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SYMMETRY AND NODES OF THE SUPERCONDUCTING GAP

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ABSTRACT - For pairing potentials which act only in the vicinity of the Fermi surface, a Fermi-surface harmonics expansion of the gap function is appropriate. After a general symmetry discussion, it is pointed-out that the first extended s-wave occuring in the Fermi-surface harmonics expansion of the gap function a) is closely related to the usual d-waves b) it can have a large number of nodes. This may reconcile the experiments which see nodes in the gap and neutron-scattering experiments which cannot resolve the anisotropy in the gap function.

I - INTRODUCTION.

There is mounting experimental evidence that the superconducting order parameter of high-temperature superconductors may have nodes on the Fermi surface. In this context, there have been many studies of so-called d-wave order parameters, $d_{x,y}$ and $d_{x^2-y^2}$. It has recently been pointed out that the so-called extended s-wave order parameter $\Delta_s(\hat{\mathbf{k}}) = \Delta_0[\cos(k_x) + \cos(k_y)]$ can also have nodes on the Fermi surface. Indeed, in a tight-binding model which includes second-neighbor hopping, the Fermi surface, when it is open, may cross the diamond-shape lines where $[\cos(k_x) + \cos(k_y)] = 0$ (Fedro *et al.* 1993).

In this paper, we discuss the symmetry classification of possible order parameters, distinguishing two kinds of order parameter basis functions: a) those which are defined over the whole Brillouin zone, b) those which are defined in a shell around the Fermi surface. In conventional superconductors, only the latter classification has been used. We also remind the reader that in either case, the symmetry does not suffice to determine the number of zeros of the gap-function because the highly non-spherical shape of the Fermi surface forbids the use of the usual spherical-harmonic classification. In the case of gaps defined in a shell around the Fermi surface, we show that when Fermi-surface harmonics are used as basis functions, the first extended s-wave state is closely related to the d-wave states. In a model with first-nearest neighbor (t) and second-nearest neighbor (t') hopping, this extended s-wave state can have eight or sixteen zeros, depending on the value of t'. We also plot the density of states in the superconducting state for various gap functions. In the conclusion, we discuss the relevance of these results for high Tc materials.

II- REFRESHER ON SYMMETRY OF THE SUPERCONDUCTING ORDER PARAMETER.

The superconducting order parameter, or gap function, must transform as an irreducible representation of the symmetry group of the Hamiltonian. Hence, it is important to keep in mind symmetry considerations. This section is based on the discussion appearing in the review by Sigrist and Ueda (1991) and is given here for the sake of completeness. After recalling the usual isotropic case, we introduce the classification appropriate for a tetragonal superconductor.

In the usual isotropic superconductors, the gap function is defined on the Fermi surface, and since the latter is spherical, the spherical harmonics can be used as a basis. Each l value then corresponds to an irreducible representation of dimension $2l + 1$ of the continuous rotation group. There is an infinite number such representations, and low-order ones usually suffice, leaving few possibilities for the number of zeros. Furthermore, the gap has the simple scaling property, $\Delta(\alpha\,\hat{\mathbf{k}}) = \alpha^l \Delta(\hat{\mathbf{k}})$ when it has the symmetry of the l'th shperical harmonic.

In a superconductor with tetragonal lattice symmetry, there are only five possible even-parity irreducible representations. They are defined in the table by reproducing one possible basis function

Irreducible representation	Basis function
Γ_1^+	$\Delta(\Gamma_1^+;\mathbf{k}) = 1$
Γ_2^+	$\Delta(\Gamma_2^+;\mathbf{k}) = k_x k_y (k_x^2 - k_y^2)$
Γ_3^+	$\Delta(\Gamma_3^+;\mathbf{k}) = k_x^2 - k_y^2$
Γ_4^+	$\Delta(\Gamma_4^+;\mathbf{k}) = k_x k_y$
Γ_5^+	$\Delta(\Gamma_5^+,1;\mathbf{k}) = k_x k_z$ $\Delta(\Gamma_5^+,2;\mathbf{k}) = k_y k_z$

Table 1: One possible basis to define each even-parity irreducible representation of the tetragonal lattice symmetry D_{4h}

Only the last representation is two-dimensional, all other ones are one-dimensional. The gap function will transform according to only one of these representations. There are now two possible spaces in which the gap function may be expanded: the full Brillouin zone, or an energy shell around the Fermi surface. In either case, an infinite set of basis functions will be needed to expand an arbitrary complex function having one of the five symmetries. Hence *the number of nodes of the gap function has little relation to its symmetry.* To simplify the discussion, we mostly consider gap functions which do not depend on the z direction.

