# Energy-momentum spectrum of some two-particle lattice Schrödinger Hamiltonians

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We determine the excitation spectrum of some one and two-particle $\mathbb{Z}^d$ lattice Schrödinger Hamiltonians. They occur as approximate Hamiltonians for the low-lying energy-momentum spectrum of diverse infinite lattice nonlinear quantum systems. A unitary staggering transformation relates the low-energy-momentum spectrum to the high-energy-momentum spectrum of the transformed operators. A feature for the one-particle repulsive delta function Hamiltonian is that, in addition to the continuous band spectrum, there is a bound state above the band, and the repulsive case spectrum and scattering can be obtained from the attractive potential case by staggering. For the two-particle pair potential Hamiltonian, there are commuting self-adjoint energy-momentum operators, and we determine the joint spectrum. For the case of a $\lambda\delta$ pair potential, and equal particle masses, for arbitrarily small $|\lambda|$, $\lambda<0$, and $d\geqslant 3$, there is no bound state for small system momentum, but a bound state exists below the band if the momentum is large. We find that the binding energy is an increasing function of the system momentum. The existence of this bound state is in contrast with the continuum case, where the Birman-Schwinger bound excludes negative-energy bound states for small couplings; this bound state is absent if the two masses are different. Other spectral results are also obtained for the large coupling case. An eigenfunction expansion that uses products of plane waves in the sum and difference coordinates is used to obtain the spectral results.

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## I. INTRODUCTION

Recent investigations have considered the low-lying excitation spectrum of lattice Hamiltonians of diverse systems with an infinite number of degrees of freedom [1–12]. Some of the Hamiltonians that have been studied are those associated with: the mass, nonlinear spring system, or lattice scalar quantum field theory; the generator of the stochastic dynamics of weakly coupled Ginzburg-Landau models; and the transfer matrix of classical ferromagnetic spin systems at high temperature.

The joint spectrum of these Hamiltonians and the momentum operators, associated with lattice translations, admit a particle interpretation and the two-particle sector is analyzed using a lattice version of a Bethe-Salpeter equation. The ladder approximation gives a good qualitative picture of the bound-state spectrum outside the two-particle band, with rigorous confirmations already accomplished in some cases, controlling perturbations beyond the ladder approximation (see, e.g., [13,5] and the basic work [14]).

The determination of elementary excitations in the above-listed systems is of vital importance, as they are related, respectively, to the time evolution of quantum fields, the relaxation to equilibrium in the stochastic models, and the falloff rate of equilibrium spin correlation functions.

In the ladder approximation, the Bethe-Salpeter equation is, roughly speaking, the nonrelativistic two-body Schrödinger resolvent equation with a repulsive or attractive delta function pair potential.

The analysis of the above infinite systems involves various restrictions on parameters of the system, i.e., small coupling constants, large single-particle mass, zero or small system momentum, etc. As the lattice two-body spectrum presents peculiar features not present in the continuum, we think it is desirable to give a more complete description of the spectral properties of one- and two-particle lattice Hamiltonians.

Within this context, we consider the two-particle Hamiltonian in $\ell_2(\mathbb{Z}^d)\times\ell_2(\mathbb{Z}^d)$ taken as

$$H_2=\frac{-\Delta_1}{2m_1}+\frac{-\Delta_2}{2m_2}+v_{12}(\vec{x}_1-\vec{x}_2)\equiv H_0+V_2, \tag{1}$$

with $\Delta_1=\Delta\otimes I$ and $\Delta_2=I\otimes\Delta$, where $m_1,m_2>0$ are the particle masses, $\vec{x}\in\mathbb{Z}^d$ and $\Delta$ is the lattice Laplacian [$\mathbf{e}^j$ being the unit vector along the $j$th direction and $f\in\ell_2(\mathbb{Z}^d)$]

$$-\Delta f(\vec{x})=2d\,f(\vec{x})-\sum_{j=1}^{d}\,[f(\vec{x}+\mathbf{e}^j)+f(\vec{x}-\mathbf{e}^j)]. \tag{2}$$

The one-particle lattice Hamiltonian, acting in the space $\ell_2(\mathbb{Z}^d)$, is

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$$H_1 = \frac{-\Delta}{2M} + v(\vec{x}) \equiv H_0 + V_1 . \qquad (3)$$

Here, $M>0$ is the particle mass and $v(\vec{x})$ is a real potential verifying $\lim_{|\vec{x}|\to\infty}|\vec{x}|^{1+\kappa}v(\vec{x})=0$ and $v(\vec{x})=v(-\vec{x})$, $\kappa>0$.

For $V_2=0$, the Hamiltonian $H_2$ has a band spectrum. The system lattice unitary translation operator commutes with $H_2$, and we can define self-adjoint momentum operators $P_j$, satisfying $[P_i,P_j]=0$, $i,j=1,\ldots,d$. Here, we will be interested in the energy spectrum of $H_1$, and the joint spectrum of $(H_2,\vec{P})$, called the energy-momentum spectrum.

We mention some features of the lattice Hamiltonians $H_1$ and $H_2$. A unitary staggering transformation (see [8]) maps low-energy spectrum to high-energy spectrum of the transformed Hamiltonians. In particular, the Hamiltonian $H_1$ of Eq. (3) with an attractive delta potential ($V=\lambda\delta,\lambda<0$) is transformed to a Hamiltonian with a repulsive delta potential ($V=\lambda\delta,\lambda>0$). For any $\lambda$ if $d=1,2$, and for suitably large $|\lambda|$, if $d\geqslant 3$), while the attractive case gives rise to a bound state below the band, there is a bound state above the band in the repulsive case.

For $H_2$ of Eq. (1), we distinguish two cases, depending on whether or not the two masses $m_1$ and $m_2$ are equal. We first consider the case $m_1=m_2$. For an attractive delta potential, we find a bound state below the band for $d=1,2$, and the binding energy increases as the system momentum increases, i.e., the bound-state curve does not approach the band. This result is in contrast to the well-known case of the nonrelativistic continuum, where the binding energy is independent of the system momentum; and the case of two particles obeying relativistic kinematics where, based on purely kinematical grounds, the binding energy decreases as the system momentum increases. For $d\geqslant 3$, and momentum zero, there is a bound state only for $\lambda$ less than a critical value $\lambda_c<0$. However, for arbitrarily small $|\lambda|$, $\lambda<0$, there is a bound state for sufficiently high momentum $|q|>q_c>0$. Here, the binding energy goes to zero as $|q|\to q_c^+$, and the bound state approaches the band. This result is in contrast with the continuum case, where the Birman-Schwinger bound (see [15]) excludes bound states for sufficiently small potentials.

