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Symmetry phase diagrams of the superconducting ground states induced by correlated hoppings interactions

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Abstract

The formation of p- and d-wave superconducting ground states on a square lattice is studied within the BCS formalism and a generalized Hubbard model, in which a second-neighbor correlated hopping (Δt_3) is included in addition to the on site and nearest neighbor repulsions. The triplet superconductivity is obtained when a small distortion of the right angles in the square lattice is introduced. This distortion can be characterized by the difference between the values of $\Delta t_3^{\pm}$ in the $x \pm y$ directions, i.e., $\delta_3 = (\Delta t_3^{+} - \Delta t_3^{-})/2$. The phase diagram is analyzed in the space of the electron density (n) and δ_3. The results show that the p- and d-channel superconductivities are respectively enhanced in the low and high electron density regions.

Keywords: Superconducting gap symmetry; Hubbard model; Two-dimensional systems

The investigation of correlated electron models that could lead to anisotropic superconducting gaps is highly motivated by the observation of d-symmetry gap in the cuprate superconductors [1] and p-wave spin-triplet superconducting state in Sr_2RuO_4 [2]. The two-dimensional behavior, present in both mentioned systems, could be essential to understand their peculiar properties. Single-band second-neighbor Hubbard models on square lattices have been proposed to describe the dynamics of the carriers on the CuO_2 [3] and RuO_2 [4] planes. Recently, we have found that the second-neighbor correlated-hopping interaction (Δt_3) is essential in the $d_{x^2-y^2}$ wave superconductivity [5] and a further small distortion of the right angles in the square lattice leads to p-wave superconductivity [6]. It is worth mentioning that a similar distortion has been observed on the surface of Sr_2RuO_4 [7]. In this article, we report the phase diagram of p- and d-wave superconducting ground states by means of a previously used generalized Hubbard model [5,6] containing nearest (t) and next-nearest neighbor (t') hoppings, correlated-hopping interactions between first (Δt) and second (Δt_3) neighbors, along with on-site (U) and nearest-neighbor (V) Coulomb interactions [5]. If we consider a small distortion of the right angles in the square lattice, the second-neighbor interactions change and their new values 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. Applying the BCS formalism [8] to our model, we obtain the following two coupled integral equations [5,6], which determine the superconducting gap (Δ_α) and the chemical potential (μ_α) for a given temperature (T) and electronic density (n),

$$1 = \frac{(4\Lambda_\alpha - V)}{N_s} \sum_{\mathbf{k}} \frac{g_\alpha(k_x)[g_\alpha(k_x) + \eta_\alpha g_\alpha(k_y)]}{E_\alpha(\mathbf{k})} \tanh\left(\frac{E_\alpha(\mathbf{k})}{2k_B T}\right), \tag{1}$$

$$n - 1 = -\frac{1}{N_s} \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k}) - \mu_\alpha}{E_\alpha(\mathbf{k})} \tanh\left(\frac{E_\alpha(\mathbf{k})}{2k_B T}\right), \tag{2}$$

where $\alpha = p$ or d, N_s is the number of sites, $\varepsilon(\mathbf{k})$ is the mean-field dispersion relation given by

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$$\varepsilon(\mathbf{k}) = (U/2 + 4V)n + 2(t + n\Delta t)[\cos(k_x a + \cos(k_y a)] + 2(t'_+ + 2n\Delta t_3^+)\cos(k_x a + k_y a) + 2(t'_- + 2n\Delta t_3^-)\cos(k_x a - k_y a), \quad (3)$$

and the single-particle excitation energy

$$E_\alpha(\mathbf{k}) = \sqrt{[\varepsilon(\mathbf{k}) - \mu_\alpha]^2 + \Delta_\alpha^2(\mathbf{k})}. \quad (4)$$

For the p-channel case, $\Lambda_p = \delta_3$, $\Delta_p(\mathbf{k}) = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$, $\eta_p = \pm 1$, and $g_p(\mathbf{k}) = \sin(ka)$; whereas for the d-channel $\Lambda_d = \Delta t_3$, $\Delta_d(\mathbf{k}) = \Delta_d[\cos(k_x a) - \cos(k_y a)]$, $\eta_d = -1$, and $g_d(k) = \cos(ka)$.

