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LETTER TO THE EDITOR

Two electrons in a one-dimensional 'rock salt' lattice with two types of on-site electron–electron correlation

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Abstract. The problem of two electrons on a one-dimensional (1D) lattice is solved for the case when the lattice unit cell contains two unequivalent sites a and b with two corresponding electron–electron correlation potentials: attractive U_a and repulsive U_b. It is shown, that the kinematics of the electron–electron scattering in such a system are remarkably different from those of the ordinary 1D Hubbard model because of the presence of the Umklapp processes. Analytical properties of the S-matrix are studied. Ground state properties and excitation spectrum are analysed as functions of U_a and U_b.

Experimental evidence that electron correlations may play an essential role in the high-temperature cuprate superconductors stimulated much theoretical work on highly correlated systems. Thus, the discovery of the presence of magnetic moments in most of the high-T_c materials together with the proposal the of the RVB theory [1], based on the Anderson theory of magnetism in transition 3d metals, were followed by intensive study of the two-dimensional Hubbard model with large positive U. Since spectroscopic experiments showed mainly p-type symmetry of the holes in the metallic regime of the cuprates [2] and Emery suggested strong hybridization of electron 3d orbitals on Cu and 2p orbitals on O [3], much theoretical work has been devoted to the extended Hubbard model and the corresponding t–J model, proposed by Rice and co-workers [4].

On the other hand, several theories assuming local attraction between electrons have been suggested to describe high-T_c superconductivity. In these theories electrons interact by means of boson exchange of various kinds. Such bosons can be phonons (for review see [5]), magnons [6, 7], excitons [8], acoustic plasmons [9] etc. Regardless of the nature of such attraction, mathematically this type of theory can be described by a negative-U Hubbard model.

The possibility of having both such types of electron correlation brought to life a hypothetical model with two correlation potentials: repulsion on copper and attraction on oxygen. There have already been some attempts to employ such a model to describe properties of high-temperature metal oxides [10, 11], but the approach used to obtain pair formation was the mean-field approximation, which may be not satisfactory in the case of sufficiently strong local attraction between particles. One

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should mention, of course, that mathematical difficulties, arising in the analysis even of the ordinary (one type of U) Hubbard Hamiltonian and even in two dimensions are enormous. In one dimension, however, exact solution is possible sometimes, as was done, for example, by Lieb and Wu [12] for the simple Hubbard chain, with the help of the Bethe *ansatz*, based on the Bethe hypothesis [13], that a N-particle wave function in one dimension can be described by a series of plane-wave exponents with coefficients to be determined from the two-particle S-matrix. From the physical point of view, this is closely related to the fact that the energy and momentum conservation laws lead to the conservation of the one-particle momenta in one-dimensional scattering of two identical particles, i.e. the corresponding *out*-momenta are the same as *in*-ones: $(p_1p_2)^{\text{out}} = (p_2p_1)^{\text{in}}$ or $(p_1p_2)^{\text{in}}$. As a result, exact properties of a many-particle system can be derived from the analysis of two-particle scattering.

The purpose of the present letter is to investigate the two-particle problem for a 1D 'rock salt' lattice (i.e. a chain, containing two sorts of unequivalent sites a and b) with two types of electron–electron correlations on the corresponding neighbouring sites: attractive, U_a, and repulsive, U_b. After constructing a two-electron wave function obeying translational properties of the lattice we determine the S-matrix of two-particle scattering. We also analyse the ground-state properties and excitations for various U_a and U_b.

