First-Brillouin-zone integration areas for anisotropic superconducting states

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First-Brillouin-zone integration areas for anisotropic superconducting states

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Abstract. In order to study the anisotropic superconductivity in two dimensional lattices, it has been recently proposed a generalized Hubbard model based on first- and second-neighbour correlated-hopping interactions. After considering this Hamiltonian within the BCS formalism, we obtain a system of two coupled integral equations, whose solution gives the superconducting gap and the chemical potential for each temperature and electronic density. This system of equations is usually solved in a numerical way, but the involved integrals over the first Brillouin zone (1BZ) consume a large amount of computing time since the integrand functions are extremely sharp around the Fermi surface (FS) especially for small pairing interactions. In this work, we report a new efficient way to carry out these integrals by dividing the 1BZ in regions delimited by curves close to the FS.

1. Introduction

The observation of $d$-wave symmetry gaps in cuprate superconductors \cite{1} and $p$-wave spin-triplet superconducting states in Sr$_2$RuO$_4$ \cite{2} has motivated the study of correlated electron systems that lead to anisotropic superconductivity. The two-dimensional behavior, present in these systems, is essential to understand their peculiar superconducting properties. Single-band second-neighbor Hubbard models on square lattices have been proposed to describe the dynamics of carriers on the CuO$_2$ \cite{3} and RuO$_2$ \cite{4} planes in La$_{2-x}$Sr$_x$CuO$_4$ and Sr$_2$RuO$_4$, respectively. Lately, we have found that the second-neighbor correlated-hopping interaction ($\Delta t_3$) is crucial for the $d_{x^2-y^2}$ wave superconductivity \cite{5} and a further small distortion of the right angles in the square lattice leads to $p$-wave superconductivity \cite{6}. It is worth mentioning that this distortion has been observed on the surface of Sr$_2$RuO$_4$ \cite{7}.

A generalized single-band Hubbard model \cite{5,6} containing first ($t$) and second ($t'$) neighbor hoppings, correlated-hopping interactions between first ($\Delta t$) and second ($\Delta t_3$) neighbors, along with on-site ($U$) and nearest-neighbor ($V$) Coulomb interactions, can be written in real and reciprocal spaces, related through a Fourier transform of the creation operators $c_{k,\sigma}^+ = \frac{1}{N_x} \sum_j \exp(ik \cdot R_j) c_{j,\sigma}^+$, as shown in Table 1.
Table 1. Generalized Hubbard Hamiltonian in the real and reciprocal spaces.

<table>
<thead>
<tr>
<th>Real space</th>
<th>Reciprocal space</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ H = t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} + t' \sum_{\langle\langle i,j \rangle\rangle} c_{i\sigma}^\dagger c_{j\sigma} + \frac{v}{2} \sum_{\langle i,j \rangle} n_i n_j + \Delta t \sum_{\langle\langle i,j \rangle\rangle} c_{i\sigma} c_{j\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t s \sum_{\langle\langle i,j \rangle\rangle} c_{i\sigma} c_{j\sigma} n_i ]</td>
<td>[ H = \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle\langle i,j \rangle\rangle} c_{i\sigma} c_{j\sigma} n_i + \sum_{k\alpha} [c(k) - \mu] c_{k\sigma}^\dagger c_{k\alpha} + \frac{1}{N_k} \sum_{k\alpha} V_{kk'} c_{k\sigma}^\dagger c_{k\alpha} c_{k'\sigma} + \frac{1}{N_k} \sum_{k\alpha} W_{kk'} c_{k\alpha}^\dagger c_{k'\sigma} c_{k'\sigma} c_{k\alpha}^\dagger</td>
</tr>
</tbody>
</table>

