \#(\sigma_{\text{disc}}(H_{\gamma,\lambda}(K)) \cap (-\infty, \mathcal{E}_K^-)), \quad (37)$$

and

$$n_+(H_{\gamma,\lambda}(K)) := \#(\sigma_{\text{disc}}(H_{\gamma,\lambda}(K)) \cap (\mathcal{E}_K^+, \infty)), \quad (38)$$

where eigenvalues are counted with multiplicities.

The threshold behaviour of the reduced determinant $\Delta_{\gamma,\lambda}(K; z)$ is governed by the coefficients

$$S_K^-(\gamma, \lambda) = \lambda(E_0 - \mathcal{E}_K^-) - \gamma^2, \quad S_K^+(\gamma, \lambda) = \lambda(\mathcal{E}_K^+ - E_0) + \gamma^2. \quad (39)$$

If $E_0 \neq \mathcal{E}_K^\pm$, the corresponding critical curves in the (γ, λ) -plane are given by

$$\lambda = \lambda_K^-(\gamma) := \frac{\gamma^2}{E_0 - \mathcal{E}_K^-}, \quad \lambda = \lambda_K^+(\gamma) := \frac{\gamma^2}{E_0 - \mathcal{E}_K^+}. \quad (40)$$

Equivalently,

$$S_K^-(\gamma, \lambda) = 0 \iff \lambda = \lambda_K^-(\gamma), \quad S_K^+(\gamma, \lambda) = 0 \iff \lambda = \lambda_K^+(\gamma).$$

The spectral classification below is based on the scalar Birman–Schwinger equation

$$\Phi_K(z) = \Psi_{\gamma,\lambda}(z), \quad (41)$$

with $\Phi_K, \Psi_{\gamma,\lambda}$ defined in (31). By Remark 1, Φ_K is strictly increasing on each of the intervals $(-\infty, \mathcal{E}_K^-)$ and $(\mathcal{E}_K^+, \infty)$, whereas $\Psi_{\gamma,\lambda}$ is strictly decreasing on every interval not containing the pole E_0 . This monotonicity is the basic tool in what follows.

4.1. The case $\mathcal{E}_K^- < E_0 < \mathcal{E}_K^+$

We begin with the case in which the molecular energy lies inside the essential band. Then the pole of $\Psi_{\gamma,\lambda}$ lies inside the band and therefore does not affect the analysis on the two spectral half-lines.

Theorem 2. Assume that

$$\mathcal{E}_K^- < E_0 < \mathcal{E}_K^+. \quad (42)$$

Then

$$n_-(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & S_K^-(\gamma, \lambda) < 0, \\ 0, & S_K^-(\gamma, \lambda) \geq 0, \end{cases} \quad (43)$$

and

$$n_+(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & S_K^+(\gamma, \lambda) > 0, \\ 0, & S_K^+(\gamma, \lambda) \leq 0. \end{cases} \quad (44)$$

Equivalently,

$$n_-(H_{\gamma,\lambda}(K)) = 1 \iff \lambda < \lambda_K^-(\gamma), \quad n_+(H_{\gamma,\lambda}(K)) = 1 \iff \lambda > \lambda_K^+(\gamma). \quad (45)$$

Proof. Since $E_0 \in (\mathcal{E}_K^-, \mathcal{E}_K^+)$, the pole of $\Psi_{\gamma,\lambda}$ lies inside the essential band and does not interfere with the spectral half-lines $(-\infty, \mathcal{E}_K^-)$ and $(\mathcal{E}_K^+, \infty)$.

Consider first the lower half-line and define

$$F_-(z) := \Phi_K(z) - \Psi_{\gamma,\lambda}(z), \quad z \in (-\infty, \mathcal{E}_K^-).$$

Because Φ_K is strictly increasing and $\Psi_{\gamma,\lambda}$ is strictly decreasing, F_- is strictly increasing. Moreover,

$$\lim_{z \rightarrow -\infty} F_-(z) = -\infty.$$

Using the threshold asymptotics of Φ_K , one obtains

$$\lim_{z \uparrow \mathcal{E}_K^-} F_-(z) = -\frac{S_K^-(\gamma, \lambda)}{E_0 - \mathcal{E}_K^-}.$$

Since $E_0 - \mathcal{E}_K^- > 0$, this limit is positive if and only if $S_K^-(\gamma, \lambda) < 0$. Hence F_- has exactly one zero in $(-\infty, \mathcal{E}_K^-)$ when $S_K^-(\gamma, \lambda) < 0$, and none otherwise. This proves (43).

