Frustrated collisions and unconventional pairing on a quantum superlattice

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Abstract – We consider the problem of scattering and binding of two interacting spin-(1/2) fermions on a one-dimensional tight-binding superlattice with a period of twice the lattice spacing. We solve the problem analytically for all ranges of parameters of the system. We find that, for the non-trivial case of singlet states, both bound and scattering wave functions consist of a generalized Bethe ansatz augmented with an extra scattering product due to “asymptotic” degeneracy. If a Bloch band is doubly occupied, the extra wave can be a bound state in the continuum corresponding to a single-particle inter-band transition. In all other cases, it corresponds to a quasi-momentum changing, frustrated collision.

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Introduction. – The study of electrons in discretized models with a periodicity larger than the lattice spacing has a broad range of physical applications. Among them, a superlattice model for ferroelectric perovskites has been proposed [1], and its rich phase diagram qualitatively explained [2]. The recent experimental advances with ultracold bosonic or fermionic atoms loaded in optical lattices provide a neat realization of superlattice Hamiltonians [3]. These may allow for experimental observation of fermionic d-wave superfluidity [4] and magnetic phases of cold spinor gases [5]. Moreover, one-dimensional electronic systems can exhibit dimerization due to Peierls’ instability [6], thus enlarging the periodicity of the system, by a factor of two, exactly [7]. There is growing interest in the theoretical and numerical understanding of the quantum phases of superlattice and dimerized models, as attested by the attention received in the recent literature [8–18]. Although essentially exact numerical calculations in one dimension can be performed, much of the physics is hidden in the numerical data, and no unambiguous physical interpretation can be given in this way. In particular, the exact origin of degeneracy in dimerized models is not known, and may only be determined via an exact analytical solution.

In this letter, we consider the problem of two-electron scattering and binding on a one-dimensional superlattice with a period of twice the lattice spacing. After introducing two different Hubbard models with non-trivial periodicity, we show that the Schrödinger equation can be solved exactly. To do so, we generalize the two-body Bethe ansatz [19] of the Hubbard model [20] in a non-trivial manner, and center our discussion on one of the models, for concreteness. We find that, surprisingly, the collision of two electrons with opposite spins either is frustrated — the scattering states are degenerate — or necessarily a bound state in the continuum is produced upon collision. We also find all (up to four) bound states of the system analytically. Our results constitute the first quantum scattering problem on a non-trivial periodic potential, and with both particles being mobile, to be solved analytically, and are also relevant to the study of dilute quantum gases in optical superlattices where two-body processes are dominant.

Periodic Hubbard models. – We start with the following general Hubbard Hamiltonian for spin-(1/2) fermions:

\begin{equation}
\hat{H} = \sum_{j,\sigma} \left[ -J_j \hat{c}_{j\sigma}^\dagger \hat{c}_{j+1\sigma} + \text{H.c.} + \lambda_j \hat{n}_{j\sigma} \right] + U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow},
\end{equation}

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where $\hat{c}_{j\sigma} (\hat{c}_{j\sigma})^\dagger$ is the creation (annihilation) operator of a fermion with spin $\sigma = \uparrow, \downarrow$ at site $j$, $\hat{n}_{j\sigma} = (\hat{c}_{j\sigma})^\dagger \hat{c}_{j\sigma}$ is the number operator, $J_j$ is the tunneling rate between adjacent sites $j$ and $j+1$, $\lambda_j$ is a single-particle potential and $U$ is the on-site interaction between fermions with opposite spin. We discuss here the case of an infinitely long lattice; the finite lattice case with periodic boundary conditions (PBC) will be considered elsewhere [21].

There are two similar but different models which leave the Hamiltonian $\hat{H}$ invariant under translations $j \to j + \tau$ ($\tau \in \mathbb{Z}$). The first is closely related to the so-called Peierls' instability [7], having a $\tau$-periodic tunneling rate $J_j = t + \delta \cos(2\pi j/\tau)$, while its single-particle potential $\lambda_j$ vanishes. The second, most commonly used, is that of a superlattice, with a constant tunneling $J_j = J > 0$ and a periodic potential $\lambda_j = \lambda \cos(2\pi j/\tau)$. We will refer to the first of these models as Peierls-Hubbard (PHM), and to the latter as ionic Hubbard (IHM).