In Table 1, \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is the creation (annihilation) operator with spin \( \sigma = \downarrow \) or \( \uparrow \) at site \( i \), \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), \( <i,j> \) and \( <<i,j>> \) respectively denote nearest- and next-nearest-neighbor sites. \( V_{kk'} \) and \( W_{kk'} \) are functions of the real-space Hamiltonian parameters as given in Reference [8]. Applying the BCS formalism [9] to the reciprocal-space Hamiltonian of Table 1, we obtain the following two coupled integral equations [8], which determine the superconducting gap \( \Delta_\alpha \) of symmetry \( \alpha = p \) or \( d \) and the chemical potential \( \mu_\alpha \) for a given temperature \( T \) and electron density \( n \).

\[
\begin{align*}
1 = \frac{1}{4\pi^2} \int_{\text{BZ}} \left[ g_a(k,\varepsilon(k)) \right]^2 \frac{E_a(k)}{2k_B^2} \tanh \left( \frac{E_a(k)}{2k_B T} \right) dk_x dk_y & \quad (2) \\
n - 1 = \frac{a^2}{4\pi^2} \int_{\text{BZ}} \frac{\varepsilon(k) - \mu_\alpha}{E_a(k)} \tanh \left( \frac{E_a(k)}{2k_B T} \right) dk_x dk_y & \quad (3)
\end{align*}
\]

where \( \varepsilon(k) = E_{MF} + 2t_{MF} \cos(k_x a) + 2t'_{MF} \cos(k_y a) + 2t_{MF} \cos(k_x a) + 2t_{MF} \cos(k_x a) + 2t_{MF} \cos(k_y a) \) is the mean-field dispersion relation, \( 1BZ \) stands for the square-lattice first Brillouin zone defined as \( \left[ -\frac{a}{2}, \frac{a}{2} \right] \times \left[ -\frac{a}{2}, \frac{a}{2} \right] \) with the lattice parameter \( a \), \( E_a(k) = \sqrt{[\varepsilon(k) - \mu_\alpha]^2 + \Delta^2(k)} \) is the quasiparticle energy with \( E_{MF} = \frac{U}{2} + 4V \), \( n \), \( t_{MF} \) and \( t'_{MF} \) are the mean-field parameters, being \( t' \equiv t' + \delta t' \) and \( \Delta t \equiv \Delta t \pm \delta t \). The pairing interaction parameters and symmetry functions for \( d- \) and \( p- \) wave superconducting states are shown in Table 2.

Table 2. Parameters for \( d- \) and \( p- \) wave symmetry superconducting states

<table>
<thead>
<tr>
<th>d-wave</th>
<th>p-wave</th>
<th>Spin state of pairs</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta_d = \Delta t_3 )</td>
<td>( \Delta_p = \delta_3 )</td>
<td>Singlet: ( \frac{1}{\sqrt{2}}(</td>
</tr>
<tr>
<td>( g_d(k_x, k_y) = \cos(k_x a) - \cos(k_y a) )</td>
<td>( g_p(k_x, k_y) = \sin(k_x a) \pm \sin(k_y a) )</td>
<td>Triplet: ( \left{ \begin{array}{c}</td>
</tr>
</tbody>
</table>

The Fermi surface (FS) is given by \( \varepsilon(k) = \mu \), which is an ellipse for \( k_x, k_y \ll \frac{a}{2} \). The main difficult to solve Equations (2) and (3) comes from their integrands, which are governed by the behavior of \( 1/E(k) \) and \( \tanh[E(k)/2k_B T] \). For example, the calculation of the superconducting critical temperature \( T_c \), defined by \( \Delta_d(T_c) = 0 \), implies that \( E(k)=0 \) on the FS. In consequence, sharp peaks appear in the integrand function along FS but they do not diverge since \( \tanh(x) = x - \frac{x^3}{3} + \frac{2x^5}{15} - \ldots \). On the other hand, for \( T=0 \), \( \tanh[E(k)/2k_B T] = 1 \) and sharp peaks appear along the FS when \( \Delta_\alpha \ll t \). In general, it can be proved that the integrand functions are well defined for all \( k \)-states and do never diverge, even for \( T=0 \). In this work, we present a method to solve the mentioned coupled integral equations when sharp peaks are present in the integrand functions.

