PROCEEDINGS

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Staggering Transformations and the Excitation Spectrum of Diverse Lattice Quantum Models*

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ABSTRACT: We consider the energy-momentum excitation spectrum of diverse lattice Hamiltonian operators: the generator of the Markov semi-group of Ginzburg-Landau models with Langevin stochastic dynamics, the Hamiltonian of a scalar quantum field theory and the Hamiltonian associated with the transfer matrix of a classical ferromagnetic spin system at high temperature. The low-lying spectrum consists of a one-particle state and a two-particle band. The two-particle spectrum is determined using a lattice version of the Bethe-Salpeter equation. In addition to the two-particle band, depending on the lattice dimension and on the attractive or repulsive character of the interaction between the particles of the system, there is, respectively, a bound state below or above the two-particle band. We show how the existence or non-existence of these bound states can be understood in terms of non-relativistic single and two-particle lattice Schrödinger Hamiltonians with a delta potential; the corresponding resolvent equations are related to the Bethe-Salpeter equation. It turns out that a staggering transformation relates the spectrum of the attractive case to the corresponding spectrum for the repulsive case for each model we analyze.

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1. Introduction

The determination of elementary excitations in physical systems is of vital importance. In quantum field theory, the spectrum of the Hamiltonian determines the nature and the masses of the particles and the time evolution of the system. In non-equilibrium statistical mechanics for systems which admit a Markovian dynamics, the excitation spectrum of the generator of the dynamics determines the rate at which the system approaches the equilibrium. In the case of equilibrium statistical mechanics for classical spin systems, a reorganization of the partition function in terms of a transfer matrix is a useful way to analyze the behavior of correlation functions; minus the logarithm of the transfer matrix is a quantum Hamiltonian operator and its spectrum gives information on the falloff rate of equilibrium correlation functions.

In a recent series of papers given in Ref. [1], we have considered the low-lying part of the excitation spectrum of diverse $\mathbb{Z}^d$ lattice quantum systems, involving an infinite number of degrees of freedom and belonging to all the three categories of models described above. We have analyzed, for various values of the dimension d: Euclidean lattice scalar quantum fields, $\mathrm{O}(N)$ ferromagnetic spin systems with nearest neighbor interactions and a Ginzburg-Landau type stochastic model with a Langevin dynamics and continuous time.

This proceedings report encompasses the separate oral presentations by each of the two authors and deals with the understanding of the spectral results emerging from the above spectral analysis and covers the material discussed in Ref. [2]. Also, some new results have been added not found elsewhere in the literature.

Using translation operators on the lattice, we can define unitary momentum operators, one for each space direction of the system under consideration. They commute with the (usually!) bounded from below 'Hamiltonian' or dynamics generator for the system, as described above, and we look at the joint spectrum for these operators. We refer to this joint spectrum as the *energy-momentum* (e-m) spectrum and we call mass spectrum its restriction to zero system momentum. We adopt the familiar quasi-particle terminology to describe this spectrum and denote by E and $\vec{p}$ the associated values energy and momenta. A curve $E = w(\vec{p})$ in this joint spectrum is called a dispersion curve.

As a general feature of the analyzed generalized e-m spectra we considered is a vacuum or lowest state, associated with no e-m excitations, i.e. zero energy and zero momentum state, and also an isolated dispersion curve $E = w_1(\vec{p})$, associated with a single particle state with mass $M \equiv w_1(\vec{p} = \vec{0})$. Above this dispersion curve is a finite band, associated with the spectrum corresponding to two unbounded particles. Going higher in the spectrum, other finite bands also exist, associated with states with three, four,..., $\ell \in I\!N$, ..., unbounded particles, which are well separated in the beginning provided the system particle mass is large enough but eventually collapse and overlap as ℓ becomes large.

This is in contrast with e.g. the case of quantum fields in the continuum where the two-particle band extends to infinity (see e.g. [3]), as a consequence of the fact that momenta are unbounded in the continuum, whereas each of its components lives in $[-\pi, \pi]$ for the lattice $\mathbb{Z}^d$.

In the weak coupling regime, this spectral pattern is completed considering other points in the spectrum corresponding to stable states of two bounded particles or, simply, bound states given by isolated dispersion curves located in the neighborhood of the two-particle band.

To analyze the spectrum of single-particles, after establishing a Feynman-Kac formula for the two-point translation invariant correlation function on the lattice and providing a spectral representation for its Fourier transform $\tilde{G}(p^0,\vec{p})$, we consider the zeros of its convolution inverse $\tilde{\Gamma}(p^0,\vec{p})$, for p^0 in the imaginary axis.

Next, using a standard hyperplane decoupling expansion in the generalized time direction (here denoted with a 0 upper index), as formulated e.g. in Ref. [4], we can use the faster decay of the inverse Fourier transform $\Gamma(x^0,\vec{x})$, in comparison with $G(x^0,\vec{x})$, to provide a meromorphic extension of $\tilde{\Gamma}(p^0,\vec{p})$ above the energy scales lying above the one particle dispersion curve.

Together with the Bethe-Salpeter (B-S) equation, the above meromorphic extension constitutes the basis of our bound state analysis. Our analysis adapts and improves, to the lattice, some of the techniques developed to study quantum field theories in the continuum (see [5]). In operator form the B-S equation reads

$$D = D_0 + D_0 K D\,, \tag{1.1}$$

and defines K. In terms of kernels, with $x_1^0 = x_2^0$, $x_3^0 = x_4^0$, we obtain

$$\begin{aligned} D(x_1,x_2,x_3,x_4) = D_0(x_1,x_2,x_3,x_4) + \textstyle\int\; & D_0(x_1,x_2,y_1,y_2)K(y_1,y_2,y_3,y_4) \\ \times\; & D(y_3,y_4,x_3,x_4)\delta(y_1^0-y_2^0)\,\delta(y_3^0-y_4^0)\,dy_1dy_2dy_3dy_4\,, \end{aligned}$$

where,

$$D_0(x_1,x_2,x_3,x_4) = \epsilon G(x_1,x_3)G(x_2,x_4) + G(x_1,x_4)G(x_2,x_3)\,,$$

with $\epsilon=-1$ if a space of anti-symmetric (fermions) 'functions' is considered, and $\epsilon=+1$ in the symmetric case, and

$$D(x_1,x_2,x_3,x_4) = S(x_1,x_2,x_3,x_4) - G(x_1,x_2)G(x_3,x_4)\,,$$

is the four-point correlation function, partially truncated for the x_1,x_2 and x_3,x_4 clusters. We remark that the equal-time restrictions allow us to mathematically control the B-S equation and is different than the customary Euclidean field theory where there are no such restrictions.

