



# The meaning of strange momentum structures in the gap

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## Abstract

The anisotropy of the superconducting gap is usually associated with the anisotropy of the pairing scattering, and in the exception of the gap symmetry structure, like the nodes, it is expected to be smooth and predictable. There is, however, the alternative approach of momentum decoupling (dominantly forward scattering), in which the anisotropy of the gap follows the anisotropy of the electronic density of states in all gap symmetries. In this last case, the gap can have strange anisotropies in addition to the symmetry-related nodes. We argue that the hump centered in the  $\Gamma$ - $X$  direction of the Bi2212 gap seen in ARPES, reflects the corresponding hump in the electronic density of states when for overdoped and/or contaminated samples the gap symmetry is switched from d-wave to s-wave and the node in this direction disappears (a situation plausible in the Momentum Decoupling regime). This correlation of the gap anisotropy with the DOS anisotropy implies a quasi-Kronecker momentum structure for the scattering amplitude. © 1999 Elsevier Science B.V. All rights reserved.

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The superconductors are classified in two principal categories: the usual simple superconductors with isotropic gap and the anisotropic superconductors with possibly unconventional order parameter symmetries like d-waves. These last superconductors are called the unconventional superconductors. The idea is that a conventional phononic mechanism will lead to an isotropic gap. A momentum dependent gap is supposed to imply an anisotropic pairing scattering. Recently, an alternative approach to unconventional superconductivity has been exploited. According to this approach, the scattering amplitude is singular in momentum space, yet it could be isotropic.

Let us consider the anisotropic Eliashberg equation in the off-diagonal sector

$$\Delta_k Z_k = \pi T \sum_m \int_{S_F} \frac{d^2 p}{S_F} N(E_F, \mathbf{p}) |g(\mathbf{k} - \mathbf{p})|^2 \times \frac{\Omega^2}{\Omega^2 + (\omega_n - \omega_m)^2} F(\Delta_p, \omega_m) \quad (1)$$

where the momentum integral is on the Fermi surface  $S_F$  and has the form of a convolution.

There are two levels of analysis of the phenomenology of unconventional superconductors. The first level consists on a study in which the exact momentum structure of the pairing scattering is not considered. The phenomenology of an anisotropic order parameter is analyzed but no constraint on the physics of the scattering kernel which leads to the

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precise order parameter is given. In that case, it is usually considered an (unphysical) separable potential

$$g(\mathbf{k} - \mathbf{p}) = g(\mathbf{k}) g(\mathbf{p}) \quad (2)$$

Then Eq. (1) becomes

$$\Delta_{\mathbf{k}} Z_{\mathbf{k}} = g^2(\mathbf{k}) \pi T \sum_m \int_{S_F} \frac{d^2 p}{S_F} N(E_F, \mathbf{p}) g^2(\mathbf{p}) \times \frac{\Omega^2}{\Omega^2 + (\omega_n - \omega_m)^2} F(\Delta_{\mathbf{p}}, \omega_m). \quad (3)$$

The  $\mathbf{k}$ -dependence of  $\Delta_{\mathbf{k}}$  is imposed by the potential  $g^2(\mathbf{k})$  and therefore any gap anisotropy is accessible, provided we consider a separable potential with the given anisotropy. This is the opposite approach to the one outlined here.

While a separable potential provides a trivial anisotropic gap solution, finding a physical scattering potential which provides such a solution is not easy. It was a success to establish that the spin-fluctuations scattering kernel provides a gap solution of the d-wave form and usually the d-wave solution has been associated to the spin fluctuations mechanism. It is not surprising that repulsive kernels will lead to gap solutions with nodes. However, the unconventional order parameters are still expected structureless far from the nodes. For example, the d-wave solution from a spin fluctuations kernel is expected to be mainly dominated by the first d-wave harmonic, the  $d_{x^2-y^2}$  in the case of the cuprates. If the gap anisotropy is imposed by the scattering amplitude, then apart from the appearance of nodes (to eliminate the repulsion effects), we do not expect structures in the anisotropy.

