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FAST TRACK COMMUNICATION

Scattering resonances and two-particle bound states of the extended Hubbard model

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Abstract
We present a complete derivation of two-particle states of the one-dimensional extended Bose–Hubbard model involving attractive or repulsive on-site and nearest-neighbour interactions. We find that this system possesses scattering resonances and two families of energy-dependent interaction-bound states which are not present in the Hubbard model with the on-site interaction alone.

(Some figures in this article are in colour only in the electronic version)

Among the tight-binding lattice models of condensed matter physics, the Hubbard model plays a fundamental role [1]. In its basic form, the Hubbard model describes particle tunnelling between adjacent lattice sites as well as short-range (contact) interaction between the particles on the same lattice site. Despite its apparent simplicity, this model is very rich in significance and implications for many-body physics on a lattice [2]. This is perhaps most profoundly manifested with numerous important experimental and theoretical achievements with cold neutral atoms trapped in optical lattice potentials [3, 4], wherein the Hubbard model is being realized with unprecedented accuracy.

The next level of generalization pertaining to, e.g., electrons in a crystal [5] or dipolar atoms [6] or molecules [7] in an optical lattice yields the extended Hubbard model involving longer range interactions between the particles on the neighbouring lattice sites. Under certain conditions, namely for hard-core bosons or strongly interacting fermions at half-filling, the extended Hubbard model can be mapped onto various lattice spin models [8] for which the Bethe ansatz is a powerful method for obtaining exact eigenstates in one dimension [9].

A remarkable Hubbard model effect demonstrated in a seminal experiment of Winkler *et al* [10] is the binding of pairs of particles into composite objects by on-site interaction, which can be either repulsive or attractive [11, 12]. In this communication, we study the one-dimensional extended Bose–Hubbard model involving attractive or repulsive on-site and nearest-neighbour interactions. Specifically, we present the complete derivation of two-particle scattering as well as bound states of the system. In general, this model is not amenable to the Bethe ansatz in its standard form [9], since for finite interaction strengths the double occupancy of lattice sites cannot be excluded. However, upon separating the centre of mass and relative motion of the two particles, we arrive at a very simple equation for the relative coordinate wavefunction, which can be solved exactly. We then find that this system possesses scattering resonances and two families of energy-dependent interaction-bound states which are not present in the Hubbard model with the on-site interaction alone.

The Hamiltonian of the extended Hubbard model reads as

$$H = \sum_j \varepsilon_j \hat{n}_j - J \sum_j \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j\right) + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) + V \sum_j \hat{n}_j \hat{n}_{j+1}, \qquad (1)$$

where $\hat{b}_j^\dagger$ ($\hat{b}_j$) is the creation (annihilation) operator and $\hat{n}_j = \hat{b}_j^\dagger \hat{b}_j$ is the number operator for a boson at the jth lattice site with energy ε_j, $J(>0)$ is the tunnel coupling between adjacent sites, and U and V are, respectively, the on-site and nearest-neighbour interactions which can be attractive or repulsive.

We seek two-particle eigenstates of Hamiltonian (1) in a homogeneous lattice, $\varepsilon_j = \varepsilon$ for all j. For convenience, we set $\varepsilon = 0$, which amounts to a shift of the zero of energy. We then expand the state vector in terms of the non-symmetrized coordinate basis $\{|x_j, y_{j'}\rangle\}$ as $|\Psi\rangle = \sum_{j,j'} \Psi(x_j, y_{j'})|x_j, y_{j'}\rangle$, where $x_j \equiv dj$ and $y_{j'} \equiv dj'$ are the particle positions and d is the lattice constant. The standard (symmetrized) bosonic basis is recovered via the transformation $|2_j\rangle = |x_j, y_j\rangle$ and $|1_j, 1_{j'}\rangle = \frac{1}{\sqrt{2}}(|x_j, y_{j'}\rangle + |y_j, x_{j'}\rangle)$ $(j \neq j')$. Defining the centre of mass $R = \frac{1}{2}(x + y)$ and relative $r = x - y$ coordinates, the two-particle wavefunction can be factorized as $\Psi(x, y) = e^{iKR}\psi_K(r)$, where the relative coordinate wavefunction $\psi_K(r)$ depends on the centre-of-mass quasi-momentum $K \in [-\pi/d, \pi/d]$ as a continuous parameter. The eigenvalue problem $H|\Psi\rangle = E|\Psi\rangle$ then reduces to the three-term difference equation

