Properties of the gap energy in the van Hove scenario of high-temperature superconductivity

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An exact transition-temperature (T_c) formula is derived within the van Hove scenario of BCS phonon-mediated pairing theory consisting of a logarithmic singularity in the density of states (DOS) at the Fermi energy. Also evaluated are a near-exact zero-temperature gap-energy expression along with an exact (numerical) temperature-dependent gap energy. Though T_c is greatly enhanced over the conventional BCS (constant DOS) value for given (weak) coupling, the zero-temperature gap-to-T_c ratio and the temperature-dependent gap energy both differ little from the BCS values.

A van Hove singularity scenario (VHS) in the electronic density of states (DOS) was initially proposed[1] to explain T_c enhancement in $A15$ superconductors over and above the T_c predicted by BCS (constant DOS) theory. Interest in this mechanism for higher T_c's was revived[2] by the discovery of high-T_c superconductivity in the cuprates.

Since the origin of cuprate superconductivity is to be found in the CuO_2 planes, which are weakly coupled together along the perpendicular axis, their electronic structure will be quasi-two-dimensional (2D). This necessarily leads to at least one VHS coinciding with a saddle point in the $\epsilon(\mathbf{k})$ surface, these saddle points being present in all 2D band structures. Within this scenario, Newns *et al.*[3] have recently given a good description in cuprates with weak-coupling BCS phonon-mediated pairing, of (a) the maximum in T_c with doping, (b) the width in doping of the T_c maximum, and (c) the isotope-shift minimum. Of particular significance in their general approach is the appearance of a T_c formula scaling with T_F (the Fermi-temperature characteristic of the material, through the carrier concentration), a phenomenon emphasized by muon-spin-relaxation measurements carried out on *all* exotic superconductors (2D-like cuprates and organics, as well as 3D-like bismuthates, Chevrel phases, heavy-fermion metals, fullerides, etc.) by Uemura *et al.*[4] A basic requirement for a BCS treatment with *any* particular DOS is that Cooper pairs do indeed exist, and this has been established[5] for the VHS.

In this paper we extend these studies by evaluating an *exact* T_c formula, a near-exact zero-temperature gap energy $\Delta(0)$, and an exact (numerical) temperature-dependent gap energy $\Delta(T)$ within the VHS approach to superconductivity. We show that the gap-to-T_c ratio varies little from the BCS (constant DOS) universal value $2\Delta(0)/k_BT_c = 3.53$, as does $\Delta(T)$, both results being at odds with recent experimental data of these two quantities.[6] Although one should start from the Eliashberg equations, Tsuei *et al.*[7] suggest that the BCS gap equation is probably a good first step.

We begin with the equation for the finite-temperature gap energy $\Delta(T)$, with a general density of states $N(E)$, namely,

$$\frac{2}{V} = \int_{E_F-\hbar\omega_D}^{E_F+\hbar\omega_D} \frac{dE}{\sqrt{(E-E_F)^2+\Delta^2(T)}} N(E) \times \tanh \frac{\sqrt{(E-E_F)^2+\Delta^2(T)}}{2k_BT_c}, \tag{1}$$

where V is a positive coupling constant representing the electron-phonon interaction, which is nonzero in a narrow shell of thickness $2\hbar\omega_D$ centered about the Fermi energy E_F. We also assume a van Hove singularity DOS of the form

$$N(E) \equiv N_0 \ln \left| \frac{E_F}{E-E_F} \right|. \tag{2}$$

Tsuei *et al.*[7] obtain an *approximate* T_c formula from (1) and (2) from the condition $\Delta(T_c) \equiv 0$, by approximating $\tanh x \simeq x$ $(x<1)$, $\tanh x \simeq 1$ $(x>1)$; we derive an *exact* T_c formula as follows. Putting $x \equiv (E-E_F)/2k_BT_c$, $Z \equiv \hbar\omega_D/2k_BT_c \equiv \Theta_D/2T_c$, and $W \equiv E_F/2k_BT_c \equiv T_F/2T_c$, in (1) and (2) with $\Delta(T_c)=0$, one obtains

$$\frac{1}{N_0V} = \int_0^Z dx \frac{\tanh x}{x} \ln \frac{W}{x}. \tag{3}$$

Integrating this by parts gives

$$\frac{1}{N_0V} = \tanh Z \ln Z \ln \frac{W}{Z} + \frac{1}{2} \tanh Z \ln^2 Z - D(Z,W), \tag{4}$$

$$D(Z,W) \equiv \int_0^Z dx \left(\ln x \ln \frac{W}{x} + \frac{1}{2} \ln^2 x \right) \mathrm{sech}^2 x. \tag{5}$$