III- GAPS DEFINED OVER THE WHOLE BRILLOUIN ZONE.

The gap functions now most commonly discussed are the extended s-wave, $\Delta_s(\hat{\mathbf{k}}) = \Delta_0[\cos(k_x) + \cos(k_y)]$ and the d-waves $\Delta_{d_{x^2-y^2}}(\hat{\mathbf{k}}) = \Delta_0[\cos(k_x) - \cos(k_y)]$ and $\Delta_{d_{xy}}(\hat{\mathbf{k}}) = \Delta_0 \sin(k_x)\sin(k_y)$. They arise very naturally in mean-field theories of the t-J model, for example, and they represent different linear combinations of nearest-neighbor pairs. They are also convenient because they have the same periodicity as the Brillouin zone. The extended s-wave, combined with the constant gap, can be seen as two terms in an expansion of a function which transforms as Γ_1^+. The d-waves transform respectively as the irreducible representations Γ_3^+ and Γ_4^+. Basis functions which belong to different representations are clearly orthogonal, whether they are integrated over the whole Brillouin zone or over the Fermi surface.

Within a given representation however, one can define several orthogonal basis expansions. The extended s-wave and the ordinary constant s-wave are orthogonal only when the $\mathbf{k}$ integration is performed over the whole Brillouin zone. Let us keep this definition of orthogonality for a while. We show now that one can expect that an extended s-wave will, in general, have many zeros. It does not have any zero on the Fermi surface at less than half-filling in the nearest-neighbor one-band Hubbard model but it was pointed out by Fedro and Koelling (1993) that when second-nearest neighbor hopping t' is included, then there may be nodes on the Fermi surface. This may be seen from figure 1,

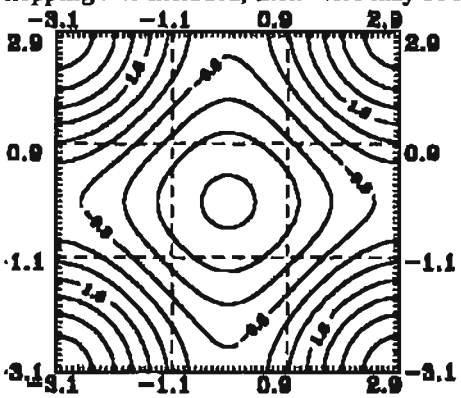


Fig.1: Fermi surface for various fillings when second-neighbor hopping $t' = 0.16t$. The dashed lines are the zeros of $\cos(k_x)\cos(k_y)$

where Fermi surfaces for a dispersion relation

$$\varepsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] + 4t'\cos(k_x)\cos(k_y) \quad (1)$$

are drawn for a variety of fillings. To see that the gap can vanish at eight points on the Fermi surface, note that the extended s-wave vanishes on a diamond (not drawn) and that for a lightly doped system, the Fermi surface is open, formed of four segments each centered around one corner of the zone.

However, it is easy to find other terms in an orthogonal basis expansion for the Γ_1^+ symmetry which have zeros for a wider range of fillings. Consider the "diagonal extended

s-wave" which may be obtained by the same linear combination as the ordinary extended *s*-wave, but with next-nearest-neighbor pairs, namely $\Delta_S(\hat{k}) = \Delta_0 \cos(k_x)\cos(k_y)$. This function vanishes on the dashed lines in figure 1, and hence it always intersects the Fermi surface, except for very low (electron or hole) fillings. In general, it will have eight nodes.

III- GAPS DEFINED OVER THE FERMI SURFACE.

