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Original article

Two-fermion lattice Schrödinger operators with first and second nearest-neighboring-site interactions

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ABSTRACT We study the Schrödinger operators $H_{\lambda\mu}(K)$ that model a two-fermion system on the three-dimensional lattice $\mathbb{Z}^3$, where total quasimomentum is fixed at $K \in \mathbb{T}^3$, and the particles interact through nearest- and next-nearest-neighbor couplings with strengths $\lambda, \mu \in \mathbb{R}$. For $K = 0$, we establish that $H_{\lambda\mu}(0)$ admits reducing invariant subspace whose restriction depends solely on the parameter $\mu \in \mathbb{R}$. This μ parameter line contains two *critical* points corresponding to the lower and upper spectral thresholds; at each of these points, the Fredholm determinant of the restricted operator vanishes. Each of these critical points divides the parameter line into two infinite intervals, where the number of eigenvalues lying below (or above) the essential spectrum remains constant. Depending on μ, the corresponding reduced operator has exactly one discrete eigenvalue, located either below the bottom or above the top of the essential spectrum. Moreover, we derive a lower bound on the number of discrete eigenvalues of $H_{\lambda\mu}(K)$ for all $K \in \mathbb{T}^3$.

KEYWORDS Two-fermion system; lattice Schrödinger operator; discrete eigenvalues; essential spectrum; reduced subspaces.

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1. Introduction

Lattice models play a central role in many areas of modern physics. Among these are the two-body and three-body lattice Hamiltonians, which represent simplified formulations of the Bose- and Fermi-Hubbard models respectively, and describe systems with fixed number of identical particles. For one-particle lattice Schrödinger operators defined on one-, two-, and three-dimensional lattices, the existence, finiteness, and localization of discrete eigenvalues relative to the essential spectrum have been established; see, for example, the one- and two-dimensional cases in [1, 2] and the three-dimensional setting in [3]. These results were subsequently extended to two-particle lattice systems. In particular, for Hamiltonians on one-, two-, and three-dimensional lattices on-site (zero-range) interactions and one-step nearest-neighbor interactions, the existence of discrete eigenvalues below and above the essential spectrum was rigorously proved. Moreover, at zero total quasi-momentum $K = 0$, the threshold phenomena such as the appearance of an eigenvalue or a virtual level at the spectral edges were analyzed in detail [4–7]. These studies also revealed a pronounced dependence on bound states on the total quasi-momentum and covered both bosonic and fermionic symmetry classes. The three-particle problem was subsequently investigated for lattice Schrödinger Hamiltonians on one- and three-dimensional lattices with zero-range (on-site) interactions. In this setting, the structure of the essential spectrum and the finiteness or infiniteness of the discrete spectrum were described, and, in the presence of a zero-range resonance in the corresponding two-particle subsystems, Efimov-type effects and asymptotic laws for the distribution of eigenvalues were established [8–14]. Moreover, these discrete Hamiltonians may be viewed as natural approximations to their continuous counterparts [15]. By discretizing configuration space, one obtains bounded operators on the lattice Hilbert spaces whose spectral behaviour approximates that of the continuous few-body Schrödinger operators in the continuum limit; this observation allows a rigorous treatment of few-body quantum systems within the framework of bounded operator theory and often simplifies technical aspects of the spectral analysis. However, unlike the continuous setting, the few-body lattice Hamiltonian does not admit a full separation of the center-of-mass motion: the lattice discretization breaks the continuous translation (and Galilean) symmetry and couples center-of-mass and relative degrees of freedom. Nevertheless, the system retains discrete translational invariance, which makes it possible to apply the Floquet-Bloch decomposition. As a result, the full lattice Hamiltonian decomposes into a direct integral of fiber operators $H(K)$ parameterized by the quasimomentum $K \in \mathbb{T}^d$, so that spectral questions may be reduced to the analysis of these fiber operators (see, for example, [16, Section 4]). In the current paper, we investigate the spectral properties of a family of Hamiltonians describing two-fermion lattice systems with nearest- and next-nearest-neighbor interactions. In particular, the Hamiltonian studied here represents the three-dimensional case of the model presented in [16]. In the momentum representation, after a von Neumann direct integral decomposition over the quasi-momentum $K \in \mathbb{T}^3$, the two-fermion system is described by the fiber Schrödinger operator (see [4, 16])

$$H_{\lambda\mu}(K) = H_0 + V_{\lambda\mu}, \qquad \lambda, \mu \in \mathbb{R}, \tag{1}$$

acting in the subspace

$$L^{2,o}(\mathbb{T}^3) = \{f \in L^2(\mathbb{T}^3) : f(-p) = -f(p)\},$$

of odd functions on the torus $\mathbb{T}^3 = (-\pi, \pi]^3$ with Haar measure.

The free Hamiltonian part is the multiplication operator

$$H_0(K)f(p) = \mathcal{E}_K(p)f(p), \quad \mathcal{E}_K(p) = \varepsilon\left(\frac{K}{2} + p\right) + \varepsilon\left(\frac{K}{2} - p\right), \quad \varepsilon(p) = 2\sum_{i=1}^{3}(1 - \cos p_i), \tag{2}$$

and interaction $V_{\lambda\mu}$ is an integral operator in $L^{2,o}(\mathbb{T}^3)$ with smooth kernel

$$v_{\lambda\mu}(p) = \mu\left(\sum_{i=1}^{3} \cos p_i\right)^2 + \mu\sum_{i=1}^{3}\cos^2 p_i + \lambda\sum_{i=1}^{3}\cos p_i - 3\mu, \qquad p \in \mathbb{T}^3,$$

in particular, the rank of $V_{\lambda\mu}$ depends on the values $\lambda, \mu \in \mathbb{R}$ and does not exceed 12.

For $K = 0$, since the operator $H_0(0)$ is multiplication by an even, permutation-symmetric function and the parity structure of $V_{\lambda\mu}$, one obtains the decomposition

$$L^{2,o}(\mathbb{T}^3) = \bigoplus_{\theta\in\{\mathrm{eeo},\mathrm{eoe},\mathrm{oee},\mathrm{ooo}\}} L^{2,\theta}(\mathbb{T}^3) \tag{3}$$

where, for example, $\theta = \mathrm{eeo}$ means that the function is even in the first two coordinates and odd in the third.

