

Van Hove Singularity and "Pseudo-Gap" in HTSC

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Received 15 September 1997

Several experimental features in the normal state of cuprates have been interpreted using a "pseudogap." We show that these results may be explained by the band structure of the CuO₂ planes in the metallic region, which exhibits saddle points (van Hove singularities).

KEY WORDS: Cuprates; van Hove singularity; pseudo-gap.

Several experiments on photoemission [1], NMR, and specific heat have been analyzed using a normal-state pseudo-gap [2]. In fact, all that is needed to interpret these data is a density of state (D.O.S.) showing a peak above the Fermi energy. To obtain the desired D.O.S. several authors [2] introduce a pseudogap in the normal state. This seems to us rather artificial; the above authors themselves write that the physical origin of this pseudogap is not understood. But it is well known that the actual electronic band structure of electrons (or holes) in the CuO₂ plane, established both theoretically and experimentally, is given in a good approximation by the following formula:

$$\xi_k = -2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a - D_e \quad (1)$$

Here, t is the transfer integral between nearest-neighbor Cu atoms. We introduce t' (the interaction with the second nearest neighbor) in order to obtain the Fermi level at the singularity for a filling factor of 0.8 electron per Cu atom, or 20% of holes in the CuO₂ plane. The Fermi level E_F is taken at $\xi_k = 0$. A saddle point appears at $\xi_k = -E_S$ (van Hove singularity, v.H.s.). So D_e represents the distance of the singularity from the Fermi level ($D_e = E_F - E_S$).

These van Hove singularities have been observed experimentally by angular resolved photoemission

(ARPES) in all five superconducting cuprates studied [3–5].

Using formula (1) we may interpret the results obtained in the *normal metallic state*. We have computed the Pauli spin susceptibility using the following formula:

$$\chi_p = \frac{\mu_0 \mu_B}{B} \int_{-\infty}^{+\infty} n(\varepsilon) (f_{FD}(\varepsilon + \mu_B B) - f_{FD}(\varepsilon - \mu_B B)) d\varepsilon \quad (2)$$

where $n(\varepsilon)$ is the D.O.S., f_{FD} the Fermi–Dirac function, B the magnetic field, μ_B the Bohr magneton, and μ_0 the vacuum permeability. The results (Fig. 1) fit well the experiments. We find a characteristic temperature T^* where the variation of χ_p vs. T goes through a maximum. We may express D_e as a function of doping $\delta p = p - p_0$, p_0 being the doping for which $E_F = E_S$; $p_0 = 0.20$ hole/copper atom in the CuO₂ plane. Figure 2 represents the various experimental points taken from Fig. 5 of [2] where the authors plot $E_g/k_B T_{c\text{Max}}$ vs. p . We see that what the authors call pseudogap is exactly our $E_F - E_S$, the distance from the Fermi level to the peak in the D.O.S.

We have also computed the electronic specific heat C_s in the normal state [7] using the same D.O.S. We find that $\gamma = C_s/T$ goes through a maximum with temperature T at a value T^* as found experimentally by Cooper and Loram [8]. In Fig. 3 we compare our computed T^* with the experimental one [8]. The agreement is excellent.

In conclusion, we are able to interpret the NMR and specific heat data in the *normal metallic state*

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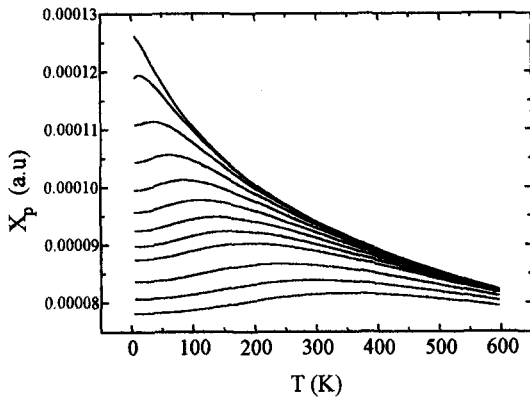


Fig. 1. Calculated Pauli spin susceptibility for $D_e=0$ (upper curve) to 70 meV (lower curve). For $D_e=0$ meV, we find the law [6] in $\ln(1/T)$; for the other doping X_p goes through a maximum with temperature T at a value T^* , then returns to the law in $\ln(1/T)$.

without invoking a pseudogap, but simply by taking into account the logarithmic singularity in the D.O.S.

The “pseudogap” observed by ARPES in the normal state of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ by Ding *et al.* [1] is a shift in the emission edge seen in the $(0, \pi)$ direction but not in the (π, π) direction. This is easily explained by the fact that the saddle points in the band structure are precisely in the $(0, \pm\pi)$ and $(\pm\pi, 0)$ directions. A more detailed calculation will be published later.