The argument for the upper half-line is analogous. Define

$$F_+(z) := \Phi_K(z) - \Psi_{\gamma, \lambda}(z), \quad z \in (\mathcal{E}_K^+, \infty).$$

Again F_+ is strictly increasing, and

$$\lim_{z \downarrow \mathcal{E}_K^+} F_+(z) = -\frac{S_K^+(\gamma, \lambda)}{\mathcal{E}_K^+ - E_0}, \quad \lim_{z \rightarrow +\infty} F_+(z) = +\infty.$$

Because $\mathcal{E}_K^+ - E_0 > 0$, there is exactly one zero in $(\mathcal{E}_K^+, \infty)$ if and only if $S_K^+(\gamma, \lambda) > 0$. This proves (44). $\square$

4.2. The case $E_0 < \mathcal{E}_K^-$

We next consider the case when the molecular energy lies below the essential band. Then the pole of $\Psi_{\gamma, \lambda}$ lies on the lower spectral side and splits the lower half-line into two monotonicity intervals.

Theorem 3. Assume that

$$E_0 < \mathcal{E}_K^-. \quad (46)$$

Then

$$n_-(H_{\gamma, \lambda}(K)) = \begin{cases} 2, & S_K^-(\gamma, \lambda) > 0, \\ 1, & S_K^-(\gamma, \lambda) \leq 0, \end{cases} \quad (47)$$

and

$$n_+(H_{\gamma, \lambda}(K)) = \begin{cases} 1, & S_K^+(\gamma, \lambda) > 0, \\ 0, & S_K^+(\gamma, \lambda) \leq 0. \end{cases} \quad (48)$$

Equivalently,

$$n_-(H_{\gamma, \lambda}(K)) = 2 \iff \lambda < \lambda_K^-(\gamma), \quad n_+(H_{\gamma, \lambda}(K)) = 1 \iff \lambda > \lambda_K^+(\gamma). \quad (49)$$

Proof. We begin with the decoupled case $\gamma = 0$. Then

$$\Delta_{\gamma, \lambda}(K; z) = (E_0 - z)(1 + \lambda a_K(z)).$$

Hence $z = E_0$ is always an eigenvalue below the essential band, while the remaining discrete spectrum is determined by $1 + \lambda a_K(z) = 0$. Since $a_K(z) > 0$ on $(-\infty, \mathcal{E}_K^-)$ and $a_K(z) < 0$ on $(\mathcal{E}_K^+, \infty)$, this equation has one solution below the band iff $\lambda < 0$, and one solution above the band iff $\lambda > 0$. This agrees with the formulas in the theorem, because for $\gamma = 0$, $S_K^-(0, \lambda) = \lambda(E_0 - \mathcal{E}_K^-)$ (negative since $E_0 - \mathcal{E}_K^- < 0$) and $S_K^+(0, \lambda) = \lambda(\mathcal{E}_K^+ - E_0)$.

Assume now that $\gamma \neq 0$. On the interval $(-\infty, E_0)$, set

$$F_1(z) := \Phi_K(z) - \Psi_{\gamma, \lambda}(z).$$

The function F_1 is strictly increasing and satisfies

$$\lim_{z \rightarrow -\infty} F_1(z) = -\infty, \quad \lim_{z \uparrow E_0} F_1(z) = +\infty.$$

Hence F_1 has exactly one zero in $(-\infty, E_0)$.

On the interval $(E_0, \mathcal{E}_K^-)$, define

$$F_2(z) := \Phi_K(z) - \Psi_{\gamma, \lambda}(z).$$

Again F_2 is strictly increasing, and

$$\lim_{z \downarrow E_0} F_2(z) = -\infty, \quad \lim_{z \uparrow \mathcal{E}_K^-} F_2(z) = -\frac{S_K^-(\gamma, \lambda)}{E_0 - \mathcal{E}_K^-}.$$

Because $E_0 - \mathcal{E}_K^- < 0$, the last limit is positive if and only if $S_K^-(\gamma, \lambda) > 0$. Therefore there is exactly one zero in $(E_0, \mathcal{E}_K^-)$ when $S_K^-(\gamma, \lambda) > 0$, and none otherwise. This proves (47).

Finally, on $(\mathcal{E}_K^+, \infty)$ the pole E_0 is irrelevant, and the same argument as in Theorem 2 shows that there is exactly one eigenvalue above the band if and only if $S_K^+(\gamma, \lambda) > 0$. This proves (48). $\square$

4.3. The case $E_0 > \mathcal{E}_K^+$

We finally consider the case when the molecular energy lies above the essential band. This is symmetric to the previous case, with the pole of $\Psi_{\gamma,\lambda}$ now lying on the upper spectral side.

