1 SCIENTIFIC HIGHLIGHT OF THE MONTH

Quasi-particles and Van Hove Scenario for the Superconducting Cuprates

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The Van Hove Scenario

In the simplest, BCS, microscopic theory of superconductivity the gap Δ in the excitation spectrum of the superconducting state is the order parameter. At zero temperature it is determined by the gap equation [1]:

$$\frac{1}{u} = \int_{\varepsilon_F}^{\hbar\omega_D+\varepsilon_F} d\varepsilon \frac{N(\varepsilon)}{2\sqrt{(\varepsilon-\mu)^2+\Delta^2}}, \tag{1}$$

where $N(\varepsilon)$ is the normal state density of states, $\mu \cong \varepsilon_F$ is the chemical potential, ε_F is the Fermi energy, ω_D is the Debye frequency, and u is the coupling constant which describes the strength of the electron-electron attraction. Here $\hbar = h/2\pi$. Usually, $N(\varepsilon)$ does not vary much on the

small energy scale of eV and thus it may be replaced in Eq. (1) by its value at the Fermi energy, $N(\varepsilon_F)$, independent of ε. Then Eq. (1) can be solved and one finds the well known result that $\Delta \approx 2\ h\ \omega_D\ \exp(-\frac{1}{uN(\varepsilon_F)})$. Evidently, this argument breaks down if $N(\varepsilon)$ varies rapidly on the scale of $h\omega_D$, as it would for ε_F near a Van Hove singularity (VHS). Typically, such a singularity is defined by $\bar{\bigtriangledown}\varepsilon_{\mathbf{k}} = 0$ and leads to a logarithmic dependence, $N(\varepsilon) \cong \ln(\varepsilon - \varepsilon_{VHS})$, of the density of state in Eq. (1). This changes the solution of Eq. (1) dramatically giving rise to a significantly larger gap Δ than the famous BCS result above. Since $k_B T_c \cong \Delta$, the larger gap Δ implies larger transition temperature T_c, and hence we conclude that T_c is enhanced if, without changing the coupling constant u, ε_F approaches the Van Hove singularity at ε_{VHS}.

As was noted by Friedel [2] and Markiewicz [3, 4] the above enhancement, which could be as much as a factor of 5 to 10, of T_c may have an important role to play in the explanation of high T_c superconductivity. In short, they have argued that whatever is the mechanism of attraction, it may be of modest strength if T_c is enhanced by the nearness of ε_F to ε_{VHS}. Over the last 10 years this Van Hove Scenario retained and even increased its attraction for two reasons. Firstly, the salient empirical fact about the high T_c superconductors turned out to be the rise and fall of T_c with the carrier concentration n, namely doping. Evidently, such behaviour can be readily explained if we assume that on doping ε_F approaches and then passes a Van Hove singularity at ε_{VHS} [4]. Secondly, in the first-principles, parameter free, calculations of the electronic structure, for most high temperature superconductors a Van Hove singularity was found near ε_F [5]. The point of this contribution is to highlight recent developments, which goes beyond merely noting that high T_c occurs in materials with ε_{VHS} near ε_F, and to report on results of actual calculations of T_c as a function of doping.

Semiphenomological Models of the Attractive Interactions

In a first-principles calculation of the electronic structure in the normal state one often seeks the wave function in the form

$$\psi_\nu(\mathbf{r}) = \sum_{L,R} \psi^\nu_{L,R} \phi_L(\mathbf{r} - \mathbf{R}), \tag{2}$$

where L and $\mathbf{R}$ label a complete set of orthogonal orbitals and the lattice sites, respectively, and solves an energy eigenvalue equation for the amplitudes $\psi^\nu_{L,R}$:

$$\sum_{L',R'} H_{LR,L'R'} \psi^\nu_{L',R'} = E_\nu \psi^\nu_{L,R}. \tag{3}$$

In the superconducting state an excitation has an amplitude, $u_\nu(\mathbf{r})$, that is a particle and another, $v_\nu(\mathbf{r})$, that is a hole and these two satisfy a coupled set of Bogoliubov-de Gennes equations [4]. The analogue of Eq. (2) is the expansion [6]

$$\begin{bmatrix} u_\nu(\mathbf{r}) \\ v_\nu(\mathbf{r}) \end{bmatrix} = \sum_{RL} \varphi_L(\mathbf{r} - \mathbf{R}) \begin{bmatrix} u^\nu_{RL} \\ v^\nu_{RL} \end{bmatrix}. \tag{4}$$

