Tunnelling couplings in discrete lattices, single particle band structure and eigenstates of interacting atom pairs

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By adjusting the tunnelling couplings over longer than nearest neighbor distances it is possible in discrete lattice models to reproduce the properties of the lowest energy band of a real, continuous periodic potential. We propose to include such terms in problems with interacting particles and we show that they have significant consequences for scattering and bound states of atom pairs in periodic potentials.

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I. INTRODUCTION

Spatially periodic potentials induced by off-resonant laser fields have been applied in numerous studies to modify the dynamics of ultra-cold bosonic gases. In the “mean-field” regime with many atoms, the potential changes the transport properties and effective mass of the atoms\cite{1, 2, 3}, in a dilute gas the lattice enables tuning of the ratio between kinetic and interaction energy and observation of a Tonks gas\cite{4, 5}, and in the limit of well confined atoms in deep lattice wells collisionally induced collapses and revivals of the matter wave mean field has been observed\cite{6}. The observation of the transition from a superfluid to a Mott insulator is a hallmark experiment on a zero temperature phase transition made possible by the use of an optical lattice\cite{7, 8, 9}.

To deal properly with the many-body aspects of the quantum state, it has been useful to approximate the motion in the periodic potential by a discrete lattice model, specifying for a single atom the atomic wave function only on positions corresponding to the potential minima of the true potential. The kinetic energy gives rise to tunnelling couplings between the sites, whereas the potential energy is described by local values of the potential on each site. If the potential attains the same value on each site, the eigenvectors of the Hamiltonian are characterized by amplitudes that experience a fixed phase rotation as one steps through the lattice. These states are (quasi-)momentum eigenstates, and their energies depend on the tunnelling coupling coefficients. The discrete lattice model with only nearest neighbor tunnelling couplings does not reproduce important features in the momentum dependence of energy in the lowest energy band of a real potential. In this paper we show that it is relatively easy to remedy this problem by incorporation of “long distance” tunnelling couplings, and we propose that such couplings be incorporated in studies of many-body dynamics in periodic potentials, since binding and collisional interactions may depend crucially on the dispersion properties of atoms in the periodic environment.

As a particular example we consider two interacting atoms, and in particular the phenomenon of repulsively bound atom pairs in optical lattices\cite{10, 11, 12, 13}. The stability of a repulsively bound pair may be understood qualitatively from the observation that the repulsive interaction gives two atoms an energy that lies within the energy band gap of free motion in the periodic potential, forcing the atoms to stay together in a discrete bound state lying above the energy continuum of scattering states. The lack of dissipative channels, unlike, e.g., the phonons in real crystals, makes the observation of repulsively bound atom pairs possible in optical lattices\cite{10}.

The paper is structured as follows. In Sec. II, we analyze the eigenstates of a single particle in a periodic potential, and we show that the lowest energy band can be obtained also from a discrete lattice model with suitably selected tunnelling couplings. In Sec. III, we turn to the description of two atoms with a short range interaction, and we identify the continuum of scattering states in the lowest Bloch band. In Sec. IV we identify the discrete states following from the attractive and repulsive binding mechanisms, and we show that these states have a number of physical properties that depend markedly on our more precise description of the band structure of the system. Sec. V concludes the paper and discusses possible consequences of incorporating its results in the treatment of many-body problems, e.g., via the Bose-Hubbard Hamiltonian.

II. SINGLE-PARTICLE DYNAMICS

We consider an atom with mass $m$ that moves in an off-resonant standing wave laser field with wave length $\lambda$. Due to the light induced energy shift, the atom experiences a potential $V(x) = V_0 \cos(2\pi x/a)$ with period $a = \lambda/2$ and potential strength $V_0$ proportional to the light intensity and inversely proportional to the optical detuning from atomic resonance. According to Bloch’s
describing atoms localized in the \( j \)th well in the lattice (to ensure constructive interference at the \( j \)th well we need a phase convention and choose \( \phi_k(x = 0) \) to be real and positive for all \( k \)). We have, for convenience, assumed a finite number \( M \) of lattice periods and periodic boundary condition on the entire system.

