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ORIGIN OF SUPERCONDUCTIVITY IN CUPRATES:THE VAN HOVE SCENARIO

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In 1987, J. LABBE and J. BOK[1] were first to propose that a logarithmic singularity in the density of states, could be a mechanism for high critical temperature superconductivity. This model explained: high Tc, the variation of the critical temperature with the density of holes in the CuO planes with a maximum when the Fermi level is exactly at the singularity, an anomalous isotope effect which is observed experimentally. We have calculated the coherence length ξ in the framework of this model and we are able to explain the observed low value in the a-b plane. For a 2D model we find that ξ=aD/Δ where a is the lattice constant, Δ the gap in the a-b plane and D the width of the singularity. We also show that including a repulsive interaction between second nearest neighbors, the Van Hove singularity is no longer at half-filling of the band but for 0.85 electron per Cu atom or 0.15 hole. This explains the separation between half-filling (magnetic state) and the concentration which puts the Fermi level at the singularity (superconductivity with maximum critical temperature). This also explains that the singularity always happens on the hole side of the half-filling.

Since the discovery of high T_c superconductivity in the cuprates there have been many atemps to build a theory that would explain its properties. In 1987 LABBE and BOK suggested that a logarithmic singularity in the density of states of the CuO 2D-band could account for a high T_c. This model also explained the variation of T_c with the density of holes (position of the Fermi level) and the experimentally observed anomalous isotope effect. In this paper we continue developing this model, first by calculating the coherence lengh ξ_0 and then by giving several arguments to explain that the concentration which puts the Fermi level at the singularity is different from half-filling of the band and is always on the hole-side of the band.

1. COHERENCE LENGTH

When we consider a two-dimensional band, such as in the CuO planes of a high T_c superconductor, there is necessarily a logarithmic Van Hove singularity:

$$n(E) = \frac{N}{2\pi^2} \ln \frac{D}{|E - E_s|} \qquad (1)$$

Highest T_c occurs when the Fermi level is equal to E_s.

If we take for simplicity a band structure

$$\epsilon_{\mathbf{k}} = E_s - 2t(\cos k_x a + \cos k_y a) \qquad (2)$$

then the band width is $W = 8t$ and for a Fermi level $E_f = E_s$ the Fermi surface is a square with four singular points at each corner. We have then the Fermi speed v_f along a side of the square:

$$v_f = \frac{2\sqrt{2}}{\hbar} ta|\sin k_x a|$$

From BCS theory we have:

$$\xi = \frac{\hbar v_f}{\pi \Delta}$$

If we take a mean Fermi speed $v_f = \frac{Wa}{4\hbar}$ we find

$$\xi_0 = \frac{aW}{4\Delta}$$

For YBaCuO, with $\Delta \simeq 20$meV and $W \simeq 2$eV we obtain $\xi_0 \simeq 25a$, i.e. 100Åwhich is too large.

Actually these calculation are not correct: when $v_f = 0$ there is a singularity in the density of state and these points should have a more important statistical weight, thus decreasing v_f. The density of state is given by:

$$n(E)dE = \int_\Gamma \frac{dk_t dk_\perp}{2\pi^2}$$

where Γ is the curve $\epsilon_k = E_s$ and k_t and $k_\perp$ are the tangential and orthogonal components of $\mathbf{k}$ in Γ's local basis. As $v_f = \frac{1}{\hbar}\mathbf{grad}_\mathbf{k}\epsilon_\mathbf{k}$ is directed perpendicularly to Γ we can write:

$$n(E) = \frac{1}{2\pi^2\hbar}\int_\Gamma \frac{dk_t}{v_f}$$

In order to calculate ξ_0 we consider a wave packet of 2Δ width in energy. This is the making of the $u_k v_k$ in BCS theory. Hence:

$$\overline{v_f} = \frac{\frac{1}{2\pi^2\hbar}\int_\Gamma \frac{dk_\perp}{v_f} v_f \times 2\Delta}{\int_{-\Delta}^{+\Delta} n(E)dE}$$

$$\hbar v_f = aD\frac{2\sqrt{2}\pi}{\ln\frac{D}{\Delta}+1}$$

$$\xi_0 \simeq \frac{aD}{\Delta}$$

We can notice that the *band* width is replaced by the *singularity* width. Experimentally we have $\xi_0 \simeq 5a$ which implies $D \simeq 5\Delta \simeq 100\text{meV}$ which seems quite reasonable.

