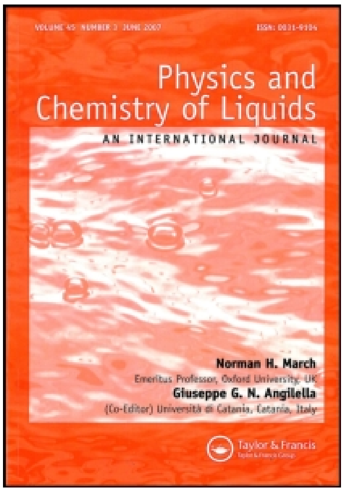

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Electron or hole liquids in high-*T_c* cuprates: evidence for *d*-wave order parameter

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ELECTRON OR HOLE LIQUIDS IN HIGH-T_c CUPRATES: EVIDENCE FOR *d*-WAVE ORDER PARAMETER

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Phillips and Jung [J.C. Phillips and J. Jung (2002). *Phil. Mag. B*, **82**, 1163] refute nodal properties of the gap function $\Delta_{\rm k}$ and propose an isotropic *s*-wave picture with electron–phonon interaction as the mechanism for high-T_c superconductivity in the cuprates. Here, we compare and contrast predictions of various physical properties with the gap function $\Delta_{\rm k}$ reflecting three scenarios: (i) isotropic *s*-wave pairing, (ii) extended *s*-wave with eight line nodes as championed quite recently by Zhao [G.M. Zhao (2001). *Phys. Rev. B*, **64**, 024503], and (iii) *d*-wave pairing. By referring to (a) scanning tunnelling microscopy imaging of a Zn impurity, supported by our own subsequent theoretical study, (b) linear decrease of T_c with non-magnetic impurity concentration, and (c) calculations on the extended *s*-wave scenario applied to tunnelling conductance, strong evidence for nodal properties of $\Delta_{\rm k}$ is given. The contentions of Phillips and Jung [J.C. Phillips and J. Jung (2002). *Phil. Mag. B*, **82**, 1163] should therefore be treated with considerable caution, isotropic *s*-wave behaviour being truly exceptional among the high-T_c cuprates.

Keywords: Fermi liquids; High-T_c cuprates; Anisotropic superconductors; Impurity effects; Tunnelling

1. BACKGROUND AND OUTLINE

In a recent paper, Phillips and Jung [1] have in their postscript drawn the sweeping conclusion, based on the tunnelling conductance experiment of Shimada *et al.* [3], that in high-T_c cuprates the isotropic *s*-wave picture with electron–phonon interaction is the appropriate mechanism and they refute interpretations based on the widely accepted *d*-wave pairing scenario. Their contention is asserted with such generality that it has prompted us to enquire as to the fingerprints that exist concerning nodal properties in the gap function $\Delta_{\rm k}$ in high-T_c cuprates. We shall focus below on two main areas: (a) non-magnetic impurity effects and (b) tunnelling conductance measurements and their interpretation, prompted by the work of Shimada *et at.* referred to above [3].

In a little more detail, and because especially of the investigation of Zhao [2], who champions the extended *s*-wave pairing scenario, we have generalized the theoretical

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studies of Sun and Maki [4] to embrace the extended *s*-wave case. This calculation of the superconducting electronic density of states, in relation to the interpretation of tunnelling conductance measurements, is reported in Section 3, following a discussion of non-magnetic impurity effects in high-T_c cuprates in Section 2. This section embraces the imaging by Pan *et al.* [5,6] of a Zn impurity in the superconducting cuprate Bi-2212 using scanning tunnelling microscopy as well as a summary of a subsequent theoretical study of our own on the charge density around such an impurity [7]. Here, reference is also made to the fact that observations on some high-T_c materials show a linear decrease of T_c with non-magnetic impurity concentration, which then excludes isotropic *s*-wave pairing for such materials by invoking the theorem of Anderson [8]. Section 4 constitutes a summary, and also contains some proposals for future directions which may distinguish not just nodal properties of Δ_{k} from isotropic *s*-wave pairing but which may help to choose between *d*-wave and extended *s*-wave scenarios, or indeed other viable choices of Δ_{k} with nodal properties.

