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1991 J. Phys.: Condens. Matter 3 6173

(http://iopscience.iop.org/0953-8984/3/32/023)

J. Phys.: Condens. Matter 3 (1991) 6173–6176. Printed in the UK

LETTER TO THE EDITOR

In-plane gap anisotropy in a van Hove superconductor

R S Markiewicz

Physics Department and Barnett Institute, Northeastern University, Boston, MA 02115 USA

Received 30 May 1991

Abstract. The van Hove singularity (VHS) model provides a unifying picture for understanding many anomalous features of high-temperature superconductors. Here, it is shown that there is an intrinsic in-plane anisotropy associated with the VHS which can explain recent observations on $Bi_2Sr_2CaCu_2O_8$.

It has been proposed that superconductivity in the new high-T_c cuprates is associated with the saddle-point van-Hove singularity (VHS) of the CuO_2 planes, at which the density-of-states (DOS) diverges logarithmically [1–7]. The VHS should also induce a number of anomalies in the normal state properties of these materials, including a normal-state resistivity which increases linearly with temperature T or frequency ω [8]. The holes within the CuO_2-plane band can be divided into two groups [5]: a high density of carriers near the Brillouin zone boundaries, which are responsible for the large DOS at the VHS (heavy, or VHS, holes) and a low density of carriers associated with parts of the Fermi surface away from the Brillouin zone boundaries (light holes). The heavy holes are nearly localized, due to strong electron–electron and electron–phonon scattering, while the light holes dominate the transport properties (resistivity, Hall effect) in these materials. The heavy holes produce the 'phenomenological polarizability' which is responsible for the marginal Fermi liquid behaviour of the normal state [9, 10].

Recently, a photoemission experiment in $Bi_2Sr_2CaCu_2O_8$ (Bi-2212) has revealed a striking anisotropy of the superconducting gap, within the a, b-plane [11]. The gap in the X direction of the Brillouin zone (away from the VHS) was close to the weak-coupling value, $2\Delta/k_B T_c \simeq 3.53$, whereas the gap along the $\bar{M}$ direction (at the VHS) was nearly twice as large, $2\Delta/k_B T_c \simeq 8$. In the $\bar{M}$ direction, there is a complication, since an electron pocket due to the Bi may overlap the Fermi level. In this paper, I will assume that this band is irrelevant, and ignore any possible complications associated with it [12].

This gap anisotropy finds a ready interpretation in terms of the VHS model, while providing additional evidence for the separation of the holes into two groups. It has long been known that gap anisotropy is directly associated with anisotropy of the effective electron–electron interaction parameter, V, and only indirectly with anisotropy of the DOS [13]. The phonon-mediated part of V may be written [14]

$$V_q = \frac{V_{q0}}{1 + V_{q0}\chi_{q0}/P_{e3}} \tag{1}$$

where V_{q0} is the unscreened interaction,

$$\chi_{q0} = -\sum_k \frac{f(E_k) - f(E_{k+q})}{E_k - E_{k+q}} \tag{2}$$

and P_{e3} is a constant estimated [14] to be 0.45 in $La_{2-x}Sr_xCuO_4$, and assumed here to be similar in Bi-2212. When the Fermi level is at the VHS, the susceptibility χ_{q0} diverges, both at $q = 0$ and at $q = Q \equiv (\pi/a, \pi/a)$, the reciprocal lattice vector which connects the two VHS. This divergence of χ leads, via (1), to a divergence of V_q at the same wave numbers. Whereas the divergence may be cut off by two-dimensional fluctuations [14], there remains a strong anisotropy in V_q.

This leads to an anisotropic gap equation [13, 15]

$$\Delta_k = \int_0^{\omega_c} \mathrm{d}\epsilon_{k'} \mathrm{d}\Omega_{k'} \frac{V_{k-k'}\Delta_{k'}N_{k'}}{\sqrt{\epsilon_{k'}^2 + \Delta_{k'}}} \tag{3}$$

where $\Omega_{k'}$ is a unit of solid angle, and $N_{k'}$ is the angle-dependent DOS in the k' direction. Near the VHS, this DOS diverges as $N_{k'} \sim 1/k'$. Thus, if k is near a VHS, Δ_k is large due to two contributions to (3): (i) the term $V_0 N_k$, from the region near the same VHS, $k' \simeq k$, and (ii) the term $V_Q N_{k'}$, when k' is near the second VHS. This gap can be considerably larger than the gap in the usual isotropic VHS models [1–3, 6], since the DOS divergence, of the form $N(E) \simeq \ln(B/E)$ with B the electronic bandwidth, is here enhanced by the divergence in V_q. On the other hand, if k is not near a VHS, Δ_k is much smaller, since the V_q connecting it to a VHS is not divergent.

