Effective Mass of Bound and Resonant Two-Electron Pairs in a Simple Cubic Lattice

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Effective masses m^* of bound 2-electron pairs on a simple cubic lattice were investigated within tUWJ model within symmetry channels. Linear increase of m^* with $|W|$ for intersite pairs and nonlinear behavior and sign change of m^* in case of pairs with on-site component were found. $|m^*|$ turned out to be larger than twice free electron mass.

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1. Introduction

A good candidate for mechanism of high temperature superconductivity (HTS) is the Bose condensation of tightly bound pairs. Thus the properties of single pair are a good starting point for investigations of HTS in the strong coupling limit. An important property is the pair's ability to move, described by its effective mass m^* . Although HTS materials are often considered two-dimensional (2D) they have in fact quasi-2D, strongly anisotropic 3D structure. There are also other strongly correlated 3D materials exhibiting superconductivity, like heavy fermion superconductors, Chevrel phases or doped BaBiO₃ [1]. That warrants investigation of 3D systems. Current paper reports calculations of pair's effective mass within tUWJ model on "generic" simple cubic (sc) lattice.

2. Formalism

We shall start with tUWJ Hamiltonian $H = H_0 + H_1$ in standard denotations

$$H = \sum_{\langle i,j \rangle} \sum_{\sigma} t_{i,j} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{\mathbf{I}} n_{i,\uparrow} n_{i,\downarrow} + \frac{W}{2} \sum_{\langle i,j \rangle} \sum_{\sigma, \sigma'} n_{i,\sigma} n_{j,\sigma'} + \frac{J}{2} \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j),$$

where $\langle \dots \rangle$ means summation over nearest neighbors (nn), H_0 — the hopping part — is the first term in the right hand side of the above equation, the rest describes interaction part H_1 . The solution of the Schrödinger equation $(H_0 + H_1)|\psi\rangle = E|\psi\rangle$ can be formally expressed as $|\psi\rangle = G_0 H_1 |\psi\rangle$ with the Green function (GF):

$$G_0 = (E - H_0)^{-1} = \frac{1}{N} \sum_{\mathbf{k}} \frac{|\mathbf{k}\rangle \langle \mathbf{k}|}{E - E_{\mathbf{k}}}, \quad (1)$$

where $|\mathbf{k}\rangle$ symbolically denotes eigenstates of H_0 , which are, in fact, the states of two particles with fixed center-of-mass momentum $\mathbf{K}$ and relative momentum $\mathbf{k}$:

$|\mathbf{K}\mathbf{k}\sigma_1\sigma_2\rangle = c_{\mathbf{K}/2+\mathbf{k},\sigma_1}^{\dagger} c_{\mathbf{K}/2-\mathbf{k},\sigma_2}^{\dagger} |0\rangle$. The eigenenergy of H_0 is given by

$$E_{\mathbf{K},\mathbf{k}}^{\text{sc}} = -4t \left(\cos \frac{K_x}{2} a_x \cos k_x a_x + \cos \frac{K_y}{2} a_y \cos k_y a_y + \cos \frac{K_z}{2} a_z \cos k_z a_z \right),$$

where a_x, a_y, a_z are lattice constants. On the other hand, H_1 is diagonal within the local orbitals basis in direct space. As we assume periodic boundary conditions the center of mass momentum $\mathbf{K}$ is conserved quantity, and we can introduce orthogonal "mixed" basis

$$|\mathbf{K}\mathbf{r}\sigma_1\sigma_2\rangle =$$

$$\frac{1}{\sqrt{N}} \sum_{\mathbf{r}'} \exp(i\mathbf{K} \cdot (\mathbf{r}' + \mathbf{r}/2)) c_{\mathbf{r}',\sigma_1}^{\dagger} c_{\mathbf{r}'+\mathbf{r},\sigma_2}^{\dagger} |0\rangle,$$

where N is number of lattice sites and $\mathbf{r}$ denotes *relative* distance between electrons in a pair. We create singlets and triplets

$$|S^{\mathbf{K}}(\mathbf{r})\rangle = (|\mathbf{K}\mathbf{r}\uparrow\downarrow\rangle - |\mathbf{K}\mathbf{r}\downarrow\uparrow\rangle) / \sqrt{2(1 + \delta_{\mathbf{r},0})},$$