The quantities D, D_0 and K can be taken as matrix operators depending on the specific model. Formally, we have $K = D_0^{-1} - D^{-1}$, and we remark that after taking into account the cancellation in D^{-1} due to its Gaussian-like (Wick theorem satisfied but with fully renormalized 'propagators'!) equivalent contribution D_0^{-1} the B-S equation puts into evidence a (channel) two-particle irreducible structure for K connecting the two clusters x_1,x_2 and x_3,x_4. To see this in our formalism, we use the hyperplane decoupling expansion method (see [4]), as before, allowing us to go above and near the two-particle threshold which is twice the mass M of the single particle.

Using translation invariance on the lattice to pass first to difference coordinates, we can re-write the B-S equation in terms of the lattice relative coordinates $\xi = x_2 - x_1$,

$\eta = x_4 - x_3$ and $\tau = x_3 - x_2$. In terms of $(\vec{\xi}, \vec{\eta}, \tau)$, and taking the Fourier transform in τ only, the B-S equation becomes

$$\hat{D}(\vec{\xi}, \vec{\eta}, k) = \hat{D}_0(\vec{\xi}, \vec{\eta}, k) + \int \hat{D}_0(\vec{\xi}, \vec{\xi}', k) \hat{K}(-\vec{\xi}', -\vec{\eta}', k) \hat{D}(\vec{\eta}', \vec{\eta}, k)\, d\vec{\xi}' d\vec{\eta}' \,.$$

$\hat{K}(-\vec{\xi}', -\vec{\eta}', k)$ acts as an energy-dependent non-local potential in the non-relativistic lattice Schrödinger operator analogy.

The bound state analysis can then be done in a first step by considering L, the ladder approximation to K. This corresponds to a local potential approximation, which is determined by keeping only the diagonal parts D_d of D and $D_{0,d}$ of D_0. Once the ladder approximation analysis is done, in Refs. [1, 5] it is shown how perturbations to the ladder approximation can be controlled to go beyond the ladder approximation and establish spectral results for the full model.

To finish the description of our main spectral results, we make precise how the bound state appears, if so, relatively to the two-particle band.

In all the models we considered in [1], we worked in the weak coupling regime and, adopting the functional 'integral' formalism, we were able to express the model by a measure on the space of field configurations (or spins) which, depending on the case, is or is not a weak perturbation of a Gaussian. Let us convey that the plus sign of the perturbation parameter (say $\lambda \in \mathbb{R}$, $|\lambda| << 1$) corresponds to a system with a repulsive interacting potential and an attractive potential for $\lambda < 0$.

For small $|\lambda|$, a bound state may or may not exist, depending on the system dimension d. When it exists, it is below the band if λ is negative and above the band if λ is positive. The distance from the band, i.e. the binding energy of this state, vanishes when $|\lambda| \searrow 0$. This situation is depicted in Figure 1, and holds for all the models we considered but one. In the general scenario, we have either the (mostly known) bound state below the band for the attractive case, in which there is a decreasing in the energy of the particle pair, or the energy increasing bound state above the band, for the repulsive case. For the exceptional case of a scalar lattice field model with non-local interactions given in [1], we can have both bound states simultaneously, no matter which sign of λ we consider. Furthermore, we can observe that the bound state below the band and the one above the band are approximately symmetrically located with respect to the center of the two-particle band. Moreover, for small momentum, $0 < |\vec{p}| << 1$, we show that the dispersion curve $E = w_{2,\uparrow}$ for the bound state above the band is concave while that of the bound state below the first band, $E = w_{2,\downarrow}$, is convex.

It is natural to ask if there is some underlying reason for the above two-particle spectral phenomenon. We show here that this phenomenon has its roots in the spectral behavior of a one-particle non-relativistic $\mathbb{Z}^d$ lattice Schrödinger operator with a delta potential at the origin given by

$$H_1 \equiv H_0 + V \ ,$$

where $H_0 = -\Delta$ is minus the lattice Laplacian and $V(\vec{x}) = \lambda\, \delta(\vec{x})$, which are both bounded operators.

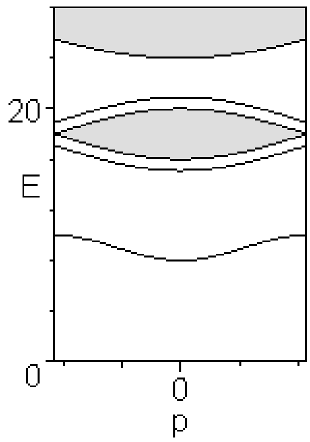

Figure 1: The approximate *e-m* spectrum for H_1, in the case $d = 1$. E denotes the energy and p the one-dimensional momentum for some fixed value of $|\lambda|$. We clearly see the one particle dispersion curve (lowest curve) and the two-particle band (first band from bottom to top) encircled by two-particle bound state dispersion curves. For $\lambda < 0$, only the isolated bound state lower dispersion curve appears; for $\lambda > 0$, only the isolated upper curve appears. The picture indicates in the highest part the beginning of the second band, corresponding to three unbounded particles, which in turn is well separated from the first band if the single particle mass is large enough.