where the spinor $\begin{bmatrix} u^{\nu}_{RL} \\ v^{\nu}_{RL} \end{bmatrix}$ satisfies the Bogoliubov-de Gennes equations:

$$\sum_{RL} \begin{bmatrix} H_{R'L',RL} - \mu\delta_{R'L',RL} & \Delta_{R'L',RL} \\ \Delta^{*}_{RL,R'L'} & -H_{R'L',RL} + \mu\delta_{R'L',RL} \end{bmatrix} \begin{bmatrix} u^{\nu}_{RL} \\ v^{\nu}_{RL} \end{bmatrix} = E_{\nu} \begin{bmatrix} u^{\nu}_{RL} \\ v^{\nu}_{RL} \end{bmatrix}. \tag{5}$$

which is the analogue of Eq. (3). The pairing potential, which in the simple BCS theory is the gap Δ, can be calculated from the pairing amplitude:

$$\chi_{RL,R'L'} \equiv \sum_{\nu} \left[1 - f\left(E_{\nu}\right)\right] u^{\nu}_{RL}\, {v^{\nu}_{R'L'}}^{*} - f\left(E_{\nu}\right) u^{\nu}_{R'L'}\, {v^{\nu}_{RL}}^{*}, \tag{6}$$

using the relation:

$$\Delta_{RL,R'L'} = \sum_{R_1L_1} \sum_{R'_1L'_1} K_{RL,R'L';\,R_1L_1,R'_1L'_1}\; \chi_{R_1L_1,R'_1L'_1}, \tag{7}$$

where the kernel K describes the electron-electron attraction.

In the normal state H depends on the amplitudes $\psi^{\nu}_{L,R}$. For instance this relationship may be that implied by the Local Density Approximation (LDA). Thus, as is well known, Eq. (3) is a self-consistant field problem. Typically, solving the Kohn-Sham equation using the LMTO method takes this form.

It turns out that Eq. (5), which describes the superconducting ground state, can also be regarded as a Kohn-Sham equation of density functional theory with the apropriate broken (gauge) symmetry. In fact this theory is analogous to spin-density functional theory with the pairing amplitude, χ, replacing the magnetization density m as the order parameter.

Evidently, the principle new feature of the superconductivity problem is the interaction kernel K, which is largely unknown. Nevertheless, progress can be made by parametrizing it in terms of phenomenological constants [6]. In fact what appears to be a useful approach is to simplify Eq. (7) by keeping only the diagonal parts of K and using the coefficients in

$$\Delta_{RL,R'L'} = K_{RL,R'L'}\; \chi_{RL,R'L'}, \tag{8}$$

as adjustible parameters. In any given practical calculations, so far, only one of these parameters was allowed to be nonzero and its value was fixed by demanding that the critical temparature T_c, above which $\chi_{RL,R'L'}$, and therefore $\Delta_{RL,R'L'}$, work out to be zero, agrees with experiments. In short, the strategy for calculating the electronic structure in the superconducting state is to take a Hamiltonian matrix (function of the amplitudes and orbitals) which works well in the normal state and add to it the one parameter (K) pairing potential Δ.

T_c versus Doping

The first implementation of the above procedure [6, 7] was based on H corresponding to the eight-band model of Andersen *et al.* [8] for the high T_c cuprates ($YBa_2Cu_3O_7$). Interestingly, from the point of view of our present concern the bands resulting from this H featured a