For pairing potentials which act only in the vicinity of the Fermi surface, P.B. Allen (1976) has suggested and discussed in detail an expansion in polynomials which he called "Fermi-surface harmonics". This expansion basis has the advantages of being infinite, orthonormal for integration over the Fermi surface, and cell periodic (each term has the periodicity of the Brillouin zone). It is also adapted to the specific shape of the Fermi surface and is a natural generalization of the spherical harmonics. The Fermi-surface harmonics of order *l* consist of all independent polynomials of order *l* made up of the three components of the velocity on the Fermi surface. Instead of $2l + 1$ functions, as for the spherical harmonics, one finds $(l + 1)(l + 2)/2$ independent polynomials of order *l*. As for spherical harmonics, a gap of order *l* obeys, $\Delta(\alpha\,\hat{\mathbf{v}}) = \alpha^l \Delta(\hat{\mathbf{v}})$ where $\hat{\mathbf{v}}$ is the direction of the velocity on the Fermi surface. Contrary to the spherical harmonics, a given irreducible representation of the point group of the lattice must be expanded with many *l* values.

Table II presents all six $l = 2$ polynomials, and their corresponding symmetry. Compared with spherical harmonics, the only unusual polynomials appear for the Γ_1^+ representation. They are $l = 2$ polynomials, so one would be tempted to include them in the *d*-waves, but in the present context this *d*-wave, *s*-wave nomenclature is in any case only suggestive, and not really appropriate. Usage in the heavy-fermion literature (Sigrist and Ueda, 1991) would call the polynomials occuring in the Γ_1^+ representation extended *s*-waves since, after the usual totally symmetric *s*-wave, they are the first polynomials appearing in an orthogonal-basis expansion of this symmetry.

Repr.	$l = 2$ Fermi-surface harmonic
Γ_1^+	$\Delta(\Gamma_1^+;\hat{\mathbf{v}}) = v_x^2 + v_y^2 - \langle v_x^2 + v_y^2 \rangle$ and $\Delta(\Gamma_1^+;\hat{\mathbf{v}}) = v_z^2 - \langle v_z^2 \rangle - [(v_x^2 + v_y^2 - \langle v_x^2 + v_y^2 \rangle) \times (\langle v_z^2(v_x^2 + v_y^2) \rangle - \langle v_z^2 \rangle \langle v_x^2 + v_y^2 \rangle)]$
Γ_2^+	First basis function occurs at $l = 4$
Γ_3^+	$\Delta(\Gamma_3^+;\hat{\mathbf{v}}) = v_x^2 - v_y^2$
Γ_4^+	$\Delta(\Gamma_4^+;\hat{\mathbf{v}}) = v_x v_y$
Γ_5^+	$\Delta(\Gamma_5^+,1;\hat{\mathbf{v}}) = v_x v_z$ $\Delta(\Gamma_5^+,2;\hat{\mathbf{v}}) = v_y v_z$

Table II: The six $l = 2$ Fermi-surface harmonics arranged according to the corresponding irreducible representation of the tetragonal lattice symmetry. Brackets $\langle\rangle$ stand for averages over the Fermi surface. The polynomials here are orthogonal but they are not normalized.

As before, assume that we can neglect the *z* direction, *i.e.* that the mass in this direction may be taken as infinite so that $v_z = 0$. There are then only three possible cases to consider.

Figure 2 shows the gap for these three cases when the band is as in Eq.(1) with $t' = 0.16t$. The *d*-wave cases have a nodal structure identical to that of the spherical harmonics. The extended *s*-wave has eight nodes.

Figure 3 shows that in the case $t' = 0.45$, a value often quoted as a good description of the Fermi surface for the *92 K* superconductor, the extended *s*-wave case can have up to sixteen nodes when the filling is not too low! By contrast, the nodes for the *d*-waves do not change their number or location. They are not shown here.