We know, for the attractive case ($\lambda < 0$), that this Schrödinger Hamiltonian has a continuous spectrum in the interval $[0, 4d]$, which is the same as the spectrum for minus the Laplacian on the lattice $\mathbb{Z}^d$. Below the continuous spectrum, there is a negative-energy bound state at $-E_b$, $E_b > 0$, for $d = 1, 2$, and any coupling constant. For $d \geq 3$, a negative energy bound state appears only for λ below a critical value λ_c. Not so familiar is the spectrum for the repulsive case ($\lambda > 0$); there is the same continuum spectrum as before but there is also an isolated bound state above $4d$, the top of the continuous spectrum, at $E_a = 4d + E_b$.

We find that there is a transformation that interchanges high and low momenta (equivalently, small and large gradients in configuration space) and maps the attractive Hamiltonian to the repulsive one and vice-versa. This transformation is the well-known *staggering* transformation. In classical and quantum statistical mechanics, for example, it relates ferromagnetic and anti-ferromagnetic spin systems.

The main observation is that, at zero spatial system momentum, the B-S equation (1.1), is, roughly speaking, a relative coordinate lattice Schrödinger operator resolvent equation

$$(H_1 - zI)^{-1} = (H_0 - zI)^{-1} - (H_0 - zI)^{-1}\, V\, (H_1 - zI)^{-1}\,, \tag{1.2}$$

with a nonlocal potential. D^0 corresponds to the free resolvent, D to the interacting resolvent and K to minus the potential V.

In the ladder approximation, the nonlocal potential nearly is a local delta potential in the models we consider. The spectral relationship induced by the staggering transformation is exact in the non-relativistic case but it is only approximate for our models. The bound states above and below the two-particle band are not necessarily equidistant from the band, as for the non-relativistic one-particle system. However, staggering transformations consist of an useful tool to determine the low-lying part of the spectrum for the repulsive case, once it is known for the attractive one, and vice-versa.

Before we close the section, we remark that the role of staggering transformations can not only be put into evidence for the case of the single-particle Schrödinger Hamiltonian H_1 but also for a two-particle Schrödinger Hamiltonian H_2 with a delta pair potential; of which we will see that H_1 is a special case, corresponding to zero spatial system momentum. We discuss these two Hamiltonians in the sequel.

The above formulation using staggering transformations gives a mathematical description of the spectral results for bound states. It turns out that there is also a nice physical interpretation as the time-dependent Schrödinger eigenvalue equation is the same as the normal mode equation for polarized oscillations of an infinite mass-spring system on the lattice with an isotopic point-like defect at the origin, for the one-particle Hamiltonian H_1, or a line or hyperplane of defects for the two-particle Hamiltonian H_2. Much effort was devoted to the study of these classical vibrations. For example, see the Refs. [6, 7].

Similar problems appear in the study of quantum spin chains (see Refs. [8, 9, 10, 11, 12]).

2. Delta Function Potential and Staggering

The *e-m* spectral behavior around the two-particle band, at zero spatial system momentum (i.e. mass spectrum), for the various models described in the introduction can be understood in terms of the spectral properties of a $\mathbb{Z}^d$ lattice Schrödinger Hamiltonian H_1 for a non-relativistic particle in a delta potential at the origin, i.e., with $\vec{x} = (x^1, \ldots, x^d) \in \mathbb{Z}^d$,

$$H_1 \equiv H_0 + V = -\Delta + V \quad ; \quad V(\vec{x}\,) = \lambda\delta(\vec{x}\,)\,, \tag{2.1}$$

where H_1 acts in $\ell_2(\mathbb{Z}^d)$, the space of square summable functions on the lattice, and Δ is the lattice Laplacian ($\mathbf{e}^j$ being the unit vector along the j th direction)

$$-\Delta f(\vec{x}\,) = 2d\, f(\vec{x}\,) - \sum_{j=1}^{d} f(\vec{x} + \mathbf{e}^j) - \sum_{j=1}^{d} f(\vec{x} - \mathbf{e}^j) \quad ; \quad f \in \ell_2(\mathbb{Z}^d)\,. \tag{2.2}$$

We point out that, unlike the continuum, the lattice delta potential is a bounded operator in any d.

The resolvent equation (1.2) is a good approximation to the ladder approximation of the relative coordinate lattice B-S equation of the models described above with the ladder kernel of the B-S equation corresponding to $-V$, $(H_1 - z)^{-1}$ to D and $(H_0 - z)^{-1}$ to D^0.

To determine the spectral properties of the Hamiltonian H_1 of (2.1), we first define a unitary *staggering* transformation U which interchanges low and high momentum in the Fourier dual lattice, and plays a key role in understanding the relation between the spectrum of H_1 with $\lambda > 0$ and $\lambda < 0$. The staggering transformation U is defined by

$$U f(\vec{x}\,) \;=\; (-1)^{\sum_{j=1}^{d} x^j}\; f(\vec{x}\,) \quad ; \quad f \in \ell_2(\mathbb{Z}^d)\;, \tag{2.3}$$

and satisfies $U^2 = I$, $U^{-1} = U$, and its momentum space representation has the form

$$(Uf)^{\sim}\,(\vec{p}\,) \;=\; \tilde{f}(\vec{\pi} - \vec{p}\,)$$

where $\vec{p} \in \mathbf{T}^d$, the d-dimensional torus $(-\pi,\pi]^d$, $\vec{\pi}$ denotes the constant vector $(\pi,\pi,\ldots,\pi)$ and, with the usual notation for the Euclidean scalar product, we have $\tilde{f}(\vec{p}\,) = \sum_{\vec{x}\in\mathbb{Z}^d} e^{-i\vec{p}.\vec{x}}$ $f(\vec{x})$. For example, U transforms constant functions $f(\vec{x}) = c$ into $Uf(\vec{x}) \;=\; (-1)^{\sum_{j=1}^{d} x^j}\; c$. In terms of non-$\ell_2$ eigenfunctions of H_0, $f(\vec{x}) = c$ has energy eigenvalue zero and $Uf(\vec{x})$ has eigenvalue $4d$. In words, U takes smooth functions into rough (large lattice gradient) functions and vice-versa.