2. Multi-region integration method

Let us consider two particular cases, whose Hamiltonian parameters are summarized in Table 3. For the \( d- \) wave case, as occurred in \( \text{La}_2\text{Sr}_x\text{CuO}_4 \), the resulting \( T_c \) is 41K. But the \( p- \) wave superconducting state generally has a lower \( T_c \) such as in this case 1.5K observed in strontium ruthenate [2].
Table 3. Hamiltonian parameters for p- and d-wave superconductors

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Hamiltonian parameters</th>
<th>Related superconductor</th>
</tr>
</thead>
<tbody>
<tr>
<td>d-wave</td>
<td>$U = V = \delta' = \delta_3 = 0$</td>
<td>$t'/t = -0.06, \Delta t = 0.1</td>
</tr>
<tr>
<td></td>
<td>$n = 0.85$ and $\mu = -0.62</td>
<td>t</td>
</tr>
<tr>
<td>p-wave</td>
<td>$U = V = \delta' = \Delta t = \Delta t_3 = 0$</td>
<td>$t'/t = 0.4, \delta_3 = 0.13</td>
</tr>
<tr>
<td></td>
<td>$n = 1.1$ and $\mu = 1.07</td>
<td>t</td>
</tr>
</tbody>
</table>

In Figures 1 and 2 the integrand functions in a half of 1BZ are respectively shown in color scale for d- and p-wave cases. The numerical integrations of Equations (2) and (3) were performed using a variable-step Simpson’s subroutine. These integrations can be efficiently done through an eighth and fourth part of the 1BZ for d- and p-wave cases, by dividing them into six and seven regions, as shown in Figures 1 and 2, respectively.

**Figure 1** (Color online) The integrand function in color scale over half of 1BZ for the d-wave case. Orange and yellow lines indicate two contour lines obtained with $\varepsilon_1 = 1.1\mu$ and $\varepsilon_2 = 0.9\mu$ around the Fermi surface, respectively. Six integration regions in an eighth part of the 1BZ are illustrated in the Figure.

**Figure 2** (Color online) The integrand function in color scale over half of 1BZ for the p-wave case. Orange and yellow lines indicate two contour lines obtained with $\varepsilon_1 = 1.25\mu$ and $\varepsilon_2 = 0.85\mu$ around the Fermi surface, respectively. Seven integration regions in a fourth part of the 1BZ are illustrated in the Figure.

In Figure 3(a), the computing time to calculate the $T_c$ of p-wave superconducting states is shown as a function of the interaction strength ($\delta_3$) by integrating over the divided (open circles) and non-divided (open squares) 1BZ. The corresponding calculated $T_c$ in Kelvins is illustrated in Figure 3(b), considering that $t = 1$eV. The numerical calculations were performed with an integrating precision of $10^{-6}$ by using a Xeon E5-2670 with 32GB of RAM. Observe that for $\delta_3 = 0.15|t|$, leading to a $T_c < 8$K, the computing time via the non-divided 1BZ method is almost infinite.

**Figure 3** (Color online) (a) Computing time in seconds consumed to integrate Equation (2) using the divided (red open circles) and non-divided (blue open squares) 1BZ as a function of the pairing interaction strength ($\delta_3$). (b) The resulting $T_c$ versus $\delta_3$ for p-wave superconductivity obtained using the multi-region integration method.
3. Conclusions

In solid state physics, the study of superconductivity within the BCS formalism leads to two coupled integral equations whose integrands have a sharp behavior around the Fermi surface. By using the standard variable-step Simpson’s method it is almost impossible to address very low critical temperature ($T_c$) superconductivity with $p$-wave symmetry, such as Sr$_2$RuO$_4$ with $T_c=1.5$K. The multi-region integration method allows to solve these equations even for $T_c=0.05$K. It is worth mentioning that the particular 1BZ division presented in this work could be improved, which is currently in process.

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References