We now consider the case $m_1\neq m_2$, and the attractive delta potential. If $d=1,2$, there exists a bound state for any small $|\lambda|$, $\lambda<0$. For dimension $d\geqslant 3$, for all values of the system momentum, no bound state exists for small $|\lambda|$, in agreement with the continuum.

We now describe the organization of the paper. In Sec. II, we define the staggering transformation on the two-particle space and show how to separate $H_2$ into a free system Hamiltonian and a relative coordinate interacting Hamiltonian which depends on the system momentum $\vec{q}$. The separation is achieved using an eigenfunction expansion based on plane waves in the sum and difference coordinates. In this way, we establish the general grounds of our two-particle analysis for general system momentum $\vec{q}$ and masses $m_1$ and $m_2$. Using the Lippmann-Schwinger equation, in Sec. III, we determine the spectrum and the scattering for the Hamiltonian $H_1$ of Eq. (3), which describes the $\vec{q}=\vec{0}$ physics of the problem. Spectral results for $H_2$ of Eq. (1) are obtained in Sec. V for $m_1\neq m_2$ and in Sec. IV for $m_1=m_2$. Finally, in Sec. VI, some concluding remarks are made.

## II. SPECTRUM FOR $H_2$

To determine the spectrum of $H_2$, we introduce the lattice translation operator, $T_{\vec{a}}f(\vec{x}_1,\vec{x}_2)=f(\vec{x}_1-\vec{a},\vec{x}_2-\vec{a})$, with $\vec{a}\in\mathbb{Z}^d$. This operator commutes with $H_2$ and is unitary. We write $T_{\vec{a}}=\exp[i\vec{P}\cdot\vec{a}]$ which defines the self-adjoint system momentum operators $P_j$, $j=1,\ldots,d$, and system momentum $\vec{q}\in\mathbf{T}^d$, with $\mathbf{T}^d=(-\pi,\pi]^d$. Since $[P_j,H_2]=0$, we determine the joint energy-momentum spectrum of $(H_2,\vec{P})$.

We define the staggering transformation acting in the two-particle space $\ell_2(\mathbb{Z}^d)\times\ell_2(\mathbb{Z}^d)$ by

$$Uf(\vec{x}_1,\vec{x}_2)=(-1)^{\sum_{j=1}^{d}(x_1^j+x_2^j)}f(\vec{x}_1,\vec{x}_2), \qquad (4)$$

which is unitary and, since $U^2=I$, we have $U^{-1}=U$. From Eq. (4), it is easily seen that $[U,T_{\vec{a}}]=0$ and $[U,\mathcal{S}]=0$, where $\mathcal{S}$ is the projection on the symmetric (even) subspace given by $\mathcal{S}=\frac{1}{2}(I+\mathcal{P})$, where $\mathcal{P}$ is the permutation operator $\mathcal{P}f(\vec{x}_1,\vec{x}_2)=f(\vec{x}_2,\vec{x}_1)$.

For $V=\lambda\delta$, we find that $H_2$ has the following intertwining property:

$$UH_2=U\left[\frac{-\Delta\otimes I}{2m_1}+\frac{I\otimes-\Delta}{2m_2}+\lambda\delta\right]$$
$$=\left[4d\left(\frac{1}{2m_1}+\frac{1}{2m_2}\right)-\left(\frac{-\Delta\otimes I}{2m_1}+\frac{I\otimes-\Delta}{2m_2}-\lambda\delta\right)\right]U,$$

so that, for each system momentum $\vec{q}$, the negative bound-state eigenfunction for the attractive case $\lambda<0$, is transformed by $U$ into the positive bound-state eigenfunction for the repulsive case $\lambda>0$. Keeping this in mind, it is enough to determine, e.g., the spectrum below the band.

Here, we obtain the spectral representation of $H_2$ via an eigenfunction expansion. Let us first remark that, although we do not have separation of the Hamiltonian in center-of-mass and relative coordinates, as in the continuum, $H_2$ commutes with $T_{\vec{a}}$. So, we consider expanding a function $f(\vec{x}_1,\vec{x}_2)$ in terms of the non-$\ell_2$ functions

$$\psi(\vec{x}_1,\vec{x}_2,\vec{p},\vec{k})=\frac{1}{(2\pi)^{2d}}e^{i\vec{k}\cdot(\vec{x}_1+\vec{x}_2)}e^{i\vec{p}\cdot(\vec{x}_1-\vec{x}_2)}.$$

The function $\psi$ is an eigenfunction of the system momentum operator $\vec{P}$, with eigenvalue $2\vec{k}\equiv\vec{q}$. Also, $\psi$ is an eigenfunction of the free system Hamiltonian $H_0$, with eigenvalue

$$K(\vec{p},\vec{k})\equiv -\frac{1}{2m_1}\tilde{\Delta}(\vec{p}+\vec{k})-\frac{1}{2m_2}\tilde{\Delta}(\vec{p}-\vec{k})$$
$$=\frac{1}{2m_1}\sum_{j=1}^{d}2[1-\cos(p^j+k^j)]+\frac{1}{2m_2}\times\sum_{j=1}^{d}2[1-\cos(p^j-k^j)].$$

Here, we see that the eigenvalue does not split into a sum of center-of-mass and relative kinetic energy as in the continuum using center-of-mass and relative coordinates. However, $H_0$ is still a multiplication operator. It has a band spectrum for any $d$, with a finite width which can become zero if the system masses are equal and the system momentum $\vec{q}$ is equal to $\vec{\pi}\equiv(\pi,\ldots,\pi)$. Furthermore, the $\psi$'s obey the following orthogonality and completeness relations:

$$\int\int\overline{\psi}(\vec{x}_1,\vec{x}_2,\vec{p}_1,\vec{k}_1)\psi(\vec{x}_1,\vec{x}_2,\vec{p}_2,\vec{k}_2)d\vec{x}_1d\vec{x}_2=\delta(\vec{k}_1-\vec{k}_2)\delta(\vec{p}_1-\vec{p}_2);$$

$$\int_{\mathbf{T}^d}\int_{\mathbf{T}^d}\overline{\psi}(\vec{x}_1',\vec{x}_2',\vec{p},\vec{k})\psi(\vec{x}_1,\vec{x}_2,\vec{p},\vec{k})d\vec{p}d\vec{k}=\delta(\vec{x}_1-\vec{x}_1')\delta(\vec{x}_2-\vec{x}_2').$$

