Gap symmetries from the neighbor coupling in square-lattice superconductors

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(Dated: November 17, 2009)

The gap symmetries of superconductivity are studied in this work. It is found that the gap symmetries are simply determined by the 4-fold rotational symmetries of the coupling potential on neighbor sites. A local on-site coupling potential results in the on-site pairing with the conventional s-wave symmetry, but a coupling potential between the nearest neighbors or the next-nearest neighbors results in the pairing on neighbor sites with the s\(^{-}\), d\(_{x^2−y^2}\), d\(_{xy}\), or s\(_{x^2−y^2}\) gap symmetries. It is proved that both isotropic and anisotropic gap functions are allowed by the 4-fold rotational symmetries of the coupling potential. Finally a numerical computation is performed to demonstrate the gap symmetries. This neighbor coupling provides a unified picture for the gap functions of the conventional and the high Tc superconductivity.

PACS numbers: 74.20.-z

I. INTRODUCTION

A few decades of study on high-Tc superconductors confirmed the d-wave symmetry of the gap function at least in cuprate superconductors, relative to the conventional s-wave BCS gap symmetry\(^{1, 2}\). The observation of the half quantum of magnetic flux provides a direct detection to the d-wave gap symmetry in cuprates\(^{2}\). The concept of d-wave order, however, is quite misleading to the physics of superconductivity. In general, it is inferred from the antisymmetry requirement of the wave function of a Cooper pair. Since electrons are fermions the wave function of a pair of electrons must be antisymmetric under their exchange. When the spin part of the wave function is antisymmetric the real space part should be symmetric. Then it was thought that the angular momentum of a Cooper pair can only be even, i.e., \(L = 0, 2, 4, \ldots\). These quantum numbers led to the description of \(s, d, g\) wave order parameters. This picture is a good approximation for electrons on a atom, where the rotational isotropy of space allows the angular momentum to be a good quantum number. When the coupling potential between electrons is attractive on one atom it can be indeed expected to observe these gap symmetries. Nevertheless, for high-Tc superconductors, the coupling is no longer on-site attractive, but is attractive only on neighbor sites. In this case the space isotropy is broken by the crystal lattice and only the point group symmetries remain. Therefore, the concept of d-wave symmetry is not valid for high Tc superconductors\(^{3}\), which in fact should contain all components of \(L = 0, 2, 4, \ldots\). Another argument comes from the newly discovered iron-based superconductors, which have a gap symmetry \(\sim \cos k_x \cos k_y \)\(^{4, 5}\). This symmetry cannot be explained by the above s, d, g-wave interpretation. It is called an extended s-wave. Some researchers such as Yao et al claimed a \(d_{xy}\) gap symmetry on one hand and at the same work they have to admit a sign change for the gap on \(\Gamma\) and \(M\)\(^{6}\) in the Brillouin zone. It is seen that the s- or d-wave description becomes very controversial for the gap symmetries in iron-based superconductors.

In this paper I argue that the gap symmetries of square lattice superconductors in fact originate from the 4-fold rotational symmetries of the coupling potential on neighbor sites. It has nothing to do with the angular momentum. I present a theoretical analysis and a computational demonstration for this argument. It is shown that the attraction between the nearest neighbors (n.n.) or the next nearest neighbors (n.n.n.) provides a coupling for Cooper pairs, so that the gap functions of Cooper pairs take the symmetries of the coupling potential between neighbors. It is interesting to notice that most gap symmetries of square lattice superconductors can be reproduced in this mechanism.

II. GAP SYMMETRIES

The BCS coupling Hamiltonian is written as

\[
H_{BCS} = -V \sum_{kk'} c_{k \uparrow}^\dagger c_{-k \downarrow} c_{-k' \downarrow}^\dagger c_{k' \uparrow} \tag{1}
\]

Change it into the site configuration then one finds

\[
H_{BCS} = -V \sum_{ij} c_{i \uparrow}^\dagger c_{j \downarrow}^\dagger c_{j \uparrow} c_{i \downarrow} \tag{2}
\]

It comes from an on-site coupling, \(V(r_1, r_2) = V \delta(r_1 - r_2)\)\(^6\). This coupling indicates that in fact a Cooper pairing can only occur on the same site. The electrons in cuprate superconductors, however, have strong on-site repulsion due to the strong correlation as seen in the Hubbard model. One usually rules out the double occupancy through the method of Gutzwiller projection\(^{10}\).