In the case $\theta = \mathrm{ooo}$ the interaction vanishes, so this subspace does not contribute to the discrete spectrum. For each $\theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}\}$, the subspace $L^{2,\theta}(\mathbb{T}^3)$ is naturally associated with a distinguished transposition $\sigma = \sigma_\theta$ of the coordinate variables, defined by

$$\sigma_{\mathrm{eeo}}(p_1, p_2, p_3) = (p_2, p_1, p_3), \qquad \sigma_{\mathrm{eoe}}(p_1, p_2, p_3) = (p_3, p_2, p_1), \qquad \sigma_{\mathrm{oee}}(p_1, p_2, p_3) = (p_1, p_3, p_2).$$

With respect to the action of this transposition σ_θ, the space $L^{2,\theta}(\mathbb{T}^3)$ admits the orthogonal decomposition

$$L^{2,\theta}(\mathbb{T}^3) = L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3) \oplus L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3), \tag{4}$$

where

$$L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3) = \{f \in L^{2,\theta}(\mathbb{T}^3) : f \circ \sigma_\theta = f\}, \quad L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3) = \{f \in L^{2,\theta}(\mathbb{T}^3) : f \circ \sigma_\theta = -f\}.$$

We focus on the antisymmetric subspaces

$$L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3), \qquad \theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}\}$$

and, by unitary equivalence, reduce the analysis to the representative case $\theta = \mathrm{eeo}$.

Our main results are as follows:

(i) Unitary equivalence of $H_\mu^{\theta,\mathrm{asym}}(0)$ for $\theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}\}$;

(ii) Exact determination of the eigenvalues of $H_\mu^{\theta,\mathrm{asym}}(0)$ outside the essential spectrum;

(iii) Bounds on the number of eigenvalues of $H_{\lambda\mu}(K)$ for arbitrary $K \in \mathbb{T}^3$.

Further, we study the class of rank-one self-adjoint perturbations V for which the perturbed Schrödinger operator $H_\mu^{\theta,\mathrm{asym}}(0)$ possesses a prescribed number of eigenvalues lying to the left or right of its essential spectrum. The model is exactly solvable, and its discrete spectrum demonstrates the creation and annihilation of bound states triggered by small perturbations of potential V supported on finite subsets of the three dimensional lattice $\mathbb{Z}^3$. When such a phenomenon of emergence and disappearance occurs at the lower (resp. upper) edge of the essential spectrum of $H_\mu^{\theta,\mathrm{asym}}(0)$, we say that the operator is *critical* at that edge. We prove that the set of perturbations V leading to criticality consists of a single point on the parameter line. This yields a precise algebraic-geometric framework for analyzing the stability and bifurcation of bound states in the lattice Schrödinger operators. Finally, since the eigenvalues of $H_\mu^{\theta,\mathrm{asym}}(0)$ are in one-to-one correspondence with the zeros of the Fredholm determinant $\Delta_\mu(z)$ (see [7]), the problem reduces to the study of the zeros of $\Delta_\mu(z)$.

Previous works [2, 3, 7, 16] have studied the two-particle Schrödinger operator $H_{\lambda\mu}(K)$, where $K \in \mathbb{T}^d$ denotes the total quasimomentum of the two-particle system. This operator naturally emerges in the framework of the Bose-Hubbard model, which describes the quantum dynamics of two identical particles bosons or fermions on a discrete lattice $\mathbb{Z}^d$ in spatial dimensions ($1 \le d \le 3$). The particle interactions are governed by two real parameters, λ and μ, representing the strengths of the interaction at the same site and between nearest-neighbor sites, respectively. For the three-dimensional lattice $\mathbb{Z}^3$, the bosonic operator $H_{\gamma\lambda\mu}(K)$ with on-site (γ) and nearest-neighbor (λ, μ) interactions was analyzed in [17]. It was shown that its restriction to a certain invariant subspace depends only on the interaction parameters λ and μ; the mechanisms of eigenvalue emergence and disappearance are described in terms of the critical operator. Moreover, conditions ensuring the existence of exactly α eigenvalues below and β eigenvalues above the essential spectrum, with $\alpha + \beta \leq 2$, were established. For the two-dimensional lattice $\mathbb{Z}^2$, the same operator structure was considered in [18] with on-site (γ), nearest-neighbor (λ, μ), and next-nearest-neighbor (μ) interactions. It was proved that, for suitable interaction parameters, the operator has exactly seven eigenvalues outside the essential spectrum for all $K \in \mathbb{T}^2$.

The structure of the paper is as follows. In Section 2, we introduce the two-fermion Schrödinger operator in the quasimomentum representation. In Section 3, several preliminary results are established. The main results of the paper are formulated in Section 4. Finally, Section 5 is devoted to the detailed proofs of these results.

2. Schrödinger operator of a two-fermion system on lattices

2.1. The two-fermion Schrödinger operator in the quasimomentum representation

We denote by $\mathbb{T}^3 = (\mathbb{R}/2\pi\mathbb{Z})^3 \equiv (-\pi, \pi]^3$ the three-dimensional torus. It can be naturally identified with the Pontryagin dual group of $\mathbb{Z}^3$ and is equipped with the Haar measure $\mathrm{d}p$.

In the quasimomentum representation, the lattice Schrödinger operator $H_{\lambda\mu}(K), K \in \mathbb{T}^3$ of the two-fermion system acting in the subspace $L^{2,o}(\mathbb{T}^3)$ of odd functions on $\mathbb{T}^3$, $L^{2,o}(\mathbb{T}^3) = \{f \in L^2(\mathbb{T}^3) : f(-p) = -f(p)\}$ (see [4, 16]).