It is easy to show that U has the intertwining property

$$-\,\Delta \,+\, \lambda\delta \;=\; U\,\left[-1\,\left(-\Delta \,-\, \lambda\delta \,-\, 4d\right)\right]\, U^{-1}\;. \tag{2.4}$$

For example, if E is a point in the spectrum of H_1, with corresponding eigenfunction ψ for an attractive potential ($\lambda < 0$), then $-E + 4d$ and $U\psi$ are the corresponding eigenvalue and eigenfunction of H_1 with a repulsive potential ($\lambda > 0$). Thus, it is enough to consider the familiar attractive case; the repulsive case (unlike that of the one-dimensional continuum Hamiltonian) exhibits unusual spectral properties.

We now consider the spectral properties of H_1 for the attractive case $\lambda < 0$. The resolvent $(H_1 \,-\, z)^{-1}$ contains all the spectral information of H_1, and is now obtained explicitly. With an abuse of notation, the resolvent equation (1.2) in kernel form is

$$(H_1 \,-\, z)^{-1}\,(\vec{x},\vec{y}) \;=\; (H_0 \,-\, z)^{-1}\,(\vec{x},\vec{y}) \,-\, (H_0 \,-\, z)^{-1}\,(\vec{x},\vec{0})\,\lambda\,(H_1 \,-\, z)^{-1}\,(\vec{0},\vec{y})\;,$$

for $z \in \mathbb{C}$, $z \notin [\sigma(H_1) \cap \sigma(H_0)]$, where $\sigma(A)$ denotes the spectrum of A.

Setting $\vec{x} = \vec{0}$ and solving for $(H_1 \,-\, z)^{-1}\,(\vec{0},\vec{y})$, we obtain

$$\begin{aligned}(H_1 - z)^{-1}\,(\vec{x},\vec{y}) = {}& (H_0 - z)^{-1}\,(\vec{x},\vec{y}) \\ & -(H_0 - z)^{-1}\,(\vec{x},\vec{0})\,\frac{\lambda}{1 + \lambda\,(H_0 - z)^{-1}\,(\vec{0},\vec{0})}\,(H_0 - z)^{-1}\,(\vec{0},\vec{y})\,.\end{aligned} \tag{2.5}$$

In momentum space, the unperturbed Hamiltonian H_0 is the multiplication operator by the function

$$2\sum_{j=1}^{d}\left(1 \,-\, \cos p^j\right) \;\equiv\; -\tilde{\Delta}(\vec{p})$$

so that the spectrum of H_0 is the interval $[0, 4d]$, and is absolutely continuous. The resolvent of H_0 is given by, for $z \notin [0, 4d]$,

$$(H_0 \,-\, z)^{-1}\,(\vec{x},\vec{y}) \;=\; \frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{e^{i\vec{p}.(\vec{x}-\vec{y})}}{-\tilde{\Delta}(\vec{p}) \,-\, z}\,d\vec{p}\;.$$

Outside the interval $[0, 4d]$, the spectrum of H_1 arises from z singularities of (2.5). These singularities can only occur as zeroes of the denominator in (2.5), i.e. for $z = -E_b$, $E_b > 0$, we have the condition

$$\lambda\,(H_0 - z)^{-1}\left(\vec{0},\vec{0}\right) = \frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{1}{-\tilde{\Delta}(\vec{p}) + E_b}\,d\vec{p} = -1\,. \tag{2.6}$$

Hence, due to the $|\vec{p}|^2$ behavior of $-\tilde{\Delta}(\vec{p})$, for small $|\vec{p}|$, there is a unique bound state energy $-E_b$, for $d = 1, 2$ and any $\lambda < 0$. For $d \geq 3$, the integral in (2.6) converges for $E_b = 0$ so that there is a critical value for the coupling $\lambda_c < 0$ for the occurrence of a bound state.

From the Perron-Frobenius theorem for the positivity improving operator e^{-H_1} (see [13]), the associated bound and ground state eigenfunction $\psi(\vec{x})$ is positive (i.e., $\psi(\vec{x}) > 0$, for all $\vec{x}$) and, using the spectral theorem, there exists a unique spectral measure $dE(\mu)$ that allows us to write

$$(H_1 - z)^{-1} = \int_{-\infty}^{+\infty}\frac{1}{\mu - z}\,dE(\mu)$$

such that the bound state eigenfunction is given by

$$\psi(\vec{x}) = \left[\lim_{z\nearrow -E_b}\left(-(-E_b) - z\right)\,(H_1 - z)^{-1}\,(\vec{x},\vec{x})\right]^{1/2}\,,$$

and is normalized, meaning that $\sum_{\vec{x}\in\mathbb{Z}^d}|\psi(\vec{x})|^2 = 1$.

Moreover, expanding $1 + \lambda\,(H_0 - z)^{-1}(\vec{0},\vec{0})$ about $z = -E_b$, we find

$$\psi(\vec{x}) = \left[\frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{p}}{\left(-\tilde{\Delta}(\vec{p}) + E_b\right)^2}\right]^{-1/2}\frac{1}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{e^{i\vec{p}.\vec{x}}\,d\vec{p}}{-\tilde{\Delta}(\vec{p}) + E_b}$$

which is even. Also, since the above integrand admits an analytic extension to a momentum strip around the real $\vec{p}$-axis, by the Paley-Wiener theorem (see [14]) the eigenfunction $\psi(\vec{x})$ decays exponentially. Furthermore, using Stone's formula (see [15]) for $E(a') - E(a)$, $0 \leq a' \leq a < 4d$, shows that H_1 has absolutely continuous spectrum in $[0, 4d]$. Of course, $\psi(\vec{x})$ can also be obtained explicitly assuming $\psi(x) = c\rho^{|\vec{x}|}$, and solving for ρ in the eigenvalue equation $H_1\,\psi(\vec{x}) = -E_b\psi(\vec{x})$. This completes the description of H_1 for the attractive delta potential.