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Because of this strong correlation effect the conventional BCS on-site pairing is certainly not energetically preferential in the cuprate superconductors. Hence, the interaction Hamiltonian has to be changed to the coupling between neighbor sites as follows

$$H_{int} = \frac{1}{N} \sum_{ijm} V_m c_{i+m \uparrow} c_{j \downarrow} c_{j+m \uparrow}$$  \hspace{1cm} (3)

where $V_m$ is the coupling potential between two electrons (or holes) on two neighbor sites, here $m$ denote the neighbors of a fixed site. In general, only the potential values on the near neighbors, such as $V_0, V_1, V_2$, are important. In the mean field approximation the above Hamiltonian becomes

$$H_{int} = -\sum_k \left( \Delta_k c_{-k \uparrow} c_{k \downarrow} + \Delta_k^{\dagger} c_{-k \downarrow} c_{k \uparrow} \right) + E_0$$  \hspace{1cm} (4)

where $\Delta_k$ is the gap function giving by

$$\Delta_k = -\frac{1}{N} \sum_m V_m \Delta_m e^{-ik \cdot R_m}$$  \hspace{1cm} (5)

$$E_0 = -\frac{1}{N} \sum_m V_m |\Delta_m|^2$$ \hspace{1cm} (6)

with $\Delta_m = <\sum_i c_{i \uparrow} c_{i+m \downarrow}>$.

An important feature is that the range of the coupling potential gives the symmetries of the gap function, as listed in the Table I.

| $m$ | condition | $\Delta_k$ | symmetry |
|-----|-----------|------------|----------|
| n.n. | (1) | $\sim (\cos k_x + \cos k_y)$ | $s^-$ |
| n.n. | (2) | $\sim (\cos k_x - \cos k_y)$ | $d_{x^2-y^2}$ |
| n.n.n. | (1) | $\sim \cos k_x \cos k_y$ | $s_{x^2+y^2}$ |
| n.n.n. | (2) | $\sim \sin k_x \sin k_y$ | $d_{xy}$ |

In Table I n.n. denotes the nearest neighbor sites, $x = (\pm 1, 0), y = (0, \pm 1)$, condition (1) stands for the isotropic case $\Delta_x = \Delta_y$, and (2) for the anisotropic case $\Delta_x = -\Delta_y$. In the case of the next nearest neighbor sites (denoted by n.n.n.), $xy = (\pm 1, \pm 1), x\bar{y} = (\pm 1, \mp 1)$, condition (1) stands for the isotropic case $\Delta_{xy} = \Delta_{\bar{x}y}$, and (2) for the anisotropic case $\Delta_{xy} = -\Delta_{\bar{x}y}$. In the above table the gap symmetry $s_{x^2+y^2}$ has been found recently in the iron-based superconductors. Surprisingly, it is seen from the table that this neighbor coupling gives most symmetries of gap functions that have been found in various superconductors, including conventional and high-Tc superconductors with square lattices.

It should be emphasized that these gap symmetries have nothing to do with angular momenta of the Cooper pairs. They originate from the point group symmetries of the crystals of superconductors. In fact, strictly speaking, the angular momentum $\hat{L}$ of Cooper pairs is not a conserved quantity since the potential does not obey the rotational symmetries of group $R_3[3]$, which is only true for the local atomic orbitals. For the neighbor coupling the point group symmetries are much more significant than the atomic orbital symmetries.

In order to confirm the isotropy and anisotropy of $\Delta_k$ Green’s function is defined as follows,

$$< c_{\uparrow}(t) c_{\downarrow}(0) > c_{\downarrow}(t) c_{\uparrow}(0) > = -i\theta(t) [c_{\uparrow}(t), c_{\downarrow}(0)]$$ \hspace{1cm} (7)

According to the standard method of Green’s function theory one obtains

$$< c_{\uparrow}(t) c_{\uparrow}(-t) > c_{\downarrow}(t) c_{\downarrow}(-t) > = \frac{\Delta_k}{\omega^2 - \xi_k^2}, \xi_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$$ \hspace{1cm} (8)

where $\xi_k$ are the energies of free electrons, $\epsilon_k = -2t(\cos k_x + \cos k_y) + 2t' \cos k_x \cos k_y$. Then the spectrum theorem of Green’s function gives

$$< c_{-k \uparrow} c_{-k \downarrow} > c_{-k \downarrow} c_{-k \uparrow} > = \frac{1}{\pi i} Im < c_{-k \uparrow} c_{-k \downarrow} > = \pi \frac{\tanh(\xi_k/2k_B T)}{2\xi_k} |\Delta_k|$$  \hspace{1cm} (9)

