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 [1] and $p$-wave spin-triplet superconducting states in Sr$_2$RuO$_4$ [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$_2$ [3] and RuO$_2$ [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 ($\Delta t'$) is crucial for 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 this distortion has been observed on the surface of Sr$_2$RuO$_4$ [7].

A generalized single-band Hubbard model [5,6] containing first ($t$) and second ($t'$) neighbor hoppings, correlated-hopping interactions between first ($\Delta t$) and second ($\Delta t'$) 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 $c_{k,\sigma}^{\dagger} = \frac{1}{N} \sum_{\alpha} \exp(i \mathbf{k} \cdot \mathbf{R}_\alpha) c_{\alpha,\sigma}^{\dagger}$, as shown in Table 1.
Table 1. Generalized Hubbard Hamiltonian in the real and reciprocal spaces.

| Real space | Reciprocal space |
|------------|----------------|
| \( H = t \sum_{(i,j),\sigma} c_{i\sigma}^+ c_{j\sigma} + t' \sum_{(i,j),\sigma} c_{i\sigma}^+ c_{j\sigma} \) | \( H = \sum_{\mathbf{k},\sigma}[\varepsilon(\mathbf{k}) - \mu] c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N_0} \sum_{\mathbf{k},\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \) |
| \( U \sum_{(i,j)} n_{i\upsilon} n_{j\downarrow} \) | \( \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) \) |
| \( \Delta t_3 \sum_{(i,j),\sigma} c_{i\sigma}^+ c_{j\sigma} n_{i\sigma} \) | \( \frac{1}{N_0} \sum_{\mathbf{k},\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} c_{\mathbf{k}'} c_{\mathbf{k}\sigma} \) |

In Table 1, \( c_{i\sigma}^+ \) (\( c_{i\sigma} \)) is the creation (annihilation) operator with spin \( \sigma = \downarrow \) or \( \uparrow \) at site \( i \), \( n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \), \( <i,j> \) and \( <<i,j>> \) respectively denote nearest- and next-nearest-neighbor sites. \( V_{\mathbf{k},\mathbf{k}'} \) and \( W_{\mathbf{k},\mathbf{k}'} \) 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 \( n \).

\[
\begin{align*}
1 \& = -\left(\frac{V - 4\Delta_\alpha a^2}{4\pi^2}\right) \int \frac{[g_{\alpha}(\mathbf{k},a)]^2}{2E_{\alpha}(\mathbf{k})} \tanh \left( \frac{E_{\alpha}(\mathbf{k})}{2k_B T} \right) dk_x dk_y \\
n \& = -\left(\frac{a^2}{4\pi^2}\right) \int \frac{\varepsilon(\mathbf{k}) - \mu_\alpha}{E_{\alpha}(\mathbf{k})} \tanh \left( \frac{E_{\alpha}(\mathbf{k})}{2k_B T} \right) dk_x dk_y
\end{align*}
\]

where \( \varepsilon(\mathbf{k}) = E_{MF} + 2t_{MF} \cos(k_x a) + 2t'_{MF} \cos(k_y a) + 2t''_{MF} \cos(k_x a) + 2t'''_{MF} \cos(k_y a) \) is the mean-field dispersion relation, \( 1\mathbb{BZ} \) stands for the square-lattice first Brillouin zone defined as \( [-\pi/a,\pi/a] \otimes [-\pi/a,\pi/a] \) with the lattice parameter \( a \), \( E_{\alpha}(\mathbf{k}) = \sqrt{[\varepsilon(\mathbf{k}) - \mu_\alpha]^2 + \Delta_\alpha^2(\mathbf{k})} \) is the quasiparticle energy with \( E_{MF} = \left(\frac{U}{2} + 4V\right) n \), \( t_{MF} = t + n\Delta t_3 \) and \( t'^{\pm}_{MF} = t'^{+} \pm 2n\Delta t_3^{\pm} \), being \( t'^{+} = t' + \delta' \) and \( \Delta t_3^{\pm} = \Delta t_3 \pm \delta_3 \). 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

| \( d \)-wave | \( p \)-wave | Spin state of pairs |
|------------|------------|------------------|
| \( \Delta_d = \Delta t_3 \) | \( \Delta_p = \delta_3 \) | Singlet: \( \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \) |
| \( g_d(k_x, k_y) = \cos(k_x a) - \cos(k_y a) \) | \( g_p(k_x, k_y) = \sin(k_x a) \pm \sin(k_y a) \) | Triplet: \( \begin{cases} |\uparrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{cases} \) |

The Fermi surface (FS) is given by \( \varepsilon(\mathbf{k}) = \mu \), which is an ellipse for \( k_x, k_y \ll \frac{\pi}{a} \). The main difficult to solve Equations (2) and (3) comes from their integrands, which are governed by the behavior of \( 1/E(\mathbf{k}) \) and \( \tanh[E(\mathbf{k})/2k_B T] \). For example, the calculation of the superconducting critical temperature \( T_c \), defined by \( \Delta_d(T_c) = 0 \), implies that \( E(\mathbf{k}) = 0 \) on the FS. In consequence, sharp peaks appear in the integrand function along FS but they do not diverge since \( \tanh(x) = x - \frac{x^3}{3} + \frac{2x^5}{15} - \cdots \). On the other hand, for \( T = 0 \), \( \tanh[E(\mathbf{k})/2k_B T] = 1 \) and sharp peaks appear along the FS when \( \Delta_d \ll t \). 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

| Symmetry | Hamiltonian parameters | Related superconductor |
|----------|------------------------|------------------------|
| \( d \)-wave | \( U = V = \delta' = \delta_3 = 0 \) | \( t'/t = -0.06, \Delta t = 0.1|t|, \Delta t_3 = 0.055|t| \) | \( n = 0.85 \) and \( \mu = -0.62|t| \) | \( \text{La}_2\text{Sr}_2\text{CuO}_4 \) |
| \( p \)-wave | \( U = V = \delta' = \Delta t = \Delta t_3 = 0 \) | \( t'/t = 0.4, \delta_3 = 0.13|t| \) | \( n = 1.1 \) and \( \mu = 1.07|t| \) | \( \text{Sr}_2\text{RuO}_4 \) |

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](image1) (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 \( \varepsilon(k) = 1.1\mu \) and \( \varepsilon(k) = 0.9\mu \) around the Fermi surface, respectively. Six integration regions in an eighth part of the 1BZ are illustrated in the Figure.

![Figure 2](image2) (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 \( \varepsilon(k) = 1.25\mu \) and \( \varepsilon(k) = 0.85\mu \) 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 \( t = 1\text{eV} \). 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 \( T_c < 8\text{K} \), the computing time via the non-divided 1BZ method is almost infinite.

![Figure 3](image3) (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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