By (2.4), the spectrum of H_1 for the repulsive potential is $(4d + E_b) \cup [0, 4d]$. The surprising feature is the existence of a bound state above the continuous spectrum at $E_a \equiv 4d + E_b$. As the bound state eigenfunction for the attractive case is positive, the bound state eigenfunction in the repulsive case has maximum oscillation, by (2.3). We can also see the condition for the positive energy state with energy E_a from (2.6). Making the change of variables $\vec{q} = \vec{p} - \vec{\pi}$, (2.6) for the attractive potential becomes, setting $z = E_a$,

$$-\frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{1}{-\tilde{\Delta}(\vec{q}) + E_b}\,d\vec{q} = -1\,,$$

i.e. the condition for the existence of a bound state at E_a, for the repulsive potential $(\lambda > 0)$.

For comparison with the ladder approximation to the lattice B-S equation in the models considered in the ensuing sections, it is convenient to have the momentum space form of the resolvent (2.5). With $H_0 = -a\Delta$, and with $a > 0$ introduced here for later use, it reads

$$\begin{aligned}(H_1 - z)^{-1\sim}(\vec{p},\vec{q}) &= (2\pi)^d \frac{1}{-a\tilde{\Delta}(\vec{p}) - z}\,\delta(\vec{p}+\vec{q}) \\ &\quad - \frac{1}{-a\tilde{\Delta}(\vec{p}) - z}\,\frac{\lambda}{1 + \frac{\lambda}{(2\pi)^d}\int_{\mathbf{T}^d}\frac{d\vec{u}}{-a\tilde{\Delta}(\vec{u}) - z}}\,\frac{1}{-a\tilde{\Delta}(\vec{q}) - z}\,. \end{aligned} \tag{2.7}$$

Before closing the analysis for H_1, we determine the effect of the staggering transformation on the wave and scattering operators (see [16]). Making explicit the λ dependence in $H_1 \equiv H_1(\lambda)$, we define the wave operators $W_\pm(\lambda) = s - \lim_{t\to\pm\infty} e^{iH_1(\lambda)t}\, e^{-iH_0 t}$. We have, recalling that $U^{-1}H_1(\lambda)U = -H_1(-\lambda)$,

$$\begin{aligned} W_\pm(\lambda)U &= s - \lim_{t\to\pm\infty} UU^{-1}e^{iH_1(\lambda)t}UU^{-1}e^{-iH_0 t}U \\ &= U\left[s - \lim_{t\to\pm\infty} e^{-iH_1(\lambda)t}e^{iH_0 t}\right] = UW_\mp(-\lambda)\,. \end{aligned}$$

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

$$\begin{aligned} US(\lambda)U^{-1} &= UW_+(\lambda)^* UU^{-1}W_-(\lambda)U^{-1} \\ &= W_-(-\lambda)^* W_+(-\lambda) = S(-\lambda)^*\,. \end{aligned}$$

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

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

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

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

which is seen to hold for the explicit solution obtained above i.e., for $\epsilon > 0$,

$$\tilde{T}(\vec{p},\vec{k};\lambda) = \frac{\lambda}{1 + \lambda(H_0 - E - i\epsilon)^{-1}(0,0)}\,, \tag{2.8}$$

where we take the $\epsilon \searrow 0$ limit in the operator kernel.

We remark that the transition matrix can also be obtained from the Lippmann-Schwinger equation,

$$\psi(\vec{x},\vec{k}) = \phi(\vec{x};\vec{k}) - \left[(H_1 - E(\vec{k}) - i\epsilon)^{-1}V\phi(.;\vec{k})\right](\vec{x};\vec{k}) \tag{2.9}$$

where $\phi(\vec{x};\vec{k}) = e^{i\vec{k}.\vec{x}}$ is an eigenfunction of H_0, and $E \in (-2d, 2d)$. For the localized potential $V(\vec{x}) = \lambda\delta(\vec{x})$, Eq. (2.9) has the solution

$$\psi(\vec{x},\vec{k}) = \phi(\vec{x};\vec{k}) - \frac{\lambda(H_0 - E - i\epsilon)^{-1}(\vec{x},0)}{1 + \lambda(H_0 - E - i\epsilon)^{-1}(0,0)}\,. \tag{2.10}$$

The scattering amplitude is, in terms of the solution of Eq. (2.10) of the Lippmann-Schwinger equation (2.9), is given by

$$\left(\phi(.;\vec{k}'),\, V\,\psi(.,\vec{k})\right) = \lambda\phi(\vec{0},\vec{k}')\psi(\vec{0},\vec{k})\,,$$

which gives Eq. (2.8).

Furthermore, for real $F(E)$ and $D(E)$, writing the free resolvent as

$$(H_0 - E - i\epsilon)^{-1}(0,0) = F(E) - i\pi D(E)\,,$$

$D(E)$ being the density of states, we can write the differential cross section as

$$|f(E)|^2 = \frac{\lambda^2}{(1+F(E))^2 + \pi^2\lambda^2 D(E)^2}\,.$$

More explicitly, we have

$$D(E) = \frac{1}{(2\pi)^d}\int_{\mathbf{T}^d} \delta\left(E - E(\vec{q})\right)\, d\vec{q}\,, \tag{2.11}$$

and, for $\mathcal{P}$ denoting the Cauchy's principal value,

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

which has the interpretation of an electric field of a two-dimensional line charge distribution $D(E)$.