The operator $H_{\lambda\mu}(K)$ is given by

$$H_{\lambda\mu}(K) := H_0(K) + V_{\lambda\mu}, \qquad \lambda, \mu \in \mathbb{R}, \tag{5}$$

where $H_0(K)$ is the multiplication operator associated with the function defined by (2) and the potential $V_{\lambda\mu}$ is an integral operator of the form

$$\begin{aligned}[V_{\lambda\mu}f](p) = {}& \frac{\lambda}{4\pi^3}\sum_{i=1}^{3}\sin p_i \int_{\mathbb{T}^3} \sin q_i f(q)\mathrm{d}q + \frac{\mu}{4\pi^3}\sum_{i=1}^{3}\sin 2p_i \int_{\mathbb{T}^3} \sin 2q_i f(q)\mathrm{d}q + \\ & + \frac{\mu}{2\pi^3}\sum_{1\leq i<j\leq 3}\left(\cos p_i \sin p_j \int_{\mathbb{T}^3} \cos q_i \sin q_j f(q)\mathrm{d}q + \cos p_j \sin p_i \int_{\mathbb{T}^3} \cos q_j \sin q_i f(q)\mathrm{d}q\right).\end{aligned} \tag{6}$$

Both operators $H_0(K)$ and $V_{\lambda\mu}$ are bounded and self-adjoint. In scientific literature, the parameter $K \in \mathbb{T}^3$ is commonly referred to as the *two-particle quasimomentum*, while $H_{\lambda\mu}(K)$ is usually called the *discrete Schrödinger operator* associated with the two-particle Hamiltonian $\hat{\mathbb{H}}_{\lambda\mu}$.

3. Some preliminaries

3.1. Analyzing the essential spectrum of discrete Schrödinger operators

The rank of the operator $V_{\lambda\mu}$, which depends on the values of λ and μ, is at most twelve. Due to this, and by applying Weyl's theorem, the essential spectrum of $H_{\lambda\mu}(K)$ is the same as the spectrum of $H_0(K)$ for any $K \in \mathbb{T}^3$. This means that $\sigma_{\mathrm{ess}}(H_{\lambda\mu}(K))$ equals the spectrum of $H_0(K)$, i.e.,

$$\sigma_{\mathrm{ess}}(H_{\lambda\mu}(K)) = \sigma(H_0(K)) = [\mathcal{E}_{\min}(K), \mathcal{E}_{\max}(K)], \tag{7}$$

where the minimum and maximum values of the essential spectrum are given by:

$$\mathcal{E}_{\min}(K) := \min_{p\in\mathbb{T}^3} \mathcal{E}_K(p) = 4\sum_{i=1}^{3}\left(1 - \cos\frac{K_i}{2}\right) \geq \mathcal{E}_{\min}(0) = 0,$$

$$\mathcal{E}_{\max}(K) := \max_{p\in\mathbb{T}^3} \mathcal{E}_K(p) = 4\sum_{i=1}^{3}\left(1 + \cos\frac{K_i}{2}\right) \leq \mathcal{E}_{\max}(0) = 24,$$

and the function $\mathcal{E}_K(p)$ is defined as:

$$\mathcal{E}_K(p) := 4\sum_{i=1}^{3}\left(1 - \cos\frac{K_i}{2}\cos p_i\right). \tag{8}$$

3.2. Decomposition into invariant subspaces and unitary equivalence

For each $\theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}, \mathrm{ooo}\}$, let $L^{2,\theta}(\mathbb{T}^3) \subset L^{2,o}(\mathbb{T}^3)$ denote the subspaces of odd functions defined by

$$L^{2,\mathrm{eeo}}(\mathbb{T}^3) = \{f \in L^{2,o}(\mathbb{T}^3) : f(p_1,p_2,p_3) = f(-p_1,p_2,p_3) = f(p_1,-p_2,p_3)\}$$
$$L^{2,\mathrm{eoe}}(\mathbb{T}^3) = \{f \in L^{2,o}(\mathbb{T}^3) : f(p_1,p_2,p_3) = f(-p_1,p_2,p_3) = f(p_1,p_2,-p_3)\}$$
$$L^{2,\mathrm{oee}}(\mathbb{T}^3) = \{f \in L^{2,o}(\mathbb{T}^3) : f(p_1,p_2,p_3) = f(p_1,-p_2,p_3) = f(p_1,p_2,-p_3)\}$$
$$L^{2,\mathrm{ooo}}(\mathbb{T}^3) = \{f \in L^{2,o}(\mathbb{T}^3) : f(p_1,p_2,p_3) = -f(-p_1,p_2,p_3) = -f(p_1,-p_2,p_3)\}$$

for a.e $(p_1,p_2,p_3) \in \mathbb{T}^3$.

Lemma 1. *The equality*

$$L^{2,\mathrm{o}}(\mathbb{T}^3) = \bigoplus_{\theta\in\{\mathrm{eeo},\mathrm{eoe},\mathrm{oee},\mathrm{ooo}\}} L^{2,\theta}(\mathbb{T}^3) \tag{9}$$

holds true.

Proof. Let $f \in L^{2,o}(\mathbb{T}^3)$. Define the following four functions:

$$f^{\mathrm{eeo}}(p_1,p_2,p_3) = \frac{1}{4}\big[f(p_1,p_2,p_3) + f(-p_1,p_2,p_3) + f(p_1,-p_2,p_3) - f(p_1,p_2,-p_3)\big] \in L^{2,\mathrm{eeo}}(\mathbb{T}^3),$$
$$f^{\mathrm{eoe}}(p_1,p_2,p_3) = \frac{1}{4}\big[f(p_1,p_2,p_3) + f(-p_1,p_2,p_3) - f(p_1,-p_2,p_3) + f(p_1,p_2,-p_3)\big] \in L^{2,\mathrm{eoe}}(\mathbb{T}^3),$$
$$f^{\mathrm{oee}}(p_1,p_2,p_3) = \frac{1}{4}\big[f(p_1,p_2,p_3) - f(-p_1,p_2,p_3) + f(p_1,-p_2,p_3) + f(p_1,p_2,-p_3)\big] \in L^{2,\mathrm{oee}}(\mathbb{T}^3),$$
$$f^{\mathrm{ooo}}(p_1,p_2,p_3) = \frac{1}{4}\big[f(p_1,p_2,p_3) - f(-p_1,p_2,p_3) - f(p_1,-p_2,p_3) - f(p_1,p_2,-p_3)\big] \in L^{2,\mathrm{ooo}}(\mathbb{T}^3).$$

By direct calculation, we have $f = f^{\mathrm{eeo}} + f^{\mathrm{eoe}} + f^{\mathrm{oee}} + f^{\mathrm{ooo}}$.