2. IMPURITY EFFECTS IN HIGH-T_c SUPERCONDUCTORS

2.1 Electron Density Change Due to a Zn Impurity in the Bi-2212 Cuprate

Imaging of a Zn impurity in superconducting cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) using scanning tunnelling microscopy (STM) has been reported by Pan *et al.* [5,6]. Subsequent to this experiment, we have made a theoretical study of the charge density around such a non-magnetic impurity.

Our own theoretical study [7], based on the assumption of a localized impurity potential due to Zn in a high-T_c material, correlated the STM imaging with the linear response function

$$F(\mathbf{r}, \mathbf{r}', E_F) = i \int^{E_F} G(\mathbf{r}, \mathbf{r}', E) G(\mathbf{r}, \mathbf{r}', E) \, dE, \tag{1}$$

where G denotes the single-particle Green function in the superconducting phase. In momentum space, F in the normal isotropic case is characterized by a singularity at $q = 2k_{\mathrm{F}}$, with k_{F} the Fermi wave number. The singularity is smoothed out on entering the superconducting phase. For a model *d*-wave superconductor, however, such an effect is more pronounced in the fully gapped q_x and q_y directions than along $q_y = \pm q_x$. The azimuthal modulation of the Fourier transform $\tilde{F}(\mathbf{q}, E_{\mathrm{F}})$ to which this gives rise in the superconducting state is responsible for the four-lobed pattern in the density change which is observed in the above STM imaging experiment of Pan *et al.* [5,6]

Figure 1, adapted from [7], compares the forms of $\tilde{F}(\mathbf{q}, E_{\mathrm{F}})$, the left-hand corner being *s*-wave-like, while the bottom-right picture shows anisotropy in the model with *d*-wave pairing.

2.2 Sensitivity of Critical Temperature T_c to Non-magnetic Impurities in High-T_c Materials

We turn from the symmetry of the density change to the effect of non-magnetic impurities such as Zn on the critical temperature T_c. In BCS superconductors, it is

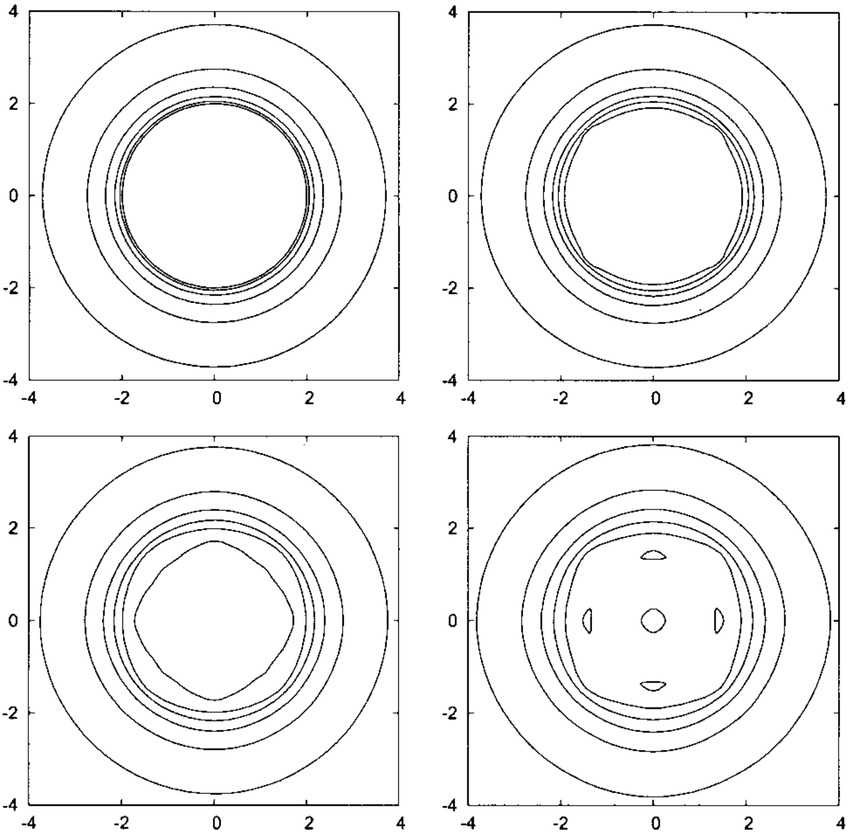

FIGURE 1 Linear response function $\tilde{F}(\mathbf{q}, E_F)$ for a d-wave superconductor in two dimensions. Actually displayed are contour plots of $\tilde{F}(\mathbf{q}, E_F)$ as a function of $\mathbf{q}/k_F$ for $\Delta_0/E_F = 0.0$ (normal state), 0.1, 0.3, 0.5 (left to right top to bottom). Redrawn from [7].