$$-J_K[\psi_K(r_{i-1}) + \psi_K(r_{i+1})] + [U\delta_{r,0} + V(\delta_{r,d} + \delta_{r,-d}) - E_K]\psi_K(r_i) = 0, \quad (2)$$

with $J_K \equiv 2J\cos(Kd/2)$ and $r_i = di$ $(i = j - j')$. The above equation admits two kinds of solutions, corresponding to the scattering states of asymptotically free particles and to the interaction-bound states of particle pairs.

We begin with the analysis of scattering solutions of equation (2). They are most straightforwardly obtained with the standard symmetrized ansatz $\psi_{K,k}(r_i \neq 0) \propto e^{-ik|r_i|} + e^{2i\delta_{K,k}} e^{ik|r_i|}$ representing plane waves undergoing a scattering phase shift $\delta_{K,k}$. This immediately yields the eigenenergies $E_{K,k} = -2J_K\cos(kd)$, which are equal to the sum of Bloch bands $\epsilon_{x,y} = -2J\cos[(K/2 \pm k)d]$ of two (asymptotically) free particles x, y with relative quasi-momentum k [11, 12]. For a given value of the centre-of-mass momentum K, and thereby J_K, the lowest $E_{K,0} = -2J_K$ and highest $E_{K,\pi} = 2J_K$ energy states are attained, respectively, at $k \to 0$ and $k \to \pi/d$. The continuum of energies $E_{K,k}$ and the corresponding density of states $\rho(E, K) \propto \partial(kd)/\partial E = [(2J_K)^2 - E^2]^{-1/2}$ are shown in figure 1. The wavefunction of scattering states is given by

$$\psi_{K,k}(0) = \cos\left(\delta^{(0)}_{K,k}\right)\frac{\cos(kd + \delta_{K,k})}{\cos\left(kd + \delta^{(0)}_{K,k}\right)}, \quad (3a)$$

$$\psi_{K,k}(r_i \neq 0) = \cos(k|r_i| + \delta_{K,k}), \quad (3b)$$

where the phase shifts $\delta^{(0)}_{K,k}$ and $\delta_{K,k}$ are defined through

$$\tan\left(\delta^{(0)}_{K,k}\right) = -\frac{U}{2J_K\sin(kd)}, \quad (4a)$$

$$\tan(\delta_{K,k}) = \frac{J_K U + [2J_K\cos(kd) + U]V\cos(kd)}{\{UV - 2J_K[J_K - V\cos(kd)]\}\sin(kd)}. \quad (4b)$$

Note that when $V = 0$, we have $\delta_{K,k} = \delta^{(0)}_{K,k}$, and the above expressions reduce to those of [11] with all the consequences discussed there. Here we examine the role of nearest-neighbour interaction $V \neq 0$ due to which the scattering amplitude $f(\delta_{K,k}) = \frac{1}{2}(e^{2i\delta_{K,k}} - 1)$ or, for that matter, the cross-section $\sigma_{K,k} = |f(\delta_{K,k})|^2 = \sin^2(\delta_{K,k})$ can exhibit novel intriguing features seen in figure 2. The cross-section vanishes at $\delta_{K,k} = 0$, which, according to equation (4b), requires $E_{K,k} = \frac{1}{2}U\left[1 \pm \sqrt{1 - 8J_K^2/(UV)}\right]$ or, more explicitly, $\cos(kd) = -U/(4J_K)\left[1 \pm \sqrt{1 - 8J_K^2/(UV)}\right]$, with the condition $8J_K^2/(UV) \leqslant 1$. The cross section attains its maximal value $\sigma_{K,k} = 1$ at $\delta_{K,k} = \pm\pi/2$, which corresponds to a pair of impenetrable (hard-core) bosons. According to equation (4b), this happens when either $\sin(kd) \to 0$ and $J_K \neq \mp UV/(U + 2V)$ (for $kd \to 0, \pi$, respectively) or $E_{K,k} = U - 2J_K^2/V$, the last equality yielding the explicit condition $\cos(kd) = J_K/V - U/(2J_K)$.

