Vertex correction to pairing at a Van Hove singularity

H. R. Krishnamurthy, D. M. Newns, P. C. Pattnaik, C. C. Tsuei, and C. C. Chi
IBM Research Division, T. J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598
(Received 20 August 1993)

We calculate in a k-averaging approximation, the vertex corrections for pairing at a Van Hove singularity mediated by an Einstein phonon. The vertex correction leads to a modest reduction in T_c, which can still reach the experimental values for realistic phonon couplings, and to a significant deepening of the dip in the isotope shift at the T_c maximum. Interference between first- and second-order vertex graphs diminishes the effect of the Coulomb interaction on T_c. The isotope-shift dip is shallower for repulsive Coulomb interaction, and deeper in the case of an attractive interaction introduced to model an excitonic contribution to pairing.

I. INTRODUCTION

One of the proposed mechanisms for achieving the high transition temperatures characteristic of cuprate superconductors involves[1-6] a combination of the logarithmic density-of-states (DOS) peak [Van Hove singularity (VHS)] associated with the saddle point in the band structure—now observed in photoemission on several materials[7]—together with a relatively high-frequency mediating excitation. The excitation considered is either an optical phonon or an electronic excitation. The transition temperature in this mechanism characteristically peaks when the Fermi level lies at the VHS, and in the case of phonon-mediated pairing it is also found[1,4] that the isotope shift has a minimum at the same point. These concepts form an explanation for the combination of the T_c maximum with an isotope shift minimum seen experimentally.[8]

This Van Hove-boosted type of phonon mechanism has been examined at the BCS (Refs. 1–4) and Eliashberg[4-6] levels, but a cause for concern is that the conditions required to give high transition temperatures (DOS peak combined with high excitation frequency) are also such as to produce larger vertex corrections[9] which are depairing in sign, and which tend to eliminate the enhancement in transition temperature generated by the VHS. In the case of Einstein phonons a rough estimate of the magnitude of the paring vertex to second order in the electron-phonon coupling energy shows that vertex corrections are down by the factor (dimensionless coupling)×(phonon frequency)×(DOS at phonon frequency), times a numerical factor:

$$\lambda_{\rm ef}\left[1-\frac{5\pi^2}{8}\lambda_{\rm ef}\frac{\omega_E}{D}\ln\left[\frac{D}{\omega_E}\right]\right]. \tag{1}$$

In (1) the first term is the Eliashberg term, and the second comes from the vertex corrections. $\lambda_{\rm ef}$ is the dimensionless coupling in the strip of width ω_E around the Fermi level [in the notation below $\lambda_{\rm ef}=(V_p/2D)\ln(D/\omega_E)$], ω_E is the Einstein phonon frequency, and D is the half-bandwidth. Taking typical values $\omega_E=0.06$ eV, $D=1$ eV, and $\lambda_{\rm ef}\sim 1$, the vertex correction in (1) is seen to be equal to the first, Eliashberg, term, which it effectively cancels. There would seem to be a strong possibility that this large depairing vertex correction effect eliminates the high transition temperature found in Eliashberg approximation at the van Hove singularity.

In this paper we address the vertex correction problem[10] numerically in a realistic but slightly simplified model. First we shall restrict ourselves to the Einstein phonon, for which in the first-order (Eliashberg) approximation only fermion propagators which are local, i.e,. summed over **k**, appear. In the second-order approximation, involving the vertex corrections, this simplification is no longer exact, but since it seems unlikely that momentum-dependent effects are significant for Einstein phonons, we make a local k-summation ansatz in order to facilitate calculation of the vertex corrections.

II. CALCULATION OF VERTEX CORRECTIONS

The procedure for calculating the vertex corrections in the case of uniform density of states has been fully detailed by Grabowski and Sham.[10] The results may be obtained by evaluating the diagrams in Fig. 1 using Nambu-Gorkov notation, keeping (for a T_c calculation) only terms up to first order in the gap. The gap insertion may lie in any of the three fermion line segments in the vertex graph in Fig. 1, yielding three conventional Feynman graph contributions[10] to the vertex function.

The interaction propagator in Matsubara notation for Einstein phonons is

$$K(i\nu_n)=\frac{V_p\omega_E^2}{\nu_n^2+\omega_E^2}, \tag{2}$$

where $\nu_n=2\pi nT$ is the even Matsubara frequency, and V_p is the phonon coupling energy. It will also be convenient to introduce the dimensionless coupling $\lambda^0=V_p/2D$.