2. POSITION OF THE SINGULARITY

When using the band structure of equation (2) we find that the logarithmic singularity, and thus the maximum T_c occurs when the band is half-filled. This is not what is observed experimentally: maximum T_c is obtained for about a 15% doping, which corresponds to a 43% filling of the band; neither is our expression of the band structure in equation (2) the most accurate one: we will now take into account the repulsive interaction between second nearest neighbors and the effects of the slight rhomboedric distortion.[2]

When taking into account the repulsive interaction with second nearest neighbors the band structure becomes:

$$\epsilon_\mathbf{k} = -2t(\cos k_x a + \cos k_y a) + 4\alpha t \cos k_x a \cos k_y a$$

where α is the ratio of the interactions between first and second nearest neighbors. The singularity occurs when $\mathbf{grad}_\mathbf{k}\epsilon_\mathbf{k} = 0$, that is for $E = -4\alpha t$: there is a shift towards low energy. The Fermi surface at the singularity is no longer a square but is rather diamond-shaped. For $\alpha = 0.1$ this corresponds to a 46% filling of the band.

On the other hand we can consider the effect of a slight rhomboedric distortion: the band structure is then:

$$\epsilon_\mathbf{k} = -2t(1+\beta)\cos k_x a - 2t\cos k_y a$$

where βt represents the difference in the interaction with first neighbors in the $\mathbf{x}$ and $\mathbf{y}$ directions. The effect is now that the singularity is splitted, one part being at energy $-2\beta t$, the other part being at $+\beta t$. The shape of the Fermi surface is also altered and the two singularities now correspond to a 45% and 55% filling.

Of course it is possible to combine both effects, and with $\alpha = 0.1$ and $\beta = 0.1$ the first singularity is at 41% and the second at 51%. We can imagine that the second one, being to close to the half-filling is destroyed by magnetic effects, so that usually superconductivity is observed only for hole-doped compounds.

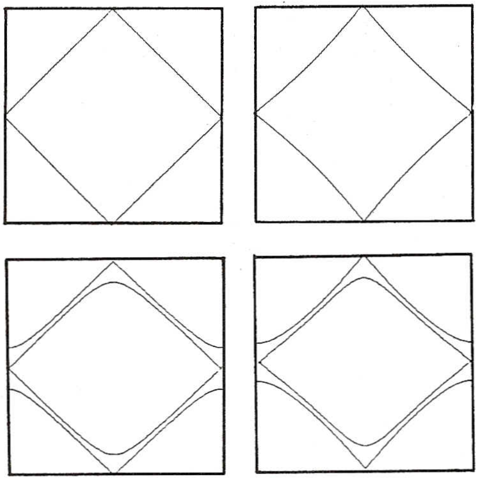

Fig 1: Fermi surface at the singularity.
From right to left and top to bottom: $\alpha=\beta=0$, $\alpha=0.1$ and $\beta=0$, $\alpha=0$ and $\beta=0.1$, $\alpha=\beta=0.1$

3. CONCLUSION

We have shown that the LABBE and BOK model can explain the coherence length ξ_0 measured in high T_c superconductors. Furthermore the relevant parameter is the *singularity* width D and not the *band* width: things happen as if the electrons were in a very narrow band. We also pointed out that the rhomboedric distortion and the second nearest neighbors interaction can explain the fact that the maximum T_c is not obtained at exactly half-filling of the band, but a little below.

1. J . LABBE and J. BOK, Europhysics lett. 3, 1225 (1987)
2. A. SANTORO and al. mat.res.bull. vol 22 no 7, 1007 (1987)