

# S-Wave Bound- and Resonant States of Two Fermions in Simple Cubic Lattice

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Resonant two-electron states are examined in attractive Hubbard model on simple cubic lattice and exact formula for scattering cross section in the limit of low density (empty lattice) is calculated. S-wave pair is considered by means of lattice Green functions (LGF). Analytical form of these functions found by Joyce is used facilitating calculations, which were greatly hindered before by the necessity of using LGF's tabulated values. It is found that the actual peak of scattering cross-section is formed on the lower band boundary in discrepancy with formulae of the theory of scattering in solids.

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## 1. Introduction

Bound and resonant states belong to a class of problems possessing exact solutions. Thus they may serve as a valuable tool to examine properties of various models, in particular those, which can be realized with great accuracy in optical lattices. They are of interest, e.g. in nuclear physics, where bound states in free space are considered, as well as in condensed matter physics, where states are formed within a crystal lattice. Also in that case exact solutions exist [1]. They were examined especially in connection with two-magnon states in ferromagnets [2, 3]. Recently the interest in bound two-particle states grows again [4–16], as they can be relevant to high-temperature superconductivity (HTS), which is supposed to be caused by Bose–Einstein condensation (BEC) of tightly bound singlet electron pairs [4, 5]. As HTS materials are quasi-two-dimensional the focus has moved onto the models with possible electron pairing on two-dimensional lattices:  $t$ – $J$  [17],  $t$ – $U$ – $J$  [18],  $t$ – $U$ – $J$ – $V$  [11, 12] and (extended) Hubbard model [4, 12, 19]. Possibility of realizing BEC in optical lattices drew attention also to one-dimension [20]. Nevertheless three dimensional models are still attracting attention in connection with materials like heavy fermion superconductors or barium bismuthates (with parent compound  $BaBiO_3$ : a Mott–Hubbard isolator with charge–density waves, which becomes superconducting upon  $K$  or  $Pb$  doping). The interest in 3d systems has been further enhanced after practical realization of BEC of bound two-fermion dimers in cold atomic gases [21] and by possibility of experimental implementing of Hubbard (and Bose–Hubbard) hamiltonians of various dimensionalities in optical lattices [21, 22].

In the times of intensive research of bound states of magnons in 3D Heisenberg model the difficulty laid in

calculating lattice Green functions — Watson-type integrals, where tedious use of tabulated values was necessary. With the advance of the theory of that integrals it became possible to express them in closed, analytic form [23], enabling precise and easy calculations.

The results of Heisenberg model show that in 3D bound states exist for large center of mass momentum, thus increasing the importance of resonant states around band bottom, which may seriously influence thermodynamics [24]. Present paper applies the analytic formulae for Green functions to calculate scattering cross-section of resonant s-wave states in the Hubbard model and shows that cross-section's actual maxima do not coincide with the approximate formulae of the theory [1].

## 2. Formulae

We start with the Hubbard Hamiltonian:

$$\hat{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} - \mu \sum_{i\sigma} \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (1)$$

We are interested in the bound- and resonant- states of two electrons in the empty lattice. They require attractive interaction, i.e.  $U < 0$ . This is a problem of scattering theory in solids, which has been developed since sixties, so below we will only cite the results of the reference [1]. The resonant wave function is given by:

$$\psi_{\mathbf{K}}(\mathbf{r}) = \frac{\Omega^{1/2}}{(2\pi)^{3/2}} \left( e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{U\mathcal{G}(E, \mathbf{r})}{D} \right). \quad (2)$$

In case of bound state the exponent term is missing. For longer ranged interactions in the Hamiltonian (e.g. next-nearest neighbor Coulomb interaction) factor  $D$  becomes a determinant (and  $\mathcal{G}$  becomes a matrix) but for Hubbard model it is just a number:

$$D = 1 - U\mathcal{G}(E, 0). \quad (3)$$

The wave function  $\psi_{\mathbf{K}}(\mathbf{r})$  is non-trivial part of wave func-

tion of two electrons with relative distance  $\mathbf{r}$  and center of mass momentum  $\mathbf{K}$ . The factor  $\exp(\mathbf{K} \cdot \mathbf{R})$ , where  $\mathbf{R}$  is position of the center of mass of the pair, is not included, as the Hamiltonian does not change  $\mathbf{K}$ . The Green function  $\mathcal{G}(E, \mathbf{r})$  is a function of momentum  $\mathbf{K}$  though:

$$\mathcal{G}(E, \mathbf{r}) = \frac{\Omega}{(2\pi)^3} \int_{-\pi}^{\pi} d^3\mathbf{k} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{E - \epsilon_{\frac{\mathbf{K}}{2} - \mathbf{k}} - \epsilon_{\frac{\mathbf{K}}{2} + \mathbf{k}}}, \quad (4)$$

where the single energy spectrum for the orthogonal lattice with lattice constants  $a_x$ ,  $a_y$  and  $a_z$  is given by:

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x a_x + \cos k_y a_y + \cos k_z a_z). \quad (5)$$

In the following we will restrict ourselves to the simple cubic lattice with  $a_x = a_y = a_z = 1$ . The Green function simplifies to:

$$\mathcal{G}(E, \mathbf{r}) = \frac{\Omega}{(2\pi)^3} \times \int \int \int_{-\pi}^{\pi} \frac{e^{i\mathbf{k} \cdot \mathbf{r}} d^3\mathbf{k}}{E + 4t(\cos k_x + \cos k_y + \cos k_z)}. \quad (6)$$

Large  $\mathbf{r}$  limit of (4) can be calculated by method of stationary phase [25], yielding  $\mathcal{G}(E, \mathbf{r} \rightarrow \infty) = \text{const.} \times U e^{i\mathbf{q}_0 \cdot \mathbf{r}} / |\mathbf{r}|$ . Now, we can extract scattering amplitude from Eq. (2):

$$f = \text{Const.} \frac{U}{1 - U\mathcal{G}(E, 0)}. \quad (7)$$

Note, that the factor multiplying constant is just a  $T$ -matrix. The differential cross-section is given by:

$$\sigma_D = |f|^2. \quad (8)$$

The actual value of constant in  $f$  doesn't matter, as we plot the values of  $\sigma_D$  with the height normalized to 1/2.

The energies of bound states  $E_0$  are given by the zeros of  $D$ , Eq. (3):

$$1 - U\mathcal{G}(E_0, 0) = 0. \quad (9)$$

For energies in the band  $D$  becomes complex and zeros of its real part (denoted also as  $E_0$ ), usually lie in the vicinity of resonant states, defined as peaks of scattering cross-section. Including the 1<sup>st</sup>-order corrections to  $E$  the position and width of the resonance are given by [1]

$$E_r = E_0 - \frac{\text{Im}(D)\text{Im}(D')}{|D'|^2}, \quad (10)$$

$$\Gamma = \frac{2\text{Im}(D)\text{Re}(D')}{|D'|^2}, \quad (11)$$

where  $D$  is given by Eq. (3) and prime denotes differentiation with respect to energy. These formulae are derived with the assumption:

$$|\text{Re}(D')| \gg |\text{Im}(D')|. \quad (12)$$

Within the band Green function Eq. (6) is divergent, what is remedied in standard way by adding an infinitesimal, imaginary part to the energy  $E$ . Analytic formula for the Green function  $\mathcal{G}(E, 0)$  was found by Joyce [23]:

$$\mathcal{G}(E, 0) = -\frac{1}{4t} \frac{4\sqrt{1 - \frac{3x_1}{4}}}{\tilde{E}\pi^2(1 - x_1)} \mathcal{K}(k_-) \mathcal{K}(k_+), \quad (13)$$

$$x_1 = -\frac{1}{2} \sqrt{1 - \frac{9}{\tilde{E}^2}} \sqrt{1 - \frac{1}{\tilde{E}^2}} + \frac{3}{2\tilde{E}^2} + \frac{1}{2}, \quad (14)$$

$$x_2 = x_1/(x_1 - 1), \quad (15)$$

$$k_{\pm}^2 = \frac{1}{2} \pm \frac{1}{4} x_2 \sqrt{4 - x_2} - \frac{1}{4} \sqrt{1 - x_2} (2 - x_2), \quad (16)$$

where  $\tilde{E} = E/(-4t)$ .  $E/(-4t)$  and  $\mathcal{K}$  is complete elliptic integral of the first kind.