Theorem 4. Assume that

$$E_0 > \mathcal{E}_K^+. \quad (50)$$

Then

$$n_-(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & S_K^-(\gamma, \lambda) < 0, \\ 0, & S_K^-(\gamma, \lambda) \geq 0, \end{cases} \quad (51)$$

and

$$n_+(H_{\gamma,\lambda}(K)) = \begin{cases} 2, & S_K^+(\gamma, \lambda) < 0, \\ 1, & S_K^+(\gamma, \lambda) \geq 0. \end{cases} \quad (52)$$

Equivalently,

$$n_-(H_{\gamma,\lambda}(K)) = 1 \iff \lambda < \lambda_K^-(\gamma), \quad n_+(H_{\gamma,\lambda}(K)) = 2 \iff \lambda > \lambda_K^+(\gamma). \quad (53)$$

Proof. If $\gamma = 0$, then $\Delta_{\gamma,\lambda}(K; z) = (E_0 - z)(1 + \lambda a_K(z))$ and $z = E_0$ is always an eigenvalue above the essential band. The equation $1 + \lambda a_K(z) = 0$ contributes one eigenvalue below the band iff $\lambda < 0$, and one additional eigenvalue above the band iff $\lambda > 0$. This matches the statement of the theorem.

Assume now that $\gamma \neq 0$. On $(-\infty, \mathcal{E}_K^-)$, the pole E_0 is absent, and the same argument as in Theorem 2 shows that there is exactly one eigenvalue below the band iff $S_K^-(\gamma, \lambda) < 0$.

For the upper half-line $(\mathcal{E}_K^+, \infty)$, the pole at E_0 splits the interval into two parts. On $(\mathcal{E}_K^+, E_0)$, define

$$F_1(z) := \Phi_K(z) - \Psi_{\gamma,\lambda}(z).$$

Then F_1 is strictly increasing and satisfies

$$\lim_{z \downarrow \mathcal{E}_K^+} F_1(z) = -\frac{S_K^+(\gamma, \lambda)}{\mathcal{E}_K^+ - E_0}, \quad \lim_{z \uparrow E_0} F_1(z) = +\infty.$$

Since $\mathcal{E}_K^+ - E_0 < 0$, there is exactly one zero in $(\mathcal{E}_K^+, E_0)$ iff $S_K^+(\gamma, \lambda) < 0$.

On (E_0, ∞) , define

$$F_2(z) := \Phi_K(z) - \Psi_{\gamma,\lambda}(z).$$

Again F_2 is strictly increasing, and

$$\lim_{z \downarrow E_0} F_2(z) = -\infty, \quad \lim_{z \rightarrow +\infty} F_2(z) = +\infty.$$

Hence F_2 has exactly one zero in (E_0, ∞) . Therefore

$$n_+(H_{\gamma,\lambda}(K)) = 1 + \mathbf{1}_{\{S_K^+(\gamma, \lambda) < 0\}},$$

which is exactly (52). □

4.4. Threshold configurations $E_0 = \mathcal{E}_K^\pm$

We now discuss the limiting situations in which the molecular energy coincides with one of the band edges. These configurations are the boundaries between the three generic regimes treated above, and the counting formulas can be obtained by taking the limits $E_0 \rightarrow \mathcal{E}_K^\pm$ in Theorems 2 – 4 while keeping track of the eigenvalue that emerges from the threshold when $\gamma \neq 0$.

Proposition 3. Assume that $K \in \mathbb{T} \setminus \{\pi\}$. Then the following assertions hold.

(i) If $E_0 = \mathcal{E}_K^-$, then

$$n_-(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & \gamma \neq 0, \\ 1, & \gamma = 0 \text{ and } \lambda < 0, \\ 0, & \gamma = 0 \text{ and } \lambda \geq 0, \end{cases} \quad (54)$$

and

$$n_+(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & \lambda(\mathcal{E}_K^+ - \mathcal{E}_K^-) + \gamma^2 > 0, \\ 0, & \lambda(\mathcal{E}_K^+ - \mathcal{E}_K^-) + \gamma^2 \leq 0. \end{cases} \quad (55)$$

(ii) If $E_0 = \mathcal{E}_K^+$, then

$$n_-(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & \lambda(\mathcal{E}_K^+ - \mathcal{E}_K^-) - \gamma^2 < 0, \\ 0, & \lambda(\mathcal{E}_K^+ - \mathcal{E}_K^-) - \gamma^2 \geq 0, \end{cases} \quad (56)$$

and

$$n_+(H_{\gamma,\lambda}(K)) = \begin{cases} 1, & \gamma \neq 0, \\ 1, & \gamma = 0 \text{ and } \lambda > 0, \\ 0, & \gamma = 0 \text{ and } \lambda \leq 0. \end{cases} \quad (57)$$