well established that T_c is insensitive to impurity concentration, a result explained by the so-called Anderson theorem [8]. But the cancellation yielding Anderson's result occurs only for an isotropic gap (see, for example, [9]). For gap functions with nodal properties, in general T_c will decrease linearly with non-magnetic impurity concentration, in agreement with numerous experimental results, such as that of Maeda *et al.* [10], on high-T_c materials, including that studied by Shimada *et al.* [3] (see also [9,11]).

However, the density change discussed in Section 2.1 and seen in STM by Pan *et al.* [5,6] is the decisive matter here, as the d-wave symmetry is directly imaged. The T_c sensitivity to non-magnetic impurity concentration is valuable supporting evidence for nodes in the gap function Δ_k.

2.3 Other Impurity Effects in Model d-Wave Superconductors

Additional impurity effects, as well as the reduction of T_c discussed in Section 2.2, were treated in the theoretical study of Sun and Maki [4]. Static spin susceptibility, superfluid density and nuclear spin lattice relaxation rate were all considered at low temperatures. A point where contact is made between their theoretical results for impurities in d-wave superconductors and experiment is in the study of superfluid density by Liang *et al.*

[12]. Their work is related to the temperature dependence of the penetration depth, a topic we raise again below in the context of possible future studies to distinguish gap functions with different nodal behaviour.

3. TUNNELLING CONDUCTANCE EXPERIMENTS AND THEIR INTERPRETATION

Tunnelling conductance experiments can be thought of as providing an indirect probe of the symmetry of the superconducting order parameter, in that the differential conductance dI/dV between a normal metal and a superconductor at low temperature is related to the superconducting density of states (SDOS) $N_s(E)$ by

$$\frac{dI}{dV} = c|T|^2 N_s(E) N_n(E), \tag{2}$$

where $N_n(E)$ is the density of states of the normal metal (usually assumed to be constant, in quasi-two-dimensional cases), T is the tunnelling matrix element, and c is a constant [13].

In the case of a quasi-two-dimensional superconductor characterized by a circular Fermi line, the normalized SDOS can be expressed as

$$\frac{N_s(E)}{N_0} = \mathrm{Re}\left\langle \frac{E}{\sqrt{E^2 - |\Delta(\theta)|^2}} \right\rangle, \tag{3}$$

where $\langle \ldots \rangle$ denotes an average over the angle θ along the Fermi line [14]. The effect of impurities can be taken into account by adding an explicit imaginary part to the energy such that $E \mapsto E - i\Gamma$ (see also [4]).

In the case of a pure s-wave symmetry gap, Eq. (3) yields the usual BCS result, characterized by no states available for tunnelling for $|E| < \Delta_0$, Δ_0 being the constant value of the gap energy over the Fermi line (Fig. 2).

On the other hand, the presence of nodes in the gap energy allows for tunnelling states also at low energy, and endows the SDOS with a characteristic V-shaped behaviour at low energy, with $N_s(E)$ vanishing linearly as $E \to 0$ [14] (Fig. 2). This is due to the possibility of exciting single-particle states out of the condensate at virtually no energy cost near the nodal points [15,16], and is generic to all models of unconventional superconductors, characterized by the presence of nodes in $\Delta(\theta)$.

In Fig. 2 we compare and contrast the energy dependence of the SDOS, Eq. (3), for an s-wave superconductor,

$$\Delta(\theta) = \Delta_0, \tag{4}$$

for a pure d-wave superconductor [4,14],

$$\Delta(\theta) = \Delta_0 \cos(2\theta), \tag{5}$$

and for an "extended" s-wave superconductor with eight line nodes, as considered by Zhao [2], where