Turning now to the time-dependent Schrödinger equation, we write

$$\Psi(\vec{x}_1,\vec{x}_2,t)=\frac{1}{(2\pi)^d}\int a(\vec{k})\phi(\vec{x}_1,\vec{x}_2,\vec{k})e^{-iE(\vec{k})t}d\vec{k},$$

where $\Psi$ satisfies $i\partial\Psi/\partial t=H_2\Psi$, if we take $\phi$ such that

$$H_2\phi=E(\vec{k})\phi, \tag{5}$$

with $\phi(\vec{x}_1,\vec{x}_2,\vec{k})=e^{i\vec{k}\cdot(\vec{x}_1+\vec{x}_2)}\chi(\vec{x}_2-\vec{x}_1,\vec{k})$ and $\chi(\vec{x},\vec{k})=(2\pi)^{-d}\int b(\vec{p},\vec{k})e^{i\vec{p}\cdot\vec{x}}d\vec{p}$. Substituting in Eq. (5), canceling the $e^{i\vec{k}\cdot(\vec{x}_1+\vec{x}_2)}$ factor, and taking the Fourier transform in the relative coordinate $\vec{x}=\vec{x}_2-\vec{x}_1$, we obtain

$$[K(\vec{p},\vec{k})-E(\vec{k})]b(\vec{p},\vec{k})+\frac{\lambda}{(2\pi)^d}\int b(\vec{p}\,',\vec{k})d\vec{p}\,'=0. \tag{6}$$

Multiplying Eq. (6) by $(K-E)^{-1}(\vec{p},\vec{k})$ and integrating over $\vec{p}$ leads to the eigenvalue equation

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{p}}{K(\vec{p},\vec{k})-E(\vec{k})}=0. \tag{7}$$

The corresponding eigenfunction is proportional to $e^{i\vec{k}(\vec{x}_1+\vec{x}_2)}\int_{\mathbf{T}^d}\{e^{i\vec{k}(\vec{x}_1-\vec{x}_2)}/[K(\vec{p},\vec{k})-E(\vec{k})]\}d\vec{p}$.

We point out that for a general potential $V(\vec{x}_1-\vec{x}_2)$, we still reduce the two-particle problem to that of solving a one-particle problem. In this case, Eq. (6) becomes, after canceling the $e^{i\vec{k}\cdot(\vec{x}_1+\vec{x}_2)}$ factor, and setting $\vec{x}\equiv\vec{x}_2-\vec{x}_1$,

$$\frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}[K(\vec{p},\vec{k})-E(\vec{k})]b(\vec{p},\vec{k})e^{i\vec{p}\cdot\vec{x}}d\vec{p}+V(\vec{x})\frac{1}{(2\pi)^d}\int b(\vec{p},\vec{k})e^{i\vec{p}\cdot\vec{x}}d\vec{p}=0.$$

Taking the Fourier transform in $\vec{x}$ gives

$$[K(\vec{p},\vec{k})-E(\vec{k})]b(\vec{p},\vec{k})+\frac{1}{(2\pi)^d}\times\int_{\mathbf{T}^d}\tilde{V}(\vec{p}-\vec{p}\,')b(\vec{p}\,',\vec{k})d\vec{p}\,'=0,$$

i.e., the time-dependent Schrödinger equation in momentum space with a kinetic energy that depends on the system momentum $\vec{q}=2\vec{k}$.

## III. SPECTRUM OF $H_2$ FOR ZERO SYSTEM MOMENTUM

For $\vec{k}=\vec{0}$, Eq. (6), with $\mu=m_1m_2/(m_1+m_2)$, is

$$\frac{-\tilde{\Delta}(\vec{p})}{\mu}b(\vec{p})+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}b(\vec{p}\,')d\vec{p}\,'=Eb(\vec{p}),$$

which is the equation $H_1\psi=E\psi$ in momentum space, taking $\mu=2M$. We point out that the above is the same equation as that obtained for normal modes of polarized classical oscillations of a monatomic isotropic crystalline lattice with an isotopiclike defect at the origin [20–23].

To derive the spectral properties of the Hamiltonian $H_1$ of Eq. (3), it is convenient to use the Laplacian in $H_0$ of Eq. (2) without the constant diagonal term, i.e., with $\Delta f(\vec{x})=\Sigma_{j=1}^d f(\vec{x}+\mathbf{e}^j)+\Sigma_{j=1}^d f(\vec{x}-\mathbf{e}^j)$. With this choice, the spectrum is given by the values of $E(\vec{q})$, corresponding to the energies of the noninteracting system, $E(\vec{q})=-1/M\Sigma_{j=1}^d\cos q^j$, $\vec{q}\in\mathbf{T}^d$, and has the energy range $[-d/M,d/M]$.

Note that if we take both $m_1$ and $m_2$ to be equal to $m>0$ in the free part $H_0$ of the Hamiltonian $H_2$ of Eq. (1), and if we set $M=m/2$ in Eq. (3), then the energy interval $[-d/M,d/M]$ also describes the momentum spectrum of the free two-particle system with relative momentum $\vec{k}$, total momentum $\vec{q}=\vec{0}$, and particle masses $m$. As it is known, the free part of $H_2$ has a band spectrum, for any fixed total momentum $\vec{q}$. This is why we refer to the energy range of $E(\vec{q})$ as a band. Also, for convenience and without spoiling the analysis for the general mass model, we will assume $2M=1$ throughout this section. The band then becomes $[-2d,2d]$.

