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Quasi-Two Dimensional Density of States and the Isotope Effect in the Superconducting Cu Oxides

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Abstract - Tsuei et al.¹ have pointed out that the correlation between a maximum in T_c and a minimum in the oxygen isotope exponent, α , observed by Crawford et al.² in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and by Franck et al.³ in $(\text{Y}_{1-x}\text{Pr}_x)\text{Ba}_2\text{Cu}_3\text{O}_7$ may be understood as a carrier density of states effect, $N(E)$. We point out here that, if the gap equation is treated in the weak coupling approximation, an $N(E)$ with an enhancement in a narrow range of energies which is symmetric about some energy E_s is sufficient to give this correlation. We discuss how such an enhancement may arise from a tight-binding description of the CuO planes.

Tsuei et al.¹ have have proposed that the doping dependence of T_c and the oxygen isotope exponent, α , observed by Crawford et al.² in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and by Franck et al.³ in $(\text{Y}_{1-x}\text{Pr}_x)\text{Ba}_2\text{Cu}_3\text{O}_7$ may be understood as a carrier density of states effect. In particular they proposed that if the density of states of the charge carriers, $N(E)$, has a van Hove singularity then a maximum in T_c and a minimum in α occur at the doping level that makes the Fermi energy coincide with a logarithmic singularity in the density of states. We point out here that this result is more general and that an $N(E)$ with an enhancement in a narrow range of energies which is symmetric about some energy E_s has the same properties. Defining $\delta = E_s - E_F$ and changing variables $\xi = E - E_F$, the weak-coupling gap equation becomes

$$1 = -\frac{V_{ph}}{2} \int_0^{\hbar\omega_D} d\xi [N(\delta + \xi) + N(\delta - \xi)] \frac{\tanh\left[\frac{\xi}{2k_B T_c}\right]}{\xi}. \quad (1)$$

Making the usual assumption $\omega_D \propto M^{-1/2}$ where M is an ion mass, the isotope exponent is easily calculated to be

$$\alpha = -\frac{\partial \ln T_c}{\partial \ln M} = -\frac{1}{2} \tanh\left[\frac{\hbar\omega_D}{2k_B T_c}\right] \frac{[N(\delta + \hbar\omega_D) + N(\delta - \hbar\omega_D)]}{\int_0^{\hbar\omega_D} d\xi \frac{[N(\xi + \delta) + N(\xi - \delta)]}{\cosh^2\left[\frac{\xi}{2k_B T_c}\right]}}. \quad (2)$$

T_C and α are functions of δ and one finds that $\partial T_C / \partial \delta = 0$ and $\partial \alpha / \partial \delta = 0$ at $\delta = 0$. This result relies only on the fact that $N(E)$ is symmetric about E_S and is independent of the exact function form for $N(E)$. The $N(E)$ used by Tsuei et al. is an example of this type of $N(E)$. Assuming, however, an $N(E)$ with a gaussian enhancement we obtain values of T_C and α that reproduce the qualitative features of the data.⁴ One may also introduce extra parameters into this simple model to take into account the effect of the Coulomb interaction: namely, the Coulomb pseudopotential, μ^* , and a characteristic electronic energy scale, E_0 . We now discuss how such an enhancement of $N(E)$ could arise from a tight-binding approximation.

The electronic structure of the CuO planes may be modelled by a single-band tight-binding Hamiltonian with nearest neighbor, t_{p1} , next nearest neighbor, t_{p1}' , and interplanar hopping, t_z . There are also strong Coulomb interactions which result in a Mott-Hubbard insulator at half-filling. However we will ignore these interactions and consider a Hamiltonian for quasiparticles which form Cooper pairs due to an attractive interaction induced by phonons as in BCS. The Hamiltonian which describes these quasiparticles is

$$H = \sum_{\mathbf{k}, \sigma} \left[-2t_{p1} \{ \cos(k_x a) + \cos(k_y a) \} + 4t_{p1}' \cos(k_x a) \cos(k_y a) - 2t_z \cos(k_z c) \right] c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (3)$$

The density of states is

$$N(E) = \sum_{\mathbf{k}} \delta[E - \xi_{\mathbf{k}}] = \sum_{\mathbf{k}} N^{2d}[E + 2t_z \cos(k_z c)] \quad (4)$$

where

$$N^{2d}(E) = \frac{2}{\pi^2 t_{p1}} \left[1 - \left(\frac{2t_{p1}'}{t_{p1}} \right)^2 \right]^{-1/2} K \left[\sqrt{\frac{1 - \left(\frac{E}{4t_{p1}} + \frac{t_{p1}'}{t_{p1}} \right)^2}{1 - \frac{E t_{p1}'}{t_{p1}^2}}} \right] \quad (5)$$

is the two-dimensional density of states, $\xi_{\mathbf{k}}$, the quasiparticle spectrum, is the expression in the brackets in Eq. (3), and $K(x)$ is an elliptic function which has a logarithmic singularity similar to that used by Tsuei et al.¹ The effect of the interplanar hopping ($t_z \neq 0$) is blunt this singularity as shown in Fig. 1 for the case where $t_{p1}' = 0$. In this case the three-dimensional density of states, $N(E)$, is flat for energies between $-2t_{p1}$ and $2t_{p1}$. Lifetime effects at T_C are also known to be significant in the cuprate superconductors⁵ and their effect is to further smooth $N(E)$.

Figure 1. Density of States for quasiparticle spectrum in Eq. (3)

There are a number of assumptions in this model which we do not address here. We have assumed that in the region of doping where the compounds are superconducting the density of states is not changing with doping and the only effect of doping is that E_F sweeps through the energy where $N(E)$ is enhanced. This is a serious assumption considering that the compounds evolve from an insulating to a superconducting state with doping. We have also assumed that the phonons may be treated in a weak-coupling approximation. These assumptions remain to be investigated.

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