The energy bands are obtained by substituting $\Psi_\sigma^j = \sum \phi_{k,s}(j)e^{i\phi_{k,s}(j)\hat{n}_{j\sigma}} |0\rangle$, with $\phi_{k,s}(j+\tau) = \phi_{k,s}(j)$, into the Schrödinger equation $\hat{H} |\Psi_\sigma^j\rangle = E_j |\Psi_\sigma^j\rangle$. For the simplest case of $\tau = 2$, considered from now on, the two models have common energy dispersions, namely $E_j(k) = (-1)^s \sqrt{2J \cos(k)} + \lambda^2$, with $s = 1, 2$ labeling the two energy bands, and where we have set $\sqrt{\lambda^2 - \lambda^2} = J$ and $\delta = \lambda/2$, provided $|\delta| < |\lambda|$. The Bloch functions $\phi_{k,s}$ are, on the other hand, different for the two models. Indeed, for the PHM $\phi_{k,s}(j+1) = \phi_{k,s}(j)$, whereas for the IHM they have

$$\frac{\phi_{k,s}(j+1)}{\phi_{k,s}(0)} = \frac{\lambda - E_j(k)}{2J \cos(k)} = \frac{-2J \cos(k)}{E_j(k) + \lambda}. \quad (2)$$

which satisfies $|\phi_{k,s}(1)| \neq |\phi_{k,s}(0)|$, and can even represent a particle occupying only one sublattice (odd or even $j$) for $\lambda/J \to \infty$ or $k = \pi/2$ (quasi-momenta are defined only mod $\pi$).

The energy dispersions of the PHM and IHM are identical and both systems have on-site interaction. Thus, if we can analytically solve one of them, the other is solvable as well. In this letter, we restrict our discussion to the IHM since, as the reader can readily check, all the formalism discussed below for this model can be applied to the PHM. We leave the solution of the PHM and further details to a forthcoming paper [21].

**Wave functions of the two-body problem.** – Consider two interacting fermions of different spin components $\sigma_1 \neq \sigma_2$ in the singlet spin state described by the IHM with period $\tau = 2$. The stationary Schrödinger equation for the two-fermion spatial wave function $|\Psi\rangle$ reads, in first quantization,

$$-J \sum_{\mu = -1,1} \left[ \Psi(j_1 + \mu, j_2) + \Psi(j_1, j_2 + \mu) \right] + \left[ \lambda(-1)^{j_1} + (-1)^{j_2} + U \delta_{j_1, j_2} - E \right] \Psi(j_1, j_2) = 0, \quad (3)$$

where the wave function is symmetric under the exchange of the spatial coordinates, $\Psi(j_1, j_2) = \Psi(j_2, j_1)$.

In the limit of a weak on-site interaction ($U = 0$), the solutions to eq. (3) are of the form $\Psi = \Psi_0$, and

$$\Psi_0(j_1, j_2) = \hat{O}_S(\phi_{k_1,s_1}(j_1)\phi_{k_2,s_2}(j_2)e^{ik_1j_1 + ik_2j_2}), \quad (4)$$

with $\hat{O}_S$ the symmetrization operator, and eigenenergies $E = E_{s_1,s_2,k_1,k_2} = E_{s_1}(k_1) + E_{s_2}(k_2)$. For a very strong interaction $|U|/J \to \infty$ the solutions correspond to “fermi-onized” wave functions [8], $\Psi = \Psi_F$, and

$$\Psi_F(j_1, j_2) = \hat{O}_A(\phi_{k_1,s_1}(j_1)\phi_{k_2,s_2}(j_2)e^{ik_1j_1 + ik_2j_2}) \times \text{sgn}(j_1 - j_2), \quad (5)$$

with $\hat{O}_A$ the antisymmetrization operator (see footnote 2) and eigenenergies given by $E_{s_1,s_2,k_1,k_2}$. Here we study the more interesting case of a finite interaction $0 < |U|/J < \infty$, for which the analytic solutions were not known previously. We discuss below all possible solutions corresponding to scattering and bound states.

