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2014 J. Phys.: Conf. Ser. 490 012221

(http://iopscience.iop.org/1742-6596/490/1/012221)

Journal of Physics: Conference Series **490** (2014) 012221 doi:10.1088/1742-6596/490/1/012221

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_2RuO_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 $La_{2-x}Sr_xCuO_4$ and Sr_2RuO_4, respectively. Lately, we have found that the second-neighbor correlated-hopping interaction (Δt_3) 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_2RuO_4 [7].

A generalized single-band Hubbard model [5,6] containing first (t) and second (t') neighbor hoppings, correlated-hopping interactions between first (Δt) and second (Δt_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 $c^{\dagger}_{\mathbf{k},\sigma} = \frac{1}{N_s}\sum_j \exp(i\mathbf{k}\cdot\mathbf{R}_j)c^{\dagger}_{j,\sigma}$, as shown in Table 1.

Table 1. Generalized Hubbard Hamiltonian in the real and reciprocal spaces.

Real space	Reciprocal space
$H = t\sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^{\dagger}c_{j,\sigma} + t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} c_{i,\sigma}^{\dagger}c_{j,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow} + \frac{V}{2}\sum_{\langle i,j\rangle} n_i n_j + \Delta t\sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^{\dagger}c_{j,\sigma}(n_{i,-\sigma}+n_{j,-\sigma}) + \Delta t_3\sum_{\langle\langle i,j\rangle\rangle,\sigma,\langle i,l\rangle\langle j,l\rangle} c_{i,\sigma}^{\dagger}c_{j,\sigma}n_l$	$H = \sum_{\boldsymbol{k},\sigma}[\varepsilon(\boldsymbol{k})-\mu]\, c_{\boldsymbol{k},\sigma}^{\dagger}c_{\boldsymbol{k},\sigma} + \frac{1}{N_S}\sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'}\, c_{\boldsymbol{k},\uparrow}^{\dagger}c_{-\boldsymbol{k}',\downarrow}^{\dagger}c_{-\boldsymbol{k}',\downarrow}c_{\boldsymbol{k},\uparrow} + \frac{1}{N_S}\sum_{\boldsymbol{k},\boldsymbol{k}',\sigma'} W_{\boldsymbol{k}\boldsymbol{k}'}\, c_{\boldsymbol{k},\sigma}^{\dagger}c_{-\boldsymbol{k}',\sigma}^{\dagger}c_{-\boldsymbol{k}',\sigma}c_{\boldsymbol{k},\sigma}$

In Table 1, $c_{i,\sigma}^{\dagger}(c_{i,\sigma})$ is the creation (annihilation) operator with spin $\sigma=\downarrow$ or $\uparrow$ at site i, $n_{i,\sigma}=c_{i,\sigma}^{\dagger}c_{i,\sigma}$, $n_i=n_{i,\downarrow}+n_{i,\downarrow}$, <i,j> and <<i,j>> respectively denote nearest- and next-nearest-neighbor sites. $V_{\boldsymbol{k}\boldsymbol{k}'}$ and $W_{\boldsymbol{k}\boldsymbol{k}'}$ 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 (Δ_α) of symmetry $\alpha=p$ or d and the chemical potential (μ_α) for a given temperature (T) and electron density (n).

$$\begin{cases} 1 = -\dfrac{(V-4\Lambda_\alpha)a^2}{4\pi^2}\iint\limits_{1BZ}\dfrac{[g_\alpha(k_x,k_y)]^2}{2E_\alpha(\boldsymbol{k})}\tanh\left(\dfrac{E_\alpha(\boldsymbol{k})}{2k_BT}\right)dk_xdk_y & (2) \\ n-1 = -\dfrac{a^2}{4\pi^2}\iint\limits_{1BZ}\dfrac{\varepsilon(\boldsymbol{k})-\mu_\alpha}{E_\alpha(\boldsymbol{k})}\tanh\left(\dfrac{E_\alpha(\boldsymbol{k})}{2k_BT}\right)dk_xdk_y & (3) \end{cases}$$

where $\varepsilon(\boldsymbol{k}) = E_{MF} + 2t_{MF}[cos(k_xa)+cos(k_ya)] + 2t'_{MF+}cos(k_xa+k_ya) + 2t'_{MF-}cos(k_xa-k_ya)$ is the mean-field dispersion relation, 1BZ stands for the square-lattice first Brillouin zone defined as $\left[-\frac{\pi}{a},\frac{\pi}{a}\right]\otimes\left[-\frac{\pi}{a},\frac{\pi}{a}\right]$ with the lattice parameter a, $E_\alpha(\mathbf{k})=\sqrt{[\varepsilon(\mathbf{k})-\mu_a]^2+\Delta_\alpha^2(\mathbf{k})}$ is the quasiparticle energy with $E_{MF}=\left(\frac{U}{2}+4V\right)n$, $t_{MF}=t+n\Delta t$ and $t'_{MF\pm}=t'_{\pm}+2n\Delta t_3{}^{\pm}$, being $t'_{\pm}=t'\pm\delta'$ 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**
$\Lambda_d=\Delta t_3$	$\Lambda_p=\delta_3$	Singlet: $\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle-\lvert\downarrow\uparrow\rangle)$
$g_d(k_x,k_y)=\cos(k_xa)-\cos(k_ya)$	$g_p(k_x,k_y)=\sin(k_xa)\pm\sin(k_ya)$	Triplet: $\begin{cases}\lvert\uparrow\uparrow\rangle\\ \lvert\downarrow\downarrow\rangle\\ \frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle+\lvert\downarrow\uparrow\rangle)\end{cases}$