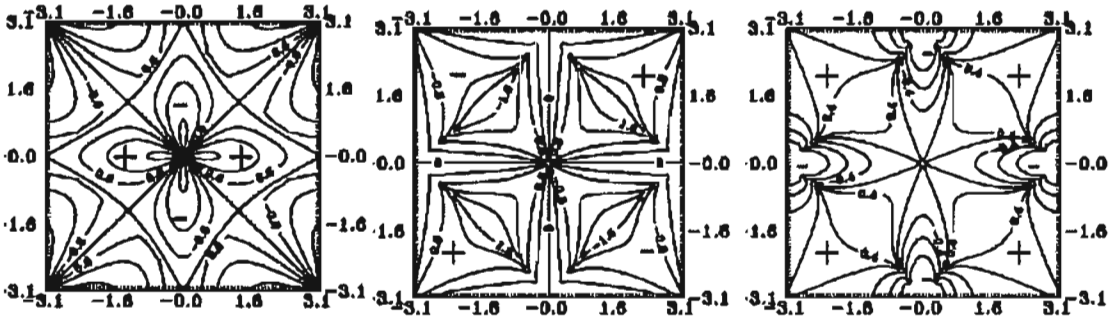
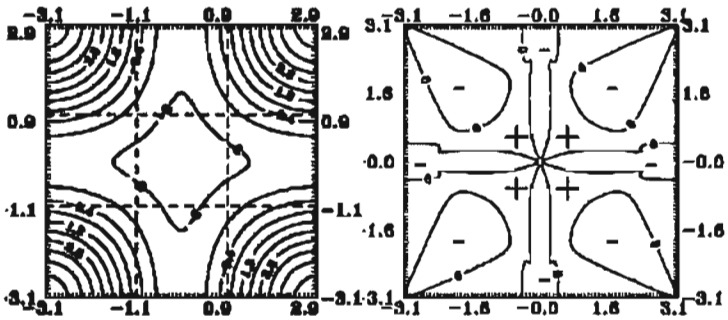


Fig.2: Contour lines for the $l = 2$ Fermi-surface harmonics. For any of the Fermi surfaces appearing in Fig.1 ($t' = 0.16t$), the value of the gap on that surface is obtained intersecting it with one of the three figures. The first two figures correspond respectively to x^2-y^2 and xy symmetry, while the last one is the extended s-wave.

Fig.3: On the left, Fermi surfaces for various fillings when $t' = 0.45t$. The corresponding nodal structure of the extended s-wave is shown on the right. As in figure 2, the value of the gap is found by intersecting a Fermi surface with the contour plot for the gap.



Finally, in figure 4 we show the electron density of states in the superconducting state. Clearly, the extended s-wave case has many more states in the gap.

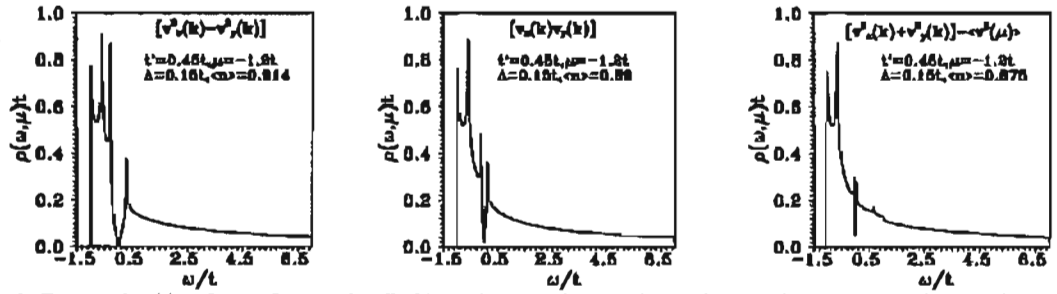


Fig.4: Electron densities of states for gaps described by various Fermi-surface harmonics. In all cases, the Fermi surface is at $-1.2t$, and the maximum value of the gap is the same. The extended s-wave case has much more sates in the gap.

V- CONCLUSION

We have shown on general grounds that the first extended s-wave gap is expected to have many nodes on the Fermi surface. In the case where the pairing potential acts only close to the Fermi surface, the choice of a basis to expand the gap in is not unique, but the most natural choice is Fermi-surface harmonics. In this case, the first extended s-wave has eight or sixteen nodes, depending on the value of the second-neighbor hopping parameter. This may reconcile the experiments which see nodes in the gap and neutron-scattering experiments which cannot resolve the anisotropy in the gap function. More calculations and detailed comparisons with experiment are called for.

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