**Scattering states.** – We first discuss the collisional states of two fermions. We invoke a periodically modulated generalization of the two-body Bethe ansatz, written in the most convenient form for our purposes, defined for all $j_1$ and $j_2$ as

$$\Psi_B(j_1, j_2) = \Psi_0(j_1, j_2) + B \Psi_F(j_1, j_2), \quad (6)$$

where $\Psi_0$ and $\Psi_F$ given by eqs. (4) and 5, and $B$ a c-number. The Bethe ansatz (6) is an exact eigenfunction, i.e. it satisfies eq. (3), if the lattice is homogeneous ($\lambda = 0$). If $\lambda$ is finite, however, for the wave function to satisfy (3) at all $j_1, j_2$, we need to add an extra wave $\Psi_1$, with its corresponding constant $C$, to the Bethe ansatz. The total wave function reads

$$\Psi(j_1, j_2) = \Psi_B(j_1, j_2) + C \Psi_1(j_1, j_2). \quad (7)$$

Clearly, $\Psi_1$ and $\Psi_B$ must be, asymptotically ($|j_1 - j_2| \geq 1$), solutions to the Schrödinger equation (3) with the same energy and total quasi-momentum $K = k_1 + k_2$, and $\Psi_1/\Psi_B \neq \text{const}$ for all $B \in \mathbb{C}$. We note that $\Psi_B$ is a linearly growing function of $|j_1 - j_2|$ for vanishing relative quasi-momentum, $k_1 = k_2$ [22]; in such a case a generalized K-dependent scattering length can be defined as $a \propto B^{-1}$ [23]; the divergence of the scattering length denotes a bound state entering or exiting the continuum. The cases of total quasi-momentum $K = 0, \pi/2$ also have to be handled with special care by taking the limits $K \to 0, \pi/2$ before using the ansatz (7) in eq. (3).

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1This is equivalent to a pair in the Bose-Hubbard model; triplet states and hard-core bosons are trivial.

2$O_{S,A}(f_{\alpha_1}(j_1)g_{\alpha_2}(j_2)) \equiv f_{\alpha_1}(j_1)g_{\alpha_2}(j_2) \pm f_{\alpha_1}(j_2)g_{\alpha_2}(j_1)$. 

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The set of band indices and quasi-momenta \( \{ s_1, s_2; k_1, k_2 \} \) for the Bethe ansatz have the corresponding energy \( E_{s_1,s_2;k_1,k_2} \). Therefore, one has to find \( \{ s_1', s_2'; k_1', k_2' \} \) so that the following two sets of conditions are fulfilled: 1) \( E_{s_1,s_2;k_1,k_2} = E_{s_1',s_2';k_1',k_2'} \); 2) if \( s_1 = s_2 \) then \( s_1' = s_2' \) or \( s_1' = s_2 = s \) and \( k_1' \neq k_1, k_2 \); 3) if \( s_1 \neq s_2 \), then \( s_1' \neq s_2' \) and \( k_1' \neq k_1, k_2 \). Once the primed set is found, one introduces the wave function (7) in eq. (3) at \( j_1 = j_2 \) even and odd, thus obtaining a set of two linear equations in \( B \) and \( C \) that can be solved analytically, giving in turn the total wave function \( \Psi \).

Since we are working with a two-band model, and the single-particle bands are mirror symmetric, \( E_s(k) = -E_s(k) \), we have to consider two different possibilities, namely intra- and inter-band scattering. These cases are qualitatively different from each other, as we shall see, and are therefore considered separately.

i) Intra-band scattering. We assume that \( \Psi_0 \), interpreted as incident wave, eq. (4), consists of two fermions with (real) quasi-momenta \( k_1 \) and \( k_2 \), occupying the same band, \( s_1 = s_2 = s \). As discussed in the previous paragraph, we have to find a non-trivial set \( \{ s_1', s_2'; k_1', k_2' \} \) corresponding to the same energy and total quasi-momentum \( K \) as the incident state. In the majority of the cases, the solution is given by a pair of complex quasi-momenta \( k_2' \equiv q = (K + \pi)/2 + i\nu \) and \( k_2'' = q^* \) (recall \( K \) is defined mod \( \pi \)), with associated band indices \( s_1' = s \) and \( s_2' = s \pm 1 \). Such solutions are outgoing bound states in the continuum, and represent an inter-band transition \( \{ s_1' \neq s_2' \} \). Note that inter-band transitions with real quasi-momenta cannot happen since we have neither external forces nor energy dissipation mechanisms. The only physically acceptable (exponentially decaying) extra wave with complex quasi-momenta is given by \( \Psi_1 \equiv \Psi_{ba}^{q,q''} \), with

\[
\Psi_{ba}^{q_1,q_2}(j_1,j_2) = \left[ \theta(j_1 - j_2)\phi_{q_1,s_1'}(j_1)\phi_{q_2,s_2'}(j_2) e^{i(k_1j_1 + k_2j_2)} \right. \\
+ \left. \bar{\theta}(j_2 - j_1)\phi_{q_1,s_2'}(j_2)\phi_{q_2,s_1'}(j_1) e^{i(k_1j_2 + k_2j_1)} \right] \\
\times e^{-|q||j_2-j_1|},
\]