$$|T_0^{\mathbf{K}}(\mathbf{r})\rangle = (|\mathbf{K}\mathbf{r}\uparrow\downarrow\rangle + |\mathbf{K}\mathbf{r}\downarrow\uparrow\rangle) / \sqrt{2},$$

$$|T_1^{\mathbf{K}}(\mathbf{r})\rangle = |\mathbf{K}\mathbf{r}\uparrow\uparrow\rangle,$$

$$|T_{-1}^{\mathbf{K}}(\mathbf{r})\rangle = |\mathbf{K}\mathbf{r}\downarrow\downarrow\rangle.$$

These states are eigenstates of H_1 in tUWJ model; we will use it as a basis for expansion of $|\psi\rangle$. This way, we will obtain singlet $\psi_{\mathbf{K}}^{(s)}(\mathbf{r}) = \langle S^{\mathbf{K}}(\mathbf{r}) | \psi \rangle$ and triplet $\psi_{\mathbf{K},\zeta}^{(t)}(\mathbf{r}) = \langle T_{\zeta}^{\mathbf{K}}(\mathbf{r}) | \psi \rangle$ wave function solutions of our 2-particle problem. For $\mathbf{r}$'s larger than the range of Coulomb interactions $\langle S^{\mathbf{K}}(\mathbf{r}) | H_1 | S^{\mathbf{K}}(\mathbf{r}) \rangle = 0$ (in the triplet case we use triplet bras and kets). Thus the nonzero "effective" part of $\langle H_1 \rangle$, hereafter denoted by $\mathbf{V}$, is small. For nn interactions it is given (in the singlet case) by 4×4 diagonal matrix with the elements $(U, W - J, W - J, W - J)$ on the diagonal. Both singlets and triplets mix states at " $\mathbf{r}$ "

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with the states at “ $-\mathbf{r}$ ”, so in fact basis is spanned only by half of the sites of the direct space.

The singlet Green function is 4×4 matrix with elements

$$G_0(E, \mathbf{K}, \mathbf{r}, \mathbf{r}') = \langle S^{\mathbf{K}}(\mathbf{r}) | G_0 | S^{\mathbf{K}'}(\mathbf{r}') \rangle = 2\delta_{\mathbf{K}, \mathbf{K}'} \sum_{\mathbf{k}} \frac{\cos \mathbf{k}\mathbf{r} \cdot \cos \mathbf{k}\mathbf{r}'}{(E - E_{\mathbf{K}, \mathbf{k}})(N\sqrt{1 + \delta_{\mathbf{r}, 0}}\sqrt{1 + \delta_{\mathbf{r}', 0}})},$$

with $\mathbf{r}, \mathbf{r}' \in \{\mathbf{0}, \mathbf{a}_x, \mathbf{a}_y, \mathbf{a}_z\}$.

The triplet GF has sin instead cos.

For $\mathbf{K}$ on some symmetry lines G_0 can be further simplified into the block-diagonal form by unitary transformation. The blocks transform according to irreducible representations of the point symmetry group of a lattice (irreps). For sc lattice (O_h group) the irreps are: A_{1g} , traditionally called s -wave (if corresponding to the site 0 or s^* , i.e., “extended s ”, if corresponding to “layer” of nn sites), E_g ($d_{x^2-y^2}$ and $d_{2z^2-x^2-y^2}$), and 3-dimensional T_{1u} , connected with three p -waves: p_x, p_y and p_z . For $\mathbf{K}$ on RΓM line $d_{x^2-y^2}$ decouples from other pairings (for anisotropic system also the other d -wave on RΓM lines). The GF for p -wave pairing is diagonal: all p -waves are decoupled from each other for arbitrary $\mathbf{K}$, yielding 3 degenerated *scalar* equations.