In the local or k-averaging approximation the normal-state electron propagator is defined as

$$G(i\omega_n)=\int d\varepsilon\frac{\rho(\varepsilon)}{i\omega_n-\varepsilon-\Sigma(i\omega_n)}, \tag{3}$$

where $\rho(\varepsilon)$ is the noninteracting DOS. In the Van Hove case

FIG. 1. Diagrams for self-energy in Nambu notation: left, Eliashberg approximation; right, vertex correction. Solid line, fermion propagator in Nambu notation, wavy line, phonon.

$$\rho(\varepsilon)=-\frac{1}{2D}\ln\left|\frac{\varepsilon-E_s}{D}\right|\Theta(D-|\varepsilon-E_s|)\ , \tag{4}$$

where $\omega_n=(2n+1)\pi T$ is the odd Matsubara frequency, and E_s is the shift of the VHS from the Fermi level (taken as energy zero). $\Sigma(i\omega_n)$ is the normal-state self-energy, given from Fig. 1 by (in a compact notation)

$$\Sigma(n)=T\sum_m K(n-m)G(m) + T^2\sum_{m,r} G(r)G(m)G(n+m-r) \times K(r-m)K(n-r)\ . \tag{5}$$

The linearized gap equation may be written

$$\Delta(n)=T\sum_m \Gamma(n,m)\frac{\mathrm{Im}G(m)\Delta(m)}{\mathrm{Im}\Sigma(m)-\omega_m}\ , \tag{6}$$

where the pairing kernel is given by[10]

$$\Gamma(n,m)=K(n-m)+T\sum_r K(n-m)[K(n-r)G(-r)G(n-m-r)+K(m-r)G(r)G(n-m+r)] + T\sum_r K(n-r)K(m-r)G(r)G(r-m-n)\ . \tag{7}$$

When the second-order terms are dropped from (5) and (7), then (5) and (6) reduce to the standard Eliashberg equations.

The numerical procedure used for calculating T_c is first, defining frequency sums within a cutoff ω_c, to iterate (5) for the normal-state self-energy. Starting from a self-energy, G is calculated using (3), the result inserted in (5), and the loop repeated. This procedure converges to high accuracy in a few iterations. Calculating Γ from (7), and inserting into (6), we have an eigenvalue equation involving eigenvector Δ, which yields T_c when the highest eigenvalue is unity.

III. RESULTS

Let us first consider how the electron-phonon coupling strength may optimally be defined in the nonuniform DOS situation. An unambiguous dimensionless measure of the electron-phonon coupling strength in the calculation is $\lambda^0=V_p/2D$, but this quantity omits the logarithmic enhancement of the DOS near the Fermi level. The Z factor yields a more physical measure of coupling strength; in Eliashberg approximation Z typically falls off monotonically from a fairly large value at low frequency, given in the case of uniform DOS as $Z(0)=1+\lambda$, to unity over a frequency range ω_E. An estimate of the effective coupling near the Fermi level can be then obtained from the excess of the Z factor over unity, more formally $\lambda_E=-\mathrm{Re}\Sigma(i\omega_0)/i\omega_0$. Finally we may introduce λ_{ef} as the electron-phonon matrix element times the DOS at the phonon frequency ω_E, giving $\lambda_{ef}=\lambda^0\ln(D/\omega_E)$.

In Fig. 2 we illustrate, for the case where the Fermi level lies at the VHS, how the Z factor $Z(i\omega_n)=1-\mathrm{Re}[\Sigma(i\omega_n)/i\omega_n]$ varies as a function of Matsubara frequency ω_n for the Eliashberg and vertex levels of approximation. The Z factor is seen in the Eliashberg case to fall off monotonically from the low-frequency value $1+\lambda_E$. However, the effect of the vertex corrections is to reduce the Z factor back towards unity, and this effect is most noticeable at the lowest frequency where the Eliashberg Z factor is largest (Fig. 2), actually giving a minimum in Z around zero frequency. The overall smaller Z is reminiscent of the BCS approximation in which $Z=1$, a result which lends some credence to use of the BCS formalism in treating superconductivity in the van Hove model.[1-4]

In Fig. 3 we compare transition temperature and isotope shift for the Eliashberg and vertex levels of approximation for pure phononic coupling. When the Fermi level lies near the van Hove the DOS is largest and the vertex corrections maximal. Hence T_c is reduced

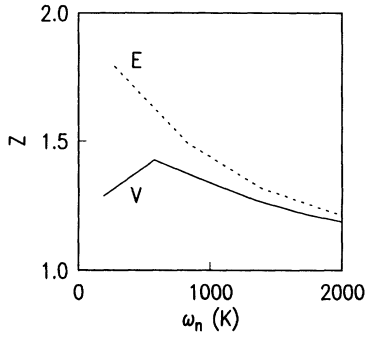

FIG. 2. Reduction in Z factor due to inclusion of vertex corrections is seen in plot of Z factor vs Matsubara frequency at T_c: dashed curve, Eliashberg approximation (labeled E); solid curve, with vertex correction included (labeled V). VHS at Fermi level, parameters are $\omega_E=700$ K, $\lambda^0=0.33$, $\lambda_{ef}=0.88$, $\lambda_E=0.79$, $D=\omega_c=10\,000$ K.