We choose the tight-binding approximation form for the initial Hamiltonian:

$$\hat{H} = -t\sum_m \{a^\dagger_{m\sigma}b_{m-1\sigma} + b^\dagger_{m\sigma}a_{m+1\sigma} + a^\dagger_{m\sigma}b_{m\sigma} + b^\dagger_{m\sigma}a_{m\sigma}\} + \sum_m \{U_a n^a_{m\uparrow}n^a_{m\downarrow} + U_b n^b_{m\uparrow}n^b_{m\downarrow}\} \tag{1}$$

where index m denotes the unit cell number with the coordinates of a and b sites equal to $x^{(a)} = 2m$ and $x^{(b)} = 2m + 1$ correspondingly (lattice parameter equals 2); t is the hopping integral between neighbouring sites. For simplicity we set the energy difference between atomic levels a and b to zero: $\varepsilon_a - \varepsilon_b \simeq 0$. We will also use the following parameterization for t and correlation potentials U_a and U_b:

$$t = 1 \qquad U_a = -\alpha \qquad \text{and} \qquad U_b = \beta.$$

The one-electron spectrum of the Hamiltonian, equation (1), consists of two bands $\varepsilon_{1,2}(k) = \mp 2\cos k$ with quasi-momentum k lying in the first Brillouin zone: $-\pi/2 \leqslant k \leqslant \pi/2$. Corresponding eigenfunctions are two-component Bloch amplitudes:

$$\psi_k(x) = \begin{pmatrix} 1 \\ \pm e^{ik} \end{pmatrix} e^{2ikm}. \tag{2}$$

It is convenient to describe the one-electron state by a set of quantum numbers $\hat{k} = (n;k)$, where $n = 1(2)$ is the band index denoting the lower (upper) band. In the following we will call these quantum numbers quasi-momenta and use $\hat{k}$ and $\varepsilon(\hat{k})$ instead of k and $\varepsilon_{1,2}(k)$ in our equations.

The two-electron state, characterized by the total quasi-momentum K and the total energy E, can be described as a superposition of pairs of one-electron states with quasi-momenta $(\hat{k}_1\hat{k}_2)$ and $(\hat{q}_1\hat{q}_2)$, satisfying the energy and momentum conservation:

$$\begin{cases} K = k_1 + k_2 \\ E = \varepsilon(\hat{k}_1) + \varepsilon(\hat{k}_2) \end{cases} \qquad \text{and} \qquad \begin{cases} K = q_1 + q_2 \pm G \\ E = \varepsilon(\hat{q}_1) + \varepsilon(\hat{q}_2) \end{cases} \tag{3}$$

where $G = \pi$ is the inverse lattice vector. Appearence of G in equation (3) reflects the fact that the total momentum of the two-particle system should be always reduced to the first Brillouin zone, where the physically different values of the total quasi-momentum K lie. Depending on the values of E and K, there are three possible types of solution of equation (3), (as illustrated by figure 1): (i) if the total energy E lies in the interval $4|\sin(K/2)| \leqslant |E| \leqslant 4\cos(K/2)$, (undashed area on figure 1), then only solutions of the left-hand side system of equation (3) exist, giving a pair of two quasi-momenta $(\hat{k}_1\hat{k}_2)$, describing two one-particle states in the same band, i.e. $n_1 = n_2$. With the energy E and momentum K satisfying: (ii) $2|\sin(K)| \leqslant |E| \leqslant 4|\sin(K/2)|$ or (iii) $|E| \leqslant 2|\sin(K)|$, (two dashed areas on figure 1) the two-particle state includes two pairs of one-particle states: $(\hat{k}_1\hat{k}_2)$ and $(\hat{q}_1\hat{q}_2)$ (solutions of the corresponding systems of equation (3)) with the same (case (ii)) or different (case (iii)) band indexes, i.e. $n_1 \neq n_2$.

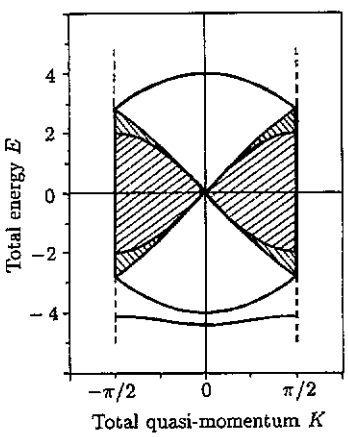

Figure 1. Two-electron states and the bound singlet states of two electrons. Undashed areas indicate the energy spectrum of triplet two-electron states (with singlet states lying only along the border). The two dashed areas correspond to the two-electron states, for which both the systems, equation (2), are soluble. The bound states energy spectrum for $\alpha = 3$, $\beta = 5$ is shown by the solid curve.

