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Spin triplet pairing and superconducting states in square lattices

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Abstract

In this work we study the pairing symmetry in a square lattice within a generalized Hubbard model, in which a second-neighbor correlated hopping is included in addition to the on-site and nearest-neighbor repulsions. When an infinitesimal distortion of the right angles in the square lattice is considered, we observe a spin triplet p-wave ground state for the case of electrons, but for holes a finite distortion is required, contrary to the d-wave case. In general, this spatial distortion induces a splitting of the doubly degenerate p-wave pairing states and one of them could become the ground state. On the other hand, this study has been extended to a finite density of electrons within the BCS formalism and the results show a maximum critical temperature of p-wave superconductivity around a 2/3 band-filling, close to the Fermi energy in the γ-band of Sr_2RuO_4 estimated by band-structure calculations.

Keywords: Spin-triplet pairing; Hubbard model; Two-dimensional systems

The recent discovery of the p-wave spin-triplet superconducting state in Sr_2RuO_4 [1] has enhanced the research of models beyond the standard BCS theory to include anisotropic superconducting gap symmetries. The two-dimensional character of this material should be essential to understand its peculiarities. Three-band Hubbard models have been proposed to describe the electron dynamics on the planes and the electronic states close to the Fermi energy can be reasonably well described by a single-band tight-binding model with next-nearest-neighbor hoppings [2]. In this work, we investigate the spin-triplet p-wave pairing and superconducting states in a generalized Hubbard model.

Let us consider a two-dimensional square lattice with a lattice parameter a and a single-band generalized Hubbard Hamiltonian for electrons as [3]

$$\begin{aligned}\widehat{H} = &-t_0 \sum_{\langle i,j\rangle\sigma} c^+_{i\sigma} c_{j\sigma} - t'_0 \sum_{\langle\langle i,j\rangle\rangle\sigma} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ &+ \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j + \Delta t \sum_{\langle i,j\rangle\sigma} c^+_{i\sigma} c_{j\sigma} (n_{i-\sigma} + n_{j-\sigma}) + \Delta t_3 \\ &\times \sum_{\substack{\langle\langle i,j\rangle\rangle\sigma \\ \langle i,l\rangle,\langle j,l\rangle}} c^+_{i\sigma} c_{j\sigma} n_{l-\sigma} \end{aligned} \quad (1)$$

where $c^+_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^+_{i\sigma} c_{i\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote respectively nearest-neighbor and next-nearest-neighbor sites. t_0 and t'_0 are positive hopping-integral parameters. When an electron-hole transformation is made in Eq. (1) via $c^+_{i\sigma} \to h_{i\sigma}$, the Hamiltonian of holes has the same form as Eq. (1), except for containing new hopping integrals for holes $t = t_0 - 2\Delta t$ and $t' = t'_0 - 4\Delta t_3$, instead of $-t_0$ and $-t'_0$ for electrons [3]. Furthermore, for the case of two fermions with a total spin $S = 1$ (triplet), the real-space wave function should be anti-symmetric under the exchange

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of particles, i.e., it should have p- or f-symmetry in the two-particle internal coordinate space. To break the degeneracy of p-wave pairing states, we consider a small distortion of the right angles in the square lattice, which leads to changes in the second-neighbor interactions, such as t' and Δt_3 terms in Eq. (1). The new values of these interactions are $t'_{\pm} \equiv t' \pm \delta'$ and $\Delta t_3^{\pm} \equiv \Delta t_3 \pm \delta_3$, where $\pm$ refers to the $\hat{x} \pm \hat{y}$ direction.

The two-particle binding energy is defined as $\Delta_2 = E_2 - 2E_1$, where E_n is the ground state energy with the appropriate symmetry corresponding to the problem of n particles and it can be calculated by using a previously developed mapping method [3]. The electron- and hole-pairing phase diagrams are respectively shown in Fig. 1(a) and (b), for $U = 6t_0$, $V = 0$, $t'_0 = 0.45t_0$, $\Delta t = 0.5t_0$, and $\Delta t_3 = 0.1t_0$. The dashed line indicates the exception of p-wave pairing states at $\delta_3 = 0$. The numerical calculations are performed in a projected square lattice of 1741 two-particle states [3]. Notice the asymmetry between pairings of electrons and of holes, where the electron triplet has a larger p-wave region and requires only an infinitesimal distortion in the second-neighbor correlated-hopping interaction (Δt_3), in contrast to the favored hole pairing with d symmetry when the distortion is small.