Proof. The proof follows by taking the limits $E_0 \rightarrow \mathcal{E}_K^-$ and $E_0 \rightarrow \mathcal{E}_K^+$ in Theorems 2 and 3 (or 4) respectively, and using the continuity of the eigenvalue counting functions with respect to E_0 as long as the thresholds are approached from the appropriate side. When $\gamma \neq 0$, the pole of $\Psi_{\gamma,\lambda}$ at E_0 forces one eigenvalue to bifurcate from the band edge, which is reflected in the first case of the counting formulas on the side where the pole is located. The explicit expressions are obtained by evaluating the limits of $S_K^\pm(\gamma, \lambda)$ and the corresponding sign conditions. $\square$

Remark 2. The threshold configurations $E_0 = \mathcal{E}_K^\pm$ are the natural boundaries between the three generic regimes. The counting formulas above are consistent with the sharp spectral transitions described by the critical coefficients $S_K^\pm(\gamma, \lambda)$ and can be obtained directly from the generic results by taking the appropriate limits.

5. Threshold states and virtual levels of the rank-one fiber operator $\mathbf{h}_\lambda(K)$

In this section we study threshold states, or virtual levels, of the auxiliary rank-one fiber operator $\mathbf{h}_\lambda(K)$. Recall that when the interchannel coupling vanishes ($\gamma = 0$), the reduced hamiltonian $H_{0,\lambda}(K)$ decouples and its fiber part reduces precisely to $\mathbf{h}_\lambda(K)$; see the proofs of Theorems 3 and 4. Although $\mathbf{h}_\lambda(K)$ is simpler than the full two-channel hamiltonian $H_{\gamma,\lambda}(K)$, its threshold behaviour is of independent interest. It clarifies the mechanism by which an eigenvalue emerges from a threshold resonance and approaches the edge of the essential spectrum when the interchannel coupling γ is turned on.

The notion of a virtual level used below is inspired by the classical functional-analytic theory developed by Yafaev for the three-dimensional continuous Schrödinger equation [24]. In that setting, virtual states are described as non-square-integrable solutions of the threshold equation which nevertheless belong to a suitable larger weighted space. The present paper deals with a one-dimensional discrete lattice model, so Yafaev's results are not applied directly. Rather, they provide a useful conceptual prototype for the functional-analytic treatment of threshold states. In our one-dimensional lattice setting, the threshold singularity is produced by the behaviour of the dispersion relation $\mathcal{E}_K(q)$ near a nondegenerate band edge. The threshold profile associated with such an edge is not an element of the physical Hilbert space $L^2(\mathbb{T})$, but it becomes admissible after passing to a suitable weighted space adapted to the singularity of the dispersion relation. Thus the construction below may be viewed as a one-dimensional discrete analogue of the general functional-analytic idea underlying Yafaev's theory.

5.1. Threshold equation and weighted spaces

For each $K \in \mathbb{T}$, consider the fiber operator

$$(\mathbf{h}_\lambda(K)g)(q) = \mathcal{E}_K(q)g(q) + \lambda \int_{\mathbb{T}} g(t) d\nu(t), \quad q \in \mathbb{T},$$

acting in the fiber space $\mathfrak{h}(K)$. After the usual identification of $\mathfrak{h}(K)$ with $L^{2,e}(\mathbb{T})$, the operator may be regarded as acting in $L^{2,e}(\mathbb{T})$. Its essential spectrum is the interval

$$\sigma_{\text{ess}}(\mathbf{h}_\lambda(K)) = [\mathcal{E}_K^-, \mathcal{E}_K^+],$$

where

$$\mathcal{E}_K^- := \min_{q \in \mathbb{T}} \mathcal{E}_K(q), \quad \mathcal{E}_K^+ := \max_{q \in \mathbb{T}} \mathcal{E}_K(q).$$

Throughout this subsection we assume $K \neq \pi$; the flat-band case $K = \pi$ is treated separately in Subsection 5.5. Then the extrema of $\mathcal{E}_K$ are nondegenerate. Let $q_-(K)$ and $q_+(K)$ be a point of minimum and a point of maximum, respectively. Thus

$$\mathcal{E}_K(q) - \mathcal{E}_K^- \asymp |q - q_-(K)|^2, \quad \mathcal{E}_K^+ - \mathcal{E}_K(q) \asymp |q - q_+(K)|^2$$

as $q \rightarrow q_\sigma(K)$, $\sigma \in \{-, +\}$.