Rather than solve (3) directly, a simplified form can be introduced, similar to the two-band model of Suhl *et al* [16]. It is assumed that the Fermi surface can be split into the two carrier groups, heavy (h) and light (l) holes, and that V_q takes on only three values V_{hh}, V_{ll}, and $V_{hl} = V_{lh}$, depending on what regions k and k' fall in. Furthermore, the average DOS of the l-holes is a constant, N_l, while the h-hole DOS is of the form $N_h = N_0 \ln(B/\epsilon)$. Then there are two coupled gaps, Δ_h and Δ_l, which satisfy [16]

$$\Delta_l(1 - \lambda_l F_l(\Delta_l)) = \Delta_h V_{lh} N_0 F_h(\Delta_h) \tag{4a}$$

$$\Delta_h(1 - \lambda_0 F_h(\Delta_h)) = \Delta_l V_{lh} N_l F_l(\Delta_l) \tag{4b}$$

where $\lambda_l = N_l V_{ll}$, $\lambda_0 = N_0 V_{hh}$,

$$F_h(\Delta) = \int_0^{\omega_c} \frac{\ln(B/\epsilon)\mathrm{d}\epsilon}{\sqrt{\epsilon^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\epsilon^2 + \Delta^2}}{2k_B T}\right) \tag{5}$$

and $F_l(\Delta)$ has the same form as (5), without the logarithmic term. As long as $V_{lh} \neq 0$, both gaps appear simultaneously at temperature T_c, given by the solution of

$$[\lambda_l - \delta\lambda^2 F_h(0)][\lambda_0 - \delta\lambda^2 F_l(0)] = \lambda_{lh}^2 \tag{6}$$

with $\lambda_{lh}^2 = V_{lh}^2 N_l N_0$, and $\delta\lambda^2 = \lambda_l\lambda_0 - \lambda_{lh}^2$. When V_{lh} is small, this can be approximated as

$$k_B T_c = \frac{eB}{2} \exp -\left(\sqrt{y^2 - 1 + 2/\lambda_0^*}\right) \tag{7}$$

with $y = \ln(B/\hbar\omega_c)$,

$$\lambda_0^* = \delta\lambda^2 \left[\lambda_l + \frac{\lambda_{lh}^2}{F_l^* \delta\lambda^2 - \lambda_0}\right]^{-1} \tag{8}$$

$F_l^* = \ln(e\hbar\omega_c/2k_B T_B)$, and T_B is the solution of the decoupled heavy holes—i.e., the solution to (7) with $\lambda_0^* \to \lambda_0$. The resulting T_c depends only weakly on λ_l, and (8) simplifies in the limit $\lambda_l \to 0$: $\lambda_0^* \to \lambda_0 + F_l^* \lambda_{lh}^2$.

A concrete example is shown in figures 1 and 2. Here it is assumed that $\lambda_0 = 0.136$, $B = 5800$ K, and $\omega_c = 500$ K. If $\lambda_{lh} = 0$, the two gaps are decoupled, and have separate transitions at $T_h = 92$ K, $T_l \simeq 1.4 \times 10^{-6}$ K (for $\lambda_l = 0.05$). Figure 1 shows how T_c increases for $\lambda_{lh} \neq 0$, and λ_l varying from -0.1 to 0.1, both for the exact equation (6) and the approximate equation (7). Figure 2 shows the two gaps as a function of T for $\lambda_l = 0.05$ and for several values of λ_{lh}. Within the BCS-like expression (5), the VHS superconducting gap is close to the BCS value $2\Delta_h(0)/k_B T_h = 3.53$, but strong coupling corrections and depairing due to real phonon scattering greatly enhance this ratio [17].

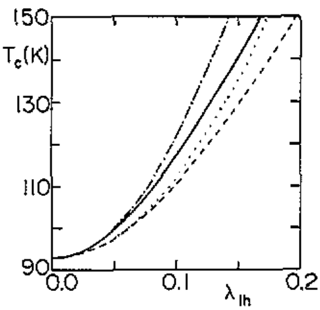

Figure 1. Superconducting transition temperature T_c versus light-hole–heavy-hole coupling parameter λ_{lh} for $\lambda_l = 0.1$ (solid curve = exact solution, (6); dot-dashed curve = approximate solution, (7)) or $\lambda_l = -0.1$ (dashed curve = exact solution; dotted curve = approximate solution).

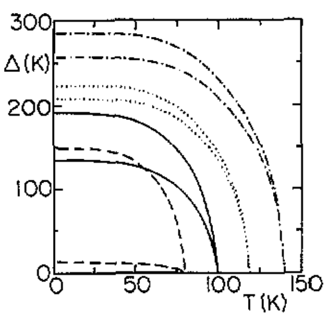

Figure 2. Superconducting gaps versus temperature for $\lambda_l = 0.05$ and $\lambda_{lh} = 0.01$ (dashed curves), 0.10 (solid curves), 0.15 (dotted curves), and 0.20 (dot-dashed curves).

Note that, since the uncoupled T_l is essentially zero, the existence of the light hole gap is entirely due to coupling with the nearly localized VHS holes. A gap ratio $\Delta_h/\Delta_l \simeq 2$, comparable to experiment [11], can be obtained with reasonable parameter values. Moreover, even though $T_l \simeq 0$, coupling to the light holes can significantly enhance T_h. This enhancement is independent of the sign of V_{lh}, and depends only weakly on the sign and magnitude of V_{ll}.

This work was supported by the Department of Energy under subcontract from Intermagnetics General Corporation. Publication 484 from the Barnett Institute.

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