The two-particle S-matrix can be obtained by solving Shrödinger's equation, which is a matrix equation for the four-component wave function $\Psi_{\sigma_1\sigma_2}(x_1, x_2)$. Then, the most general form of the two-electron wave function is given by the direct product of the one-electron wave functions, equation (2):

$$\begin{aligned}\Psi_{\sigma_1\sigma_2}(x_1 < x_2) &= A_{\sigma_1\sigma_2}(\hat{k}_1\hat{k}_2)\psi_{\hat{k}_1}(x_1)\psi_{\hat{k}_2}(x_2) - A_{\sigma_1\sigma_2}(\hat{k}_2\hat{k}_1)\psi_{\hat{k}_2}(x_1)\psi_{\hat{k}_1}(x_2) \\ &\quad + A_{\sigma_1\sigma_2}(\hat{q}_1\hat{q}_2)\psi_{\hat{q}_1}(x_1)\psi_{\hat{q}_2}(x_2) - A_{\sigma_1\sigma_2}(\hat{q}_2\hat{q}_1)\psi_{\hat{q}_2}(x_1)\psi_{\hat{q}_1}(x_2) \\ \Psi_{\sigma_1\sigma_2}(x_1 > x_2) &= A_{\sigma_2\sigma_1}(\hat{k}_2\hat{k}_1)\psi_{\hat{k}_1}(x_1)\psi_{\hat{k}_2}(x_2) - A_{\sigma_2\sigma_1}(\hat{k}_1\hat{k}_2)\psi_{\hat{k}_2}(x_1)\psi_{\hat{k}_1}(x_2) \\ &\quad + A_{\sigma_2\sigma_1}(\hat{q}_2\hat{q}_1)\psi_{\hat{q}_1}(x_1)\psi_{\hat{q}_2}(x_2) - A_{\sigma_2\sigma_1}(\hat{q}_1\hat{q}_2)\psi_{\hat{q}_2}(x_1)\psi_{\hat{q}_1}(x_2)\end{aligned} \tag{4}$$

where pairs of one-particle quasi-momenta $(\hat{k}_1\hat{k}_2)$ and $(\hat{q}_1\hat{q}_2)$ are determined from equation (3). It is easy to show that the wave function, equation (4), satisfies the Shrödinger equation for any $x_1 \neq x_2$. The corresponding eigenvalue E is given by

equation (3). From the continuity of $\Psi_{\sigma_1\sigma_2}(x_1, x_2)$ at $x_1 = x_2$, the two following equations for coefficients A can be easily derived:

$$\begin{aligned} A_{\sigma_1\sigma_2}(\hat{k}_1\hat{k}_2) - A_{\sigma_1\sigma_2}(\hat{k}_2\hat{k}_1) &= A_{\sigma_2\sigma_1}(\hat{k}_2\hat{k}_1) - A_{\sigma_2\sigma_1}(\hat{k}_1\hat{k}_2) \\ A_{\sigma_1\sigma_2}(\hat{q}_1\hat{q}_2) - A_{\sigma_1\sigma_2}(\hat{q}_2\hat{q}_1) &= A_{\sigma_2\sigma_1}(\hat{q}_2\hat{q}_1) - A_{\sigma_2\sigma_1}(\hat{q}_1\hat{q}_2). \end{aligned} \tag{5}$$