Let $h = f^{\theta_1}\overline{f^{\theta_2}}$, where $\theta_1 \neq \theta_2$ and $\theta_1, \theta_2 \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}, \mathrm{ooo}\}$. The function $h = f^{\theta_1}\overline{f^{\theta_2}}$ is odd in at least one variable, hence, its integral over $\mathbb{T}^3$ vanishes. Therefore, $\langle f^{\theta_1} f^{\theta_2}\rangle = 0$, which proves orthogonality. □

By the structure of the perturbation operator $V_{\lambda\mu}$, its restriction to $L^{2,\mathrm{ooo}}(\mathbb{T}^3)$ vanishes. Therefore, it suffices to analyze the remaining three subspaces $L^{2,\mathrm{eeo}}(\mathbb{T}^3)$, $L^{2,\mathrm{eoe}}(\mathbb{T}^3)$ and $L^{2,\mathrm{oee}}(\mathbb{T}^3)$, each admitting a decomposition into symmetric and antisymmetric components with respect to the corresponding transposition:

$$\sigma_\theta = \begin{cases} (12), & \text{if } \theta = \mathrm{eeo}, \\ (13), & \text{if } \theta = \mathrm{eoe}, \\ (23), & \text{if } \theta = \mathrm{oee}. \end{cases}$$

Lemma 2. *For any $f \in L^{2,\theta}(\mathbb{T}^3), \theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}\}$, there exists an orthogonal decomposition $f = f^{\mathrm{sym}} + f^{\mathrm{asym}}$ where f^{sym} is symmetric and f^{asym} is antisymmetric under the transposition σ.*

Proof. For $f \in L^{2,\theta}(\mathbb{T}^3)$, define:

$$f^{\mathrm{sym}} := \frac{1}{2}\left(f(p) + f(\sigma_\theta p)\right)$$
$$f^{\mathrm{asym}} := \frac{1}{2}\left(f(p) - f(\sigma_\theta p)\right)$$

These satisfy:

- $f = f^{\mathrm{sym}} + f^{\mathrm{asym}}$ (by direct computation)
- $f^{\mathrm{sym}}(\sigma_\theta p) = f^{\mathrm{sym}}(p)$ (symmetric)
- $f^{\mathrm{asym}}(\sigma_\theta p) = -f^{\mathrm{asym}}(p)$ (antisymmetric)

□

We define the symmetric and antisymmetric subspaces of $L^{2,\theta}(\mathbb{T}^3)$ with respect to the σ transposition as

$$L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3) := \left\{f \in L^{2,\theta}(\mathbb{T}^3) : f(p) = f(\sigma_\theta p)\right\},$$
$$L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3) := \left\{f \in L^{2,\theta}(\mathbb{T}^3) : f(p) = -f(\sigma_\theta p)\right\}.$$

The operator $H_0(0)$ is a multiplication operator defined by the even function $\mathcal{E}_0(p)$, that is symmetric with respect to permutation of the variables p_1, p_2, p_3. This operator acts on the space $L^{2,o}(\mathbb{T}^3)$. Hence, for each parity type θ, the subspaces $L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3)$ and $L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3)$ are invariant with respect to $H_0(0)$.

According the equalities

$$2\cos p_1 \cos q_1 + 2\cos p_2 \cos q_2 = (\cos p_1 + \cos p_2)(\cos q_1 + \cos q_2) + (\cos p_2 - \cos p_1)(\cos q_2 - \cos q_1),$$
$$2\cos p_1 \cos q_1 + 2\cos p_3 \cos q_3 = (\cos p_1 + \cos p_3)(\cos q_1 + \cos q_3) + (\cos p_3 - \cos p_1)(\cos q_3 - \cos q_1),$$
$$2\cos p_2 \cos q_2 + 2\cos p_3 \cos q_3 = (\cos p_2 + \cos p_3)(\cos q_2 + \cos q_3) + (\cos p_3 - \cos p_2)(\cos q_3 - \cos q_2),$$

the operator $V_{\lambda\mu}$ in (6) can be written as

$$[V_{\lambda\mu}f](p) = \frac{\lambda}{4\pi^3}\sum_{i=1}^{3}\sin p_i \int_{\mathbb{T}^3} \sin q_i f(q)\mathrm{d}q + \frac{\mu}{4\pi^3}\sum_{i=1}^{3}\sin 2p_i \int_{\mathbb{T}^3} \sin 2q_i f(q)\mathrm{dq}$$
$$+ \sum_{\substack{i,j,k\,\in\{1,2,3\}\\ i\neq j\neq k}} \frac{\mu}{4\pi^3}[\sin p_i(\cos p_j + \cos p_k)\int_{\mathbb{T}^3} \sin q_i(\cos q_j + \cos q_k) f(q)\mathrm{d}q$$
$$+ \sin p_i(\cos p_j - \cos p_k)\int_{\mathbb{T}^3} \sin q_i(\cos q_j - \cos q_k) f(q)\mathrm{d}q]. \tag{10}$$

From (10), it follows that the subspaces $L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3)$ and $L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3)$ are invariant subspaces of the operator $V_{\lambda\mu}$. Consequently, these subspaces are also invariant with respect to $H_{\lambda\mu}(0)$, and hence, they provide a reduction of this operator. Therefore, the spectrum of the operator $H_{\lambda\mu}(0)$ satisfies

$$\sigma\big(H_{\lambda\mu}(0)\big) = \bigcup_{\theta\in\{\mathrm{eeo},\,\mathrm{eoe},\,\mathrm{oee}\}} \sigma\big(H_{\lambda\mu}(0)\big|_{L^{2,\theta,\mathrm{sym}}(\mathbb{T}^3)}\big) \cup \sigma\big(H_{\lambda\mu}(0)\big|_{L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3)}\big). \tag{11}$$