Eventually we are led to the matrix equation for the singlet case

$$\tilde{\psi}_{\mathbf{K}} = \tilde{G}_0(E, \mathbf{K}) \tilde{V} \tilde{\psi}_{\mathbf{K}}. \quad (2)$$

Bold fonts denote that we are dealing with vectors and matrices, tilde — that the given quantity is after unitary transformation $\mathcal{U}$. Numerator of $\tilde{G}_0 = \mathcal{U}G_0\mathcal{U}^{-1}$ consists of products of the functions: 1, $\sqrt{2/3}(\cos k_x + \cos k_y + \cos k_z)$, $\cos k_x - \cos k_y$, $(\cos k_x + \cos k_y - 2\cos k_z)/\sqrt{3}$, which transform according to $s, s^*, d_{x^2-y^2}$ and $d_{2z^2-x^2-y^2}$ irreps respectively; $\tilde{V} = V$.

The condition for nontrivial solutions (of E) of Eq. (2) reads

$$\det(\mathbf{I} - \tilde{G}_0(E, \mathbf{K}) \tilde{V}) = 0, \quad (3)$$

where $\mathbf{I}$ is identity matrix. Approximating E around its minima by a free particle formula: $E - E_{\min} = \lim_{\mathbf{K} \rightarrow 0} \hbar^2 \mathbf{K}^2 / 2m^*$ we can get the effective mass m^* of pairs in a given symmetry channel.

During calculations we take advantage of the formula

$$\frac{1}{\pi^3} \iiint_0^\pi \frac{\cos(px) \cos(qy) \cos(nz) dx dy dz}{E - a \cos x - b \cos y - c \cos z} = \int_0^\infty \exp(-Et) I_p(at) I_q(bt) I_s(ct) dt,$$

where $I_n(t)$ is modified Bessel function of the first kind [2].

3. Results

The dispersion curves for pairs of different symmetries for $W/t = -10.796$, i.e. for d -wave critical W value [1], are shown in Fig. 1, together with parts of two-free electrons band (grayed out). Note the different number of

curves in different parts of the Brillouin zone (BZ), a result of degeneration. On ΓM line $d_{x^2-y^2}$ -wave pairing is decoupled from 4×4 singlet determinant, so we have 1 d -wave curve and 2 or 3 curves (for $U \geq 0$ and $U < 0$, respectively) of mixed s - d character. On ΓR and RM lines the d -wave curve is doubly degenerated on the expense of disappearing of one of s - d curves. The “shallow”, close to the band bottom, solutions of singlet determinant in the Γ point are “ d -like”, i.e., mostly $W - J$ dependent. Note their prominent degeneration at R point in BZ.

Fig. 1. Dispersion curves for $W - J = -10.796t$.

Fig. 2. $m_{pair}^*/2m_{el}$ vs. W/t , $J = 0$ for intersite pairs of various symmetries and symmetry directions in Bz. Inset: d -wave for $M\Gamma$ and ΓR lines.

Fig. 3. $m_{pair}^*/2m_{el}$ vs. W/t , $J = 0$, $U = -16t$ for on-site shallow pairs (s^*). Deep pair in the inset.

The respective effective masses (in the units of two free-electron masses) are shown in Fig. 2. The masses increase

linearly with $|W - J|$. The anisotropy of the states in various symmetry directions is well shown. Only the strongly bound s^* states for $U = 0$ are isotropic.

For $U < 0$ effective masses are isotropic and depend on W non-linearly as shown in Fig. 3. The effective mass of “shallow” states, closer to band bottom, with smaller binding energy is diverging around $W \sim U$, indicating the change of curvature of $E(K)$ relation. The “deep” states, with $E \sim U$ reach minimal m^* around $W = U$.

4. Conclusions

Dispersion curves and effective masses m^* of bound 2-electron pairs on sc lattice (in the limit of empty lattice) in the tUWJ model were found in symmetry channels. W and J always appear together as $W - J$ — they are equivalent. m^* increase with $|W - J|$ for intersite pairs, while non-linear behavior with $W - J$ of (strongly bound,

extended s^* -wave) pairs with significant on-site component is found. Effective masses of pairs are larger than masses of two free electrons. $m^*/2m_{el}$ can be close to one for shallow s^* -wave states and is the largest (≈ 25) in the case of d -wave pairs on ΓR direction. The calculations in 2D models suggest that considering second-neighbor hopping might decrease m^* [3]; similar effect could be reached by considering anisotropic lattice [4].

References

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