The causal (retarded) Green's function associated with the Hamiltonian $H_0$, is (for $\eta \to 0^+$)

$$G_0^>(\vec{x},\vec{y};E) \equiv [(E+i\eta)-H_0]^{-1}(\vec{x},\vec{y}) = \frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{e^{i\vec{q}\cdot(\vec{x}-\vec{y})}}{E+i\eta-E(\vec{q})}d\vec{q}. \tag{8}$$

An important property of the Green's function of Eq. (8) is its transformation under the one-particle unitary staggering transformation $U$. In the configuration space, we have $Uf(\vec{x})=(-1)^{\sum_{j=1}^d x^j}f(\vec{x})$; $f\in\ell_2(Z^d)$, and satisfies $U^2=I$ and $U^{-1}=U$. In words, $U$ transforms smooth functions into rough functions and vice versa. $U$ has the intertwining property $-\Delta+\lambda\delta=U[-1(-\Delta-\lambda\delta)]U^{-1}$. In momentum space, the action of the staggering transformation becomes $(Uf)^{\sim}(\vec{p})=\tilde{f}(\vec{\pi}-\vec{p})$, $\vec{p}\in\mathbf{T}^d$. From the definition of $U$, and the staggering transformation properties of the Laplacian under $U$, it follows that $G_0^>(E)$ satisfies the property

$$G_0^>(\vec{x},\vec{y};E) = -(-1)^{\sum_{j=1}^d (x^j-y^j)}G_0^<(\vec{x},\vec{y};-E), \tag{9}$$

where $G_0^<$ is the advanced Green's function which is obtained replacing $\eta$ by $-\eta$ in Eq. (8).

It is a general feature that the imaginary part of the trace of a one-particle Green's function is related to the one-particle density of states of its associated Hamiltonian [16,17]. Here, the density $D(E)$, per lattice point, of the (free-)particle states of the Laplacian, at a given energy $E$, is given by

$$D(E)=\frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}\delta(E-E(\vec{q}))d\vec{q}. \tag{10}$$

Using the staggering transformation, with $\vec{x}=\vec{y}=\vec{0}$, it follows that $D(E)$ is an even function of $E$. Also, since the eigenvalues of the Laplacian exist only for $E\in[-2d,2d]$, $D(E)$ is zero outside the band. Besides, $D(E)$ is strictly positive in $(-2d,2d)$. Near the band edges $\pm 2d$, $D(E)$ shows Van Hove singularities of the form

$$D(E)\simeq \frac{d}{(2\sqrt{\pi})^d\Gamma\left(\frac{d}{2}\right)}\left[d-\frac{E^2}{4d}\right]^{d/2-1}; \quad |E|\simeq 2d. \tag{11}$$

Although $D(E)$ may diverge at the band edges, its integral remains finite, with integral one over the band. If $d=1$, Eq. (11) holds as an equality, for any $E$. For $d=2$, $D(E)$ has jump discontinuities at the edges and has a logarithmic singularity at $E=0$. For general $d\geqslant 3$, $D(E)$ is continuous and bounded.

For $\mathcal{P}$ denoting the Cauchy's principal value, let

$$F(E)=\mathcal{P}\int_{-2d}^{2d}\frac{D(E')}{E-E'}dE',$$

which has the interpretation of an electric field of a two-dimensional line charge distribution $D(E)$. Using Eq. (10), Eq. (8) becomes $G_0^>(0,0;E)=F(E)-i\pi D(E)$. We remark that $F(E)$ is the Hilbert transform of an even and strictly positive function. It follows that $F(E)$ is odd in $(-2d,2d)$, monotonically decreasing outside the band, and continuous at least inside the band but near the edges. If $d=1$, $F(E)$ vanishes inside the band and is exceptionally given by $\mathrm{sign}(E)/\sqrt{E^2-4}$, if $|E|>2$. If $d=2$, $F(E)$ has an infinite logarithmic discontinuity at the band edges, and is bounded for $d\geqslant 3$, at least near the band edges.

From the above behavior of $G_0^>$, the spectral properties of $H_1$ can be now consistently discussed in terms of the associated Lippmann-Schwinger equation, i.e.,

$$\psi^>(\vec{x})=\phi(\vec{x};E)+\sum_{\vec{y}} G_0^>(\vec{x},\vec{y};E)V(\vec{y})\psi^>(\vec{y}), \tag{12}$$

where $\phi(\vec{x};E)$ is a suitably chosen eigenstate of $H_0$, with energy $E\in(-2d,2d)$. For the localized potential $V(\vec{x})=\lambda\delta(\vec{x})$, Eq. (12) has the solution

$$\psi^>(\vec{x})=\phi(\vec{x};E)+\frac{\lambda\phi(0;E)}{1-\lambda F(E)+i\pi\lambda D(E)}G_0^>(\vec{x},0;E). \tag{13}$$

Since $V$ is localized at $\vec{x}=0$, only free-particle states $\phi(\vec{x};E)$ having nonzero amplitudes at $\vec{x}=0$ are scattered. Taking Eq. (13), we notice that the scattered wave contains a term (a "scattering amplitude") with a factor

$$f(E)=\frac{\lambda}{[1-\lambda F(E)]+i\pi\lambda D(E)}, \tag{14}$$

which is infinite, under some circumstances. The condition for a singularity to occur in $f(E)$ is given by

$$1-\lambda F(E)=0; \quad \lambda D(E)=0. \tag{15}$$

When $E$ lies in $(-2d,2d)$, the above properties of $F(E)$ ensure that the first of these conditions can be satisfied for $d\geqslant 2$, but not for $d=1$, where $F(E)\equiv 0$ in the band. On the other hand, for $d=2$, since $F(E)$ becomes infinite at the band edges, the first condition is satisfied for any $|\lambda|$. For small enough $|\lambda|$, if $\lambda<0$, the solution occurs at some $E$ close to $-2d$, and at $E$ close to $2d$, if $\lambda>0$. A similar argument holds for $d\geqslant 3$. However, since $F(E)$ is now bounded, a critical value $\lambda_c$ exists and a solution is found, for each sign of $\lambda$, only for $|\lambda|>|\lambda_c|>0$. Regarding the second condition in Eq. (15), recall that $D(E)$ is finite and nonzero near $\pm 2d$, for all $d\geqslant 2$. For $d=2$, the only possibility for having the product $\lambda D(E)$ small is to take small enough values of $|\lambda|$. $D(E)$ is arbitrarily small, for $d\geqslant 3$, if $E$ is close enough to $\pm 2d$, where $D(E)$ vanishes. Thus, a resonance appears for small $\lambda$ in $d=2$ and for $|\lambda|$ above but near $|\lambda_c|$, for $d\geqslant 3$.