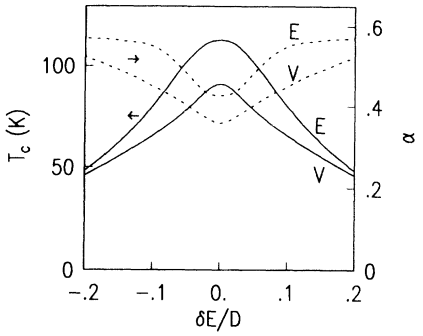

FIG. 3. Reduced T_c and deeper isotope shift minimum due to inclusion of vertex corrections is seen in plot of transition temperature (solid curves) and isotope shift (dotted curves) vs shift δE of VHS from Fermi energy: curves labeled E, Eliashberg approximation; curves labeled V, with inclusion of vertex corrections. Parameters are $\omega_E = 700$ K, $\lambda^0 = 0.40$, $\lambda_{ef} = 1.34$, $\lambda_E = 1.15$, $D = 20\,000$ K, $\omega_c = 10\,000$ K.

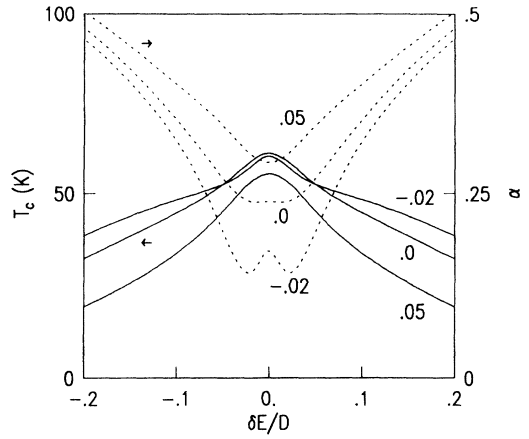

FIG. 4. Transition temperature (solid curves) and isotope shift (dotted curves) plotted vs shift δE of VHS from Fermi energy, with inclusion of vertex corrections, illustrating the effect of the Coulomb interaction, including an attractive interaction to model an excitonic pairing effect. Values of λ_e^0 are 0.05 (repulsive interaction, $\mu^* = 0.113$), 0.0, and -0.02 (attractive interaction, $\mu^* = -0.057$), curves labeled accordingly. Other parameters are $\omega_E = 700$ K, $\lambda^0 = 0.33$, $\lambda_{ef} = 0.88$, $\lambda_e = 0.79$, $D = \omega_c = 10\,000$ K.

significantly relative to Eliashberg in this region, the reduction being less significant away from the VHS where the DOS is lower. Nevertheless, T_c's of order 90 K may still be obtained of realistic couplings $\lambda_{ef} \sim \lambda_E \sim 1$. The isotope shift is also affected by the vertex correction, and acquires a more significant dip at the T_c maximum, in contrast to the shallow minimum in the Eliashberg case.[11]

Next we consider the effect of including an electronic interaction. To introduce a repulsive Coulomb interaction, we add a constant term to the phononic kernel (2):

$$K(\nu_n) \rightarrow K(\nu_n) - V_e \ , \tag{8}$$

where V_e is positive in the repulsive case, and may be parameterized in terms of the coupling constant $\lambda_e^0 = V_e/2D$, or in terms of μ^* which may be defined (for Fermi level at the VHS) as

$$\mu^* = \frac{\lambda_e^0 \ln(D/\omega_E)}{1 + (\lambda_e^0/2)\ln^2(D/\omega_E)} \ . \tag{9}$$

More speculatively, we may also model an attractive electronic (excitonic) interaction by introducing a negative sign for V_e.

In Fig. 4 are illustrated the effects of both a repulsive and attractive Coulomb interaction [for larger values of the interaction V_e with an attractive sign the iteration procedure involving Eqs. (3) and (5) is unstable]. The predominant effect of a small Coulomb interaction from the vertex graph is via the interference term, in which the second diagram in Fig. 1 contains one Coulomb and one phonon interaction line. This interference term is potentially opposite in sign to the conventional Eliashberg Coulomb term (first diagram in Fig. 1), so the two effects combined tend to cancel out the effects of the Coulomb interaction—in principle, the Coulomb effect on T_c could even be counterintuitive in sign, if the vertex contribution were the dominant one.

It is seen from the numerical example presented in Fig. 4 that, due to the above-mentioned cancellation between the Eliashberg and vertex graphs when the Fermi level lies right at the VHS, there results a very small counterintuitive reduction in T_c from an attractive Coulomb interaction, and a very modest reduction in T_c in the case of a repulsive interaction. On the other hand, when the Fermi level is displaced significantly away from the VHS, the Coulomb effect on T_c is larger and now the repulsive (attractive) Coulomb interaction lowers (raises) T_c as expected unintuitively—the Eliashberg term is now seen to be the dominant one again.