There is an alternative approach to anisotropic superconductivity, that is the *momentum decoupling* regime in which phonons [1,2] could be the pairing mediators despite the unconventional gap symmetries. If the electronic system is in the proximity of a phase separation instability, a singularity starts to develop at  $\mathbf{q} \rightarrow 0$  in the effective scattering amplitude [2,3]. In that case we can write to a first approximation

$$g(\mathbf{k} - \mathbf{p}) \approx g \delta(\mathbf{k} - \mathbf{p}) \quad (4)$$

with  $\delta$  being the Kronecker function. With this kernel the gap is given by

$$\Delta_{\mathbf{k}} Z_{\mathbf{k}} = g^2 N(E_F, \mathbf{k}) \pi T \sum_m \frac{\Omega^2}{\Omega^2 + (\omega_n - \omega_m)^2} \times F(\Delta_{\mathbf{p}}, \omega_m) \quad (5)$$

The momentum structure is imposed by the angularly resolved electronic density of states (ARDOS) on the Fermi level  $N(E_F, \mathbf{k})$ . If correlation effects are neglected or absorbed into an effective tight-binding description then

$$N(E_F, \mathbf{k}) \approx \left| \frac{1}{\nabla_{\xi_{\mathbf{k}}} \xi_{\mathbf{k}}} \right|_{E_F} \quad (6)$$

where  $\xi_{\mathbf{k}}$  is the tight-binding dispersion. In a physical situation, the momentum range of the interaction must allow an energy range bigger than the level spacing of our system in order to make sense the definition of a density of states, and therefore the effective scattering amplitude is not strictly a Kronecker function, which is, however, useful to illustrate the effects.

When the gap anisotropy is imposed by the anisotropy of the ARDOS, then, in addition to the momentum structure related to the gap symmetry (the nodes), and for any gap symmetry, we can obtain new structures in the momentum dependence of  $\Delta_{\mathbf{k}}$ . If we adopt the traditional view of anisotropies imposed by the anisotropy of the scattering, these additional strange structures that could appear in angularly resolved photoemission spectroscopy (ARPES) are totally unexpected and may appear as ‘wrong’ experimental points. A characteristic example is in our opinion the hump structure in the  $\Gamma$ - $X$  direction of Bi2212 (the diagonal direction) reported by Ding et al. [4] in 1995, which apparently persists in recent data of Vobornik et al. [5] on overdoped samples. Let us consider for example a simple tight-binding dispersion that could be relevant in the oxides.

$$\xi_{\mathbf{k}} = t_1(\cos k_x + \cos k_y) + t_2 \cos k_x \cos k_y + \dots \quad (7)$$

with first, second and possibly third nearest neighbors hopping on a square lattice.

We show on the left column of Fig. 1 the Fermi surface corresponding to various hopping situations. On the right column of the same figure, we show the

corresponding angular dependence of  $N(E_F, \mathbf{k})$ . The angle  $\phi$  is measured from the  $X-\bar{M}$  axis around the  $X$  point (group conventions are associated with