where, in general, \( q_n \equiv q_n + iv \), and \( \theta \) (\( \bar{\theta} \)) is the step function being zero (one) at \( j_1 = j_2 = 0 \). In fig. 1 we plot the density \( |\Psi|^2 \) for a significant case \( \lambda/J = U/J = 2 \) in which all the parameters of the Hamiltonian are in competition. As observed, the contribution of the bound state in the continuum (8) is appreciable at small inter-particle distances, while the wave function behaves, for \( |j_1 - j_2| \gg 1 \), as the periodically modulated Bethe ansatz \( \Psi_B \).

This surprising result implies that paired states can be created upon two-body collisions on a superlattice even without external forces, phonons or dissipation, and are due to the combination of the band structure and finite interactions. These states should play a non-negligible role in the many-electron problem; we have verified that the ground state of the system, with PBC, at half-filling (4 lattice sites) and quarter-filling (8 sites) is always a partially paired state for any non-zero \( \lambda \) and \( U > 0 \) [21].

There are, on the other hand, cases for which the extra wave \( \Psi_1 \) has real quasi-momenta \( k_1' \) and \( k_2' \). It has now the simple form

\[
\Psi_1(j_1,j_2) = \hat{O}_S(\phi_{k_1',s_1'}(j_1)\phi_{k_2',s_2'}(j_2) e^{i(k_1j_1 + k_2j_2)}).
\]

By energy conservation, it is obvious that the associated band indices correspond to \( s_1' = s_2' = s \). The energies and total quasi-momenta for which bound states in the continuum or scattered extra waves are needed can be inferred from fig. 2, where the spectrum is plotted for \( \lambda/J = U/J = 2 \). In the figure, the regions of the \( s = 2 \) (\( s = 1 \)) continuum with energies below (above) the dotted line (see the discussion on bound states below).
to cases for which the extra wave has real quasi-momenta. These regions are already very small—but dense—for the value of $\lambda$ under consideration. We note that as $\lambda/J$ gets larger, it becomes less likely that $\Psi_1$ corresponds to a scattered wave. Since, for these cases, we can construct two different wave functions (with $\Psi_F$ corresponding to $k_1, k_2$ or $k_1', k_2'$) or any superposition thereof having the same total quasi-momentum and energy, these states are degenerate (frustrated).

ii) Inter-band scattering. The two incident fermions, with quasi-momenta $k_1$ and $k_2$ are now in different bands, $s_1 \neq s_2$. Energy conservation implies that $\Psi_1$ has band indices $s_1' \neq s_2'$, and the non-trivial outgoing quasi-momenta $k_1', k_2'$ are always real — there is no bound state in the continuum — and as a consequence inter-band scattering states are always degenerate. The extra wave has again the simple form of eq. (9), and the total wave function $\Psi$, eq. (7), is calculated by substitution in the Schrödinger equation at $j_1 = j_2$, as we have already explained.

**Bound states.** — The system under consideration also supports bound states — exponentially decaying wave functions in the relative coordinate $|j_1 - j_2|$ with energies outside the continuum for each total quasi-momentum $K$ — for both attractive and repulsive on-site interaction (if $U > 0$, these are sometimes called antibound states [24]). Due to the periodicity of the Hamiltonian, we need, as for the case of scattering states, two constants so that the Schrödinger equation (3) can be satisfied for all $j_1, j_2$. We propose the following ansatz for the wave function:

$$\Psi(j_1, j_2) = \Psi_{\text{bs}}^q_1 q_2(j_1, j_2) + B \Psi_{\text{bs}} q_2^1 q_2^2(j_1, j_2),$$

with $q_n = \ell_n + iv$, $\tilde{q}_n = \ell_n + i\pi$, total quasi-momentum $K = \ell_1 + \ell_2 = \ell_1 + \ell_2$ (see footnote 3), and $\Psi_{\text{bs}}$ given by eq. (8). Since the two wave functions in eq. (10) must have, asymptotically, the same energies, we get a relation between $q_n$ and $\tilde{q}_n$; necessarily, the band indices of the functions $\Psi_{\text{bs}}$ are unequal (except for $K = 0$ for which one of the functions $\Psi_{\text{bs}}$ has $s_1 = s_2$, $|v| < \infty$, and the other has $s_1 \neq s_2$ with $v = \infty$). The constant $B$ is then calculated for $j_1 = j_2 = j$ even (or odd), and $q_n$. $\tilde{q}_n$ are varied self-consistently until the Schrödinger equation (3) is satisfied for $j$ even and odd, which yields the desired bound-state energy. Although it is possible to solve this problem for general $q_n$ and $\tilde{q}_n$, it is simpler to distinguish all possible cases for which eq. (10) is a solution to eq. (3). There are three different types of bound states, based on the combinations of $q_1, \tilde{q}_1$, as explained below.