$$\Delta(\theta) = \Delta[p + \cos(4\theta)], \tag{6}$$

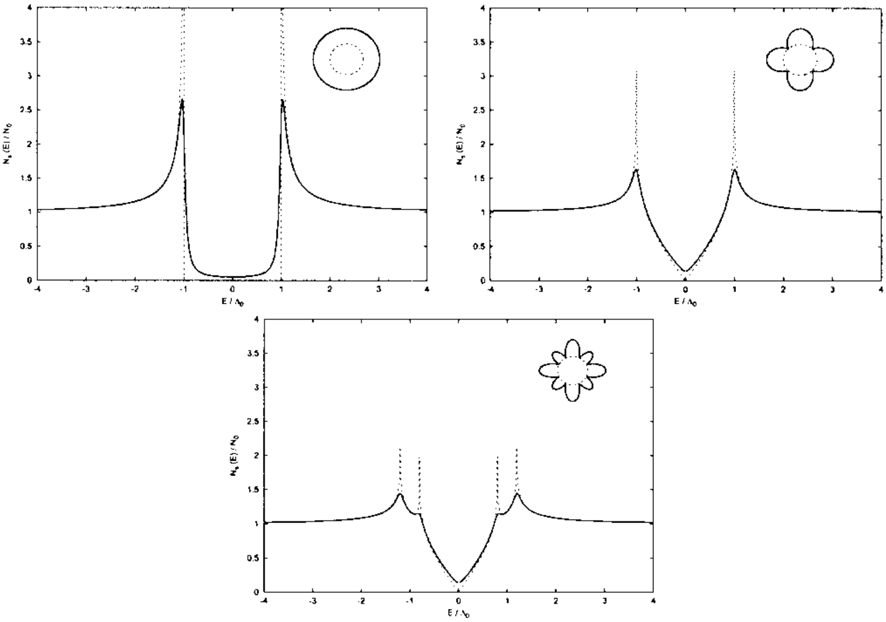

FIGURE 2 Normalized superconducting density of states $N_s(E)/N_0$ as a function of E/Δ_0 for a pure *s*-wave, pure *d*-wave, and for an "extended *s*-wave" superconductor, with $p = 0.2$ (left to right, bottom to top). Dashed lines refer to pure superconductors, whereas continuous lines refer to superconductors in the presence of impurities ($\Gamma/\Delta = 0.05$). Insets show a schematic plot of the gaps considered here (continuous lines), with respect to the Fermi line (dashed line).

with $0 \leq p < 1$, in order to have nodes along the Fermi line. Evidence of doping-dependent pairing symmetry in cuprate superconductors on the basis of tunnelling experiments has been recently reported by Yeh *et al.* [17] (see also [18]). In contrast, no dependence of the gap function on hole concentration is asserted by the experiment of Renner *et al.* [19].

It is important to note that any model gap function of the kind $\Delta(\theta) = \Delta_0[p + \cos(n\theta)]$, with n an even integer, gives rise to the *same* SDOS, according to Eq. (3). In particular, the SDOS corresponding to Zhao's "extended" *s*-wave with eight line nodes ($n = 4$) [2] is identical to that related to $s + d$-wave symmetry ($n = 2$). Therefore, an interpretation of tunnelling experiments based on such an approximate model gap is likely only to reveal whether or not there are nodes in the gap function, regardless of their number, as the detailed θ dependence of the gap energy affects the differential conductance only via the anisotropy dependence of the tunnelling matrix element [2,20]. More accurate models would of course specify the full momentum dependence of the gap energy over the whole of the first Brillouin zone.

Both the pure *d*- and the "extended" *s*-wave symmetries are characterized by a V-shaped, linear behaviour at low energies, which would be destroyed by an *s*-wave component with $p > 1$ (Fig. 2, dashed lines). In addition to this feature, which is generic to any gap containing node lines, no matter what their number may be, the "extended" *s*-wave gap is characterized by a second peak at some energy $E < \Delta_0$, depending on p. Such a structure would be obtained also in the case of an $s + d$-wave gap [17,18]. A non-zero impurity concentration ($\Gamma \neq 0$) has the effect of smearing the logarithmic divergences in $N_s(E)$ into finite-height peaks, and the cusp at low energy into a parabolic arc, which gives rise to a non-zero differential conductance at zero bias (Fig. 2, continuous lines).

The V-shaped behaviour at low energy, possibly rounded off by impurities, typical of either pure *d*-wave or ''extended'' s-wave superconductivity, and in general of any gap with nodal lines, can be recognized e.g. in the tunnelling spectra of Renner *et al.* in under- and overdoped Bi-2212 [19], which we take as a representative example of the literature on tunnelling experiments in the cuprates.