By evaluating all matrix elements

\[
J_d \equiv -H_{j,j+d} = -\langle w_j | \mathcal{H} | w_{j+d} \rangle = \int dx \ w_0(x)^* \left( -\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) w_d(x),
\]

where we have used the translational invariance of the problem, the Hamiltonian can be explicitly rewritten in the Wannier basis,

\[
\mathcal{H} = -\sum_{j,d} J_d |w_j\rangle\langle w_{j+d}| + |w_{j+d}\rangle\langle w_j|.
\]

So far no approximations were done except for the omission of the higher bands, which can be reintroduced in the formalism if needed. The Hilbert space is now represented by a discrete basis of localized Wannier states, and it is only a matter of re-interpretation to read Eq. (4) as a discrete lattice model of the problem.

To interpret \( J_d \) in terms of the band structure, we insert the expression for the Wannier functions (2) into the integral for \( J_d \) and obtain

\[
J_d = -\frac{1}{M} \sum_{k,q} \int dx \ \phi_q(x)^* \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \times \phi_k(x)e^{ikad} = -\frac{1}{M} \sum_k E(k)e^{ikad}.
\]

where we observe that the \( J_d \) amplitudes are the Fourier coefficients of the band structure. The band structure is an even function of \( k \) and therefore

\[
E(k) = -J_0 - 2 \sum_{d>0} J_d \cos(kad).
\]

Without loss of generality we can set \( J_0 = 0 \) in the following.

The application of lattice models which include only nearest neighbor tunnelling couplings only provide us with a simple cosine shaped band structure, as depicted in Fig. 1 (dashed line). Including more \( J_d \) terms, the \( J_d \)-values are compared to \( J_1 \) in the insert of Fig. 1 gives a more accurate energy dispersion as indicated by the dash-dotted line in the figure. As the lattice strength is ramped up in the limit of strong potentials \( V_0 >> E_R \), the importance of the higher \( J_d \) values decreases and only \( J_1 \) differs significantly from zero. For \( J_2 \) to be less than 1\% of \( J_1 \), \( V_0 \) has to exceed 5.32\( E_R \).

We observe that in the opposite limit where \( V_0 \to 0 \), \( J_d \) coincides with the Fourier transform of the free space energy dispersion parabola, i.e. \( J_d = -\frac{\hbar^2}{2m} (ad)^{-2}(-1)^d \), with absolute values plotted as filled circles in the insert of Fig. 1.

Fig. 1 clearly shows significant and well known differences between the real band structure and the simple cosine dependence found for nearest neighbor tunnelling models. These differences are visible if one tries to perturb and excite motion in the system, and as we shall see in the following section they also have important consequences for the states of interacting atoms in the periodic potential.
III. ATOMIC SCATTERING STATES IN THE LATTICE

We now proceed to the two-body problem and find the eigenstates $\psi(x,y)$ of a pair of particles moving on the lattice with discrete one-dimensional position coordinates $x$ and $y$, and interacting by short range interactions. The Hamiltonian of this system is assumed to be of the form

$$H = -\sum_d J_d (\Delta_x^{(d)} + \Delta_y^{(d)} + 4) + U \delta_{x,y}$$

(7)

where the action of the “$d^{th}$ Laplacians” on a wave function are given by $\Delta_x^{(d)} f(x) = (f(x + ad) + f(x - ad) - 2f(x))$ with step size $ad$. The sum over the discrete Laplacians incorporates the tunnelling terms $\Delta^{(d)}$ which in turn describe both the kinetic energy and the periodic potential energy of the particles, i.e. the full dynamics of independent particles in the lattice. The interaction between particles should be computed as a matrix element between products of Wannier states of the real physical atoms are asymptotically free. As in normal scattering theory, the continuum part of the Hamiltonian $\hat{H}$, thus provides also the spectrum of interacting atoms on the lattice. This is due to the flatness of the cosine potential.

We will first discuss the scattering states, where the atoms are asymptotically free. As in normal scattering theory, the continuum part of the Hamiltonian $\hat{H}$, and the sum of the single particle Hamiltonians of non-interacting particles are unitarily equivalent. This implies that the energy spectrum is given by simple addition of contributions from two identical band structure calculations as the ones shown in Fig. 1. We can also solve the scattering problem explicitly and find the two-body wave function in terms of the center-of-mass, and relative coordinate, $z = x - y$. Note that the problem of particles moving in the full cosine potential does not separate in these coordinates, but in the lattice model, the Hamiltonian does not explicitly depend on the shape of the lattice potential wells (the interaction is built into the "Laplacian" and the Wannier functions making up the discrete states), and separation is possible. When we apply the Hamiltonian to the wave function Ansatz, $\psi(x,y) = e^{ikz} \psi_K(z)$, for each value of $K$ we have to solve the one-body Schrödinger equation for the relative position coordinate,

$$\left( -2 \sum_{d>0} \cos(\frac{1}{2}Kda)J_d (\Delta_z^{(d)} + 2) + U \delta_{z,0} \right) \psi_K(z)$$

$$= E \psi_K(z).$$

(9)