The explicit determination of the quantities $D(E)$ and $F(E)$ has been the subject of much research. For $d = 1$, by elementary integration, we obtain

$$\left\{\begin{array}{l} D(E) = \left\{\begin{array}{ll} \left[\pi\sqrt{1-E^2}\right]^{-1}, & |E| < 2 \\ 0, & |E| > 2 \end{array}\right. \\ F(E) = \left\{\begin{array}{ll} 0, & |E| < 2 \\ \frac{\mathrm{sign}(E)}{\sqrt{E^2-1}}, & |E| > 2 \end{array}\right. \end{array}\right. \quad ; \quad d = 1\,.$$

For $d = 2$, a non-trivial analysis allows $F(E)$ and $D(E)$ to be expressed completely in terms of the complete elliptic integral of the first kind $K(u) \equiv \int_0^{\pi/2}(1 - u^2\sin^2\theta)^{-1/2}d\theta$. As given in [17, 18, 19, 20, 21], we obtain

$$\left\{\begin{array}{l} D(E) = \left\{\begin{array}{ll} \pi^{-2}\,K(\frac{1}{2}\sqrt{4-E^2}), & |E| < 4 \\ 0, & |E| > 4 \end{array}\right. \\ F(E) = \left\{\begin{array}{ll} \pi^{-1}\mathrm{sign}(E)K(|E|/2), & 0 < |E| < 4 \\ \pi^{-1}\mathrm{sign}(E)K(2/|E|), & |E| > 2 \\ 0, & E = 0 \end{array}\right. \end{array}\right. \quad ; \quad d = 2\,.$$

A compact representation for $d = 3$ has been found only recently. A deep structural result of Ref. [22] has been discovered which allows $D(E)$ and $F(E)$ to be also expressed in terms of the function K. In this case, we have, for $|E| < 6$,

$$\begin{cases} D(E) = \pi{-}1\, G_I(E) \\ F(E) = G_R(E) \\ \lim_{\epsilon \searrow 0} G(E \pm i\epsilon) \equiv G_R(E) + iG_I(E) \\ G(E) = \dfrac{1-9\zeta^4}{E(1-\zeta)^3(1+3\zeta)} \left[\dfrac{2}{\pi} K(\alpha)\right]^2 \\ \alpha^2 = \dfrac{16\zeta^2}{(1-\zeta)^3(1+3\zeta)} \quad , \quad \zeta \equiv \left(1+\sqrt{1-\dfrac{9}{E^2}}\right)^{-1/2} \left(1+\sqrt{1-\dfrac{1}{E^2}}\right)^{1/2} \end{cases} \quad ; \quad d = 3\,.$$

These representations allow the determination of the scattering amplitude $f(E)$ for all values of the energy E and the coupling constant λ. The scattering amplitudes exhibit Lorentzian resonances, bumps (non-Lorentzian), dips and extinction. Also, one can see manifestations of Van Hove singularities.

The relationship with quantum mechanical Hamiltonians does not stop here. We also consider, to be closer to the particle contents of the B-S equation (1.1), the two-particle Hamiltonian in $\ell_2(\mathbb{Z}^d) \times \ell_2(\mathbb{Z}^d)$ taken as

$$H_2 \;=\; \frac{-\Delta_1}{2m_1} \;+\; \frac{-\Delta_2}{2m_2} \;+\; v_{12}(\vec{x}_1 - \vec{x}_2) \;\equiv\; H_0 + V_2\,, \tag{2.12}$$

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 Δ is the lattice Laplacian as before.

For $V_2 = 0$, the Hamiltonian H_2 has also 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 joint spectrum of $\left(H_2, \vec{P}\right)$, i.e. the e-m spectrum.

For H_2 of Eq. (2.12), we distinguish two cases, depending on whether or not the two masses m_1 and m_2 are equal. We will 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 $d \geq 3$, and momentum zero, there is a bound state only for λ 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 to the continuum case, where the Birman-Schwinger bound (see [13]) excludes bound states for sufficiently small potentials.

Next, we 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 $d \geq 3$, for all values of the system momentum, no bound state exists for small $|\lambda|$, in agreement with the continuum.

3. Spectrum for H_2: Generalities

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 $T_{\vec{a}} = \exp{[i\vec{P}.\vec{a}]}$ 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

$$U\, f(\vec{x}_1, \vec{x}_2) = (-1)^{\sum_{j=1}^{d} (x_1^j + x_2^j)}\, f(\vec{x}_1, \vec{x}_2)\,, \tag{3.1}$$

which is unitary and, since $U^2 = I$, we have $U^{-1} = U$. From Eq. (3.1), 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

$$\begin{aligned} U\, H_2 &= U\, \left[\tfrac{-\Delta \otimes I}{2m_1} + \tfrac{I \otimes -\Delta}{2m_2} + \lambda\delta \right] \\ &= \left[4d \left(\tfrac{1}{2m_1} + \tfrac{1}{2m_2} \right) - \left(\tfrac{-\Delta \otimes I}{2m_1} + \tfrac{I \otimes -\Delta}{2m_2} - \lambda\delta \right) \right] U\,, \end{aligned}$$

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-ℓ_2 functions

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

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

$$\begin{aligned} K(\vec{p}, \vec{k}\,) &\equiv -\tfrac{1}{2m_1}\, \tilde{\Delta}(\vec{p} + \vec{k}\,) - \tfrac{1}{2m_2} \tilde{\Delta}(\vec{p} - \vec{k}\,) \\ &= \tfrac{1}{2m_1} \textstyle\sum_{j=1}^{d}\, 2\, \left[1 - \cos(p^j + k^j) \right] \\ &\quad + \tfrac{1}{2m_2} \textstyle\sum_{j=1}^{d}\, 2\, \left[1 - \cos(p^j - k^j) \right]\; . \end{aligned}$$

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 ψ's obey the following orthogonality and completeness relations