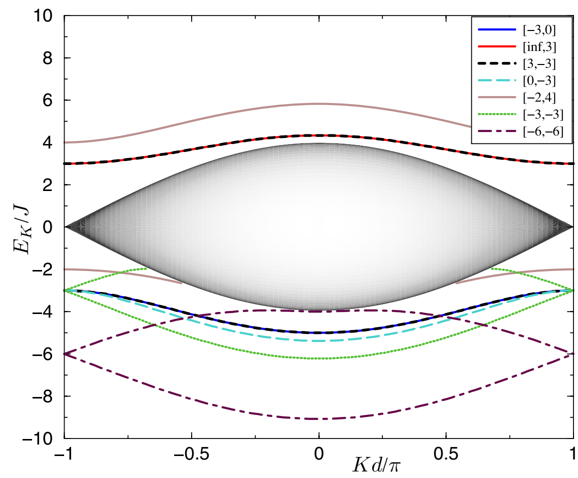

Figure 1. Energies versus the centre-of-mass momentum K for a pair of bosons in a 1D lattice described by the extended Hubbard model. The continuum spectrum corresponds to energies $E_{K,k}$ of the scattering states, with the shading proportional to the density of states $\rho(E, K)$. The lines correspond to energies E_K of the two particle bound states for various values of interaction strengths $[U/J, V/J]$.

At the edges of the scattering band, $kd \to 0, \pi$, we can define generalized 1D scattering lengths $a_K^{(0,\pi)}$ via [12, 13, 14]

$$a_K^{(0,\pi)} = -\lim_{kd\to 0,\pi} \frac{\partial\delta_{K,k}}{\partial k} = \frac{UV - 2J_K(J_K \mp V)}{UV \pm J_K(U + 2V)}d. \quad (5)$$

Thus, the scattering length a_K vanishes at the bottom of scattering band, $k \to 0$, when $J_K = \frac{1}{2}[V \pm \sqrt{V(2U + V)}]$, and at the top of the band, $k \to \pi/d$, when $J_K = -\frac{1}{2}[V \pm \sqrt{V(2U + V)}]$, with the condition $V(2U + V) \geqslant 0$. The scattering length diverges when $J_K = \mp W$ for $kd \to 0, \pi$, where $W \equiv UV/(U + 2V)$. In other words, the divergence of $a_K^{(0,\pi)}$ occurs when the centre-of-mass quasi-momentum $|K|$ is equal to

$$K_R = \frac{2}{d}\arccos\left(\mp\frac{W}{2J}\right), \quad (6)$$

with the condition $0 \leqslant \mp W/2J \leqslant 1$ for $kd \to 0, \pi$, respectively. As will become apparent from the proceeding discussion, K_R indicates the emergence of scattering resonances associated with the bound states (see figure 3).

We now consider the two-particle bound states. Using the exponential ansatz $\psi_K(r_i \neq 0) \propto \alpha_K^{|i|-1}$ in equation (2), after

