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Fermionic bound states on a one-dimensional lattice

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We study bound states of two fermions with opposite spins in an extended Hubbard chain. The particles interact when located both on a site or on adjacent sites. We find three different types of bound states. Type U is predominantly formed of basis states with both fermions on the same site, while two states of type V originate from both fermions occupying neighboring sites. Type U and one of the states from type V are symmetric with respect to spin flips. The remaining one from type V is antisymmetric. V states disappear by merging with the two-particle continuum below some critical wave number. All bound states become compact for wave numbers at the edge of the Brillouin zone.

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I. INTRODUCTION

Advances in experimental techniques of manipulation of ultracold atoms in optical lattices make it feasible to explore the physics of few-body interactions. Systems with few quantum particles on lattices have new unexpected features as compared to the condensed-matter case of many-body interactions, where excitation energies are typically small compared to the Fermi energy. In particular, a recent experiment explored the repulsive binding of bosonic atom pairs in an optical lattice [1], as predicted theoretically decades earlier [2,3] (see also [4] for a review). In this work, we study binding properties of fermionic pairs with total spin zero. We use the extended Hubbard model, which contains two interaction scales—the on site interaction U and the nearest-neighbor intersite interaction V. The nonlocal interaction V is added in condensed-matter physics to emulate remnants of the Coulomb interaction due to nonperfect screening of electronic charges. For fermionic ultracold atoms or molecules with magnetic or electric dipole-dipole interactions, it can be tuned with respect to the local interaction U by modifying the trap geometry of a condensate, additional external dc electric fields, combinations with fast rotating external fields, etc. (for a review and relevant references see [5]).

The Brief Report is organized as follows. We first describe the model and introduce the basis we use to write down the Hamiltonian matrix to be diagonalized. Then we derive the quantum states of the lattice containing one and two fermions, with opposite spins in the latter case. We study the obtained bound states for two fermions. We obtain analytical expressions for the energy spectrum of the bound states. Some of the bound states are characterized by a critical momentum below which they dissolve with the two-particle continuum.

II. MODEL AND BASIS CHOICE

We consider a one-dimensional lattice with f sites and periodic boundary conditions described by the extended Hubbard model with the following Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_U + \hat{H}_V, \tag{1}$$

where

$$\hat{H}_0 = -\sum_{j,\sigma} \hat{a}^\dagger_{j,\sigma}(\hat{a}_{j-1,\sigma} + \hat{a}_{j+1,\sigma}), \tag{2}$$

$$\hat{H}_U = -U\sum_j \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}, \quad \hat{n}_{j,\sigma} = \hat{a}^\dagger_{j,\sigma}\hat{a}_{j,\sigma}, \tag{3}$$

$$\hat{H}_V = -V\sum_j \hat{n}_j\hat{n}_{j+1}, \quad \hat{n}_j = \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow}. \tag{4}$$

$\hat{H}_0$ describes the nearest-neighbor hopping of fermions along the lattice. Here the symbols $\sigma = \uparrow, \downarrow$ stand for a fermion with spin up or down. $\hat{H}_U$ describes the onsite interaction between the particles, and $\hat{H}_V$ describes the intersite interaction of fermions located at adjacent sites. $\hat{a}^\dagger_{j,\sigma}$ and $\hat{a}_{j,\sigma}$ are the fermionic creation and annihilation operators satisfying the corresponding anticommutation relations: $\{\hat{a}^\dagger_{j,\sigma}, \hat{a}_{l,\sigma'}\} = \delta_{j,l}\delta_{\sigma,\sigma'}$ and $\{\hat{a}^\dagger_{j,\sigma}, \hat{a}^\dagger_{l,\sigma'}\} = \{\hat{a}_{j,\sigma}, \hat{a}_{l,\sigma'}\} = 0$. Note that throughout this work we consider U and V as positive, which leads to bound states located below the two-particle continuum. A change in the sign of U, V will simply swap the energies.

Hamiltonian (1) commutes with the number operator $\hat{N} = \Sigma_j \hat{n}_j$ whose eigenvalues are $n = n_\uparrow + n_\downarrow$, i.e., the total number of fermions in the lattice. We consider $n=2$, with $n_\uparrow = 1$ and $n_\downarrow = 1$. Therefore we construct a basis starting with the eigenstates of $\hat{N}$. We use a number state basis $|\Phi_n\rangle = |n_1; n_2, \ldots, n_f\rangle$ [3], where $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ represents the number of fermions at the ith site of the lattice. $|\Phi_n\rangle$ is an eigenstate of the number operator $\hat{N}$ with eigenvalue $n = \Sigma_{j=1}^f n_j$.