Multiplying both sides of (4) by $2\coth Z$, adding $\ln^2(W/Z)$, and rearranging, leads to

$$\left[\frac{1}{N_0V} + D(Z,W) \right] 2\coth Z + \ln^2 \frac{W}{Z} = \ln^2 W, \tag{6}$$

which on exponentiation leaves the exact (implicit) T_c formula given by

$$T_c = \frac{1}{2} T_F \exp\left\{ - \left[\left(\frac{1}{N_0 V} + D\left(\frac{\Theta_D}{2T_c}, \frac{T_F}{2T_c}\right) \right) 2 \coth \frac{\Theta_D}{2T_c} + \ln^2 \frac{T_F}{\Theta_D} \right]^{1/2} \right\}. \quad (7)$$

This result was found to give T_c values roughly 15% *smaller* than Eq. (3) of Ref. 7, for a given N_0V, Θ_D, and T_F, as shown below.

As one is also interested in the gap-to-T_c ratio $2\Delta(0)/k_BT_c$ predicted by the van Hove scenario, we shall derive an expression for $\Delta(T)$ at $T = 0$ using (1) and (2). Thus

$$\frac{2}{N_0 V} = \int_{E_F-\hbar\omega_D}^{E_F+\hbar\omega_D} \frac{dE}{\sqrt{(E-E_F)^2 + \Delta^2(0)}} \ln \left| \frac{E_F}{E - E_F} \right|. \quad (8)$$

Putting $\xi \equiv E - E_F$, integrating by parts, and simplifying gives

$$\frac{1}{N_0 V} = \ln\left(\frac{E_F}{\hbar\omega_D}\right) \sinh^{-1}\left(\frac{\hbar\omega_D}{\Delta(0)}\right) + \int_0^{\hbar\omega_D} \frac{d\xi}{\xi} \sinh^{-1} \frac{\xi}{\Delta(0)}. \quad (9)$$

Since one can typically expect $\hbar\omega_D/\Delta(0) > 1$, the expansion

$$\sinh^{-1} x = \ln|2x| + \sum_{k=0}^{\infty} \frac{(-1)^{k+1}(2k)!}{2^{2k}(k!)^2 2k x^{2k}} \quad (x > 1) \quad (10)$$

may be employed in the integral term of the right-hand side of (9) if the integral is broken up into *two* integrals, from 0 to $\Delta(0)$ and from $\Delta(0)$ to $\hbar\omega_D$. The first such integral then gives

$$A_1 \equiv \int_0^1 \frac{dy}{y} \sinh^{-1} y \simeq 0.955202. \quad (11)$$

The second integral will involve the expansion

$$\int \frac{dx}{x} \sinh^{-1} \frac{x}{a} = \frac{1}{2} \ln^2(2x/a) - \frac{(a/x)^2}{8} + \frac{3(a/x)^4}{128} - \cdots \quad (x > a). \quad (12)$$

Hence, neglecting terms of order $\Delta(0)^2$ and higher, (9) becomes

$$\frac{1}{N_0 V} = \ln \frac{E_F}{\hbar\omega_D} \sinh^{-1} \frac{\hbar\omega_D}{\Delta(0)} + A_1 + \frac{1}{2} \ln^2 \frac{2\hbar\omega_D}{\Delta(0)} + A_2 + O\left(\left[\frac{\Delta(0)}{\hbar\omega_D}\right]^2\right), \quad (13)$$

where

$$A_2 \equiv \tfrac{1}{2}\ln^2 2 - \tfrac{1}{8} + \tfrac{3}{128} - \cdots \simeq 0.132735. \quad (14)$$

Solving for $\Delta(0)$ by exponentiation gives the near-exact expression

$$\Delta(0) \simeq 2k_BT_F \exp\{-[2/N_0V + \ln^2(T_F/\Theta_D) - 1.64]^{1/2}\}. \quad (15)$$