On the other hand, the real-space Hamiltonian [Eq. (1)] can be rewritten in the momentum space by making a Fourier transform of the creation and annihilation operators [4]. Within the BCS formalism, the equations for determining the p-channel superconducting gap $[\Delta(\mathbf{k}) = \Delta_p(\sin(k_x a) + \sin(k_y a))]$ and the chemical potential (μ) are [4]

$$\mathbf{1} = -\frac{(V - 4\delta_3)}{N_s} \sum_{\mathbf{k}} \frac{\sin(k_x a)[\sin(k_x a) + \sin(k_y a)]}{E(\mathbf{k})} \times \tanh\left(\frac{E(\mathbf{k})}{2k_B T}\right), \tag{2}$$

$$n - 1 = -\frac{1}{N_s} \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k}) - \mu}{E(\mathbf{k})} \tanh\left(\frac{E(\mathbf{k})}{2k_B T}\right) \tag{3}$$

where n is the density of particles, N_s is the total number of sites, the single excitation energy is given by

$$E(\mathbf{k}) = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta^2(\mathbf{k})},$$

and

$$\varepsilon(\mathbf{k}) = (U/2 + ZV)n + 2(t + n\Delta t)[\cos(k_x a) + \cos(k_y a)] + 2(t'_+ + 2n\Delta t_3^+)\cos[(k_x + k_y)a] + 2(t'_- + 2n\Delta t_3^-) \times \cos[(k_x - k_y)a].$$

In particular, the critical temperature (T_c) can be determined by $\Delta_p(T_c) = 0$ and its results are shown in Fig. 2 for $V = -0.39t_0$, $t'_0 = 0.45t_0$, $\Delta t = 0.5t_0$, $\Delta t_3 = 0.05t_0$, $\delta' = 0.001t_0$, $\delta_3 = 0.01t_0$ and arbitrary U. Notice that there is a maximum around $n = 4/3$ (corresponding to 2/3 band-filling), in agreement with the Fermi energy estimated by the band theory [5]. The value of T_c decreases as the inter-atomic interaction (V) diminishes and it remains finite even for $V = 0$.

In summary, we have studied s-, p-, and d-wave pairings in a square lattice within the generalized Hubbard model. We observe that an infinitesimal distortion in the square lattice or in the second neighbor interactions can induce a p-symmetry spin-triplet electron pairing, but not for the p-wave hole pairing. This fact agrees with the sign of the low temperature Hall coefficient observed in Sr_2RuO_4 [6]. On the other hand, the finite density calculation reveals a much lower T_c for the

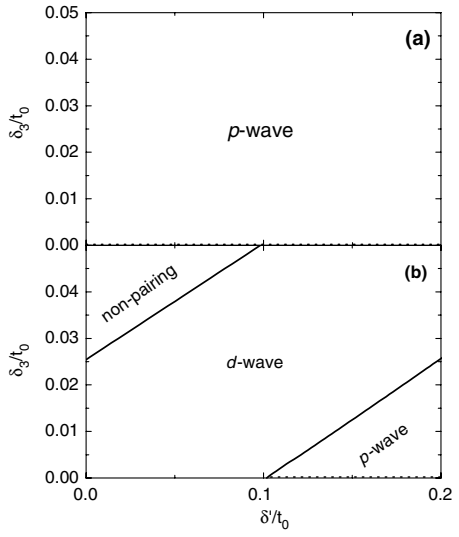

Fig. 1. (a) Electron and (b) hole pairing phase diagrams in a distortion strength space. The dashed lines denote the absence of p-wave pairing at $\delta_3 = 0$.

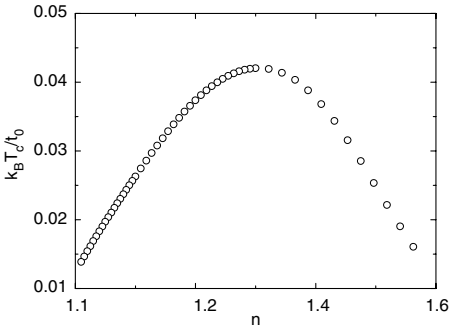

Fig. 2. Critical temperature (T_c) as a function of the electron density (n) for $V = -0.39t_0$, $t'_0 = 0.45t_0$, $\Delta t = 0.5t_0$, $\Delta t_3 = 0.1t_0$, $\delta' = 0.001t_0$ and $\delta_3 = 0.01t_0$.

p-channel in comparison with that of d-channel, in qualitative agreement with experiment results.

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