### 3. Results

The results of the calculations are shown in the following figures. Figure 1 shows the general rule how the bound and resonant states are created [26]: we seek the zeros of  $D$ , Eq. (3), in the form  $1/U = \mathcal{G}(E, 0)$ , i.e. we seek a point where the line  $1/U$  (straight, horizontal) crosses the real part of  $\mathcal{G}(E, 0)$  (thick dashed). The energy of that crossing,  $E_0$ , is shown by a vertical, dotted line. At that energy the delta peak of  $\sigma_D$  occurs indicating bound state. In the figure we can see dot-dashed line in its place, indicating  $E_r$ , Eq. (10); as there are no corrections connected with the imaginary part of  $\mathcal{G}$  (with  $\text{Im}(\mathcal{G})$  shown as a full, thick line), it occurs at the same place as  $E_0$ .

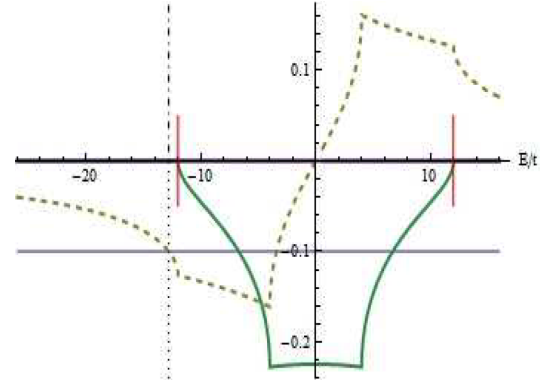


Fig. 1. Plots of  $1/U$  for  $U/t = -10$  (horizontal line),  $\text{Re}(\mathcal{G})$  (thick dashed line),  $\text{Im}(\mathcal{G})$  (thick full line),  $E_0$  indicated by a vertical, dotted line,  $E_r$ , Eq. (10), indicated by vertical dot-dashed line, vertical bars on the ordinate axis denote band boundaries.  $\mathcal{G}$  plotted for center of mass momentum  $\mathbf{K} = 0$ .

In Fig. 2,  $|U|$  is decreased, so that  $1/U$  can cross  $\text{Re}(\mathcal{G})$  within the band, in the region of  $\text{Re}(\mathcal{G}') < 0$ , where resonances can exist [2]. Note the large discrepancy between  $E_0$  and  $E_r$ . The resonance width (11) is much larger than the actual width of  $\sigma_D$ .

$|U|$  is further decreased in Fig. 3:  $E_0$  moves towards smaller  $|E|$  values, so does  $E_r$ , yet the actual peak in scattering cross section remains fixed at the band boundary! Thus formula (10) fails.

In Fig. 4  $|U|$  is so small that  $1/U$  does not cross  $\text{Re}(\mathcal{G})$  at all. Surprising thing is, that the resonant peak of  $\sigma_D$  remains, despite Eq. (9) is not fulfilled, even in its real

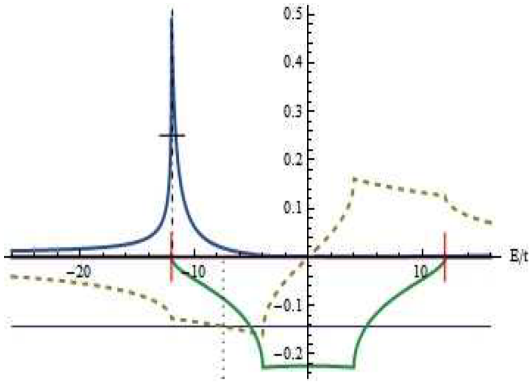


Fig. 2. Differential cross-section (full, thick, positive line) Eq. (8), normalized to the height 1/2, for  $U/t = -7$ . Horizontal bar in the middle of dot-dashed line depicts resonance width, Eq. (11). The rest of denotations as in Fig. 1.

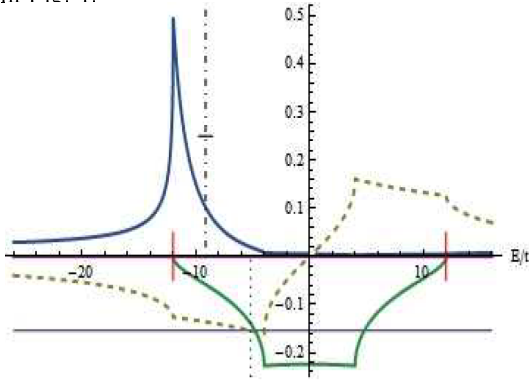


Fig. 3. Differential cross-section for  $U/t = -6.5$ . Denotations as in Fig. 2.

part;  $Re(1 - U\mathcal{G})$  has minimum at  $E_0$  and that apparently suffices to sustain the resonant structure. That minimum coincides with the minimum of  $Re(\mathcal{G})$ , where both  $E_0$  and  $E_r$  are placed, but the  $\sigma_D$  peak remains fixed at the band boundary.