On the other hand, there are instances of tunnelling experiments on the cuprates, such as that of Shimada *et al.* [3], which have been interpreted in terms of strongly correlated *s*-wave symmetry [1,3]. However, Shimada *et al.* already cautioned that ''*if the angular distribution of the tunnelling current is highly anisotropic*, *we cannot definitely exclude a d-wave state*'' [3]. Indeed, anisotropy effects due to the directional dependence of the tunnel matrix elements that describe the tunnelling barrier tend to be relevant, especially for unconventional superconductors [20].

4. SUMMARY AND PROPOSED FUTURE DIRECTIONS

In Sections 2 and 3, we have presented evidence, both from experiment and based on theoretical models, that numerous high-T_c cuprates have nodal properties in the gap function Δ_{k}. We have focussed here principally on two areas: non-magnetic impurity effects in Section 2 and tunnelling conductance in Section 3. Fingerprints of the nodal properties of Δ_{k} are clear in the scanning tunnelling microscopy measurement of Pan *et al.* [5,6] on a Zn impurity in a Bi-2212 high-T_c cuprate, and supporting evidence is contained in our own theoretical study of the electron density distribution around such an impurity [7]. Furthermore, in the same area of impurity effects, we know from the theorem of Anderson [8] that for isotropic *s*-wave superconductors, non-magnetic impurity scattering has no effect on T_c. There is a body of evidence for high-T_c cuprates that T_c decreases linearly with impurity concentration [11] (see also [9]), which excludes the isotropic *s*-wave scenario in all materials where such a decrease has been observed.

Section 3 treats, quite briefly, tunnelling conductance experiments and their interpretation. A simple model is used to calculate here the superconducting electronic density of states in an extended *s*-wave scenario to complement the earlier study of Sun and Maki [4] on *d*-wave pairing. While we do not expect, in the light of our theoretical study, tunnelling conductance to distinguish decisively between extended *s*-wave and *d*-wave pairing, clear fingerprints exist of nodal properties, as evidenced in the measurements of Renner *et al.* [19]. However, we do not see such fingerprints in the tunnelling results of Shimada *et al.* [3], on which Phillips and Jung [1] base their contentions, though in their original paper Shimada *et al.* [3] explicitly write, as quoted above, that they cannot definitely exclude *d*-wave pairing. Our conclusion here then is that in very numerous samples of high-T_c cuprates, isotropic *s*-wave pairing is excluded by experiment. The sample used by Shimada *et al.* [3] is an instance in which the isotropic *s*-wave picture advocated by Phillips and Jung [1] presently remains viable.

While, at most, a few high-T_c cuprates obey the Phillips–Jung isotropic *s*-wave proposal, it remains, of course, of considerable interest to distinguish between extended *s*-wave and *d*-wave scenarios, or other viable choices of Δ_{k} having nodal properties. In this context, two further areas come to mind as worthy of future investigation.

The first of these concerns the relation between critical temperature T_c, Cooper pair binding energy ε and coherence length ξ. Very recently [21], we have solved the Bethe–Goldstone equation for general orbital angular momentum ℓ and have thereby found the Cooper pair binding energy as a function of coherence length and ℓ. For $\ell = 0$ the usual BCS-type relation between ε and ξ is regained, but for $\ell \neq 0$, ε saturates as a function of ξ^{-2}. Since ε is related to $k_B T_c$, this saturation accords with that we found empirically for heavy Fermion materials ($\ell = 1$) and possibly also for high-T_c cuprates [22]. Here then is a further fingerprint of nodal properties of Δ_k.

The second area worthy of future study is prompted by Zhao's work [2]. The aspect we propose is concerned with the Meissner effect and related properties: in particular transverse magnetic moment and temperature dependence of penetration depth. To date, the evidence presented by Zhao [2] appears to be strongly in favour of the extended s-wave scenario. However, it may be that while very general arguments are now available [23] (see also [24,25]) showing that the Meissner effect (and also flux quantization) follow from three basic assumptions: (i) off-diagonal long-range order (ODLRO) in the two-particle density matrix, (ii) gauge covariance, and (iii) thermodynamic stability, the form of ODLRO involving intimate knowledge of the Ginzburg–Landau wave-function for a gap function Δ_k with nodal properties may be required before a decisive choice can be made between the various nodal schemes of Δ_k. But the present work confirms, beyond reasonable doubt, that Δ_k in the dominant body of high-T_c cuprates has such nodal properties.

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