Let us denote by $V_\mu^{\theta,\mathrm{asym}}$ the restriction of the operator $V_{\lambda\mu}$ to the antisymmetric subspaces $L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3)$; note that this restriction does not depend on λ, since the coupling constant λ appears only in the symmetric part of $V_{\lambda\mu}$. Applying the representation (10) of the $V_{\lambda\mu}$ yields

$$[V_\mu^{\mathrm{eeo,asym}}f](p) = \frac{\mu}{4\pi^3}\sin p_3(\cos p_2 - \cos p_1)\int_{\mathbb{T}^3} \sin q_3(\cos q_2 - \cos q_1) f(q)\mathrm{d}q,$$

$$[V_\mu^{\mathrm{eoe,asym}}f](p) = \frac{\mu}{4\pi^3}\sin p_2(\cos p_3 - \cos p_1)\int_{\mathbb{T}^3} \sin q_2(\cos q_3 - \cos q_1) f(q)\mathrm{d}q,$$

$$[V_\mu^{\mathrm{oee,asym}}f](p) = \frac{\mu}{4\pi^3}\sin p_1(\cos p_3 - \cos p_2)\int_{\mathbb{T}^3} \sin q_1(\cos q_3 - \cos q_2) f(q)\mathrm{d}q.$$

Let us introduce the notation

$$H_\mu^{\theta,\mathrm{asym}}(0) := H_{\lambda\mu}(0)\mid_{L^{2,\theta,\mathrm{asym}}(\mathbb{T}^3)} = H_0 + V^{\theta,\mathrm{asym}}.$$

Lemma 3. *Let*

$$\mathbb{U}_1 : L^{2,\mathrm{eoe,asym}}(\mathbb{T}^3) \to L^{2,\mathrm{eeo,asym}}(\mathbb{T}^3), \qquad \mathbb{U}_2 : L^{2,\mathrm{oee,asym}}(\mathbb{T}^3) \to L^{2,\mathrm{eeo,asym}}(\mathbb{T}^3)$$

be the permutation operators defined for almost all $(p_1, p_2, p_3) \in \mathbb{T}^3$ *by*

$$(\mathbb{U}_1 f)(p_1, p_2, p_3) = f(p_1, p_3, p_2), \qquad (\mathbb{U}_2 f)(p_1, p_2, p_3) = f(p_2, p_3, p_1).$$

Then

$$\mathbb{U}_1 V_\mu^{\mathrm{eoe,asym}}\mathbb{U}_1^* = V_\mu^{\mathrm{eeo,asym}}, \qquad \mathbb{U}_2 V_\mu^{\mathrm{oee,asym}}\mathbb{U}_2^* = V_\mu^{\mathrm{eeo,asym}}.$$

Consequently, the Hamiltonians

$$H_\mu^{\theta,\mathrm{asym}}(0), \qquad \theta \in \{\mathrm{eeo}, \mathrm{eoe}, \mathrm{oee}\},$$

are unitarily equivalent, and hence have identical spectra. It is therefore sufficient to analyze the case $\theta = \mathrm{eeo}$.

Proof. The operators $\mathbb{U}_1$ and $\mathbb{U}_2$ are unitary since coordinate permutations preserve the Lebesgue measure on $\mathbb{T}^3$. By construction, $V_\mu^{\theta,\mathrm{asym}}$ is defined by the same formula $\mathcal{V}_\mu$, with the role of the variables permuted according to θ. Conjugating $V_\mu^{\mathrm{eoe,asym}}$ by $\mathbb{U}_1$ relabels the coordinates (p_2, p_3), yielding $V_\mu^{\mathrm{eeo,asym}}$, and similarly for $\mathbb{U}_2$. Since $H_\mu^{\theta,\mathrm{asym}}(0)$ is the sum of the same free part and the corresponding $V_\mu^{\theta,\mathrm{asym}}$, these conjugation relations extend directly to the full Hamiltonians, proving their unitary equivalence. □

Remark 1. *This lemma establishes that the Hamiltonians associated with the labels* eeo, eoe *and* oee *are unitarily equivalent, as they differ only by permutations of coordinates. Consequently, their spectra coincide, and it is sufficient to carry out the spectral analysis for any one of these Hamiltonians.*

Remark 2. *The main objective of this work is to characterize the eigenvalues of* $H_\mu^{\mathrm{eeo,asym}}(0)$ *that lie outside the essential spectrum. In particular, we aim to estimate the number of eigenvalues of the operator* $H_{\lambda\mu}(K)$ *for any* $K \in \mathbb{T}^3$.

4. Main results of the work

It is known that the essential spectrum of the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ coincides with the interval $[0, 24]$. To identify discrete eigenvalues of $H_\mu^{\mathrm{eeo,asym}}(0)$, we aim to derive an implicit equation using Fredholm determinant theory. To determine the discrete eigenvalues, it suffices to consider the eigenvalue equation

$$H_\mu^{\mathrm{eeo,asym}}(0)f = zf$$

for $z \in \mathbb{R} \setminus [0, 24]$ and nontrivial functions $f \in L^{2,\mathrm{eeo,asym}}(\mathbb{T}^3)$. The Fredholm determinant associated with the operator $H_\mu^{\mathrm{eeo,asym}}(0)$, denoted by $\Delta_\mu(z)$, is given by

$$\Delta_\mu(z) = 1 + \mu a(z), \tag{12}$$

where

$$a(z) = \frac{1}{4\pi^3} \int\limits_{\mathbb{T}^3} \frac{\sin^2 p_1 (\cos p_3 - \cos p_2)^2 \mathrm{d}p}{\mathcal{E}_0(p) - z}. \tag{13}$$

Lemma 4. *A number $z \in \mathbb{R} \setminus [0, 24]$ is an eigenvalue of the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ if and only if the condition*

$$\Delta_\mu(z) = 0 \tag{14}$$

is satisfied. Furthermore, within $\mathbb{R} \setminus [0, 24]$ the function $\Delta_\mu(z)$ admits at most one root.