We explain the shift between the observed experimental optimum T_c , where $p=0.16$ instead of 0.20,

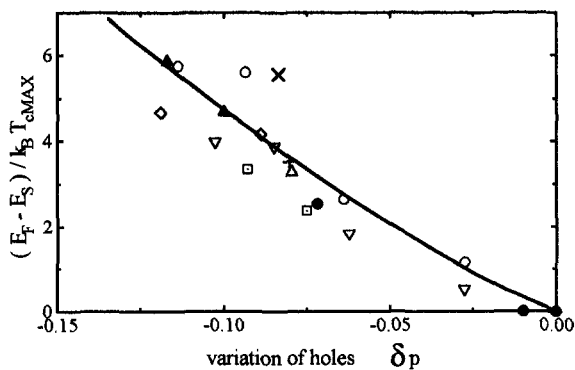


Fig. 2. $D_e = E_F - E_S$ divided by $k_B T_{cMAX}$ ($T_{cMAX} = 110$ K) vs. variation of the hole density calculated from the band structure of formula (1): solid line. The different symbols are the same as in Fig. 5 of [2]; they represent the values of the so-called normal pseudogap divided by $k_B T_{cMAX}$ ($E_g/k_B T_{cMAX}$) obtained from NMR on different compounds. Our calculations are made with a transfer integral $t = 0.25$ eV; δp is taken as zero for $p = 0.20$.

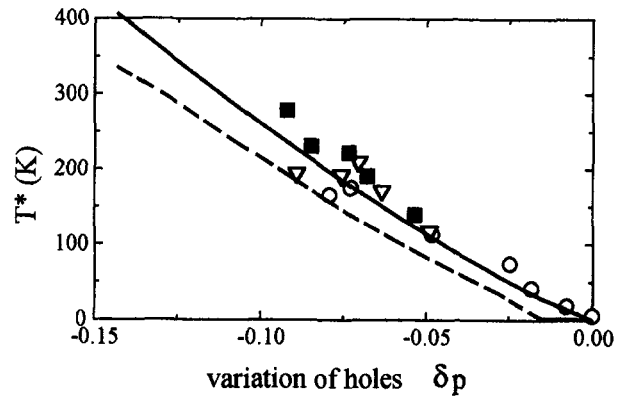


Fig. 3. The temperature, T^* , where the calculated χ_p (dashed line) and the specific heat (solid line) go through a maximum, vs. δp . For comparison we show the results presented in Fig. 27 of [8]. The symbols are the same (solid squares: from thermoelectric power; circles: from specific heat; triangles: from NMR Knight shift data).

and the expected optimum T_c at $E_F = E_S$ or $D_e = 0$, by the fact that in our first calculations [9] we have not taken into account the variation of the 3D screening parameter $q_0 a$ as a function of D_e . These calculations are in progress and show the competition between the effect of the position of the v.H.s. and the value of $q_0 a$ for getting the optimum T_c , this competition depending on the compound. When the overdoping increases, i.e., the density of free carriers increases, $q_0 a$ increases too, and in our model this leads to a decrease in T_c (Fig. 4). This is why for $D_e = 0$, or number of holes = 0.20, we do not have the optimum T_c ,

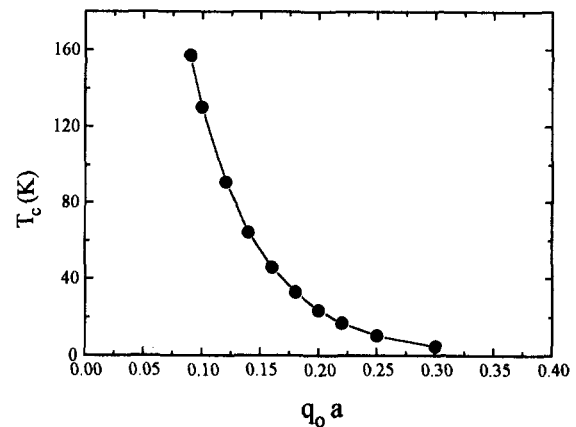


Fig. 4. Variation of the critical temperature T_c as a function of the screening parameter $q_0 a$. This calculation is made with the Bouvier-Bok model [9] for $E_F = E_S$.

and why the logarithmic law for χ_p is found in the overdoped range. In the underdoped range with respect to the observed optimum T_c (i.e., density of free carriers decrease), q_0a decreases too, but the Fermi level departs too far from the singularity to obtain high T_c . In this way our results agree completely with the experimental observations.

Note that our model is valid only in the metallic state. It has been shown by Boebinger *et al.*, [10] that LaSrCuO, for example, undergoes a metal-insulator transition in the underdoped regime as a function of temperature in the normal state. This insulator-metal transition appears at a temperature lower than what we call T^* in this paper. Of course our model is not valid for very low doping levels.

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