The main difficulty to solve Eqs. (1) and (2) comes from their integrands, which are governed by the behavior of $1/E_\alpha(\mathbf{k})$ shown in Fig. 1 for $U = V = \delta = 0$, $t' = -0.6|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.15|t|$, $\delta_3 = 0.11|t|$, $n = 0.8$, $\Delta_\alpha = 0.00154|t|$, and $\mu_\alpha = 0.147|t|$. Using this set of parameters, the plots for $\alpha = p$ and $\alpha = d$ are visually indistinguishable, hence in Fig. 1 only the first case is presented. Observe that the sharp peaks located at the Fermi surface defined by $\varepsilon(\mathbf{k}) = \mu_\alpha$ are two orders of magnitude larger than the corresponding values in the rest of the first Brillouin zone. Then, the superconducting ground-state properties are mainly determined by the Fermi surface. This fact seems to be in accordance to the BCS theory [8]. Also, it can be proved that the integrands in Eqs. (1) and (2) do never diverge.

On the other hand, the energy of the superconducting ground state (W_α) per site at $T = 0$ can be written as [9]

$$W_\alpha = \frac{1}{N_s}\sum_{\mathbf{k}}[\varepsilon(\mathbf{k}) - E_\alpha(\mathbf{k})] + \frac{\Delta_\alpha^2}{4\Lambda_\alpha - V} + (n-1)\mu_\alpha - \left(\frac{U}{4} + 2V\right)n^2. \quad (5)$$

The phase diagram, shown in Fig. 2, between p- and d-wave superconducting ground states has been obtained

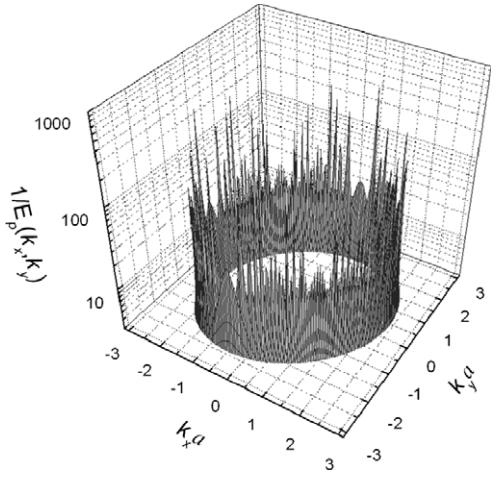

Fig. 1. Integrand $1/E_\alpha(\mathbf{k})$ plotted over the first Brillouin zone for $U = V = \delta = 0$, $t' = -0.6|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.15|t|$, $n = 0.8$, $\Delta_p = 0.00154|t|$, $\mu_p = 0.147|t|$, and lattice parameter a.

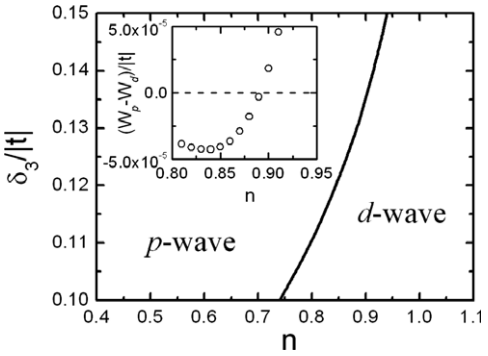

Fig. 2. Superconducting ground-state phase diagram in the space of electron density (n) and δ_3 for $U = V = \delta = 0$, $t' = -0.6|t|$, $\Delta t = 0.5|t|$, and $\Delta t_3 = 0.15|t|$. Inset: Difference of ground state energies ($W_p - W_d$) versus n for the same parameters and $\delta_3 = 0.13|t|$.

by comparing W_p and W_d, as illustrated in the inset of Fig. 2 for $U = V = \delta = 0$, $t' = -0.6|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.15|t|$ and $\delta_3 = 0.13|t|$. Notice that the p- and d-channel superconductivities are, respectively, enhanced in the low and high electron density regions. This fact is in agreement with the hole nature of carriers observed in cuprate superconductors [1]. Moreover, for a given n, the p-wave superconductivity is enhanced by δ_3 and at the same time the d-channel is being suppressed, since the anisotropy between $\hat{x} + \hat{y}$ and $\hat{x} - \hat{y}$ grows.

In summary, we have presented a generalized Hubbard model which allows studying p- and d-wave superconductivities within the same framework. The application of the BCS formalism to this kind of correlated electron models leads to the coupled Eqs. (1) and (2), whose integrals can be efficiently calculated by isolating the region around the Fermi surface. Finally, the superconducting ground-state phase diagram suggests that the number of nodes in the single-particle wavefunction could be relevant in the determination of pairing symmetry, i.e., electron- and hole-like wavefunctions could favour p- and d-wave superconductivities, respectively.

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