The proof of this lemma is quite standard (cf., e.g., [3, 7]).

Lemma 5. *The functions $\Delta_\mu(z)$ and $a(z)$ defined in $\mathbb{R} \setminus [0, 24]$ are real-valued. Moreover, $a(z)$ is strictly increasing and positive in $(-\infty, 0)$, strictly increasing and negative in $(24, +\infty)$, and satisfies the following asymptotic relations:*

$$\lim_{z \nearrow 0} a(z) = a(0), \quad \lim_{z \searrow 24} a(z) = -a(0), \quad \lim_{z \to \pm\infty} a(z) = 0,$$

and

$$\lim_{z \nearrow 0} \Delta_\mu(z) = 1 + a(0)\mu, \quad \lim_{z \searrow 24} \Delta_\mu(z) = 1 - a(0)\mu, \quad \lim_{z \to \pm\infty} \Delta_\mu(z) = 1.$$

Proof. The asymptotic formulas for the function $a(z)$, defined in (13) can be proved as in Lemma 4.7 of [16]. Hence, we omit the corresponding calculations. The asymptotic behavior of the function $\Delta_\mu(z)$ follows directly from (12) together with the asymptotic of $a(z)$. □

Remark 3. *The value $a(0)$ is given by the integral representation (see (13))*

$$a(0) = \frac{1}{4\pi^3} \int_{\mathbb{T}^3} \frac{\sin^2 p_1 (\cos p_3 - \cos p_2)^2}{\mathcal{E}_0(p)} \, dp.$$

A numerical evaluation using a standard quadrature on a uniform grid (with mesh size $N \times N \times N$ and convergence check in N) gives

$$a(0) \approx 0.0891,$$

with accuracy about 10^{-4} (stable under further grid refinement).

The following theorem presents the first main result of this paper, which gives one a complete description of the discrete spectrum of the operator $H_\mu^{\mathrm{eeo,asym}}(0)$.

Theorem 1. *Let $\mu \in \mathbb{R}$. Then the following statements hold for $H_\mu^{\mathrm{eeo,asym}}(0)$.*

(i) *For any $\mu \in [-\frac{1}{a(0)}, \frac{1}{a(0)}]$ the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ has no eigenvalues outside the essential spectrum.*

(ii) *For any $\mu < -\frac{1}{a(0)}$ the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ has a unique simple eigenvalue $z(\mu; 0) < 0$ and the associated eigenfunction can be written as*

$$f_\mu(p) = C \frac{\sin p_3 (\cos p_2 - \cos p_1)}{\mathcal{E}_0(p) - z(\mu; 0)}, \quad p \in \mathbb{T}^3, \tag{15}$$

where $C \in \mathbb{R}$ is a (nonzero) normalization constant.

(iii) *For any $\mu > \frac{1}{a(0)}$, the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ has a unique simple eigenvalue $z(\mu; 0) > 24$ and the associated eigenfunction can be written as*

$$f_\mu(p) = C \frac{\sin p_3 (\cos p_2 - \cos p_1)}{z(\mu; 0) - \mathcal{E}_0(p)}, \quad p \in \mathbb{T}^3, \tag{16}$$

where $C \in \mathbb{R}$ is a (nonzero) normalization constant.

4.1. Critical operators

To clarify the mechanisms responsible for eigenvalue emergence and annihilation, we introduce the notion of a *critical* operator.

Definition 1. *We say that the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at a point $\mu_0 \in \mathbb{R}$ if the map*

$$\mathbb{R} \ni \mu \ \mapsto \ \mathrm{tr}\ E_{H_\mu^{\mathrm{eeo,asym}}(0)}\left(\mathbb{R} \setminus \sigma_{\mathrm{ess}}(H_\mu^{\mathrm{eeo,asym}}(0))\right) \tag{17}$$

is discontinuous at μ_0. Here $E_H(\cdot)$ denotes the spectral projection of the operator $H_\mu^{\mathrm{eeo,asym}}(0)$.

Similarly, we say that $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at an endpoint $z = 0$ or $z = 24$ of the essential spectrum if there exist points $\mu_0^{(-)}, \mu_0^{(+)} \in \mathbb{R}$ such that the maps

$$\begin{aligned} &\mathbb{R} \ni \mu \ \mapsto \ \mathrm{tr}\ E_{H_\mu^{\mathrm{eeo,asym}}(0)}\left((-\infty, \inf \sigma_{\mathrm{ess}}(H_\mu^{\mathrm{eeo,asym}}(0)))\right), \textit{and} \\ &\mathbb{R} \ni \mu \ \mapsto \ \mathrm{tr}\ E_{H_\mu^{\mathrm{eeo,asym}}(0)}\left((\sup \sigma_{\mathrm{ess}}(H_\mu^{\mathrm{eeo,asym}}(0)), \infty)\right) \end{aligned} \tag{18}$$

are discontinuous at $\mu_0^{(-)}$ and $\mu_0^{(+)}$, respectively.

Remark 4. *Since the map in* (17) *takes only integer values, we obtain the following equivalent characterization: The operator $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at $\mu_0 \in \mathbb{R}$ if the number of its eigenvalues outside the essential spectrum fails to remain constant in any neighborhood of μ_0. Likewise, $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at the lower endpoint $z = 0$ (resp. the upper endpoint $z = 24$) if there exists $\mu_0 \in \mathbb{R}$ such that the number of eigenvalues below (resp. above) the essential spectrum is not constant in any neighborhood of μ_0.*

The following theorem provides a precise characterization of the criticality of the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ in terms of the real parameter μ.

Theorem 2. *The operator $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at the lower threshold $z = 0$ (resp., the upper threshold $z = 24$) of the essential spectrum if and only if the leading asymptotic terms of the determinant $\Delta_\mu(z)$ at the corresponding endpoint satisfy*

$$1 + a(0)\mu = 0 \quad \textit{(resp., } 1 - a(0)\mu = 0\textit{)}.$$

In other words, the determinant $\Delta_\mu(z)$ vanishes at $z = 0$ or $z = 24$ according to these asymptotics.