For $z \notin [\mathcal{E}_K^-, \mathcal{E}_K^+]$, the eigenvalue equation

$$(\mathbf{h}_\lambda(K) - z)g = 0$$

is equivalent to

$$(\mathcal{E}_K(q) - z)g(q) + \lambda c = 0, \quad c := \int_{\mathbb{T}} g(t) d\nu(t),$$

hence to the representation

$$g(q) = -\frac{\lambda c}{\mathcal{E}_K(q) - z}.$$

Accordingly, the discrete spectrum outside the essential band is determined by the scalar equation

$$\Delta_\lambda(K; z) = 0, \quad \Delta_\lambda(K; z) := 1 + \lambda a_K(z), \quad (58)$$

where

$$a_K(z) := \int_{\mathbb{T}} \frac{d\nu(q)}{\mathcal{E}_K(q) - z}.$$

At a threshold energy $E = \mathcal{E}_K^\sigma$, the formal threshold profile is

$$g(q) \sim \frac{1}{\mathcal{E}_K(q) - \mathcal{E}_K^\sigma}.$$

Since the extremum is nondegenerate, this yields

$$g(q) \sim \frac{\text{const}}{|q - q_\sigma(K)|^2} \quad \text{as } q \rightarrow q_\sigma(K).$$

Such a function does not belong to $L^2(\mathbb{T})$. Therefore threshold states cannot be treated in the usual Hilbert space and must instead be described in a suitable weighted space.

To this end, define the weight

$$w_{K,\sigma}(q) := (1 - \cos(q - q_\sigma(K)))^2, \quad \sigma \in \{-, +\}.$$

Then

$$w_{K,\sigma}(q) \asymp |q - q_\sigma(K)|^4 \quad \text{as } q \rightarrow q_\sigma(K).$$

This choice is natural, since the threshold profile behaves like $|q - q_\sigma(K)|^{-2}$, and therefore

$$|g(q)|^2 w_{K,\sigma}(q) \asymp \text{const} \quad \text{as } q \rightarrow q_\sigma(K).$$

Thus the weighted space captures precisely the borderline singularity of a threshold state.

Definition 1 (Weighted threshold space). *For each $K \in \mathbb{T}$ and $\sigma \in \{-, +\}$, define*

$$\mathcal{L}_{K,\sigma}^w(\mathbb{T}) := \left\{ f : \mathbb{T} \rightarrow \mathbb{C} \text{ measurable} : \int_{\mathbb{T}} |f(q)|^2 w_{K,\sigma}(q) d\nu(q) < \infty \right\}.$$

If one works in the even sector, the corresponding space is

$$\mathcal{L}_{K,\sigma}^{w,e}(\mathbb{T}) := \left\{ f \in L^{2,e}(\mathbb{T}) : \int_{\mathbb{T}} |f(q)|^2 w_{K,\sigma}(q) d\nu(q) < \infty \right\}.$$

Lemma 2. *For each $K \in \mathbb{T}$ and $\sigma \in \{-, +\}$, the space $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$ is a Hilbert space with inner product*

$$\langle f, g \rangle_{\mathcal{L}_{K,\sigma}^w} = \int_{\mathbb{T}} f(q) \overline{g(q)} w_{K,\sigma}(q) d\nu(q).$$

Moreover, $L^2(\mathbb{T})$ is a dense proper subspace of $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$, and the embedding

$$L^2(\mathbb{T}) \hookrightarrow \mathcal{L}_{K,\sigma}^w(\mathbb{T})$$

is continuous.

Proof. Define $(U_{K,\sigma}f)(q) := w_{K,\sigma}(q)^{1/2}f(q)$. Then $U_{K,\sigma}$ is an isometric isomorphism from $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$ onto $L^2(\mathbb{T})$, which proves completeness.

Since $0 \leq w_{K,\sigma}(q) \leq 4$, we have

$$\|f\|_{\mathcal{L}_{K,\sigma}^w}^2 = \int_{\mathbb{T}} |f(q)|^2 w_{K,\sigma}(q) d\nu(q) \leq 4\|f\|_{L^2}^2,$$

hence $\|f\|_{\mathcal{L}_{K,\sigma}^w} \leq 2\|f\|_{L^2}$. Thus the embedding is continuous.