Finally, our wave function must satisfy the Shrödinger equations with the same energy E (which follows from equation (1)) at $x_1 = x_2$, when the electrons have the same coordinates. The corresponding equations for the sites a and b of the unit cell m are of the form:

$$\begin{aligned} &-\Big\{\Psi_{\sigma_1\sigma_2}(2m, 2m-1) + \Psi_{\sigma_1\sigma_2}(2m-1, 2m) + \Psi_{\sigma_1\sigma_2}(2m, 2m+1) \\ &\qquad + \Psi_{\sigma_1\sigma_2}(2m+1, 2m)\Big\} - \alpha\delta_{\sigma_1,-\sigma_2}\Psi_{\sigma_1\sigma_2}(2m, 2m) = E\Psi_{\sigma_1\sigma_2}(2m, 2m) \\ &-\Big\{\Psi_{\sigma_1\sigma_2}(2m+1, 2m+2) + \Psi_{\sigma_1\sigma_2}(2m+2, 2m+1) + \Psi_{\sigma_1\sigma_2}(2m+1, 2m) \\ &\qquad + \Psi_{\sigma_1\sigma_2}(2m, 2m+1)\Big\} + \beta\delta_{\sigma_1,-\sigma_2}\Psi_{\sigma_1\sigma_2}(2m+1, 2m+1) \\ &\quad = E\Psi_{\sigma_1\sigma_2}(2m+1, 2m+1). \end{aligned} \tag{6}$$

Equations (5) and (6) must be solved now as a set of four linear equations on eight undefined coefficients A in equation (4). As a result of the solution, we determine four of these constants as linear combinations of the others:

$$\begin{aligned} A_{\sigma_2\sigma_1}(\hat{k}_2\hat{k}_1) &= S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}\{(\hat{k}_1\hat{k}_2)(\hat{q}_1\hat{q}_2)\}A_{\sigma_1'\sigma_2'}(\hat{k}_1\hat{k}_2) \\ &\quad + \tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}\{(\hat{k}_1\hat{k}_2)(\hat{q}_1\hat{q}_2)\}A_{\sigma_1'\sigma_2'}(\hat{q}_1\hat{q}_2) \end{aligned} \tag{7}$$

(expressions for $A_{\sigma_i\sigma_j}(\hat{q}_i\hat{q}_j)$ are the same as those in equation (7) after the substitution $\hat{k} \leftrightarrow \hat{q}$). Here we assume summation over spin indexes σ_1' and σ_2'. Coefficients $S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ and $\tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ have the physical meaning of S-matrices of electron–electron scattering. While $S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ describes processes with conservation of the initial one-particle momenta $\hat{k}_1$ and $\hat{k}_2$ (electrons exchange their quasi-momenta), $\tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ corresponds to the Umklapp processes, in which the total momentum $k_1 + k_2$ is reduced by the magnitude of the inverse lattice vector $G = \pi$, so that the *out*-momenta $\hat{q}_1$ and $\hat{q}_2$ are to be determined from equation (3). To write down the explicit form of matrices S and $\tilde{\mathbf{S}}$ it is convenient to use the following parameterization of the one-particle momenta:

$$l_i = \pm\sin(k_i) \qquad \text{and} \qquad \mu_i = \pm\sin(q_i)$$

where signs $+(-)$ correspond to the band indexes $n_i = 1(2)$, respectively.

With such parameterization, solutions for matrices $S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ and $\tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ are given by:

$$\begin{aligned} S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}\{l\mu\} &= \frac{l(\mu + \xi/2\mathrm{i})}{(\eta/2)^2 + (\mu + \xi/2\mathrm{i})(l + \xi/2\mathrm{i})}\delta_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2} \\ &\quad + \frac{(\eta/2)^2 + (\mu + \xi/2\mathrm{i})\xi/2\mathrm{i}}{(\eta/2)^2 + (\mu + \xi/2\mathrm{i})(l + \xi/2\mathrm{i})}\delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1} \\ \tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}\{l\mu\} &= \mathrm{i}\frac{\mu(\eta/2)}{(\eta/2)^2 + (\mu + \xi/2\mathrm{i})(l + \xi/2\mathrm{i})}\delta_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2} \\ &\quad - \mathrm{i}\frac{\mu(\eta/2)}{(\eta/2)^2 + (\mu + \xi/2\mathrm{i})(l + \xi/2\mathrm{i})}\delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1} \end{aligned} \tag{8}$$

where $\eta = \beta + \alpha/2$, $\xi = \alpha - \beta/2$, $l = l_1 - l_2$ and $\mu = \mu_1 - \mu_2$.