Figure 5 displays what happens with further decrease of  $|U|$ . The sharply defined "peak" disappears, yet there

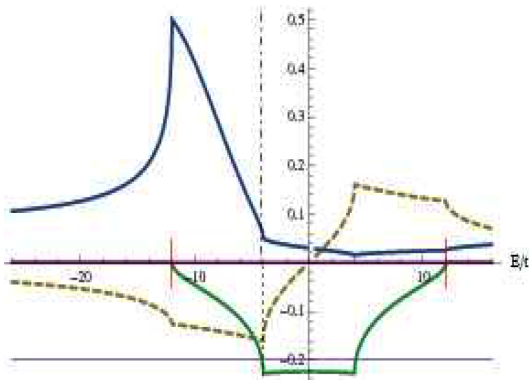


Fig. 4. Differential cross-section for  $U/t = -5$ . Denotations as in Fig. 2.

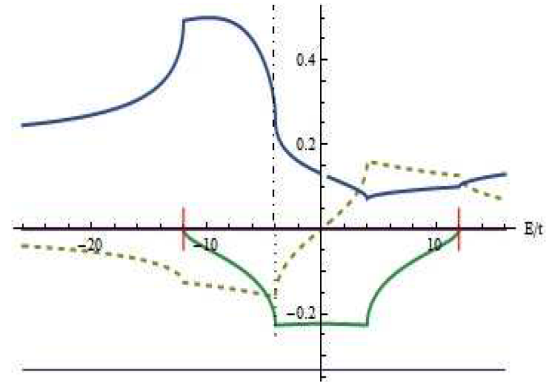


Fig. 5. Differential cross-section for  $U/t = -3$ . Denotations as in Fig. 2.

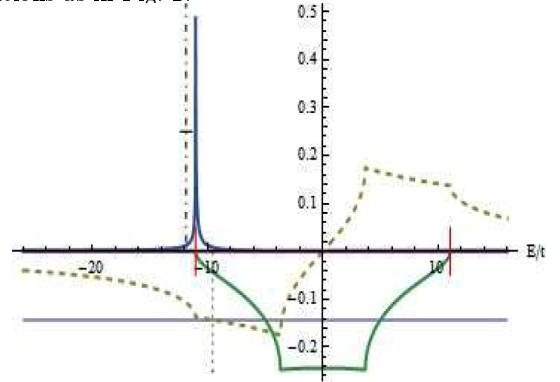


Fig. 6. Differential cross-section for  $U/t = -7$  and center of mass momentum  $\mathbf{K} = 0.8\sqrt{3}$  along  $\Gamma R$  line of sc lattice. The rest of denotations as in Fig. 2.

remains an elevated value of  $\sigma_D$  between the band boundary and the minimum of  $Re(\mathcal{G})$ .

The effect of the increasing center of mass momentum  $\mathbf{K}$  is shown in Fig. 6: the resonant peak is still fixed at the band boundary.  $E_r$  indicates erroneously bound state below the band, instead of resonant one.

#### 4. Conclusions

In conclusion we have performed calculations of s-wave scattering cross-section of resonant two-electron states in attractive Hubbard model on simple cubic lattice, in the limit of empty lattice. We took advantage of analytical formulae for the three dimensional lattice Green functions [23] and used the theory of scattering in solids [1]. The main results are: i) showing the persistence of resonance structures, even when the resonant condition  $Re(1 - U\mathcal{G}) = 0$  is *not* fulfilled, ii) showing that the resonant peak, when defined, remains fixed at the lower band boundary for all  $U < 0$  and  $\mathbf{K}$  values, iii) the traditional formulae for the position of resonant peak,  $E_r$ , and its width  $\Gamma$  fail in case of s-wave pairs in Hubbard model.

The author ascribes discrepancy between  $E_r$  and the actual peak of  $\sigma_D$  to the violating inequality (12). As it

is connected with the shape of  $\mathcal{G}(0)$  the same effect will be probably found in case of extended Hubbard model.

Note, that for  $U > 0$  we obtain figures analogical to the ones described in the current paper but symmetrically reflected relative to the vertical coordinate axis.

The results of present work may be also relevant to the research of bound magnon states in Heisenberg model [27].

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