Combining the above equation and (5) one obtains the gap equation

$$\Delta_k = -\sum_q V(k - q) \frac{\tanh(\xi_q/2k_B T)}{2\xi_q} |\Delta_q|$$ \hspace{1cm} (10)

where $V(q)$ are the fourier components given by $V(q) = (1/N) \sum_m V_m e^{-ik \cdot R_m}$. Under the 4-fold rotations, $R$, of the point group symmetries of the potential $U(m)$ this equation transforms in the following way (see Appendix),

$$\Delta_{R_k} = -\sum_q V(k - q) \frac{\tanh(\xi_q/2k_B T)}{2\xi_q} |\Delta_{R_q}|$$ \hspace{1cm} (11)

Compare the above equation with the gap equation (10) one finds that solutions with the following two symmetries exist:

$$\Delta_{R_k} = \pm \Delta_k$$ \hspace{1cm} (12)

Therefore, both conditions (1) and (2) in Table I can be realized, that is, both the isotropic case and the anisotropic one are allowed. It is then confirmed that various gap symmetries listed in Table I are allowed by the neighbor coupling. A real system selects one of the symmetries with the lowest energy, or the largest gap magnitude.

The symmetries revealed in (12) are called respectively conventional and unconventional superconductivity in literatures[11]. In this paper it is proved that both these two symmetries are in fact a conclusion of the 4-fold rotational symmetries of the coupling potential on the square lattice superconductors.

The gap symmetries can be checked by numerical calculations. The gap equation (10) is solved self-consistently through iterations from a guessed initial gap function. It is found that this equation has stable solutions for a wide range of parameters. Two examples are...
shown in Fig. 1 for the $d_{x^2-y^2}$ and the $s_{x^2+y^2}$ gap symmetries. With the same parameters one also finds $s^-$ and $d_{xy}$ gap symmetries from a different guessed initial gap function, but their magnitudes of gap functions are a few orders smaller. That is to say, the two symmetries shown in Fig. 1 are most energetic preferential for the given parameters. Further computations show that different guessed initial gap functions lead to different gap symmetries, but the gap function with the largest magnitude is almost determined by the neighbor coupling with lowest potential value. Thus the earlier theoretical analysis of this paper is further demonstrated by these calculations. It is concluded that the gap symmetries of cuprate superconductivity are in fact due to the neighbor coupling with 4-fold rotational symmetries of crystals of superconductors. The gap symmetries provide information for the coupling range of Cooper pairs. Comparing with the on-site coupling of the conventional $s$-wave BCS superconductivity the Cooper pairs of high-Tc superconductors can distribute on two neighbors, including the n.n. and the n.n.n. neighbors. The size of the Cooper pairs is determined by the minimum of the coupling potential. The neighbor coupling probably provides a unified phenomenological model for the BCS and the high-Tc superconductivity.

III. CONCLUSION

In conclusion, it is found that the gap symmetries are simply determined by the 4-fold rotational symmetries of the coupling potential on neighbor sites. A local on-site coupling potential results in the on-site pairing with the conventional $s$-wave symmetry, but a n.n. or n.n.n. coupling potential results in the pairing on neighbor sites with the $s^-$, $d_{x^2-y^2}$, $s_{x^2+y^2}$ symmetries. It is proved that both isotropic and anisotropic gap functions are allowed by the 4-fold rotational symmetries of the coupling potential. Finally a numerical computation is performed to demonstrate the gap symmetries. The solutions of the gap equation are very stable for a wide range of parameters.

This work was supported by the National Natural Science Foundation of China (Grant No. 10874049), the State Key Program for Basic Research of China (No. 2007CB925204) and the Natural Science Foundation of Guangdong province (No. 07005834).

Appendix

Eq. (11) can be proved in the following way. From (11) one has

$$\Delta_{Rk} = -\frac{1}{N} \sum_{qm} V_m e^{i(q-Rk)\cdot m} \frac{\tanh(\xi_q/2k_BT)}{2\xi_q} \Delta_q$$

$$= -\frac{1}{N} \sum_{qm} V_m e^{i(R^{-1}q-k)\cdot R^{-1}m} \frac{\tanh(\xi_q/2k_BT)}{2\xi_q} \Delta_q$$

$$= -\frac{1}{N} \sum_{qm} V_m e^{i(q-k)\cdot m} \frac{\tanh(\xi_q/2k_BT)}{2\xi_q} \Delta_{Rq}$$

$$= -\sum_{q} V(k-q) \frac{\tanh(\xi_q/2k_BT)}{2\xi_q} \Delta_{Rq}$$

where the symmetry $\xi_{Rq} \approx \xi_q$ has been used since the value of $\xi_q$ depends weakly on $\Delta_q$ and $\epsilon_{Rq} = \epsilon_q$.

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