To see that the inclusion is proper, set $f(q) := w_{K,\sigma}(q)^{-1/2}$. Then $|f(q)|^2 w_{K,\sigma}(q) = 1$, so $f \in \mathcal{L}_{K,\sigma}^w(\mathbb{T})$. On the other hand, since $w_{K,\sigma}(q)^{-1/2} \asymp |q - q_\sigma(K)|^{-2}$ as $q \rightarrow q_\sigma(K)$, we have $f \notin L^2(\mathbb{T})$. Finally, density of $L^2(\mathbb{T})$ in $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$ follows from the identification via $U_{K,\sigma}$. $\square$

Remark 3. The terminology “virtual level” is used here in the same spirit as in Yafaev’s rigorous theory of virtual states for the three-dimensional continuous Schrödinger equation [24]. The present lattice model is one-dimensional and discrete, and therefore the singular structure of the threshold state, the natural weighted space, and the spectral consequences are different from those in the continuous three-dimensional case. Nevertheless, the underlying functional-analytic principle is analogous: the threshold state is detected not as an ordinary eigenvector of the Hilbert-space operator, but as a generalized threshold solution whose singularity is controlled by an appropriate weight. This provides the conceptual link between the present classification of threshold resonances for $\mathbf{h}_\lambda(K)$ and the classical theory of virtual levels.

5.2. Threshold eigenvalues and threshold resonances

At threshold, the quantity

$$\int_{\mathbb{T}} g(t) d\nu(t)$$

need not be well defined for singular states of the form $(\mathcal{E}_K - \mathcal{E}_K^\sigma)^{-1}$. For this reason the threshold equation must be understood in a weak, or formal Lippmann–Schwinger, sense.

Definition 2 (Threshold equation). Let $E = \mathcal{E}_K^\sigma$, $\sigma \in \{-, +\}$. We say that g is a threshold solution of $\mathbf{h}_\lambda(K)$ at E if there exists a constant $c \neq 0$ such that

$$(\mathcal{E}_K(q) - E)g(q) + \lambda c = 0 \quad \text{for a.e. } q \in \mathbb{T}. \quad (59)$$

Equivalently,

$$g(q) = -\frac{\lambda c}{\mathcal{E}_K(q) - E}. \quad (60)$$

Definition 3 (Threshold eigenvalue and threshold resonance). Let $E = \mathcal{E}_K^\sigma$, $\sigma \in \{-, +\}$. A nontrivial threshold solution g is called

- a threshold eigenfunction if $g \in L^2(\mathbb{T})$;
- a threshold resonance if

$$g \in \mathcal{L}_{K,\sigma}^w(\mathbb{T}) \setminus L^2(\mathbb{T}).$$

If the analysis is restricted to the even sector, $L^2(\mathbb{T})$ is replaced throughout by $L^{2,e}(\mathbb{T})$.

Remark 4. The above definition separates two qualitatively different threshold states. A threshold eigenfunction is genuinely square integrable and therefore belongs to the underlying Hilbert space. By contrast, a threshold resonance fails to be square integrable, but its singularity is exactly mild enough to be captured by the weighted space $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$.

5.3. Existence of threshold resonances

The next result gives the threshold classification for the rank-one fiber operator $\mathbf{h}_\lambda(K)$.

Proposition 4. Assume $K \in \mathbb{T} \setminus \{\pi\}$ and $\lambda \neq 0$. Then, for each $\sigma \in \{-, +\}$, the threshold equation (59) at $E = \mathcal{E}_K^\sigma$ has a nontrivial solution

$$g_\sigma(q) = -\frac{\lambda c}{\mathcal{E}_K(q) - \mathcal{E}_K^\sigma}, \quad c \neq 0.$$

Moreover,

$$g_\sigma \in \mathcal{L}_{K,\sigma}^w(\mathbb{T}) \setminus L^2(\mathbb{T}).$$

Consequently, $\mathcal{E}_K^\sigma$ is a threshold resonance of $\mathbf{h}_\lambda(K)$, but not a threshold eigenvalue.

Proof. Fix $\sigma \in \{-, +\}$ and choose any $c \neq 0$. Then the function

$$g_\sigma(q) := -\frac{\lambda c}{\mathcal{E}_K(q) - \mathcal{E}_K^\sigma}$$

satisfies (59) by construction.

We prove the claim for $\sigma = -$; the proof for $\sigma = +$ is identical. Since $K \neq \pi$, the minimum of $\mathcal{E}_K$ is nondegenerate. Hence there exist $q_-(K) \in \mathbb{T}$ and a constant $C_K^- > 0$ such that

$$\mathcal{E}_K(q) - \mathcal{E}_K^- \sim C_K^- |q - q_-(K)|^2 \quad \text{as } q \rightarrow q_-(K).$$

Therefore

$$g_-(q) \sim \frac{\text{const}}{|q - q_-(K)|^2}, \quad q \rightarrow q_-(K),$$

and hence

$$|g_-(q)|^2 \sim \frac{\text{const}}{|q - q_-(K)|^4}.$$

This is not integrable in one dimension, so $g_- \notin L^2(\mathbb{T})$.