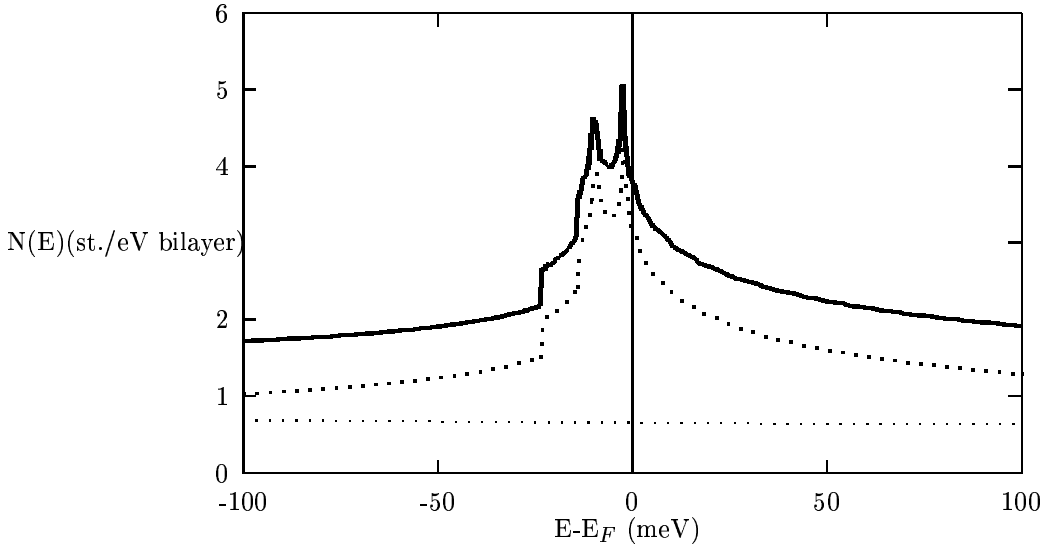

Figure 1: The normal-state density of states in the neighbourhood of the Fermi level for the eight odd (thick dots) and eight even (thin dots) CuO_2 plane-bands of $YBa_2Cu_3O_7$, as well as their sum (full curve). The two logarithmic van Hove singularities are due to the saddle-points of the odd plane-band near respectively X and Y. Here 'odd' and 'even' refer to the symmetry of the wave functions with respect to the mirror plane between the two CuO_2 layers of the bilayer.

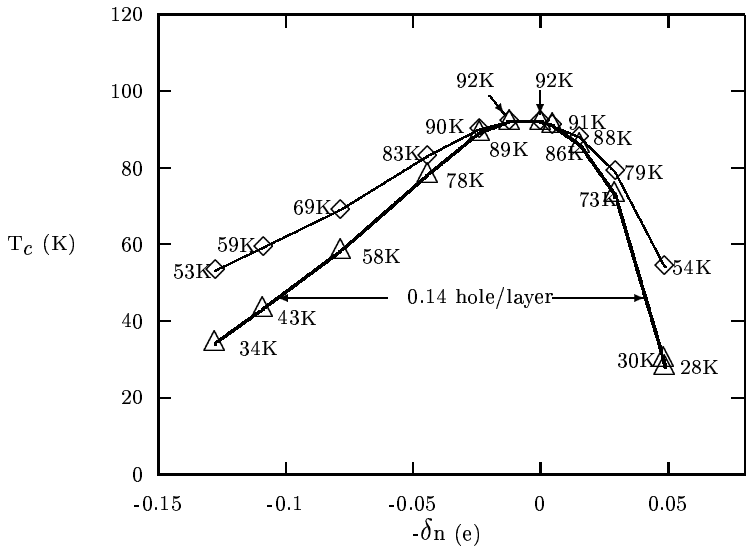

Figure 2: T_c versus deviation of the number of holes from that at optimal doping for the CuO_2 bilayer of $YBa_2Cu_3O_7$. The thick solid curve with triangles corresponds to the intra-layer nearest-neighbour Cu $d_{x^2-y^2}$–Cu $d_{x^2-y^2}$ scenario (d–wave superconductivity), while the thin solid curve with diamonds represents the on-site Cu $d_{x^2-y^2}$–Cu $d_{x^2-y^2}$ scenario (s–wave superconductivity). On both curves T_c's corresponding to different hole concentrations are marked.

prominent (bifurcated) Van Hove singularity. A consequence of this is the two sharp peaks in the density of states shown in Fig. 1.

On introducing the electron-electron attraction, the scenario which turned out to be most interesting was the one in which the interaction, K, operated between electrons, with opposite spins, on nearest neighbour Cu sites, occupying $d_{x^2-y^2}$ orbitals. The coupling constant which gives T_c=92K turned out to be K=0.68 eV. With this one phenomenological constant fixed, a number of other physical properties, such as the low temperature specific heat and the quasi-particle spectra, were calculated in good, quatitative agreement with experiments [6].

At this stage the scene was set to investigate the influence of Van Hove singularities on the superconducting properties in the context of a realistic description of the electronic structure in the normal state. To mimic the effects of doping the chemical potential was changed as one would in making a rigid band argument but of course the interaction constant K was kept the same. The very encouraging result for the T_c vs. doping is shown in Fig. 2. Evidently, the Van Hove scenario works and, suprisingly, the width of the peak is in good agreement with the width of 0.15 holes per layer found empirically.