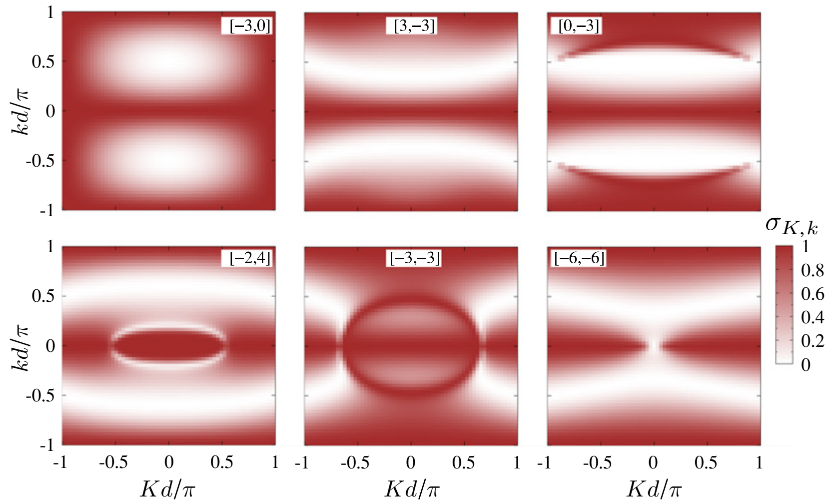

Figure 2. Two-particle scattering cross-section $\sigma_{K,k}$ versus the centre-of-mass K and relative k quasi-momenta for several values of interaction strengths $[U/J, V/J]$. Flipping simultaneously the sign of both U and V is equivalent to shifting $k \to k + \pi/d$.

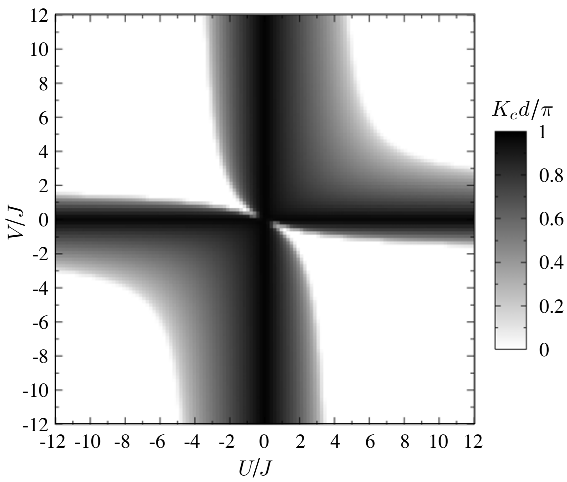

Figure 3. The U, V diagram for the existence of the second bound solution $|\alpha_K^{(2)}| < 1$ of equation (7) with $K_c < |K| \leqslant \pi/d$, with shading proportional to $K_c \in [0, \pi/d]$.

little algebra, we obtain

$$J_K V \alpha_K^3 + \left(VU - J_K^2\right)\alpha_K^2 + J_K(V+U)\alpha_K + J_K^2 = 0. \tag{7}$$

Solutions of equation (7) with $|\alpha_K| < 1$ determine the normalized bound states

$$\psi_K(0) = \mathcal{N}\frac{2J_K\alpha_K}{U\alpha_K + J_K\left(\alpha_K^2 + 1\right)} \equiv \mathcal{N}\varphi_K, \tag{8a}$$

$$\psi_K(r_i \neq 0) = \mathcal{N}\alpha_K^{|i|-1}, \tag{8b}$$

where $\mathcal{N} \equiv \left[\varphi_K^2 + 2/\left(1-\alpha_K^2\right)\right]^{-1/2}$, with the energies given by

$$E_K = -J_K\frac{1+\alpha_K^2}{\alpha_K}. \tag{9}$$

Note that complex solutions of equation (7) do not correspond to the bound states, even if $|\alpha_K| < 1$, since the energy (9) should be real.

It can be shown that equation (7) admits at most two solutions corresponding to the bound states. Obviously, for noninteracting particles $U = V = 0$, there can be no bound state. For $U \neq 0$ and $V = 0$ [11] and for $U = 0$ and $V \neq 0$, there is only one bound solution $\alpha_K^{(1)}$ at any K. For any other values of U, $V \neq 0$, the first bound solution $\alpha_K^{(1)}$ exists at any K and the second bound solution $\alpha_K^{(2)}$ exists at $|K| > K_c$, where the critical K_c is shown in figure 3 and is defined as

$$K_c = \begin{cases} K_R & \text{if} \quad |W/2J| \leqslant 1 \\ 0^- & \text{otherwise.} \end{cases} \tag{10}$$

We thus see that the scattering length diverges when the second bound state approaches the edge of the scattering continuum. This signifies the appearance of the scattering resonance at $|K| = K_R$, which is determined by equation (6) under the condition $|W/2J| \leqslant 1$. When, however, this condition is not satisfied, no scattering resonance is present, and the second bound state exists for all $K \in [-\pi/d, \pi/d]$ with the energy below or above the scattering continuum depending on whether $W \equiv UV/(U+2V)$ is negative or positive, respectively (see figure 1).