Table I lists values of the dimensionless coupling N_0V consistent with the two typical high-T_c values of 40 K and 90 K cited in Ref. 7, along with the Θ_D and T_F values quoted there, as given by the BCS (constant DOS) T_c formula $T_c = 1.13 \exp^{-1/N_0V}$ and by the exact T_c formula (7). We note that the exact T_c formula (7) requires values of N_0V only moderately larger than those of Ref. 7, and roughly one-quarter those needed with the BCS T_c formula. We see that in (13) the magnitude of the lowest-order neglected term is only about 15% the lowest-order term retained, for the specific case $N_0V = 0.164$, $\Theta_D = 300$ K, $T_F = 8807$ K, and less than 1% of the dominant term. Also listed in the last column are the gap-to-T_c ratios $2\Delta(0)/k_BT_c$ resulting from (7) and (15). These values are somewhat larger than the BCS (constant DOS) value of $2\pi/e^\gamma \simeq 3.53$, where γ is the Euler constant, though definitely smaller than experimental values as high as 12 that have been reported[6] for Y-Ba-Cu-O and Bi-Sr-Ca-Cu-O. The modest increase of our $2\Delta(0)/k_BT_c$ over the BCS value of 3.53 is consistent with the variation of from about 4 down to about 2.8 obtained[8] with a power-law DOS $N(E) = N_0(E - E_F)^\alpha$,

TABLE I. Dimensionless coupling N_0V consistent with two typical high-T_c values characteristic of La-Sr-Cu-O and Y-Ba-Cu-O, respectively, for some typical Debye (Θ_D) and Fermi (T_F) characteristic temperature values as cited in Ref. 7, using (a) the BCS (constant DOS) T_c formula $T_c = 1.13\Theta_D e^{-1/N_0V}$, (b) approximate T_c formula of Ref. 7 with a VHS DOS, and (c) exact T_c formula (7). Gap-to-T_c ratio $2\Delta(0)/k_BT_c$ evaluated with (7) and (15) is also listed.

T_c (K)	Θ_D (K)	T_F (K)	N_0V			$2\Delta(0)/k_BT_c$
			BCS	Ref. 7	Eq. (7)	
40	400	5548	0.412	0.093	0.100	3.64
(La-Sr-Cu-O)	500	5548	0.378	0.088	0.095	3.66
	754	5580	0.327	0.082	0.086	3.53
	300	8807	0.754	0.148	0.164	3.60
90	400	8807	0.620	0.130	0.143	3.63
(Y-Ba-Cu-O)	754	8807	0.445	0.106	0.115	3.68

TABLE II. Temperature dependence of gap energy $\Delta(T)/\Delta(0)$ vs T/T_c in the BCS (constant DOS) theory as reported in Ref. 9 compared with the BCS (VHS DOS) of the present work.

T/T_c	$\Delta(T)/\Delta(0)$		% deviation
	BCS (Ref. 9)	Eqs. (1) and (2)	
1.0	0.0	0.0	0.0
0.98	0.2436	0.2447	0.5
0.92	0.4749	0.4769	0.4
0.86	0.6117	0.6141	0.4
0.80	0.7110	0.7135	0.4
0.74	0.7874	0.7897	0.3
0.68	0.8471	0.8493	0.3
0.62	0.8939	0.8958	0.2
0.56	0.9299	0.9315	0.2
0.50	0.9569	0.9582	0.1
0.40	0.9850	0.9857	0.1
0.30	0.9971	0.9973	0
0.20	0.9999	0.9999	0
0.0	1.0	1.0	0

as α is varied from about -0.8 to $+0.8$, but apparently excluding $\alpha = 0^-$, which corresponds to the VHS DOS (2) employed here. The present paper has been motivated in part by this omission as well as by the need to rule out a singular behavior in the gap-to-T_c ratio in the vicinity of $\alpha = 0$ as a possible explanation for the "anomaly" reported in Ref. 8.

Finally, from (1) with (2) can also be deduced, without approximation, the temperature dependence of the gap energy, viz., $\Delta(T)/\Delta(0)$ vs T/T_c. This was evaluated numerically and is compared in Table II with the BCS (constant DOS) results in Ref. 9. Our results correspond to the largest gap-to-T_c value of Table I, namely to $T_c = 90$ K, $\Theta_D = 754$ K, $T_F = 8807$ K, and $2\Delta(0)/k_BT_c = 3.68$. This case was found to present the largest numerical deviation from the BCS $\Delta(T)$ results and is seen to be *at most about* 0.5%.

In conclusion, we report an exact T_c formula which follows from the BCS gap equation with a VHS DOS. This formula produces T_c values about 15% smaller than the approximate T_c formula of Ref. 7, for given Θ_D, T_F, and N_0V values. A near-exact expression for $\Delta(0)$ along with the exact T_c formula gives a gap-to-T_c ratio $2\Delta(0)/k_BT_c$ deviating very little from the BCS (constant DOS) value of 3.53. Finally, the corresponding exact temperature dependence gap energy $\Delta(T)$ differs at most by only about 0.5% from the BCS function.

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