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# Boson-exchange superconductor model with a Van Hove singularity

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## Abstract

A realistically-shaped electron–boson interaction Eliashberg spectrum  $\alpha^2F(\omega)$  is shown to be crucial in determining superconducting transition temperatures when the Fermi-energy shift from a Van Hove saddle-point singularity lies between the minimum and maximum boson frequencies in  $\alpha^2F(\omega)$ . © 1999 Published by Elsevier Science B.V. All rights reserved.

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A Van Hove scenario (VHS) consisting of a saddle-point singularity at energy  $\epsilon_{\text{VH}}$  in the vicinity of the Fermi energy  $\epsilon_{\text{F}}$  in Eliashberg superconductors is the simplest model of a rapidly-varying electronic density of states (EDOS)  $N(\epsilon)$  [1–12]. Eliashberg superconductivity is caused by charge carriers pairing mediated via some kind of *bosonic excitations* in the correlated electron-ion system. Although the analogous Migdal theorem (allowing neglect of vertex corrections to many-body-perturbation-theoretic Feynmann diagrams) has been proved only for *phonon* mediation, Eliashberg equations are still useful as a first approximation [13,14]. Hopefully, vertex corrections, if important, can be included within effective kernels without modifying the form of the basic equations [13–15].

The behavior of the superconducting transition temperature,  $T_c$ , as a function of the shift  $t \equiv |\epsilon_{\text{F}} - \epsilon_{\text{VH}}|$ , was considered [1] in a modified Eliashberg theory that includes a non-constant EDOS [16–18]. It was found that for large  $t$ , i.e.,  $t > \omega_{\text{max}}$ ,  $T_c$  is insensitive to the EDOS singularity and identical to the familiar McMillan  $T_c$ -formula. But  $T_c$  changes radically if a peak in  $N(\epsilon)$  is close to  $\epsilon_{\text{F}}$ . Qualitatively,  $T_c$  depends only *weakly*, in either extreme  $t < \omega_{\text{min}}$  or  $t > \omega_{\text{max}}$ , on the fine-structure of the frequency distribution of the assumed electron–boson interaction spectrum function  $\alpha^2F(\omega)$  of Eliashberg theory. Any dependence on the  $\alpha^2F(\omega)$  fine structure enters the  $T_c$ -equation only via an average boson frequency  $\omega_{\text{in}}$ , the mass-renormalization factor  $\lambda$ , and possibly through the first few moments of  $\alpha^2F(\omega)$ , [17] – the Coulomb pseudopotential  $\mu_*$  being taken as zero. Thus, two different spectra leading to identical  $\lambda$  and  $\omega_{\text{in}}$  parameters results in *nearly* equal  $T_c(t)$  for either  $t < \omega_{\text{min}}$  and  $t > \omega_{\text{max}}$ . However, the more interesting and realistic case when  $\epsilon_{\text{F}}$  is shifted from  $\epsilon_{\text{VH}}$  by some finite value [10] such that  $\omega_{\text{min}} < t < \omega_{\text{max}}$  has not been studied.

In this Letter we elucidate the effect upon  $T_c$  of a *realistically*-structured  $\alpha^2 F(\omega)$ , for  $t$  lying within the interval  $(\omega_{\min}, \omega_{\max})$ . We ignore all complications arising from possible structural instabilities in a VHS (for an excellent review see [7]), and assume the simplest model for the EDOS, namely  $N(\epsilon) = N_0 \ln(2W/|\epsilon - t|)$  over the entire range of  $\epsilon$  [1,5]. This model may be relevant for any type intermediate boson such as excitons, plasmons, paramagnons, etc., e.g., in cuprate superconductors where  $\epsilon_F$  is closely pinned to the  $\epsilon_{\text{VH}}$  of  $N(\epsilon)$  as now firmly established experimentally [7]. We need not assume that the singular  $N(\epsilon)$  originates from the intrinsic band structure of CuO-planes. Indeed, flat regions of the band structure – leading to singularities in  $N(\epsilon)$  – may arise from the complex electron-electron interactions in *high- $T_c$ -oxides*, but we do not exclude that an intermediate boson necessary for the Eliashberg formalism would be provided by these interactions [19]. Furthermore, one need not specify precisely the interaction spectrum  $\alpha^2 F(\omega)$  which may be *any function of  $\omega$*  over the interval  $(\omega_{\min}, \omega_{\max})$  and zero otherwise. Effects of strong gap-anisotropy found in some high- $T_c$  materials are not considered, although the symmetry of the order parameter may yet prove to be d-wave. If so, the present work would merely suggest the need of more careful consideration of the possible consequences from the ‘ $\epsilon_F$  to  $\epsilon_{\text{VH}}$ -vicinity’ in the corresponding Eliashberg theory. For *s-wave-type symmetry* these effects could be qualitatively included in the treatment given below within the spirit of [20] (see also [21]) – i.e., by means of a mean-square anisotropy factor  $a^2$ .