In general, analytic expressions for the bound solutions of equation (7) are too cumbersome for detailed inspection, but several special cases yield simple instructive results. (i) With only the on-site interaction $U \neq 0$ and $V = 0$, there is one bound solution $\alpha_K^{(1)} = (U - E_K)/(2J_K)$ with the corresponding energy $E_K = \text{sgn}(U)\sqrt{U^2 + 4J_K^2}$, as was discussed in [11]. (ii) With very strong on-site interaction $|U| \to \infty$ and $V \neq 0$, the first bound solution is trivial, $\alpha_K^{(1)} = 0$ and $E_K = U$, representing an infinitely bound pair. The second more relevant 'fermionized' [15] solution $\alpha_K^{(2)} = -J_K/V$ and $E_K = V + J_K^2/V$ describes a pair of hard-core bosons, $\psi_K(0) = 0$, which are bound by the nearest-neighbour interaction V provided $|J_K/V| < 1$ [16]. Note that in this limit we have $W = V$, and the last condition for the existence of the second bound state again reduces to $|K| > K_c$. (iii) Finally, a rather curious and simple case is

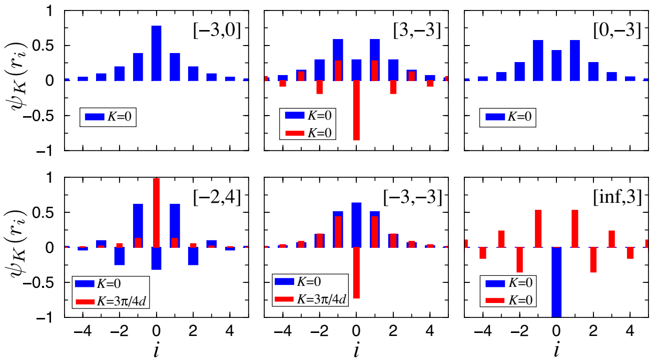

Figure 4. Relative coordinate wavefunctions $\psi_K(r_i)$ of the two-particle bound states for several values of interaction strengths $[U/J, V/J]$. Thick (blue) bars correspond to the first bound solution of (7) at $K = 0$. Thinner (red) bars correspond to the second bound solution at $K = 0$, if it exists for all K, or at $K = 3\pi/4d$, if it exists for $|K| > K_c$ (cf figures 1 and 3).

realized with $U = -V$. The first bound solution is similar to that in (i), but with U replaced by V, $\alpha_K^{(1)} = (V - E_K)/(2J_K)$ and the energy $E_K = \mathrm{sgn}(V)\sqrt{V^2 + 4J_K^2}$, which corresponds to binding mainly by the off-site interaction. The second bound solution is similar to that in (ii), but now with V replaced by U, $\alpha_K^{(2)} = -J_K/U$ and $E_K = U + J_K^2/U$, provided $|J_K/U| < 1$ (note that now $W = U$). This solution corresponds to the on-site interaction binding.

More generally, when the on-site U and off-site V interactions have different signs, the first bound state is associated mainly with the stronger (in absolute value) interaction and the second bound state with the weaker one. When, however, U and V have the same sign and comparable strength, the bound states have a mixed nature in the sense that both interactions significantly contribute to the binding. To illustrate the foregoing discussion, in figure 4 we show the wavefunctions of bound states for several cases pertaining to the on-site, off-site and mixed binding, while the corresponding energy dispersion relations are plotted in figure 1.

To conclude, we have derived a complete solution of the two-body problem in a one-dimensional extended Hubbard model. We have found that depending on the strength of the on-site and nearest-neighbour interactions, this system possesses one or two families of bound states as well as scattering resonances corresponding to the degeneracy of the bound and scattering states. Our results pertaining to the on- and off-site pairing mechanisms might be relevant to the studies of high-T_c superconductivity [5] and to the more recent quest to realize related physics with cold trapped atoms or molecules in optical lattices [17, 18].

Acknowledgments

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