The effect on the isotope shift of the relatively small values of the Coulomb interaction in Fig. 4 is quite interesting. The attractive interaction deepens the isotope shift minimum, while the repulsive Coulomb interaction

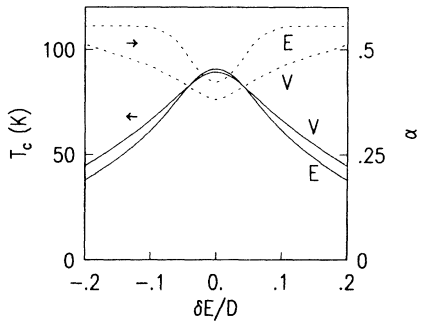

FIG. 5. Transition temperature (solid curves) and isotope shift (dotted curves) plotted vs shift δE of VHS from Fermi energy, for Eliashberg (curves labeled E) and inclusion of vertex corrections (curves labeled V), illustrating cancellation of vertex effect on T_c by a large repulsive Coulomb interaction. Parameters $\omega_E = 700$ K, $\lambda^0 = 0.60$, $\lambda_{ef} = 2.0$, $\lambda_E = 1.58$, $\lambda_e^0 = 0.12$ (repulsive interaction, $\mu^* = 0.24$), $D = 20\,000$ K, $\omega_c = 10\,000$ K.

makes the dip shallower.

The cancellation associated with the vertex correction with one Coulomb and one phonon interaction is expressed in another way in Fig. 5, illustrating results for a rather large repulsive Coulomb interaction. With this choice of parameters the vertex correcting has little effect on T_c, due to cancellation between the diagram with one Coulomb and one phonon interaction, and the diagrams with two phonons and two Coulomb interaction lines.

IV. CONCLUSION

The zeroth-order conclusion from this study is that while phonon vertex corrections are depairing in sign, nevertheless they do not eliminate the strong phononic pairing at a VHS. When realistic values of D in the range 1–2.5 eV are used, together with realistic values of the coupling constant, T_c's in the experimental range for the cuprates are possible.

The effect of the vertex corrections on the isotope shift is significant. The dip in the isotope shift at the maximum T_c becomes more pronounced when they are included, in contrast with the relatively shallow dip obtained in the Eliashberg approximation. The isotope shift results are indeed more similar to the BCS approximation, consistent with the reduced Z factor produced by the vertex corrections.

The Coulomb interaction, normally repulsive, may be also be made attractive as a crude way to model an excitonic pairing contribution. The vertex contribution to first order in a relatively weak Coulomb interaction interferes with the Eliashberg Coulomb contribution so that at the T_c maximum the Coulomb effect on T_c can be small—or, in principle, even counterintuitive in sign. On the other hand, away from the T_c maximum the vertex contribution is relatively smaller and the intuitive reduction in T_c by a repulsive (or increase in T_c by an attractive) Coulomb interaction occurs.

The Coulomb interaction also has a strong effect on the isotope shift, the shift at the T_c maximum being reduced in the presence of a relatively weak attractive interaction, and increased by a repulsive interaction.

From these results it is clear that the Eliashberg approximation is useful as a rough guide to the values of T_c to be expected form phononic pairing, but it cannot be relied on more quantitatively, in particular, the isotope shift when vertex corrections are included has a more pronounced minimum than expected from the Eliashberg approximation, in better agreement with the experimental data.

The foregoing results to not trivially reproduce the observed sharp maximum in T_c as a function of Fermi level location together with a deep isotope shift minimum. But if the excitonic attractive contribution were localized near the T_c maximum, as in the saddle-point pairing[12] excitonic mechanism, then T_c would peak sharply and also, from Fig. 4, the isotope shift might have a deep minimum. It remains, however, to demonstrate these conjectures in an explicit calculation at the vertex level of approximation. Of course we recognize the existence of other effects, such as anharmonic phonons, which may further reduce the isotope effect.

One final speculation regarding the interesting phenomenon of interference between the first-order diagram in Fig. 1 when the interaction is Coulombic and the second-order diagram to first order in the Coulomb interaction, which as observed above tends to nullify the effect of Coulomb repulsion, is that it may also occur in other narrow band systems, for example, C_{60}-based systems.

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[11]The present model, in which (3) is evaluated numerically, differs slightly from an earlier approximation (Refs. 4 and 6) in which the step-function cutoff was replaced by a Lorentzian cutoff, and the integral evaluated via a contour. The contour method takes in negative regions of the log and yields a slightly smaller overall coupling constant for the same λ^0. At large δE the numerical model is found systematically to give an isotope shift somewhat greater than the BCS ($\alpha=0.5$) values (see Fig. 3, for example).

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