It is readily verified that plane wave functions of the form $\psi_K^d(z) = e^{ikz}$ are eigenfunctions of the unperturbed Hamiltonian $H_0 = -2 \sum_{d>0} \cos(\frac{1}{2}Kda)J_d (\Delta_z^{(d)} + 2)$ with energies

$$\epsilon_K(k) = -4 \sum_{d>0} J_d \cos(\frac{1}{2}Kad) \cos(kad).$$

(10)

As noted above, the spectrum of scattering states, but not the scattering wave functions themselves, are independent of the short range scattering potential, and Eq. (10) thus provides also the spectrum of interacting atoms on the lattice. This spectrum is displayed in Fig. 2(a)-(c) with inclusion of different numbers of tunnelling coefficients $J_d$. The different shades of grey in the figure show the density of states. For fixed center-of-mass momentum $K$ the density of states has a peak around the maximal and minimal energy. This is due to the flatness of the cos(kad) function in Eq. (10) near its extremal values. A complete degeneracy in $k$ can be observed due to the front factor $\cos(\frac{1}{2}Kda)$ in Eq. (10), when only nearest neighbor coupling is included and $K = \pm \pi/a$. This degeneracy, however, is lifted by the amount $\Delta_{E=\pi/a} = 8 \sum_{m} (-1)^m J_{2m}$ in Fig. 2(b)-(c).

Another pronounced feature in the spectra of Fig. 2 is the extra van Hove singularity in the scattering states for values of the center-of-mass momentum close to $K = \pm \pi/a$. To see where it comes from we note that the non-interaction system separate, so we could have chosen a product wave function $\Psi = \psi_{q_1}(x)\psi_{q_2}(y)$ with total energy $E(q_1) + E(q_2)$, where $q_j$ is the quasi-
momentum of the individual atoms and $E$ is the one-body band structure. If we infer the center-of-mass quasi-momentum $K = q_1 + q_2$ and relative motion quasi-momentum $k = (q_1 - q_2)/2$, we can see that this is indeed the same energy $\epsilon_K(k)$ as derived above

$$\epsilon_K(k) = E(q_1 = \frac{K}{2} + k) + E(q_2 = \frac{K}{2} - k)$$

$$= -2 \sum_{d>0} J_d \left( \cos \left( \frac{K}{2} + k \right) d + \cos \left( \frac{K}{2} - k \right) d \right)$$

$$= -4 \sum_{d>0} J_d \cos \frac{Kad}{2} \cos kad.$$

(11)

The extra van Hove singularities can be understood from Fig. 3 where the band structure for each atom is plotted together with the total energy as a function of the relative momentum $k$. The extra van Hove singularity around $K = \pm \pi/a$ in Fig. 2(b)-(c) is due to the appearance of a local minimum in the two-body energy spectrum at $k = \pi/a$. This phenomenon sets in when $\frac{\partial^2 \epsilon_K}{\partial k^2}(k = \pi/a) = 0$ as shown in Fig. 3(c), where $K = 0.4 \pi/a$. We note that $\frac{\partial^2 \epsilon_K}{\partial k^2}(k = 0) = 0$ and $\frac{\partial^2 \epsilon_K}{\partial k^2}(k = \pi/a) = 0$ cannot be simultaneously fulfilled when the band structure is a pure cosine function, i.e., when only nearest neighbor tunneling is included in the model. When $K = \pm \pi/a$, as in figure 3(f), the energy minima at $k = 0$ and $k = \pi/a$ are degenerate and therefore we see only two maxima in the density of state in Fig. 2(c).

In the next section we include the atom-atom interaction, $V(z) = U\delta_{z,0}$, to account for bound states.