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

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 Ψ satisfies $i\frac{\partial \Psi}{\partial t} = H_2\, \Psi$, if we take ϕ such that

$$H_2\, \phi = E(\vec{k})\, \phi\,, \tag{3.2}$$

with $\phi(\vec{x}_1, \vec{x}_2, \vec{k}) = e^{i\vec{k}.(\vec{x}_1+\vec{x}_2)}\chi(\vec{x}_2 - \vec{x}_1, \vec{k}\,)$ and $\chi(\vec{x}, \vec{k}\,) = (2\pi)^{-d} \int b(\vec{p}, \vec{k})e^{i\vec{p}.\vec{x}}\, d\vec{p}$. Substituting in Eq. (3.2), cancelling the $e^{i\vec{k}.(\vec{x}_1+\vec{x}_2)}$ factor, and taking the Fourier transform in the relative coordinate $\vec{x} = \vec{x}_2 - \vec{x}_1$, we obtain

$$[K(\vec{p}, \vec{k}\,) - E(\vec{k}\,)]b(\vec{p}, \vec{k}) + \frac{\lambda}{(2\pi)^d} \int b(\vec{p}\,', \vec{k})\, d\vec{p}\,' = 0\,. \tag{3.3}$$

Multiplying Eq. (3.3) by $(K - E)^{-1}(\vec{p}, \vec{k})$ and integrating over $\vec{p}$ leads to the eigenvalue equation

$$1 + \frac{\lambda}{(2\pi)^d} \int_{\mathbf{T}^d} \frac{d\vec{p}}{K(\vec{p}, \vec{k}\,) - E(\vec{k})} = 0\,. \tag{3.4}$$

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. (3.3) becomes, after cancelling the $e^{i\vec{k}.(\vec{x}_1+\vec{x}_2)}$ factor, and setting $\vec{x} \equiv \vec{x}_2 - \vec{x}_1$,

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

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

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

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

Next, we show that the spectrum of the Hamiltonian H_1 is obtained from the spectrum of H_2, at zero system momentum. Indeed, for $\vec{k} = \vec{0}$, Eq. (3.3), with $\mu = m_1 m_2/(m_1 + m_2)$, 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 isotopic-like defect at the origin [6, 7].

4. Spectrum of H_2 for Unequal Masses

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

$$1 + \lambda \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{g(p,q) \, - \, z} \, dp = 0 \, , \tag{4.1}$$

where

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

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. (4.1) becomes

$$1 + \lambda \, \frac{-1}{2[z - w_+(q)]^{1/2} \; [z - w_-(q)]^{1/2}} = 0 \, , \tag{4.2}$$

with solutions

$$w_\pm(q) = \frac{1}{\mu} \;\pm\; \left[\frac{\cos^2(q/2)}{\mu^2} + \frac{\sin^2(q/2)}{\gamma^2} \right]^{1/2} \quad , \tag{4.3}$$

$\mu = m_1 \, m_2 \, (m_1 + m_2)^{-1}$ and $\gamma = m_1 \, m_2 \, (m_2 - m_1)^{-1}$. 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

$$\epsilon = -\frac{(w_+ - w_-)}{2} + \frac{1}{2} \, \left[(w_+ - w_-)^2 + \lambda^2 \right]^{1/2} \; . \tag{4.4}$$

The results for unequal masses and $d = 1$ are depicted in Figure 2.

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

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

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 $d \geq 3$. This agrees with the Birman-Schwinger bound (see [13]). 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 ($\lambda < 0$).

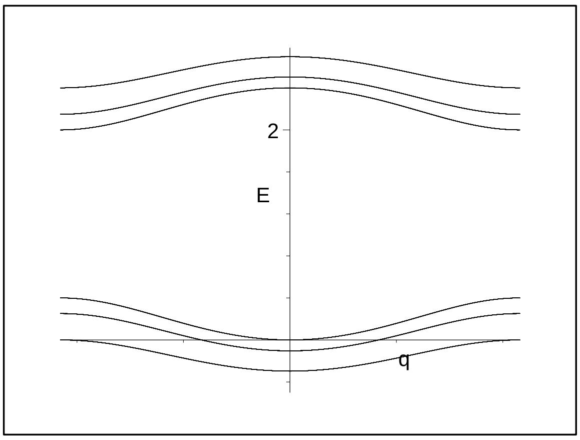

Figure 2: The energy-momentum spectrum for the case $d = 1$ and unequal masses, with $m_2 = 0.2\, m_1$. E is the energy and q the one-dimensional momentum variable, for some fixed value of $|\lambda|$. The most inner curves are the band envelopes. All its interior points also belong to the spectrum. 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.

5. Spectrum of H_2 for Equal Masses

In the case of equal masses, γ 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 $\mu = 1/4$. Eq. (3.3) becomes, for system momentum $\vec{q} = 2\vec{k}$,

$$4\sum_{j=1}^{d} \cos\frac{q^j}{2}(1-\cos p^j)b(\vec{p}) + \frac{\lambda}{(2\pi)^d}\int b(\vec{p}')d\vec{p}' = \left[E - \left(4d - 4\sum_{j=1}^{d}\cos\frac{q^j}{2}\right)\right] b(\vec{p})\,, \quad (5.1)$$

which is the momentum space form of the normal mode equation for classical polarized oscillations of an anisotropic crystalline lattice with a point defect [6, 7, 17, 18, 20, 21]. 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. (5.3) below].

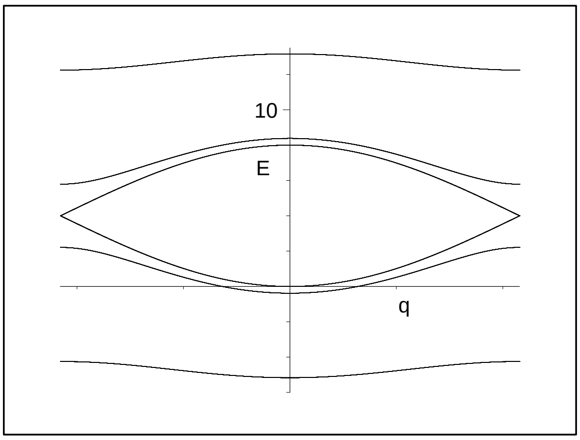

Figure 3: The equal mass energy-momentum spectrum for the case $d = 1$. E is the energy and q the one-dimensional momentum variable, for some fixed value of $|\lambda|$. The most inner curves are the band envelopes. All its interior points also belong to the spectrum. For $\lambda < 0$, only the isolated 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.