For $\beta = -\alpha$, corresponding to the case of a 1D lattice with one type of electron correlation (simple Hubbard chain), $\tilde{\mathbf{S}}$ vanishes and for $\mathbf{S}$ we obtain the well-known result of Lieb and Wu [12].

Matrices $S^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ and $\tilde{S}^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2}$ provide a complete picture of electron–electron scattering on a one-dimensional lattice with two types of electron–electron correlation. The kinematics of the scattering in terms of l_i and μ_i follow from the conservation laws, equation (3), i.e. μ_1 and μ_2 are related to l_1 and l_2 as follows:

$$\begin{cases} |\mu_1 - \mu_2| = \sqrt{(l_1 + l_2)^2 \mp 4\sqrt{1 - l_1^2}\sqrt{1 - l_2^2}} \\ (\mu_1 + \mu_2)(l_1 + l_2) = -\left[\sqrt{1 - l_1^2} \pm \sqrt{1 - l_2^2}\right]^2 . \end{cases} \tag{9}$$

Here the upper (lower) sign corresponds to the same (different) one-electron band indexes: $n_1 = n_2 = n_1' = n_2'$ ($n_1 \neq n_2$ and $n_1' \neq n_2'$).

If the initial one-particle momenta $\hat{k}_1$ and $\hat{k}_2$ describe electrons in the same band (i.e. $n_1 = n_2$) and parameters l_1 and l_2 satisfy

$$(l_1 + l_2)^2 \leqslant 4\sqrt{1 - l_1^2}\sqrt{1 - l_2^2} \tag{10}$$

then solutions for μ_1 and μ_2, derived from equation (9), are complex, with non-zero imaginary parts. To eliminate the corresponding divergent terms, arising from exponents with complex quasi-momenta $\hat{q}_1$ and $\hat{q}_2$ in the expression for our wave function, equation (4), we set $A_{\sigma_i\sigma_j}(\hat{q}_i\hat{q}_j) = A_{\sigma_i\sigma_j}(\hat{q}_j\hat{q}_i) = 0$, and for four other constants A we immediately get:

$$\begin{aligned} A_{\sigma_1\sigma_2}(\hat{k}_1\hat{k}_2) &= A_{\sigma_1\sigma_2}(\hat{k}_2\hat{k}_1) = C^{(\mathrm{T})} + C^{(\mathrm{S})}\delta_{\hat{k}_1,\hat{k}_2} \\ A_{\sigma_2\sigma_1}(\hat{k}_2\hat{k}_1) &= A_{\sigma_2\sigma_1}(\hat{k}_1\hat{k}_2) = C^{(\mathrm{T})} - C^{(\mathrm{S})}\delta_{\hat{k}_1,\hat{k}_2}. \end{aligned} \tag{11}$$

Here coefficients $C^{(\mathrm{T})}$ and $C^{(\mathrm{S})}$ define respectively anti-symmetric (triplet) and symmetric (singlet) parts of the two-electron coordinate wave function, given by equation (4). The corresponding region of two-electron states is shown on figure 1, where only triplet states exist within the undashed area, and singlet states with $\hat{k}_1 = \hat{k}_2$ are realized on its border. For the rest of the $(\hat{k}_1\hat{k}_2)$ pairs (those which do not satisfy equation (10)) solutions μ_1 and μ_2, derived from equation (9) are real, so that the corresponding momenta $\hat{q}_1$ and $\hat{q}_2$ together with $\hat{k}_1$ and $\hat{k}_2$ represent the set of the *out*-states, into which the initial electrons with momenta $\hat{k}_1$, $\hat{k}_2$ can be scattered.