Type I: bound states with energies below the first bound-state band with $s_1 = s_2 = 1$ or above the first bound-state band. These correspond to $q_1 = K/2 + iv$ and $\tilde{q}_1 = (K + \pi/2)/2 + iv$, with $v \neq \tilde{v}$. Therefore, the real parts of the quasi-momenta are fixed while $v$ and $\tilde{v}$ are calculated self-consistently with $B$.

Type II: energies in one of the band gaps and total quasi-momenta $K \in (-\varphi, \varphi)$, with $0 < \varphi < \pi/2$ depending on the value of $U/J$ and $\lambda/J$. These have $q_1 = (K + \pi)/2 + iv$ and $\tilde{q}_1 = (K + \pi)/2 + i\pi - v$, with $v \neq \tilde{v}$, and then to their calculation is analogous to that of type I.

Type III: energies in one of the band gaps and total quasi-momenta $K \in (-\pi/2, -\varphi) \cup (\varphi, \pi/2)$, with $0 < \varphi < \pi/2$ being the same number as for type II if bound states of that type exist in their range of quasi-momenta. These have $q_1 = \ell + iv$ and $\tilde{q}_1 = \ell - iv$. One has to calculate, for a given starting value of $\ell$, the relation between $v$ and $\ell$ so that the energy is real, and then to iterate self-consistently until the Schrödinger equation is satisfied.

All bound states for $\lambda/J = U/J = 2$ are plotted in fig. 2, where we clearly identify three different bound-state bands. The first one corresponds to a pair bound from the lowest scattering band with $s_1 = s_2 = 1$, and lies in the first band gap. The second band of bound states is in the second band gap, and binding energies are evidently smaller than those for the first bound band, since they are bound from the $s_1 \neq s_2$ bands. The density-modulation prevents high occupancy of two particles at the same lattice site if they are in different bands. The third band, above the continuum with $s_1 = s_2 = 2$, is similar (although not equivalent) to the first bound-state band. The dotted line in fig. 2 is the minimum (in absolute value) of the energy $E_{1,2,q,q''}$ with $q = (K + \pi/2)/2 + iv$ for each value of the total quasi-momentum $K$, and therefore denotes the boundaries $\pm \varphi$ between bound states of type II and III. We note that, for larger values of $U/J$ (not shown), there can be up to four bound states at certain values of the total quasi-momentum.

**Conclusions.** — We have found that, on a one-dimensional superlattice, the non-trivial underlying periodicity has important implications for the two-body problem. We have derived exact, analytical solutions for the wave functions which show, unambiguously, that partial pairing of fermions after their scattering occurs over a large range of parameters of the model studied, and corresponds to hitherto unexplored bound states in the continuum. These states appear only if the incident particles occupy the same band. In the case in which the two fermions occupy different bands, collisions produce a phase shift, but also a second outgoing wave corresponding to quasi-momenta being different from the incident ones. This implies that inter-band scattering is frustrated, and the spectrum is degenerate. Given the fact that, in models that can be solved with the Bethe ansatz [19,20], the two-body phase shifts determine the whole physics at the many-body level, it is conceivable that the implications of our two-particle solutions will influence the many-body problem. A simple generalization of our results to include periodic boundary conditions shows that the two-body ground states in finite lattices with repulsive interaction correspond to partially paired states with a bound state in the continuum [21]. Our exact

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3If $K = \pi/2$ there is no non-trivial ($\Psi \neq 0$) bound state.
Frustrated collisions and unconventional pairing on a superlattice

solutions are also of relevance to ultracold, low-density gases in optical superlattices where the physics is most influenced by pairwise collisions; they represent a novel advance in the field of few-body physics on a lattice, which have attracted much interest recently (see [25] and references therein). Moreover, for bosons, our wave functions can be used to construct trial functions of product (Jastrow) type for the many-body problem [26] in the dilute regime.

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