To observe the fermionic character of the considered states, any two-particle number state is generated from the vacuum $|O\rangle$ by first creating a particle with spin down and then a particle with spin up: e.g., $\hat{a}^\dagger_{2,\uparrow}\hat{a}^\dagger_{1,\downarrow}|O\rangle$ creates a particle with spin down on site 1 and one with spin up on site 2, while $\hat{a}^\dagger_{2,\uparrow}\hat{a}^\dagger_{2,\downarrow}|O\rangle$ creates both particles with spin down and up on site 2.

Due to periodic boundary conditions Hamiltonian (1) commutes also with the translation operator $\hat{T}$, which shifts all lattice indices by one. It has eigenvalues $\tau=\exp(ik)$, with Bloch wave number $k=\frac{2\pi\nu}{f}$ and $\nu=0,1,2,\ldots,f-1$.

III. SINGLE-PARTICLE SPECTRUM

For the case of having only one fermion (either spin up or spin down) in the lattice ($n=1$), a number state has the form $|j\rangle=\hat{a}^{\dagger}_{j,\sigma}|O\rangle$. The interaction terms $\hat{H}_U$ and $\hat{H}_V$ do not contribute. For a given wave number k, the eigenstate to Eq. (1) is therefore given by

$$|\Psi_1\rangle = \frac{1}{\sqrt{f}}\sum_{s=1}^{f}\left(\frac{\hat{T}}{\tau}\right)^{s-1}|1\rangle. \quad (5)$$

The corresponding eigenenergy

$$\varepsilon_k=-2\cos(k). \quad (6)$$

IV. TWO FERMIONS WITH OPPOSITE SPINS

For two particles, the number state method involves $N_s=f^2$ basis states, which is the number of ways one can distribute two fermions with opposite spins over the f sites including possible double occupancy of a site. Below we consider only cases of odd f for simplicity. Extension to even values of f is straightforward.

We define basis states to a given value of the wave number k,

$$|\Phi_1\rangle = \frac{1}{\sqrt{f}}\sum_{s=1}^{f}\left(\frac{\hat{T}}{\tau}\right)^{s-1}\hat{a}^{\dagger}_{1,\uparrow}\hat{a}^{\dagger}_{1,\downarrow}|O\rangle, \quad (7)$$

$$|\Phi_{j,+}\rangle = \frac{1}{\sqrt{f}}\sum_{s=1}^{f}\left(\frac{\hat{T}}{\tau}\right)^{s-1}\hat{a}^{\dagger}_{j,\uparrow}\hat{a}^{\dagger}_{1,\downarrow}|O\rangle, \quad (8)$$

$$|\Phi_{j,-}\rangle = \frac{1}{\sqrt{f}}\sum_{s=1}^{f}\left(\frac{\hat{T}}{\tau}\right)^{s-1}\hat{a}^{\dagger}_{1,\uparrow}\hat{a}^{\dagger}_{j,\downarrow}|O\rangle, \quad (9)$$

$$1<j\leq (f+1)/2. \quad (10)$$

Note, that the sign $\pm$ discriminates between states, where the distance from the spin-up particle to the spin-down particle with increasing lattice site index is smaller (larger) than vice versa. Note that distances are measured by scanning the (periodic) chain in the direction of increasing lattice site number, passing a given particle (say with spin up) and then counting the distance to the spin-down particle. In the limit of an infinite system the two signs discriminate between states where the spin-up particle is to the left or right of the spin-down one.

Therefore, a complete wave function is given by

$$|\Psi_2\rangle = c_1|\Phi_1\rangle + \sum_{j=2}^{f+1/2} c_{j+}|\Phi_{j,+}\rangle + \sum_{j=2}^{f+1/2} c_{j-}|\Phi_{j,-}\rangle. \quad (11)$$

Any vector in our given Hilbert space is then spanned by the numbers $|c_1,c_{2+},c_{2-},c_{3+},\ldots\rangle$.