According to the min-max principle, the number of eigenvalues of the operator $H_{\lambda\mu}(K)$ located outside the essential spectrum is not fixed but remains bounded above by twelve.

Theorem 3. *Assume that $K \in \mathbb{T}^3$ and $(\lambda, \mu) \in \mathbb{R}^2$.*

(i) *If $\mu < -\dfrac{1}{a(0)}$, then the operator $H_{\lambda\mu}(K)$ has at least three eigenvalues located below the essential spectrum.*

(ii) *If $\mu > \dfrac{1}{a(0)}$, then the operator $H_{\lambda\mu}(K)$ has at least three eigenvalues located above the essential spectrum.*

5. Proofs of the main results

We first prove the following lemma on the roots of the function Δ_μ, which will be used to establish the main result.

Lemma 6. *Let $\mu \in \mathbb{R}$.*

(i) *If $\mu < -\dfrac{1}{a(0)}$, then the function $\Delta_\mu(\cdot)$ has a unique root $\xi_1(\mu)$ in $(-\infty, 0)$.*

(ii) *If $\mu \in [-\dfrac{1}{a(0)}, \dfrac{1}{a(0)}]$, then the function $\Delta_\mu(\cdot)$ has no roots in $\mathbb{R} \setminus [0, 24]$.*

(iii) *If $\mu > \dfrac{1}{a(0)}$, then the function $\Delta_\mu(\cdot)$ has a unique root $\xi_2(\mu)$ in $(24, +\infty)$.*

Proof. Let us prove the item (i). If $\mu < -\dfrac{1}{a(0)}$, then according to Lemma 5

$$\lim_{z \nearrow 0} \Delta_\mu(z) < 0$$

and

$$\lim_{z \to -\infty} \Delta_\mu(z) = 1.$$

Hence there exists a number $\xi_1(\mu)$ in $(-\infty, 0)$ such that

$$\Delta_\mu(\xi_1(\mu)) = 0.$$

Since the rank of the operator $V_\mu^{\mathrm{eeo,asym}}$ is equal to one, there exists a unique root.

If $\mu \in [-\frac{1}{a(0)}, \frac{1}{a(0)}]$, then according to Lemma 5, the inequalities

$$\lim_{z \nearrow 0} \Delta_\mu(z) > 0, \quad \lim_{z \searrow 24} \Delta_\mu(z) > 0$$

hold. Since

$$\lim_{z \to \pm\infty} \Delta_\mu(z) = 1,$$

the functions $\Delta_\mu(\cdot)$ has no roots.

Finally, if $\mu > \frac{1}{a(0)}$, then according to Lemma 5,

$$\lim_{z \searrow 24} \Delta_\mu(z) < 0$$

and

$$\lim_{z \to +\infty} \Delta_\mu(z) = 1.$$

Hence there exists a number $\xi_2(\mu)$ in $(24, +\infty)$ such that

$$\Delta_\mu(\xi_2(\mu)) = 0.$$

Since the rank of the operator $V_\mu^{\mathrm{eeo,asym}}$ is equal to one, there exists a unique root. □

Proof of Theorem 1 follows from Lemma 4 and 6. □

Proof of Theorem 2. We establish the result for the lower threshold; the case of the upper threshold follows by a similar argument.

Let μ_0^- be a point such that $1 + a(0)\mu = 0$. By Theorem 1, parts (i) and (ii), for every neighborhood of μ_0^- there exists a value of μ for which the number of eigenvalues of $H_\mu^{\mathrm{eeo,asym}}(0)$ lying below the essential spectrum is not constant. Equivalently, by Remark 4, the mapping

$$V_\mu^{\mathrm{eeo,asym}} \longmapsto \operatorname{tr} E_{H_\mu^{\mathrm{eeo,asym}}(0)}\big((-\infty, \inf \sigma_{\mathrm{ess}}(H_\mu^{\mathrm{eeo,asym}}(0)))\big)$$

is discontinuous at μ_0^-. According to Definition 1, this implies that whenever the equality $1 + a(0)\mu = 0$ holds, the operator $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at the lower threshold of the essential spectrum.

Conversely, assume that $H_\mu^{\mathrm{eeo,asym}}(0)$ is critical at the lower edge of the essential spectrum. Then there exists a point μ_0^- at which the function

$$V_\mu^{\mathrm{eeo,asym}} \longmapsto \operatorname{tr} E_{H_\mu^{\mathrm{eeo,asym}}(0)}\big((-\infty, \inf \sigma_{\mathrm{ess}}(H_\mu^{\mathrm{eeo,asym}}(0)))\big)$$

is discontinuous. Suppose that $\mu_0^- \neq -\frac{1}{a(0)}$. In this case, by Theorem 1, parts (i) and (ii), one can find a neighborhood $U(\mu_0^-)$ in which the number of eigenvalues of $H_\mu^{\mathrm{eeo,asym}}(0)$ lying below its essential spectrum does not vary, contradicting the assumption of criticality. From this contradiction, it follows that $\mu_0^- = -\frac{1}{a(0)}$. □

5.1. Analysis of the discrete spectrum of the operator $H_{\lambda\mu}(K)$

For any $n \geq 1$, we define two quantities: $e_n(K; \lambda, \mu)$ and $E_n(K; \lambda, \mu)$. These are defined using a min-max approach.

The first quantity, $e_n(K; \lambda, \mu)$, is the largest lower bound for the expectation value of the operator $H_{\lambda\mu}(K)$ with respect to a normalized vector ψ, where ψ is orthogonal to a set of $n-1$ vectors $\phi_1, \ldots, \phi_{n-1}$ from the space $L^{2,o}(\mathbb{T}^3)$.

The second quantity, $E_n(K; \lambda, \mu)$, is the smallest upper bound for the same expectation value, under the same conditions.