We can now investigate the ground-state and low-energy excitations of our two-particle system. If one of the electron–electron correlation potentials corresponds to the on-site attraction, singlet bound states of two electrons exist in the system. The energy spectrum $E(K)$ of these states can be obtained from the poles of $\mathbf{S}$-matrix. The corresponding equation, derived from equation (8), is of the form:

$$\begin{aligned} &\sqrt{E^2 - 16\cos^2\frac{K}{2}}\sqrt{E^2 - 16\sin^2\frac{K}{2}} \\ &\quad + \frac{\beta - \alpha}{2}\left\{\sqrt{E^2 - 16\cos^2\frac{K}{2}} + \sqrt{E^2 - 16\sin^2\frac{K}{2}}\right\} - \alpha\beta = 0. \end{aligned} \tag{12}$$

Each such bound state is formed by two pairs of complex one-particle momenta (the so-called *strings*, discussed in [14]):

$$k_{1,2} = \frac{K}{2} \pm i\gamma \qquad q_{1,2} = \frac{K}{2} - \frac{G}{2}\sin(K) \pm i\tilde{\gamma}.$$

where $E = -4\cos K/2\coth\gamma = -4|\sin K/2|\coth\tilde{\gamma}$. The corresponding spectrum, derived from equation (12) for $\alpha = 3$ and $\beta = 5$, is shown on figure 1.

Analysis of equation (12) shows that, whereas for the values of the total momentum lying near the Brillouin zone boundary, solutions of equation (12) exist even for arbitrary weak attraction, the ground state (with $K = 0$) will be a bound state only if α and β obey:

$$\alpha \geqslant \frac{2\beta}{\beta + 2}. \tag{13}$$

In the opposite case the ground state will be a non-bound state of two electrons with quasi-momenta $k_1 = k_2 = 0$. It follows from (4) and (11) that the corresponding two-particle state will be a singlet, in agreement with the theorem proved by Lieb and Mattis [15]. Figure 2 shows two corresponding regions on the (α, β)-plane.

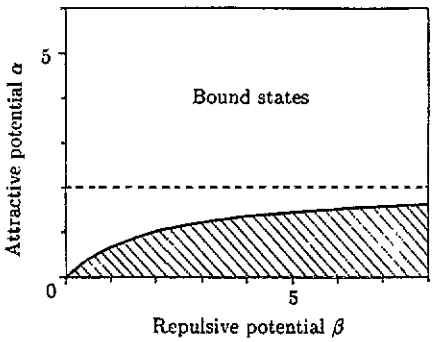

Figure 2. The ground-state phase diagram.

In conclusion, we have analysed the two-electron problem for a chain with two sorts of on-site electron–electron correlation: attractive U_a and repulsive U_b on the neighbouring sites a and b, respectively. The S-matrix of electron–electron scattering was derived. It was shown that translational properties of the lattice result in remarkably different (from that of the simple Hubbard chain) kinematics of electron–electron scattering. Presence of the Umklapp processes leads to the appearence of extra (in addition to those participating in the scattering as *initial*) one-electron momenta. It does not rule out, of course, the possibility of obtaining an exact solution to the many-electron problem, but the ordinary Bethe *ansatz* should be modified to account for additional one-particle quasi-momenta which will subsequently appear in the N-particle wave function.

We have also investigated ground-state properties of such a two-electron system and obtained the ground-state phase diagram (see figure 2). Equation (13) indicates that the ground-state properties of the system with both types of electron–electron interaction (attractive and repulsive) depend on competition between the correlation

potentials. It may happen that for a many-particle system this competition can result in dependence of the ground-state properties upon the total concentration of particles. Thus, if the bare correlation energies in the Hamiltonian, equation (1), are such that (α, β) lie near the critical curve, equation (13), renormalization of the interaction, which can arise from doping of the system by additional electrons, will lead to the dramatic change in the ground-state properties, for example, to the decay of initially bound pairs. As a result, the system would lose its superconducting properties, associated with formation of the bound states. We believe that this phenomenon, if exists, could be an explanation for the disappearance of superconductivity with doping, as observed in high-T_c cuprate superconductors.

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