The Fermi surface (FS) is given by $\varepsilon(\boldsymbol{k})=\mu$, 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 $\tanh[E(\mathbf{k})/2k_BT]$. For example, the calculation of the superconducting critical temperature (T_c), defined by $\Delta_\alpha(T_c)=0$, 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 $T=0$, $\tanh[E(\mathbf{k})/2k_BT]=1$ 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 $\boldsymbol{k}$-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 $La_{2-x}Sr_xCuO_4$, 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 $\mu = -0.62\|t\|$	$La_{2-x}Sr_xCuO_4$
p-wave	$U = V = \delta' = \Delta t = \Delta t_3 = 0$ $t'/t = 0.4,\ \delta_3 = 0.13\|t\|$ $n = 1.1$ and $\mu = 1.07\|t\|$	Sr_2RuO_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.

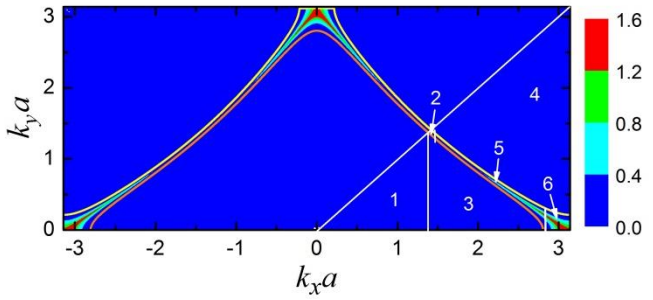

Figure 1 (Color online) The integrand function in color scale over half of 1BZ for the *d*-wave case. Orange and yellow lines indicate two contour lines obtained with $\varepsilon(\boldsymbol{k}) = 1.1\mu$ and $\varepsilon(\boldsymbol{k}) = 0.9\mu$ around the Fermi surface, respectively. Six integration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

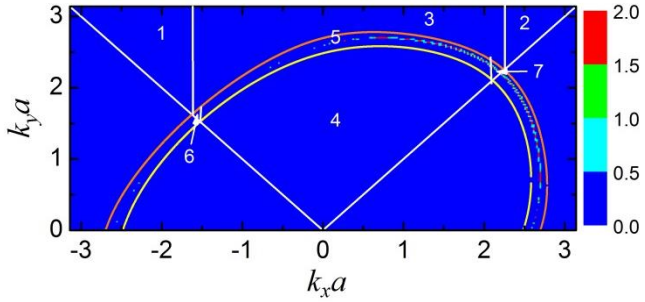

Figure 2 (Color online) The integrand function in color scale over half of 1BZ for the *p*-wave case. Orange and yellow lines indicate two contour lines obtained with $\varepsilon(\boldsymbol{k}) = 1.25\mu$ and $\varepsilon(\boldsymbol{k}) = 0.85\mu$ around the Fermi surface, respectively. Seven integration 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 (δ_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.

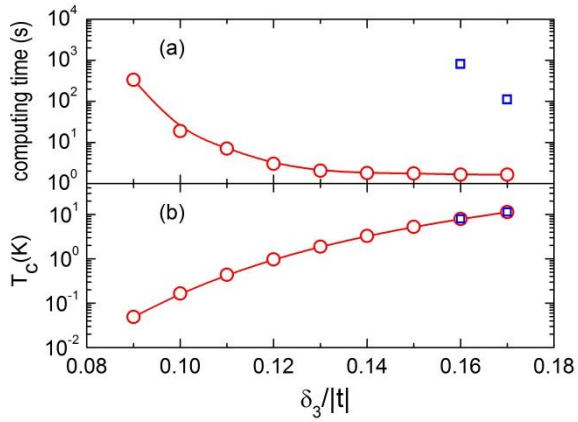

Figure 3 (Color online) (a) Computing time in seconds consumed to integrate Equation (2) using the divided (red open circles) and non-divided (blue open squares) 1BZ as a function of the pairing interaction strength (δ_3). (b) The resulting T_c versus δ_3 for *p*-wave superconductivity obtained using 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_2RuO_4 with T_c=1.5K. The multi-region integration method allows to solve these equations even for T_c=0.05K. It is worth mentioning that the particular 1BZ division presented in this work could be improved, which is currently in process.

Acknowledgment

This work has been partially supported by CONACyT-103219, CONACyT-131596, UNAM-IN102511, UNAM-IN107411, and the UNAM-UNACAR exchange project. Computations have been performed at KanBalam and NES of DGCTIC, UNAM.

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