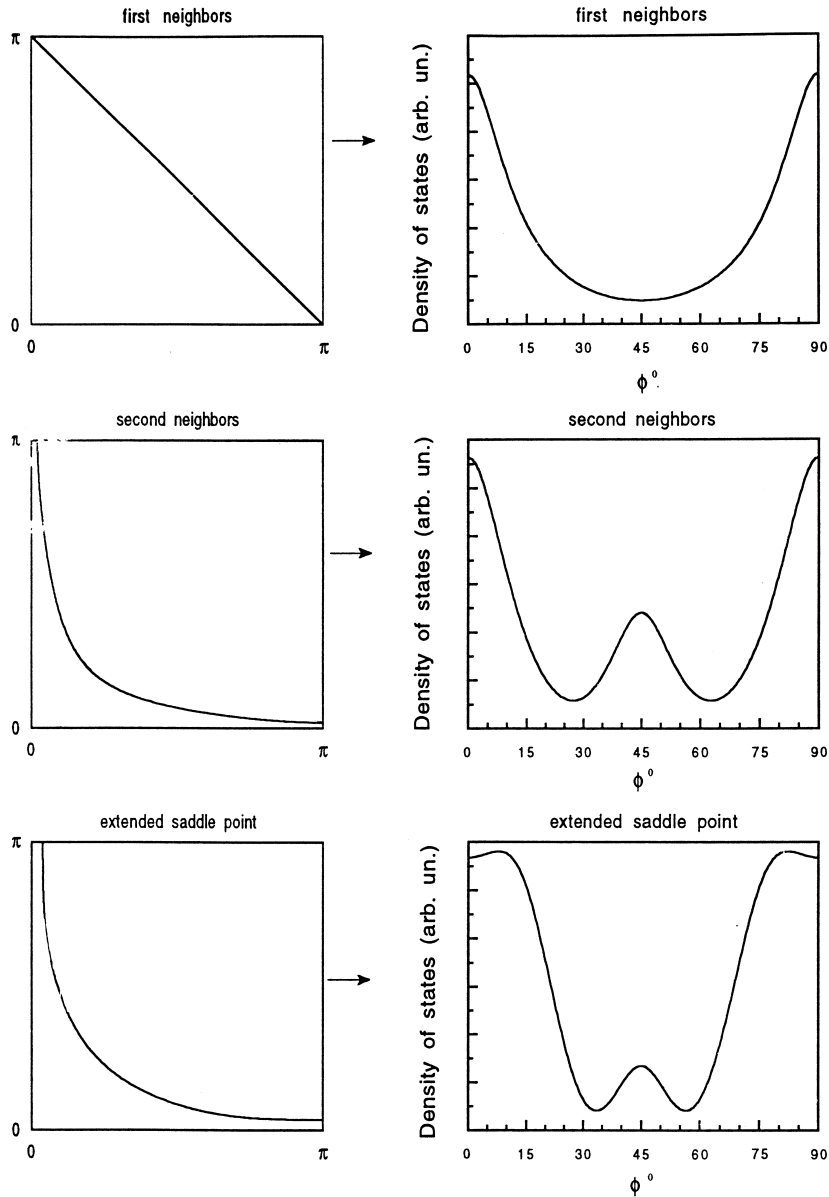


Fig. 1. The Fermi surface on a first quadrant of the Brillouin zone (left column) and the corresponding angular dependence of the electronic density of states on the Fermi surface  $N(E_F, \mathbf{k})$  (right column) for different typical tight binding dispersions used to approximate electronic structure of the cuprates. The upper panels correspond to the nearest neighbors hopping model, the middle panel to a model with second nearest neighbors which better fits the bending of the Fermi surface seen experimentally, and the lower panel to a model with hopping terms up to the fifth nearest neighbors that could also fit the extended character of the van-Hove singularities. The local maximum or hump of  $N(E_F, \mathbf{k})$  in the diagonal characterizes any tight-binding fit of the experimental Fermi surface.

Bi2212). When only nearest-neighbors hopping is considered, the Fermi surface is a line connecting the  $\bar{M}$  points. In that case the ARDOS  $N(E_F, \mathbf{k})$  has maxima at the  $\bar{M}$  points and a minimum in the diagonal  $\Gamma$ - $X$  direction. However, if we already add next nearest neighbors hopping to better fit the experimental Fermi surface the ARDOS has a local maximum in the diagonal. This hump of the ARDOS is very similar to the hump of the gap reported by ARPES. Since the Kronecker function is defined as the only unity function of the convolution product, if the gap (the result of the convolution) has the form of  $N(E_F, \mathbf{k})$  (one of the convoluted functions) then the scattering amplitude (the other convoluted function) has necessarily the form of a Kronecker function.

In conclusion, when strange structures appear in the momentum dependence of the gap, then one should explore the possibility to be in the Momentum Decoupling regime in which case these anisotropies reflect the anisotropy of the electronic dispersion. If the angularly resolved density of states reported by ARPES, has the same strange momentum structures with the superconducting gap measured by the same experiments, then as a result of functional analysis, these ARPES experiments definitely establish that the relevant scattering potential has a momentum dependence close to a Kronecker function. This is true irrespective of the gap symmetry. The hump structure reported in the  $\Gamma$ - $X$  direction of overdoped (and/or polluted) Bi2212 could naturally reflect the analogous hump of the momentum dependence of the electronic density of states establishing the Kronecker structure of the effective scattering. In fact, because of impure samples and/or overdoping it is plausible (in the momentum decou-

pling regime) to switch from a d-wave gap to a gap without node in this direction [2] in which case the hump will appear more clearly. Consistently with this picture for the hump structure, we can also explain with this type of scattering the momentum dependence of the anomalous dip structure above the gap [1,6–8], the temperature dependence of the anisotropy in overdoped Bi2212 samples [1] the large orthorhombicity effects in YBCO without involving the chains [9,10] etc.

As for the physical meaning of a scattering potential having a Kronecker form, it could indicate the proximity of the electronic system to a phase separation instability, possibly driven by the phonons [2,3]. The interlayer tunnelling mechanism of Anderson and collaborators [11] is effectively  $q = 0$  pairing between the planes and can be viewed as an additional pairing term having exactly the Kronecker form.

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