According to the min-max principle, we have the inequalities $e_n(K; \lambda, \mu) \leq \mathcal{E}_{\min}(K)$ and $E_n(K; \lambda, \mu) \geq \mathcal{E}_{\max}(K)$.

Since the rank of the operator $V_{\lambda\mu}$ is at most twelve, one can choose a set of twelve vectors, $\phi_1, \phi_2, \ldots, \phi_{12}$, from its range. Consequently for all $n \geq 13$, the following equalities hold: $e_n(K; \lambda, \mu) = \mathcal{E}_{\min}(K)$ and $E_n(K; \lambda, \mu) = \mathcal{E}_{\max}(K)$.

Lemma 7. *Assume that $n \geq 1$ and $i \in \{1, 2, 3\}$. The following two properties hold:*

(i) *For fixed values of K_j where $j \neq i$, the function*

$$K_i \mapsto \mathcal{E}_{\min}((K_1, K_2, K_3)) - e_n((K_1, K_2, K_3); \lambda, \mu)$$

is non-increasing in the interval $(-\pi, 0]$ and non-decreasing in $[0, \pi]$.

(ii) *Similarly, for fixed K_j with $j \neq i$, the function*

$$K_i \mapsto E_n((K_1, K_2, K_3); \lambda, \mu) - \mathcal{E}_{\max}((K_1, K_2, K_3))$$

also exhibits the same monotonic behavior, being non-increasing in $(-\pi, 0]$ and non-decreasing in $[0, \pi]$.

Proof. We may,without loss of generality, assume that $i = 1$. Let $\psi \in L^{2,o}(\mathbb{T}^3)$ be an arbitrary vector. Consider the quadratic form associated with shifted operator $(H_0(K) - \mathcal{E}_{\min}(K))$:

$$((H_0(K) - \mathcal{E}_{\min}(K))\psi, \psi) = \int_{\mathbb{T}^3} \sum_{i=1}^{3} \cos \tfrac{K_i}{3} \left(1 - \cos q_i\right)|\psi(q)|^2 \, \mathrm{d}q, \quad K := (K_1, K_2, K_3).$$

If we regarded expression as a function of the single variable $K_1 \in \mathbb{T}$, it is evident that it is non-decreasing in $(-\pi, 0]$ and non-increasing in $[0, \pi]$. This monotonicity follows directly from the properties of the cosine function. Since the potential operator $V_{\lambda\mu}$ does not depend on K, the corresponding function

$$K_1 \mapsto e_n(K; \lambda, \mu) - \mathcal{E}_{\min}(K)$$

inherits the same monotonic behavior. Therefore,for each $n \geq 1$, this function is non-decreasing in $(-\pi, 0]$ and non-increasing in $[0, \pi]$.

An entirely analogous argument applies to the functions

$$K_i \mapsto E_n(K; \lambda, \mu) - \mathcal{E}_{\max}(K),$$

demonstrating the monotonicity of the shifted eigenvalues from above. □

Theorem 4. *Let $\lambda, \mu \in \mathbb{R}$. Suppose that the operator $H_{\lambda\mu}(0)$ has n eigenvalues (counting multiplicities) located below (respectively, above) its essential spectrum. Then, for every $K \in \mathbb{T}^3$, the operator $H_{\lambda\mu}(K)$ also possesses at least n eigenvalues lying below (respectively, above) its essential spectrum.*

Proof. We rely on Lemma 7, which establishes certain monotonicity properties of the eigenvalues with respect to K. Specifically, for any $K \in \mathbb{T}^3$ and any integer $m \geq 1$, the following inequalities hold:

$$0 \leq \mathcal{E}_{\min}(0) - e_m(0; \lambda, \mu) \leq \mathcal{E}_{\min}(K) - e_m(K; \lambda, \mu),$$

$$E_m(K; \lambda, \mu) - \mathcal{E}_{\max}(K) \geq E_m(0; \lambda, \mu) - \mathcal{E}_{\max}(0) \geq 0.$$

Assume that for some $\lambda, \mu \in \mathbb{R}$, the value $e_n(0; \lambda, \mu)$ is a discrete eigenvalue of the operator $H_{\lambda\mu}(0)$. By definition of a discrete eigenvalue, this implies

$$\mathcal{E}_{\min}(0) - e_n(0; \lambda, \mu) > 0.$$

Combining this observation with the inequalities above, we immediately deduce that for any $K \in \mathbb{T}^3$, the eigenvalue $e_n(K; \lambda, \mu)$ remains strictly below $\mathcal{E}_{\min}(K)$, i.e.,

$$e_n(K; \lambda, \mu) < \mathcal{E}_{\min}(K).$$

Since the eigenvalues are arranged in increasing order,

$$e_1(K; \lambda, \mu) \leq \ldots \leq e_n(K; \lambda, \mu) < \mathcal{E}_{\min}(K),$$

it follows that the operator $H_{\lambda\mu}(K)$ possesses at least n discrete eigenvalues lying below its essential spectrum.

An entirely analogous argument applies to the eigenvalues $E_n(K; \lambda, \mu)$, establishing the corresponding result for eigenvalues above the essential spectrum. □

Proof of Theorem 3 will prove by combining the results of Theorem 4 and Theorem 1. □

6. Conclusion

In this work, we performed a detailed spectral analysis of the two-fermion lattice Schrödinger operators $H_{\lambda\mu}(K)$ on the three-dimensional lattice $\mathbb{Z}^3$ with nearest- and next-nearest-neighbor interactions. By reducing the problem to invariant subspaces and studying the associated Fredholm determinant, we identified two critical spectral points that determine the behavior and number of discrete eigenvalues. Our results demonstrate that the reduced operator possesses exactly one discrete eigenvalue depending on the interaction strength and provide explicit bounds for the number of eigenvalues for arbitrary quasimomentum. Furthermore, we described a class of rank-one self-adjoint perturbations that induce the creation or annihilation of bound states, offering a clear algebraic-geometric framework for understanding stability and bifurcation phenomena. These findings deepen the understanding of spectral properties of lattice Schrödinger operators and contribute to the mathematical foundations of interacting quantum systems.

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