In the same way, bound states of the Hamiltonian $H_1$ correspond to singularities of scattering amplitudes, regarded as functions of $E$. When both conditions of Eq. (15) are simultaneously satisfied, the Lippmann-Schwinger Eq. (12) may present nontrivial solutions even when $\phi(\vec{x};E)$ is set to be a null function, which is the case if $E$ is outside $[-2d,2d]$. In fact, letting $\phi(\vec{x};E)\equiv 0$ in Eq. (12), we find, for the bound states,

$$\psi_b(\vec{x})=\lambda G_0^>(\vec{x},0;E_b)\psi_b(0). \tag{16}$$

Provided that $\psi_b(0)\neq 0$, a nontrivial solution emerges when $1-\lambda G_0^>(0,0;E_b)=[1-\lambda F(E_b)]+i\lambda D(E_b)=0$, which is equivalent to Eq. (15). As before, the first of these conditions can always be met, for some $E$, provided that $\lambda$ is suitably chosen. The second one requires, consistently with the vanishing of $\phi(\vec{x};E)$, the bound-state energy $E_b$ to satisfy $|E_b|>2d$, where $D(E)$ vanishes. Since $F(E)$ is odd and monotonically decreasing outside $[-2d,2d]$, a unique finite bound-state solution $E=E_b(\lambda)$ exists either for the attractive and the repulsive potentials. For $\lambda<0$, we have $E_b(\lambda)\equiv E_b^{\downarrow}(\lambda)<-2d$ and the corresponding binding energy is $\epsilon=-2d-E_b^{\downarrow}(\lambda)$. By staggering [since $F(E)$ is odd], for $\lambda>0$, it follows that $E_b(\lambda)\equiv E_b^{\uparrow}(\lambda)=-E_b^{\downarrow}(-|\lambda|)>2d$ and the binding energy is obviously the same. For $d\leqslant 2$, where $F(E)$ diverges near the band edges, a bound state exists for any value of $\lambda$. For $d\geqslant 3$, where $F(E)$ is bounded, a bound state still exists but only for $\lambda$ depending on a critical value $\lambda_c$. Staggering guarantees, for each of the cases, either attractive or repulsive, a symmetrical pattern around the band $[-2d,2d]$. Knowing the spectrum for one of these two cases, the other one is obtained by reflection about the middle of the band $E=0$. For a physical interpretation for the existence of the (nonintuitive) bound state, for $\lambda>0$, in terms of a system of classical oscillators, see [19].

Turning to the bound state wave functions, from Eq. (16), we see that the bound-state wave functions are determined by $G_0^>(0,\vec{x},E_b)$. The asymptotic behavior, for large $|\vec{x}|$ and $E_b<-2d$, is dominated by $\vec{q}\simeq 0$ in Eq. (8), leading to, for $|\vec{x}|\to\infty$,

$$G_0^>(0,\vec{x},E_b)\simeq-\frac{2}{(2\sqrt{\pi})^d}\left(\frac{\sqrt{\epsilon}}{2|\vec{x}|}\right)^{d/2-1}K_{d/2-1}(\sqrt{\epsilon}|\vec{x}|), \tag{17}$$

where $K_\nu=K_{-\nu}$ is the modified Bessel function of order $\nu$ and $\epsilon>0$ is the binding energy. Thus, apart from a normalization, for large $|\vec{x}|$, the wave function for the $\lambda<0$ case satisfies

$$\psi_b^{\downarrow}(\vec{x})\simeq|x|^{1-d/2}K_{d/2-1}(\sqrt{\epsilon}|\vec{x}|),$$

which shows that it is exponentially decreasing, the decay rate being uniform in $\vec{x}$ and depending only on $d$ (and on the mass $m$). Using the transformation property of $G_0^>$ under the staggering transformation, it follows that

$$\psi_b^{\uparrow}(\vec{x})\simeq(-1)^{\Sigma_{j=1}^d x^j}|x|^{1-d/2}K_{d/2-1}(\sqrt{\epsilon}|\vec{x}|)$$

describes the asymptotic behavior of wave function of the bound state with positive energy ($\lambda>0$). It is worth noting that these asymptotic formulas are valid only when $\epsilon\ll 4d$ that is, the limit of weak binding. In this limit, the appearance of the bound states can be understood from the hybridization of $\vec{q}$ states associated with energies close to $\pm 2d$. Also, we remark that if the binding energy $\epsilon$ is large compared to $4d$, an exponential decay behavior at $|\vec{x}|\to\infty$ persists for any of the $\psi_b(\vec{x})$. This can be seen applying the Payley-Wiener theorem [18], using the analyticity properties on a strip about the real axis of the Fourier transform of $G_0^>$. However, a closer examination shows that the decay rate depends on the direction, and the asymptotic behavior is not isotropic.

If $d=1$, $G_0^>(0,x;E)$ can be explicitly calculated for any value of $x$. We obtain, for $\alpha=\cosh^{-1}(1+\epsilon/2)>0$, $G_0^>(0,x;E_b)=\text{const.}\,e^{-\alpha|x|}$. This equation agrees with Eq. (17), with $d=1$, except for the fact that $\alpha\neq\sqrt{\epsilon}$. The condition $\alpha\simeq\sqrt{\epsilon}$ is only recovered in the limit of weak binding $\epsilon\approx 0$.

Before closing this section, we determine the effect of the staggering transformation on the wave and scattering operators (see [24]). Making explicit the $\lambda$ dependence in $H_1\equiv H_1(\lambda)$, we define the wave operators $W_\pm(\lambda)=s-\lim_{t\to\pm\infty}e^{iH_1(\lambda)t}e^{-iH_0t}$. We have, recalling that $U^{-1}H_1(\lambda)U=-H_1(-\lambda)$,

$$W_\pm(\lambda)U=s-\lim_{t\to\pm\infty}UU^{-1}e^{iH_1(\lambda)t}UU^{-1}e^{-iH_0t}U$$

$$=U[s-\lim_{t\to\pm\infty}e^{-iH_1(\lambda)t}e^{iH_0t}]=UW_\mp(-\lambda).$$

For the scattering operator $S(\lambda)\equiv W_+(\lambda)^*W_-(\lambda)$, we find

$$US(\lambda)U^{-1}=UW_+(\lambda)^*UU^{-1}W_-(\lambda)U^{-1}$$

$$=W_-(-\lambda)^*W_+(-\lambda)=S(-\lambda)^*.$$

In terms of the Fourier transform of the transition matrix $\tilde{T}(\vec{p},\vec{k};\lambda)$,

$$\tilde{S}(\vec{p},\vec{k})=\delta(\vec{p}-\vec{k})-2\pi i\,\delta(E(\vec{p})-E(\vec{k}))\tilde{T}(\vec{p},\vec{k};\lambda)$$

and $\tilde{S}(\vec{p},\vec{k})$ is the Fourier transformed kernel of $S$. By considering the effect of a staggering transformation in momentum space, for $\vec{p}\neq\vec{k}$ but $E(\vec{p})=E(\vec{k})$, we have

$$\tilde{T}(\vec{p},\vec{k};\lambda)=-\overline{\tilde{T}}(\vec{\pi}-\vec{k},\vec{\pi}-\vec{p};-\lambda),$$

which is seen to hold for the explicit solution obtained above, i.e.,

$$\tilde{T}(\vec{p},\vec{k};\lambda)=\lambda[1-\lambda G_0^>(0,0;E(\vec{k}))]^{-1}. \tag{18}$$