IV. REPULSIVELY AND ATTRACTIVELY BOUND STATES

The bound states of the system can be obtained from the Green’s function solution of the Schrödinger equation (9). We first solve the problem in the absence of the interaction,

$$(E - H_0)G^0_K(E, z) = \delta_{z,0}$$

(12)

to obtain the unperturbed Green’s function. The full Green’s function in position space can now be obtained

$$G_K(E, z) = G^0_K(E, z) + \int dz' G^0_K(E, z')V(z')G_K(E, z')$$

$$= G^0_K(E, z) + G^0_K(E, z)UG_K(E, z = 0)$$

$$= G^0_K(E, z) \frac{1}{1 - UG^0_K(E, z = 0)}$$

$$= \frac{G^0_K(E, z)}{1 - UG^0_K(E, z = 0)}.$$  

(13)

Whenever there is a bound state $G_K$ has a pole, therefore the bound state energies are determined solely by the interaction strength $U$ and the unperturbed Green’s function

$$1 = UG^0_K(E_b, z = 0).$$

(14)

The unperturbed Green’s function, in turn, is readily obtained from the momentum space representation, $G^0_K(E, z) = (2\pi)^{-1} \int dk G^0(E, k)e^{ikz}$,

$$G^0_K(E, k) = \frac{1}{E - \epsilon_K(k) + i\eta}, \quad (\eta \to 0^+).$$

(15)

The integral of Eq. (15) can be found analytically if $\epsilon_K(k)$ is a simple cosine, and in the general case it can be computed numerically and the solution to Eq. (14) can be found by a simple numerical search.

We can combine Eqs. (12) and (14) to obtain the relation

$$(E - H_0)G^0_K(E_b, z) = \frac{1}{G^0_K(E_b, z = 0)}\delta_{z,0}G^0_K(E_b, z)$$

$$= U\delta_{z,0}G^0_K(E_b, z).$$

(16)

This shows that $G^0_K(E_b, z)$ is itself a solution to the Schrödinger equation, i.e., it provides directly the bound state wave function $\psi_K(z)$, and $G^0_K(E_b, k)$ provides the wave function $\psi_K(k)$ in momentum space.

There are discrete bound states for both positive and negative $U$ corresponding to repulsive and attractive interaction, respectively. The energy of the repulsively and attractively bound atom pairs lie above and below the scattering continuum as plotted in Fig. 2. The repulsively bound pair state was recently experimentally demonstrated by Winkler et al. [10].
If we only include \( J_1 \) we have the following symmetry in the continuum spectrum, Eq. (16),

\[
\epsilon_K(k) = -\epsilon_K(k + \pi/a).
\]  

This implies, according to Eq. (15), when \( E \) is outside the scattering continuum,

\[
G^0_K(E, k) = -G^0_K(-E, k + \pi/a),
\]

and hence

\[
1 = U G^0_K(E_{ab}(K), z = 0) = (-U) G^0_K(-E_{ab}(K), z = 0) = (-U) G^0_K(E_{rb}(K), z = 0),
\]

which relates the repulsively \((rb)\) and attractively \((ab)\) bound atom pair energies:

\[
E_{ab}(K) = -E_{rb}(K).
\]  

Eq. (16) now implies, if we include only \( J_1 \), that the attractively and repulsively bound wave functions are related by

\[
\psi^{ab}_K(k) = \psi^{rb}_K(k + \pi/a).
\]

This symmetry is also pointed out in [12], but it is important to note that when the higher \( J_d \) tunnelling couplings are included, Eq. (17) and hence the following equations (20)(21) are no longer valid.

The shape of the band structure is altered when \( J_{d>1} \) are included, but more importantly the wave functions are altered significantly, compare Figs. 4 and 5.

In Fig. 4 only \( J_{d=1} \) is included. As one would expect the bound states are composed of the quasi-momentum components lying closest in energy to the bound state. In the region around \( K = 0 \) this correspond to relative momentum \( k = \pi/a \) and the formation of bound pairs can in this region be explained by the fact that the peak in \( k \)-distribution corresponds to the individual atoms having quasi-momentum \( q_1 = q_2 = \pi/a \). Here the effective mass is negative and therefore a repulsive force causes attraction [13]. As \( K \) approaches \( \pm \pi/a \) the scattering states with different relative momenta become degenerate in energy and the momentum distribution of the bound state goes from a peaked function Fig. 4(a) to a constant function (b), which corresponds to a delta function in relative coordinate (f).