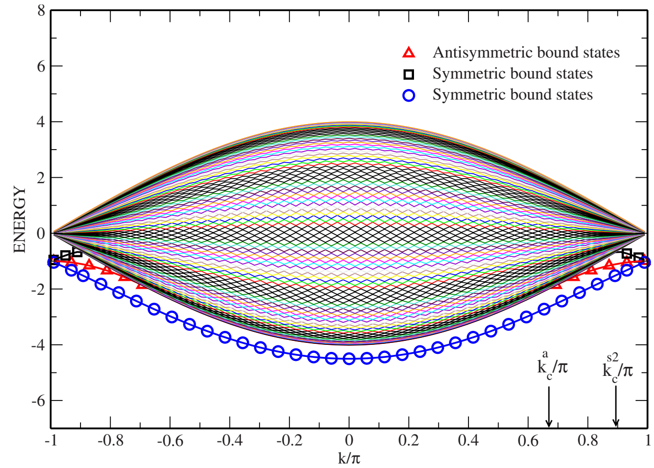

FIG. 1. (Color online) Energy spectrum of the two fermion states. The eigenvalues are plotted as a function of the wave number k. Here $U=1$, $V=1$, and $f=101$. Symbols are from analytical derivation; lines are the result of numerical diagonalization. The arrows indicate the location of the critical wave numbers (see text).

Next we calculate the matrix elements of Hamiltonian (1) in the framework of basis (11). We arrive at a $f\times f$ matrix with elements $H(i,j)$ $(i,j=1,\ldots,d)$,

$$H(i,j)=-\begin{pmatrix} U & q & q & 0 & \ldots & & & \\ q^* & V & 0 & q & 0 & \ldots & & \\ q^* & 0 & V & 0 & q & 0 & \ldots & \\ 0 & q^* & 0 & 0 & 0 & q & 0 & \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ & \ldots & 0 & q^* & 0 & 0 & 0 & q \\ & & \ldots & 0 & q^* & 0 & 0 & p \\ & & \ldots & 0 & & q^* & p & 0 \end{pmatrix}. \quad (12)$$

Here $q=1+\tau$ and $p=\tau^{-(f+1)/2}+\tau^{-(f-1)/2}$.

In Fig. 1 we show the energy spectrum of Hamiltonian matrix (12) obtained by numerical diagonalization for the interaction parameters $U=2$ and $V=2$ and $f=101$. At $U=0$ and $V=0$, the spectrum is given by the two fermion continuum, whose eigenstates are characterized by the two fermions independently moving along the lattice. In this case the eigenenergies are the sum of the two single-particle energies,

$$E^0_{k_1,k_2}=-2[\cos(k_1)+\cos(k_2)], \quad (13)$$

with $k_{1,2}=\pi\nu_{1,2}/(f+1)$, where $\nu_{1,2}=1,\ldots,f$. The Bloch wave number $k=k_1+k_2 \mod 2\pi$. Therefore, if $k=\pm\pi$, the continuum degenerates into points. The continuum is bounded by the hull curves $h_{\pm}(k)=\pm 4\cos\frac{k}{2}$. The same two-particle continuum is still observed in Fig. 1 for nonzero interaction. However, in addition to the continuum, we observe one, two, or three bound states dropping out of the continuum, which depends on the wave number. For any nonzero U and V, all three bound states drop out of the continuum at $k=\pm\pi$. One of them stays bounded for all values of k. The two other ones merge with the continuum at some critical value of $|k|$ upon approaching $k=0$ as observed

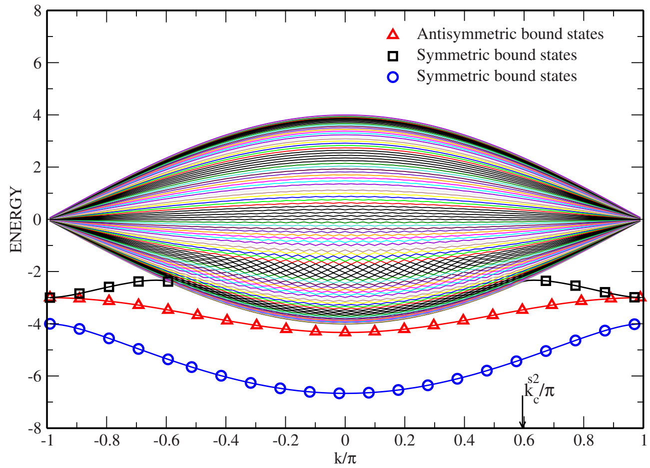

FIG. 2. (Color online) Energy spectrum of the two fermion states. The eigenvalues are plotted as a function of the wave number k. Here $U=4$, $V=3$, and $f=101$. The symbols are from analytical derivation; lines are the results of numerical diagonalization. The arrow indicates the location of the critical wave number (see text).

in Fig. 1. Note that for $k=\pm\pi$ and $U=V$, all three bound states are degenerate.