Effects of Disorder

A serious, general, objection one can raise against the above arguments is that doping, inevitably, brings with it disorder which will smear out, and render ineffective, the Van Hove singularity. To investigate the force of this criticism Litak *et al.* [9] have studied the effect of disorder scattering on the Van Hove scenario on the basis of a model with reduced realism. In fact, they have used a one band, extended, negative U Hubbard model which, in the Hartree-Fock-Gorkov approximation, gave rise to a simplified version of the Bogoliubov-de Gennes equation in Eq. (5). The disorder was introduced into the problem by allowing the site energies, ε_i, to take values $\delta/2$ and -$\delta/2$ randomly, and it was treated in the Coherent Potential Approximation (CPA) [10]. The calculations were performed for nearest neighbour hopping on a square lattice for which the normal state featured the well known prototype of Van Hove singularity at the band center. The way the corresponding peak is smeared by disorder is illustrated in in Fig. 3, where we show the density of states for different strength, δ, of disorder as calculated by the CPA procedure in the normal state.

Thus the question is "how does this gradual broadening of the central peak affects the doping dependence of the transition temperature T_c?". For the particular case at hand this is answered in Fig. 4 where we show the results of the CPA calculation for the superconducting state. Evidently, with increasing disorder the enhancement of T_c by the Van Hove singularity fades gradually in agreement with the experiments depicted in Fig. 5. Thus, we conclude that simple calculations support the suggestion that the high T_c in the cuprates comes about as a result of a relatively weak pairing force being enhanced by the closeness of a Van Hove singularity to the Fermi energy.

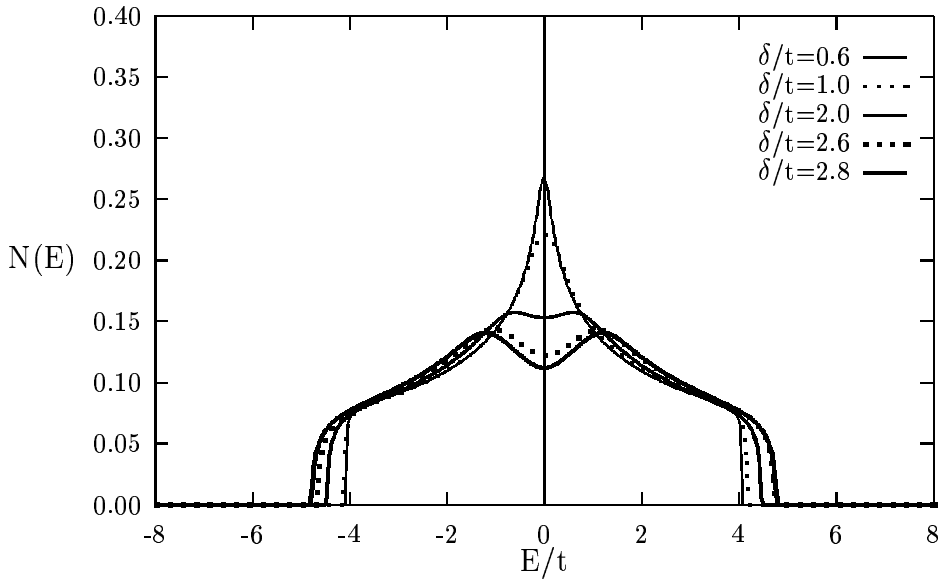

Figure 3: Density of states $N(E)$ for a normal state with various disorder strengths $\delta = \epsilon_A - \epsilon_B$ ($A_{0.5}$ $B_{0.5}$).