Note that the on-shell limit (diagonal part) Eq. (18) gives $f(E)$ of Eq. (14).

### IV. SPECTRAL RESULTS FOR $H_2$: UNEQUAL MASSES

For $d=1$, we have the eigenvalue equation

$$1+\lambda\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{1}{g(p,q)-z}dp=0, \tag{19}$$

where

$$g(p,q)=\frac{1}{2m_1}[2d-2(\cos(q/2)\cos p-\sin(q/2)\sin p)]$$
$$+\frac{1}{2m_2}[2d-2(\cos(q/2)\cos p+\sin(q/2)\sin p)]$$
$$\equiv a\cos p+b\sin p+c.$$

But

$$\int_{-\pi}^{\pi}\frac{dp}{\alpha\cos(p+r)-\zeta}=\frac{-\pi}{(\zeta-\alpha)^{1/2}(\zeta+\alpha)^{1/2}}$$

with $a=\alpha\cos r$, and $b=\alpha\sin r$ and $\zeta=z-c$, so that Eq. (19) becomes

$$1+\lambda\frac{-1}{2[z-w_+(q)]^{1/2}[z-w_-(q)]^{1/2}}=0, \tag{20}$$

with solutions

$$w_\pm(q)=\frac{1}{\mu}\pm\left[\frac{\cos^2(q/2)}{\mu^2}+\frac{\sin^2(q/2)}{\gamma^2}\right]^{1/2}, \tag{21}$$

$\mu=m_1m_2(m_1+m_2)^{-1}$ and $\gamma=m_1m_2(m_2-m_1)^{-1}$. Note that $w_\pm(\vec{q})$ are precisely, respectively, the upper and lower envelopes for the band, i.e. the energy envelopes for two particles with total system momentum $\vec{q}$. For the attractive case, $\lambda<0$, letting $z=w_-(q)-\epsilon$, $\epsilon>0$, we have a bound state with binding energy

$$\epsilon=-\frac{(w_+-w_-)}{2}+\frac{1}{2}[(w_+-w_-)^2+\lambda^2]^{1/2}. \tag{22}$$

The results for unequal masses and $d=1$ are depicted in Fig. 1.

For dimension $d$ and system momentum $\vec{q}=\vec{\pi}$, the bound state equation is

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{p}}{\sum_{j=1}^{d}\left(\frac{1}{\mu}+\frac{\sin p^j}{\gamma}\right)-z}=0,$$

or, with $z=d(1/\mu-1/\gamma)-\epsilon$, the binding energy $\epsilon>0$ verifies

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{p}}{\sum_{j=1}^{d}\frac{1}{\gamma}(\sin p^j+1)+\epsilon}=0,$$

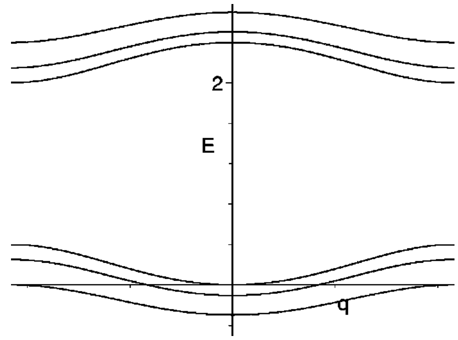


FIG. 1. The energy-momentum spectrum for the case $d=1$ and unequal masses, with $m_2=0.2m_1$. The most inner curves are the band envelopes. All its interior points also belong to the spectrum. Its lower and upper envelopes do not coincide at $q=\pm\pi$. For $\lambda<0$, only the isolated bound state lower dispersion curves appear; for $\lambda>0$, only the isolated upper curves appear. The curves closest to the band describe bound states for $\lambda^2=26$ and the farthest curves are for $\lambda^2=80$. These curves change concavity for some momentum value. Also, the band envelopes change from convex to concave. The gaps between each pair of symmetrical curves and the band are equal, and the binding energies increase as the system momentum increases.

which, noting that $1+\sin p^j$ can be replaced by $1-\cos p^j$, has a solution for $\lambda<0$, $|\lambda|$ arbitrarily small, only for $d=1,2$, but not for $d\geqslant3$. This agrees with the Birman-Schwinger bound (see [15]). The band width at $\vec{q}=\vec{\pi}$ is $2d/\gamma$.

To close, we remark that the staggering transformation allows us to obtain spectral results for the repulsive delta function potential ($\lambda>0$) from those of the attractive case ($\lambda<0$).

### V. SPECTRAL RESULTS FOR $H_2$: EQUAL MASSES

In the case of equal masses, $\gamma$ becomes $+\infty$. This is the case relevant to the correspondence with the infinite nonlinear lattice quantum models, since the resolvent of this Hamiltonian is similar to what occurs in the Bethe-Salpeter equation. This is why our analysis is more complete here. Without loss of generality, setting $2m_1=2m_2=1$, we have $\mu=1/4$. Equation (6) becomes, for system momentum $\vec{q}=2\vec{k}$,

$$4\sum_{j=1}^{d}\cos\frac{q^j}{2}(1-\cos p^j)b(\vec{p})+\frac{\lambda}{(2\pi)^d}\int b(\vec{p}\,')d\vec{p}\,'$$
$$=\left[E-\left(4d-4\sum_{j=1}^{d}\cos\frac{q^j}{2}\right)\right]b(\vec{p}), \tag{23}$$

which is the momentum space form of the normal mode equation for classical polarized oscillations of an anisotropic