Upon increasing U and V, we observe that a second bound-state band separates from the continuum for all k (Fig. 2). At the same time, when $U\neq V$, the degeneracy at $k=\pm\pi$ is reduced to two.

Finally, for even larger values of U and V, all three bound-state bands completely separate from the continuum (Fig. 3).

V. SYMMETRIC AND ANTISYMMETRIC STATE REPRESENTATION

In order to obtain analytical estimates on the properties of the observed bound states, we use the fact that the Hamiltonian for a two fermion state is invariant under flipping the spins of both particles. We define symmetric basis states

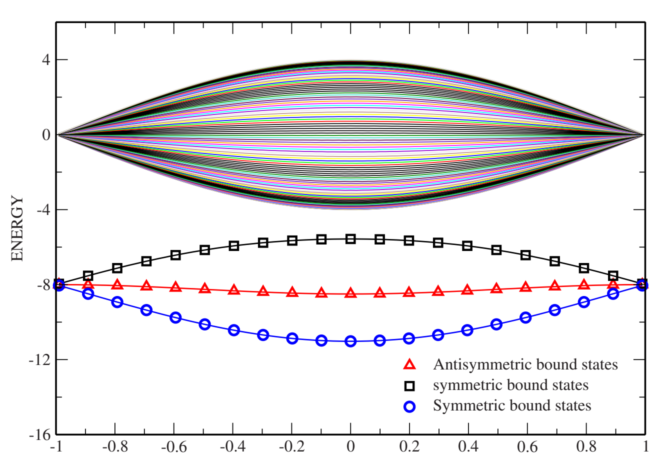

FIG. 3. (Color online) Energy spectrum for the two fermion states. The eigenvalues are plotted as a function of the wave number k. Here $U=8$, $V=8$, and $f=101$. The symbols are from analytical derivation; lines are the results of numerical diagonalization.

$$|\Phi_{j,s}\rangle = \frac{1}{\sqrt{2}}(|\Phi_{j,+}\rangle + |\Phi_{j,-}\rangle) \tag{14}$$

and antisymmetric states

$$|\Phi_{j,a}\rangle = \frac{1}{\sqrt{2}}(|\Phi_{j,+}\rangle - |\Phi_{j,-}\rangle). \tag{15}$$

Note that $|\Phi_1\rangle$ is a symmetric state as well. Then matrix (12) can be decomposed into irreducible symmetric and antisymmetric ones,

$$H^s(i,j) = -\begin{pmatrix} U & q\sqrt{2} & & & & \\ q^*\sqrt{2} & V & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & p \end{pmatrix}, \tag{16}$$

$$H^a(i,j) = -\begin{pmatrix} V & q & & & & \\ q^* & 0 & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & -p \end{pmatrix}. \tag{17}$$

The rank of the matrix H^s is $(f+1)/2$, while the rank of H^a is $(f-1)/2$.

VI. ANTISYMMETRIC BOUND STATES

The antisymmetric states exclude double occupation. Therefore the spectrum is identical with the one of two spinless fermions [3]. Following the derivations in [3] we find that the antisymmetric bound state, if it exists, has an energy

$$E_2^a(k) = -\left[V + \frac{4}{V}\cos^2\left(\frac{k}{2}\right)\right]. \tag{18}$$

This result is valid as long as the bound-state energy stays outside of the continuum. The critical value of k at which validity is lost, is obtained by requesting $|E_2^a(k)|=|h_\pm(k)|$. It follows that $V=2\cos(\frac{k}{2})$. Therefore the antisymmetric bound state merges with the continuum at a critical wave number

$$k_c^a = 2\arccos\left(\frac{V}{2}\right), \tag{19}$$

setting a critical length scale $\lambda_c^a=\frac{2\pi}{k_c^a}$. For $V=1$ it follows that $k_c^a/\pi\approx 0.667$ (see Fig. 1).