On the other hand,

$$w_{K,-}(q) \sim \frac{1}{4} |q - q_-(K)|^4 \quad \text{as } q \rightarrow q_-(K),$$

and therefore

$$|g_-(q)|^2 w_{K,-}(q) \sim \text{const}.$$

Hence $g_- \in \mathcal{L}_{K,-}^w(\mathbb{T})$. We conclude that $g_- \in \mathcal{L}_{K,-}^w(\mathbb{T}) \setminus L^2(\mathbb{T})$, that is, $\mathcal{E}_K^-$ is a threshold resonance and not a threshold eigenvalue. $\square$

Remark 5. The notion of threshold resonance used here is based on the existence of a nontrivial threshold solution in the weighted space $\mathcal{L}_{K,\sigma}^w(\mathbb{T})$. This is conceptually different from the behaviour of the scalar determinant $\Delta_\lambda(K; z)$ at $z = \mathcal{E}_K^\sigma$. In the present rank-one model, the formal threshold profile $(\mathcal{E}_K - \mathcal{E}_K^\sigma)^{-1}$ exists for every $\lambda \neq 0$, whereas the equation $\Delta_\lambda(K; z) = 0$ governs genuine eigenvalues outside the essential spectrum. Note that $\Delta_\lambda(K; z)$ has no zero at the threshold because $a_K(z)$ diverges, so the threshold is not an eigenvalue in the usual sense.

5.4. Discrete spectrum outside the essential band

Although threshold resonances exist in the above weighted sense, the discrete spectrum outside the essential band is still determined by the scalar equation (58). The following statement is standard.

Theorem 5. Assume $K \in \mathbb{T} \setminus \{\pi\}$. Then:

- (i) if $\lambda < 0$, the operator $\mathbf{h}_\lambda(K)$ has exactly one eigenvalue below $\mathcal{E}_K^-$ and no eigenvalues above $\mathcal{E}_K^+$;
- (ii) if $\lambda > 0$, the operator $\mathbf{h}_\lambda(K)$ has exactly one eigenvalue above $\mathcal{E}_K^+$ and no eigenvalues below $\mathcal{E}_K^-$;
- (iii) if $\lambda = 0$, the operator $\mathbf{h}_\lambda(K)$ has no discrete spectrum outside $[\mathcal{E}_K^-, \mathcal{E}_K^+]$.

Proof. For $z \notin [\mathcal{E}_K^-, \mathcal{E}_K^+]$, eigenvalues are precisely the zeros of

$$\Delta_\lambda(K; z) = 1 + \lambda a_K(z), \quad a_K(z) = \int_{\mathbb{T}} \frac{d\nu(q)}{\mathcal{E}_K(q) - z}.$$

The function $a_K(z)$ is continuous and strictly increasing on each of the intervals $(-\infty, \mathcal{E}_K^-)$ and $(\mathcal{E}_K^+, \infty)$. Moreover,

$$a_K(z) > 0 \quad \text{for } z < \mathcal{E}_K^-, \quad a_K(z) < 0 \quad \text{for } z > \mathcal{E}_K^+,$$

and $a_K(z) \rightarrow 0$ as $|z| \rightarrow \infty$. Therefore, if $\lambda < 0$, the equation $1 + \lambda a_K(z) = 0$ has exactly one solution on $(-\infty, \mathcal{E}_K^-)$ and none on $(\mathcal{E}_K^+, \infty)$. If $\lambda > 0$, the situation is reversed. Finally, if $\lambda = 0$, the equation has no solution outside the essential spectrum. $\square$

Corollary 2. Let $z_\lambda(K)$ denote the unique discrete eigenvalue from Theorem 5. Then

$$z_\lambda(K) \uparrow \mathcal{E}_K^- \quad \text{as } \lambda \rightarrow 0^-,$$

and

$$z_\lambda(K) \downarrow \mathcal{E}_K^+ \quad \text{as } \lambda \rightarrow 0^+.$$

Thus the isolated eigenvalue approaches the corresponding threshold as the coupling tends to zero.