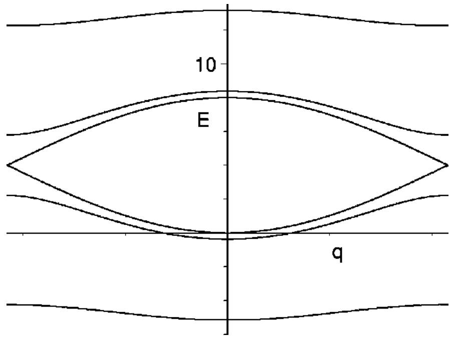


FIG. 2. The equal mass energy-momentum spectrum for the case $d=1$. The most inner curves are the band envelopes. All its interior points also belong to the spectrum. For $\lambda<0$, only the isolated bound-state lower dispersion curves appear; for $\lambda>0$, only the isolated upper curves appear. The upper envelope for the band is concave and the lower one convex. They join each other at $q=\pm\pi$. The curves closest to the band describe bound states for $\lambda^2=1.6$ and the farthest curves are for $\lambda^2=34$. These curves change concavity for momentum close to $\pm\pi$. The gaps between each pair of symmetrical curves and the band are equal, and the binding energies increase as the system momentum increases.

crystalline lattice with a point defect [20,21,23]. The anisotropy depends on the direction of the system momentum; for $\vec{q}=\vec{0}$, the first term is the isotropic kinetic energy $-2\tilde{\Delta}(\vec{p})$.

The eigenvalue equation becomes

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{p}}{4d-4\sum_{j=1}^{d}\cos(q^j/2)\cos p^j-E}=0,$$

which leads to the equation for the binding energy [see Eq. (25) below].

We first take $d=1$. Eqs. (19) to (22) hold in the $\gamma\to\infty$ limit. Solving the bound state equation gives $\epsilon=-\frac{1}{2}(w_+(q)-w_-(q))+\frac{1}{2}[(w_+(q)-w_-(q))^2+\lambda^2]^{1/2}$, which determines $E_b(q)$. From this solution, we see that this bound state curve does not intersect the band for all values of $q$.

As for the one-particle case, we now consider the effect of a staggering transformation on the two-particle Hamiltonian. For $d=1$, this will give us a bound state curve, for the repulsive case, above the band at $z=w_+(q)-\epsilon$, $\epsilon>0$, with gap $\epsilon$ given by the same expression as above, for the attractive case. The final result for $d=1$ is summarized in Fig. 2.

Let us turn to the cases $d\geqslant 2$. Setting $f(\vec{p},\vec{q})=4d-4\Sigma_{j=1}^{d}\cos(q^j/2)\cos p^j$, the condition for a bound state is

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{1}{f(\vec{p},\vec{q})-z}d\vec{p}=0. \tag{24}$$

To determine the bound state below the band, in the attractive case, $\lambda<0$, with fixed $\vec{q}$, it is convenient to define $f_{min}(\vec{q})\equiv\min_{\vec{p}\in\mathbf{T}^d}f(\vec{p},\vec{q})=\Sigma_{j=1}^{d}4(1-\cos q^j/2)$ and set $z(\vec{q})=f_{min}(\vec{q})-\epsilon(\vec{q})$, $\epsilon>0$, being the binding energy. The bound state condition of Eq. (24) becomes

$$1+\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{1}{4\sum_{j=1}^{d}\cos(q^j/2)(1-\cos p^j)+\epsilon}d\vec{p}=0. \tag{25}$$

Note that the integrand in Eq. (25) is positive and is a continuous function of $\epsilon>0$.

Another important observation is that, for any $d$ and any $\lambda$, there is always a solution $\epsilon(\vec{\pi})=|\lambda|$ to Eq. (25), for $\vec{q}=\vec{\pi}$. This is a trivial matter since the kinetic energy term vanishes. The eigenvalue equation is simply $\lambda\,\delta(\vec{x})\psi(\vec{x})=E'\psi(\vec{x})$, $E'=4-d=z-4d=\lambda=-\epsilon$, which has the multiplicity one eigenfunction $\delta(\vec{x})$ with eigenvalue $E'=\lambda$ and the infinite multiplicity eigenvalue zero with eigenfunctions $\delta(\vec{x}-\vec{u})$, $\vec{u}\neq\vec{0}$. For $\vec{q}=\vec{\pi}$, the band is a single point (see Fig. 2). The fact that the bound-state wave function is localized in a single point is to be compared with the bound-state (given below) wave function for $\vec{q}=\vec{0}$, which has exponential decay. This last result is in agreement with the results of Sec. III. All these results follow from the Payley-Wiener theorem [18].

We now give an interesting physical interpretation of the above result. Note that the $\cos q^j/2$ factor in the kinetic-energy term in Eq. (23) is the inverse of a directional mass which increases for increasing system momentum, and which, in turn, lowers the energy. Note that this makes the equal mass case different from the unequal mass case. Due to the unequal mass term, the operator does not have an interpretation of an anisotropic one-particle lattice Schrödinger. Also, another difference between the equal and unequal mass cases is that the band collapses to a single point, at $\vec{q}=\vec{\pi}$, when the masses are equal. For example, in $d=1$, we can interpret the $H_2$ eigenvalue equation as an equation for classical polarized oscillations for particles in a two-dimensional lattice with defects along a diagonal line through the origin (zero relative coordinate). The bound states correspond to a multiplicity one normal mode having nonzero displacements only along the line of defects. There is also an infinite number of other normal modes, along parallel diagonal lines, for which the nonzero particle displacements only occur on the line. These are the modes that correspond to the coalescent point of the band.

Back to the general case, if $d=2$ and $\vec{q}\neq\vec{\pi}$, the integral diverges as $\epsilon\searrow 0$. Since the integrand is strictly monotone in the binding energy $\epsilon>0$, there is a unique bound-state solution for each $\lambda<0$, which does not intersect the band. For $d\geqslant 3$, the integral in Eq. (25) converges absolutely and remains finite as $\epsilon\searrow 0$. It defines a positive and even function of $\vec{q}$ and, for fixed $\vec{q}$ is strictly monotone decreasing for increasing $\epsilon$. Using the parity property on the components of $\vec{q}$, we concentrate our analysis to non-negative components $q^j$, $j=1,\ldots,d$. For fixed $\lambda$, differentiating Eq. (25) with respect to $q^j$, $j=1,\ldots,d$, shows that the components of the gradient of the solutions $\epsilon(\vec{q})$ are continuous and non-negative, vanishing only at $\vec{q}=\vec{0}$. In words, the binding energy increases as the system momentum increases. This is in contrast to the nonrelativistic continuum case, where the binding energy is independent of the system momentum. Also, in the case of particles obeying relativistic kinematics, the binding energy of two particles decreases as the system momentum increases.