Equation (18) is in excellent agreement with the numerical data in Figs. 1–3 (cf. open triangles). We also note that the antisymmetric bound state is located between the two symmetric bound states, which we discuss next.

VII. SYMMETRIC BOUND STATES

A bound state can be searched for by assuming an unnormalized eigenvector to Eq. (16) of the form

$|c,1,\mu,\mu^2,\mu^3,\ldots\rangle$ with $|\mu|\equiv\rho\leq 1$. We obtain

$$Ec = -Uc - \sqrt{2}q^*,$$

$$E = -\sqrt{2}qc - V - q^*\mu,$$

$$E = -\frac{q}{\mu} - q^*\mu. \tag{20}$$

It follows that $\mu=\rho\exp(ik/2)$ and

$$E_2^s(k) = -2\left(\rho + \frac{1}{\rho}\right)\cos k/2. \tag{21}$$

The parameter ρ satisfies a cubic equation,

$$a\rho^3 + b\rho^2 + c\rho + d = 0 \tag{22}$$

with the real coefficients a, b, c, and d given by $a=2V\cos(\frac{k}{2})$, $b=4\cos^2(\frac{k}{2})-UV$, $c=2(U+V)\cos(\frac{k}{2})$, and $d=-4\cos^2(\frac{k}{2})$. An analytic solution to Eq. (22) can be obtained but is cumbersome to be presented here. We plot the results in Figs. 1–3 (cf. open circles and squares). We obtain excellent agreement. Note that one root of Eq. (22) has $|\rho|>1$ and is therefore not of interest here.

At the Brillouin zone edge $k=\pm\pi$ cubic Eq. (22) is reduced to a quadratic one, and can be solved to obtain finally $\rho\to 0$ and

$$E_2^{s1}(k\to\pm\pi) = -U, \quad E_2^{s2}(k\to\pm\pi) = -V. \tag{23}$$

In particular we find for $k=\pm\pi$ that $E_2^{s2}=E_2^a$. In addition, if $U=V$, all three bound states degenerate at the zone edge.

If $V=0$, cubic Eq. (22) is reduced to a quadratic one in the whole range of k and yields [3]

$$E_2^{s1}(k) = -\sqrt{U^2 + 16\cos^2(k/2)}. \tag{24}$$

Next we determine the critical value of k for which the bound state with energy E_2^{s2} is joining the continuum. Since at this point $\rho=1$, we solve Eq. (22) with respect to k_c and find

$$k_c^{s2} = 2\arccos\left(\frac{UV}{2(U+2V)}\right) \tag{25}$$

setting another critical length scale $\lambda_c^s=\frac{2\pi}{k_c^s}$. E.g., for $U=V=1$ $k_c^{s2}/\pi\approx 0.89$, in excellent agreement with Fig. 1. For $U=4$ and $V=3$ we find $k_c^{s2}/\pi\approx 0.59$ confirming numerical results in Fig. 2.

VIII. CONCLUSIONS

Two fermionic particles with opposite spin allow for three different types of bound states on a one-dimensional lattice with onsite U and nearest-neighbor V interaction. Two of them are symmetric with respect to spin flips, and one is antisymmetric. The antisymmetric bound state is characterized by a critical wave number separates wave numbers with bound states from wave numbers without. It follows from Eq. (19) that this happens for $V<2$. For larger values of V the whole wave-number space becomes available for antisymmetric bound states, similar to one of the symmetric bound states for any nonzero U. The second symmetric bound state also observes a critical wave number. It follows from Eq. (25) that this happens for $U<4V/(V-2)$, while the whole wave-number space becomes available otherwise. It could be a challenging task to observe these different phases with one, two, or three bound states experimentally by tuning U, V, and k.

When a bound-state band merges with the continuum, the bound state dissolves in the continuum as a quasibound state. The corresponding scattering problem has been discussed in several papers to relate it to Feshbach resonances, which sensitively control the two-body interaction between atoms [6]. In particular, two interacting bosons were discussed in Ref. [7], and a scattering theory for two fermions can be found in [8].

Partially attractive potentials with different signs of U and V can be easily implemented as well. We expect some of the bound-state bands to be located above the two-particle continuum. For higher lattice dimensions more nearest neighbors have to be taken into account, similar to an increase in the interaction range. In these cases, we expect consequently more bound states to appear.

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