We first take $d = 1$. Eqs. (4.1) to (4.4) hold in the $\gamma \to \infty$ limit. Solving the bound state equation gives $\epsilon = -\frac{1}{2}(w_+(q) - w_-(q)) + \frac{1}{2}\left[(w_+(q) \ - w_-(q))^2 + \lambda^2\right]^{1/2}$, 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 ϵ given by the same expression as above, for the attractive case. The final result for $d = 1$ is summarized in Figure 3.

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

$$1 + \frac{\lambda}{(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{f(\vec{p}, \vec{q}) - z}\, d\vec{p} \ = \ 0 \ . \tag{5.2}$$

To determine the bound state below the band, in the attractive case, $\lambda < 0$, with fixed $\vec{q}$, it is convenient to define $f_{min}(\vec{q}) \ \equiv \ \min_{\vec{p} \in \mathbf{T}^d} \ f(\vec{p}, \vec{q}) \ = \ \sum_{j=1}^{d} 4(1 - \cos q^j/2)$ and set $z(\vec{q}) = f_{min}(\vec{q}) - \epsilon(\vec{q})$, $\epsilon > 0$, being the binding energy. The bound state condition of Eq. (5.2) becomes

$$1 + \frac{\lambda}{(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{4\sum_{j=1}^{d} \cos(q^j/2)(1 - \cos p^j) + \epsilon}\, d\vec{p} = 0 \tag{5.3}$$

Note that the integrand in Eq. (5.3) is positive and is a continuous function of $\epsilon > 0$.

Another important observation is that, for any d and any λ, there is always a solution $\epsilon(\vec{\pi}) = |\lambda|$ to Eq. (5.3), 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 Figure 3). 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 section 2. All these results follow from the Payley-Wiener theorem [14].

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. (5.1) 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 $d \geq 3$, the integral in Eq. (5.3) 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 ϵ. Using the parity property on the components of $\vec{q}$, we concentrate our analysis to nonnegative components q^j, $j = 1, \ldots, d$. For fixed λ, differentiating Eq. (5.3) 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 nonnegative, 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 λ solution to Eq. (5.3) with $\vec{q} = \vec{0}$ in the limit $\epsilon \searrow 0$, i.e.

$$1 + \frac{\lambda_c(\vec{0})}{(2\pi)^d} \int_{\mathbf{T}^d} \frac{1}{4\sum_{j=1}^d (1 - \cos p^j)} \, d\vec{p} = 0 \,. \tag{5.4}$$

This is similar to the continuum results where the Birman-Schwinger bounds (see [13]) excludes bound states below a critical coupling. Thus, using the continuity in ϵ, 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 ϵ to show the existence of a solution for each $\vec{q}$ up to $\vec{q}$ near $\vec{\pi}$. We remark that, from Eq. (5.4), 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 λ_c is the critical value determined by $\lambda_c = \min_{\vec{q}\in\mathbf{T}^d} \lambda_c(\vec{q})$.

In contrast to the continuum case, we now show, for $d \geq 3$, $\lambda < 0$ and $|\lambda|$ 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 $\epsilon(\vec{q}) \simeq -\lambda + 2\sum_{j=1}^d \left(q^j - \pi\right)$. 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 $2\sum_{j=1}^d \left(q^j \pm \pi\right) = \lambda$. 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 $2\sum_{j=1}^d \left(q^j + \pi\right) = \lambda$. 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 $h(\vec{p}, q^1) = 4\cos(q^1/2)\left(1 - \cos p^1\right) + 4\left(1 - \cos p^2\right) + 4\left(1 - \cos p^3\right)$. We consider small negative λ. For $q^1 = 0$, the integral is finite for $\epsilon \geq 0$ 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 Figure 4.

6. 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 $d \geq 3$, 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 phenomenon like condensation in some real system is a good question to be analyzed.

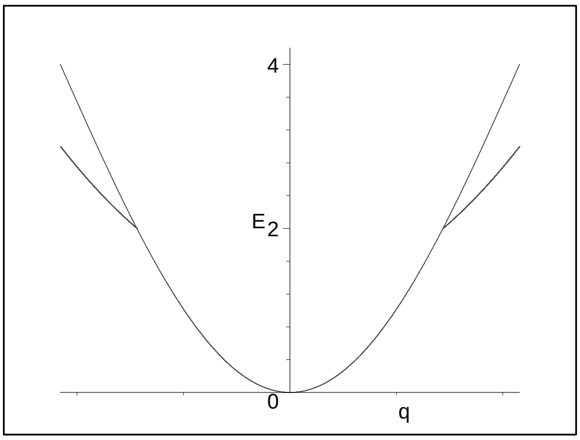

Figure 4: The approximate energy-momentum spectrum for the attractive case $d = 3$, small coupling and equal masses. The system momentum is $\vec{q} = (q^1 \equiv q, 0, 0)$ and E is the energy for some fixed value of $|\lambda|$. The upper curve is the band lower envelope, and we see that a bound state only occurs for $q > 0$.

Also, we have developed a framework within which the effect on the spectrum can be determined for more general potentials. 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 in Refs. [1].

Moreover, it would be relevant to extend the present analysis and consider the role played by staggering transformations in multi-phase regions and exactly soluble models, as well as to investigate degeneracies in multi-component cases (see [1]) and the existence of soliton-anti-soliton solutions for space lattice classical nonlinear wave equations and their quantum analogues.

Finally to make contact with the main topic of this conference, we think it would be interesting to investigate the existence of bound states above and below the two-particle band in exactly soluble lattice models.

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