Setting $\vec{q}=\vec{0}$, a negative bound-state solution exists provided that $\lambda<\lambda_c(\vec{0})<0$, where $\lambda_c(\vec{0})$ is the $\lambda$ solution to Eq. (25) with $\vec{q}=\vec{0}$ in the limit $\epsilon\searrow 0$, i.e.,

$$1+\frac{\lambda_c(\vec{0})}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{1}{4\sum_{j=1}^{d}(1-\cos p^j)}d\vec{p}=0. \tag{26}$$

Thus, using the continuity in $\epsilon$, we extend the argument and a solution $\epsilon(\vec{q})$ is shown to exist for a neighborhood of $\vec{q}=\vec{0}$. A new critical value $\lambda_c(\vec{q})<0$ emerges at each $\vec{q}$. In this way, we can iterate the use of continuity in $\epsilon$ to show the existence of a solution for each $\vec{q}$ up to $\vec{q}$ near $\vec{\pi}$. We remark that, from Eq. (26), we also know that the components of the gradient of $\lambda_c(\vec{q})$ are continuous, positive, finite, and strictly increasing functions, for all $\vec{q}\neq\vec{\pi}$), the final conclusion is that a bound-state curve, which never intercepts the band, is present at least provided that $\lambda<\lambda_c$, where $\lambda_c$ is the critical value determined by $\lambda_c=\min_{\vec{q}\in\mathbf{T}^d}\lambda_c(\vec{q})$.

We now show, for $d\geqslant 3$, $\lambda<0$ and $|\lambda|$ is arbitrarily small, that there is a region of $\vec{q}$ space contained in $(-\pi,\pi]^d$, and containing $\vec{q}=\vec{\pi}$, such that a bound-state exists. We know there is a bound-state solution for $\vec{q}=\vec{\pi}$ and $[\partial\epsilon/\partial q^j](\vec{\pi})=2$, so that, for $\vec{q}\simeq\vec{\pi}$, we have $\epsilon(\vec{q})\simeq-\lambda+2\Sigma_{j=1}^{d}(q^j-\pi)$. That means there is a bound state for $\vec{q}$ near $\vec{\pi}$. The vanishing of the binding energy $\epsilon(\vec{q})$ determines, approximately, the hyperplane $2\Sigma_{j=1}^{d}(q^j\pm\pi)=\lambda$. Thus, a bound state exists for the region of $\vec{q}$ space bounded by the boundary of the hypercube $(-\pi,\pi]^d$, but bounded away from it, and the hyperplane. Besides, we know the binding energy vanishes for $\epsilon(\vec{q})=0$. Thus, there is a bound state for a region in $\vec{q}$ space bounded by the cube $(-\pi,\pi]^d$ and the hyperplane $2\Sigma_{j=1}^{d}(q^j+\pi)=\lambda$. A more detailed picture of the zero binding-energy surface can be obtained numerically. As an example of a bound state emerging away from zero system momentum, we consider $d=3$ and $q^2=q^3=0$. Then the bound-state equation becomes

$$1+\frac{\lambda}{(2\pi)^3}\int_{\mathbf{T}^3}\frac{d\vec{p}}{h(\vec{p},q^1)+\epsilon}=0,$$

for $h(\vec{p},q^1)=4\cos(q^1/2)(1-\cos p^1)+4(1-\cos p^2)+4(1-\cos p^3)$. We consider small negative $\lambda$. For $q^1=0$, the integral is finite for $\epsilon\geqslant 0$ such as there is no bound state. On the other hand, for $q^1=\pi$, the integral reduces to a two-dimensional integral which diverges as $\epsilon\searrow 0$, and there is a unique bound-state solution. By continuity in $q^1$, the bound state persists down to some minimal value of $q^1>0$. We remark that there is a Birman-Schwinger-type bound below this critical $q^1$ value. The approximate bound-state curve is shown in Fig. 3.

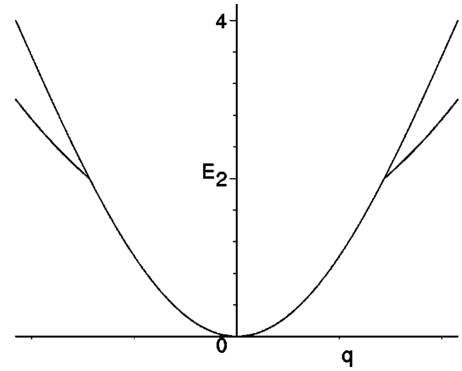


FIG. 3. The approximate energy-momentum spectrum for the attractive case $d=3$, small coupling, and equal masses. The system momentum is $\vec{q}=(q^1\equiv q,0,0)$. The upper curve is the band lower envelope, and we see that a bound state only occurs for $q>0$.

## VI. CONCLUSIONS

Emphasizing how the use of staggering transformations can be important in understanding the low-lying spectrum of quantum lattice systems, we have obtained interesting spectral features for the (one- and) two-particle Schrödinger operator on $\mathbb{Z}^d$, with a delta potential, which are expected to occur in some infinite lattice nonlinear quantum systems. Among other results which are hard to guess on the basis of pure intuition, we show that a bound state can appear, if $d\geqslant 3$, if the system momentum is sufficiently high, for both the attractive and the repulsive cases, in all dimensions. Also, even if the strength of the potential is arbitrarily small, the higher is the system momentum in these cases, the more stable the pair becomes. Whether this could favor a phenomenonlike condensation in some real system is a good question to be analyzed.

Also, we have developed a framework within which the effect on the spectrum can be determined for more general potentials. Also, here we considered perturbation of Laplacians, but more general kinetic-energy operators, as occur in the infinite lattice systems mentioned in the Introduction, can also be analyzed with our methods.

It would be interesting to get a complete picture of the zero binding-energy surfaces, even in the ladder approximation, for the stochastic model, the nonlinear mass spring system and the spin system described above.

## ACKNOWLEDGMENTS

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