In Fig. 5 \( J_d \) up to \( d \leq 6 \) has been included in obtaining the \( k \)- and \( r \)-distributions of the repulsively bound states. As discussed previously; when the extra van Hove singularity sets in Fig. 5(a), the two-body spectrum broadens around \( k = \pi/a \) and this can also be observed in the decomposition of the bound states fig. 5(c). In Fig. 5(e) we clearly see the consequences of lifting the \( k \)-degeneracy at \( K = \pm \pi/a \). The momentum distribution is no longer constant but instead peaked around the two momenta \( k = \pm \pi/2a \) which compose the top of the scattering band, as can be seen in Fig. 5(f).

In the experiment by Winkler et al. [10] the atoms were prepared in the \( K = 0 \) bound state. We suggest that by exposing the system to a force field the bound pairs can be prepared in any \( K \)-state. This can be realised in practice by chirping the lattice lasers so the lattice potential is accelerated in the laboratory frame [15]. To investigate the effect on the two-atom states, we make

**FIG. 4:** Repulsively bound states obtained with nearest neighbor interaction only. First column shows \( \psi_k(k) \) and the second \( \psi_k(z) \) both obtained from Eqs. 15-16, see text for details.

**FIG. 5:** Repulsively bound states obtained with six nearest neighbor interactions included. First column shows \( \psi_k(k) \) and the second \( \psi_k(z) \) both obtained from Eqs. 15-16, see text for details.
the new time dependent Ansatz
\[ \Psi(x, y, t) = e^{iK(t)x} \psi(x - y, t) \]  
with a time dependent center-of-mass quasi-momentum, \( K(t) \). Inserting this Ansatz into the time dependent Schrödinger equation with the Hamiltonian (7) and the linear term due to the force, \(- F \cdot (x + y)\), we obtain
\[ i\hbar \frac{\partial}{\partial t} \psi(z, t) = \left( -2 \sum_{\delta > 0} \cos(\frac{1}{2} K(t)da)J_d \left( \Delta_\delta^z + 2 \right) + U\delta_{z,0} \right) \psi(z, t) \]  
if we choose
\[ K(t) = \frac{2F}{\hbar}. \]  
Since there is an energy gap between the bound state and the scattering states, we may apply the adiabatic approximation to Eq. (23) and simply replace \( \psi(x - y, t) \) by the eigenstate \( \psi_K(x - y) \) of Eq. (9) with \( K = K(t) \). Provided we accelerate the lattice slowly enough we can thus explore all the wave functions \( \psi_K(x - y) \) of the system with \( K = 2Ft/\hbar \).

V. DISCUSSION

The states and energies of particles in periodic potentials depend on the details of these potentials. We have in this paper shown that the lowest band in the single particle band structure in such a potential can be described very accurately with a discrete lattice model with tunnelling couplings to a sufficiently high number of remote sites. Such modelling may be particularly important when one studies scattering processes where energy and momentum are conserved. We have previously studied the break-up of a single condensate as a four wave mixing process [10], which cannot take place if the band structure is a simple cosine function. In the present work we described the continuum of scattering states of atoms interacting by a short range attractive or repulsive interaction, and we identified the two-atom repulsively and attractively bound states.

Simple models for the periodic potentials may be of particular interest when systems with a large number of particles are studied. In this case, one has recourse to second quantization, and the restriction to a discrete set of Wannier states is a first step towards an accurate treatment of the many-body properties, e.g., how the atoms distribute themselves among potential wells. See ref. [11] for a whole list of projects for further studies. So far many problems were dealt with by the Bose-Hubbard Hamiltonian. [8, 14, 17, 18, 19, 20], either solved exactly numerically or exposed to further simplifying approximations. Based on the experience of the present work, we suggest that in cases where collisions with momentum and energy conservation play a role, one should extend the conventional Bose-Hubbard Hamiltonian with only nearest neighbor tunnelling to include also tunnelling terms over longer distances, \[ \mathcal{H} = - \sum_{\delta \neq 0} J_d (\hat{a}^\dagger_j \hat{a}_{j+\delta} + \hat{a}^\dagger_{j+\delta} \hat{a}_j) + U \hat{a}^\dagger_j \hat{a}^\dagger_{j^\prime} \hat{a}_{j^\prime} \hat{a}_j, \] as depicted in Fig. 6. This modified Hamiltonian, or further extended with non-local interaction terms [21, 22], would seem to be a good starting point for detailed studies of collisions and instabilities in moving condensates in periodic potentials. We are currently pursuing such studies, including also the interplay of repulsive binding and real molecular binding of atoms in optical lattices.

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