Proof. This follows immediately from the monotonicity of $a_K(z)$ and the equation $1 + \lambda a_K(z_\lambda(K)) = 0$. Indeed, as $\lambda \rightarrow 0^\pm$, the zero must move toward the point where $a_K(z)$ becomes unbounded, namely the corresponding band edge. $\square$

5.5. The exceptional flat-band case $K = \pi$

We now treat the degenerate situation $K = \pi$. The dispersion relation becomes constant:

$$\mathcal{E}_\pi(q) \equiv 4, \quad q \in \mathbb{T}.$$

Hence the free fiber operator is a scalar multiple of the identity, and the essential spectrum collapses to the single point

$$\sigma_{\text{ess}}(\mathbf{h}_\lambda(\pi)) = \{4\}.$$

The rank-one perturbation takes the form

$$(\mathbf{h}_\lambda(\pi)g)(q) = 4g(q) + \lambda \int_{\mathbb{T}} g(t) d\nu(t).$$

Thus the operator splits into a direct sum of the constant function (the zero mode) and its orthogonal complement. Indeed, write

$$L^2(\mathbb{T}) = \mathbb{C}\mathbf{1} \oplus \{\mathbf{1}\}^\perp,$$

where $\mathbf{1}(q) \equiv 1$. Then for any g orthogonal to $\mathbf{1}$, we have

$$\mathbf{h}_\lambda(\pi)g = 4g,$$

so the whole orthogonal complement is an eigenspace with eigenvalue 4. On the one-dimensional subspace spanned by $\mathbf{1}$, the operator acts as

$$\mathbf{h}_\lambda(\pi)\mathbf{1} = 4\mathbf{1} + \lambda\mathbf{1} = (4 + \lambda)\mathbf{1}.$$

Therefore the spectrum of $\mathbf{h}_\lambda(\pi)$ is

$$\sigma(\mathbf{h}_\lambda(\pi)) = \{4\} \cup \{4 + \lambda\},$$

where the eigenvalue 4 has infinite multiplicity (the whole orthogonal complement), and the eigenvalue $4 + \lambda$ is simple with eigenvector $\mathbf{1}$.

Consequently:

- If $\lambda = 0$, the operator reduces to the free one: all states have energy 4 (the essential spectrum).
- If $\lambda \neq 0$, the eigenvalue $4 + \lambda$ is isolated and lies outside the essential spectrum if and only if $\lambda \neq 0$. Specifically, for $\lambda < 0$ we have $4 + \lambda < 4$, giving a discrete eigenvalue below the essential point; for $\lambda > 0$ we have $4 + \lambda > 4$, giving a discrete eigenvalue above.

The threshold analysis in this flat-band case is trivial because there is no continuous band. The notions of threshold eigenvalue and threshold resonance become degenerate. Nevertheless, one may still consider the formal threshold profile at $E = 4$. The equation

$$(\mathcal{E}_\pi(q) - 4)g(q) + \lambda c = 0$$

reduces to $\lambda c = 0$. Hence a nontrivial threshold solution exists only if $\lambda = 0$, in which case any function g with zero mean is a solution (in fact an eigenfunction). For $\lambda \neq 0$, the only solution is $g \equiv 0$. Thus the flat-band case exhibits a different behaviour: the threshold is not a resonance for $\lambda \neq 0$ but rather the essential spectrum is a single point that also supports an embedded eigenvalue when $\lambda = 0$.

Remark 6. From the perspective of the limit $K \rightarrow \pi$ with $K \neq \pi$, the band edges satisfy $\mathcal{E}_K^- \rightarrow 4$ and $\mathcal{E}_K^+ \rightarrow 4$. The discrete eigenvalue $z_\lambda(K)$ approaches 4 as $K \rightarrow \pi$ for any fixed $\lambda \neq 0$, in agreement with the fact that for $K = \pi$ the eigenvalue becomes $4 + \lambda$ (which is not equal to 4 unless $\lambda = 0$). The apparent discontinuity is resolved by noting that the essential spectrum collapses, so the notion of “outside the essential band” changes.

6. Conclusion

We have provided a complete spectral analysis of the fiber hamiltonians $H_{\gamma,\lambda}(K)$ in the constant-profile case. By exploiting the rank-two nature of the perturbation, we reduced the eigenvalue problem to a 2×2 linear system and obtained a scalar Fredholm determinant whose zeros give the discrete spectrum. The explicit form of the lattice Green function $a_K(z)$ allowed us to compute threshold asymptotics and to classify the discrete spectrum below and above the essential band in terms of the critical coefficients $S_K^\pm(\gamma, \lambda)$. The results cover all generic positions of E_0 relative to the band, as well as the threshold configurations $E_0 = \mathcal{E}_K^\pm$. The flat-band case $K = \pi$ was treated separately.

In addition, we studied the rank-one fiber operator $\mathbf{h}_\lambda(K)$, which serves as a simplified model. We showed that for $K \neq \pi$ the band edges are threshold resonances (not eigenvalues) in a natural weighted L^2 space, and we characterized its discrete spectrum. The flat-band case $K = \pi$ exhibits a degenerate essential spectrum and an extra isolated eigenvalue.

These results form a solid foundation for further investigations, such as the analysis of the full two-channel model with a non-constant profile $\alpha(q)$, or the study of resonances and scattering theory.

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