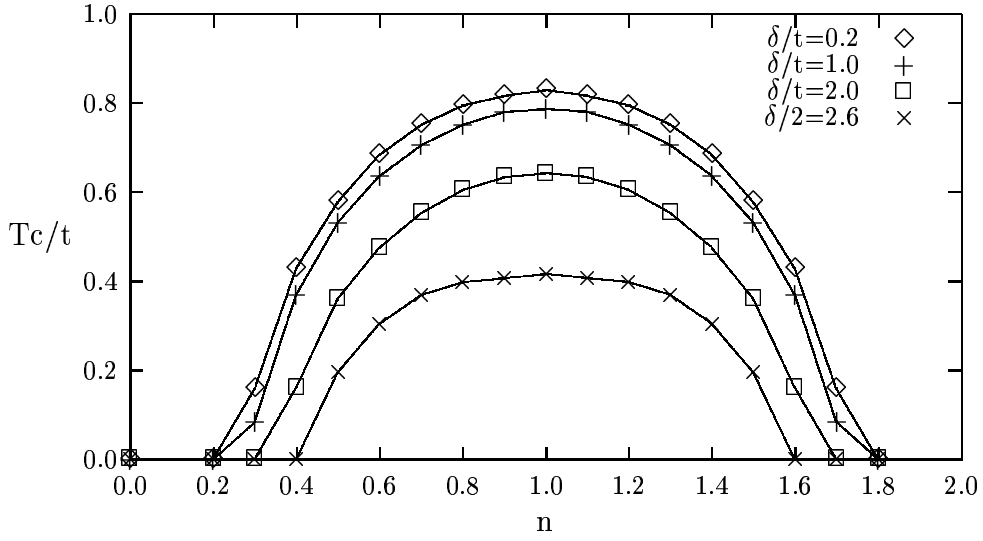

Figure 4: Critical temperature T_c vs. band filling n for d wave superconductors with a number of disorder strengths δ.

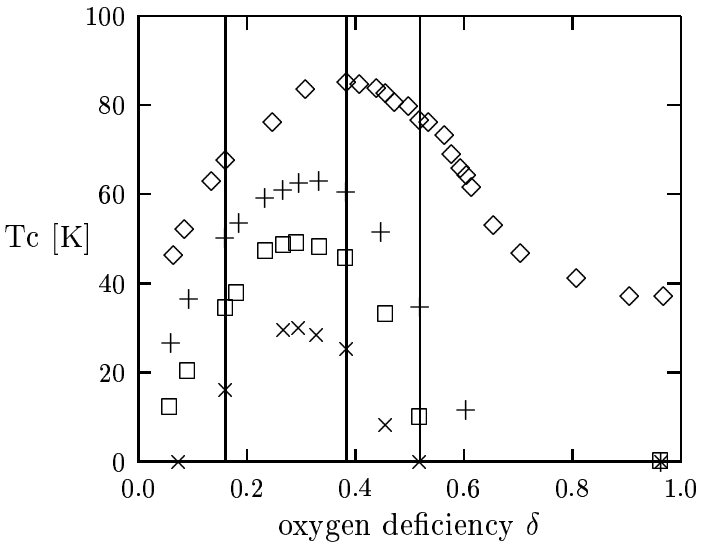

Figure 5: Critical temperature T_c as a function of oxygen deficiency δ for $Y_{0.8}Ca_{0.2}Ba_2(Cu_{1-y}Zn_y)_3O_{7-\delta}$ with $y = 0$ ($\diamond$), $y = 0.02$ (+), $y = 0.04$ ($\square$), $y = 0.06$ ($\times$) [11].

References

[1] M.Tinkham, 'Introduction to Superconductivity' (Second eddition Krieger, 1980).

[2] J. Friedel, J. Phys. Condens. Matter **1** (1989) 7757.

[3] R.S. Markiewicz and B.C.Giessen, Physica C **160** (1989) 497.

[4] R.S. Markiewicz, J. Phys. Chem. Solids **58** (1997) 1173.

[5] D.L. Novikov and A.J.Freeman, in J. Klamut, B.W. Veal, B.M. Dabrowski, P.W. Klamut, M. Kazimierski (Eds.), 'Recent Developments in High Temperature Superconductivity' (Springer Verlag 1996).

[6] B.L. Gyorffy, Z. Szotek, W.M. Temmerman, O.K.Andersen, and O. Jepsen, Phys. Rev. B **58**, 1025-1042 (1998).

[7] Z. Szotek, B.L. Gyorffy, W.M. Temmerman, and O.K. Andersen, Phys. Rev. B **58**, 522-526 (1998).

[8] O.K. Andersen, O. Jepsen, A.I. Liechtenstein, and I.I. Mazin, Phys. Rev. B **49**, 4145 (1994).

[9] G. Litak, A.M. Martin, B.L. Gyorffy, J.F. Annett, K.I. Wysokinski, Physica C **309** (1998) 257-262.

[10] G. Litak, K.I. Wysokinski, R. Micnas, S. Robaszkiewicz, Physica C **199** (1992) 191.

[11] C. Bernhard, J.L. Tallon, C. Bucci, R. De Renzi, G, Guidi, G.V.M. Willians and Ch. Niedermayer, Phys. Rev Lett. **77**, 2304 (1996).