The Migdal-Eliashberg theory including all the complexities of band structure has been developed by Garland [22]. Ignoring interband and anisotropy effects modifies the relevant equations in a way that incorporates the energy dependence of  $N(\epsilon)$  and leads to equations very similar to those of standard Eliashberg theory. A popular method of analytically solving the Eliashberg equations valid for general  $N(\epsilon)$  [16–18] is described in [1] where the basic gap  $\Delta(i\omega_n)$  and mass renormalization  $\tilde{Z}(i\omega_n)$  functions are related, near  $T = T_c$ , through

$$\Psi(i\omega_n) = \Psi^{\circ}(i\omega_n) + \nu\pi T_c \sum_{m=-\infty}^{+\infty} K(i\omega_n, i\omega_m) \Psi(i\omega_m), \quad (1)$$

where  $\Psi(i\omega_n) \equiv \Delta(i\omega_n)\tilde{Z}(i\omega_n)/\Delta(0)Z(0)$ , and  $\omega_m$  are the Matsubara frequencies. The free term and the kernel in (1) are determined by specific  $\alpha^2 F(\omega)$  and  $N(\epsilon)$  which enter through known functions  $I(\omega_n, \omega_m)$  and  $\tilde{N}(|\tilde{\omega}_m|)$  determined in [1] (see, also [16–18]), namely

$$\Psi^{\circ}(i\omega_n) = I(\omega_n, 0) + \kappa [I(\omega_n, 0) - 1],$$

$$K(i\omega_n, i\omega_m) = [I(\omega_n, \omega_m) - I(\omega_n, 0)I(0, \omega_m)] \frac{Z(0)}{\tilde{Z}(i\omega_m)} \frac{\tilde{N}(|\tilde{\omega}_m|)}{|\omega_m|}.$$

Here  $\tilde{\omega}_n = \omega_n \tilde{Z}(i\omega_n)$ ,  $\lambda = 2 \int_0^{\infty} \frac{d\omega}{\omega} \alpha^2 F(\omega)$ , and  $\nu = \lambda/Z(0)$ , while  $Z(0) = 1 + \lambda$  is the renormalization factor associated with  $N(\epsilon) = \text{const}$ . Then,  $T_c$  emerges as an eigenvalue of the equation  $\Psi(0) = 1$ .

Note, however, that *the exact transformation* used to arrive at (1) was suggested in [23] and is essentially a regularization procedure for integral equations with divergent kernels. Following Refs. [1,24,25] one generates a series for  $\Psi(i\omega_n)$  from  $\Psi^{\circ}(i\omega_n)$ , which is a zero-order approximation that will be successful depending on the nature of the sum in (1) and provided the constant  $\nu$  is small. For intermediate-coupling  $\lambda < 1.5$  ( $\nu < 0.6$ ) and  $\omega_{ph} > \pi T_c$ , it was shown [24,25] that the zero-order approximation already leads to rather accurate expressions for  $T_c$ . The exact value of  $\kappa$  is proportional to the weak pseudopotential  $\mu_*$  [1], which for simplicity is initially taken as zero. As to the function  $\tilde{Z}(\omega_n)$ , following [14] we neglect its frequency-dependence and put

$$\tilde{Z}(0) = Z(0) + \frac{1}{\ln(2W/t)} \int_0^{\infty} \frac{d\omega^2}{t^2 - \omega^2} \ln\left(\frac{\omega}{t}\right) \alpha^2 F(\omega_2)$$

as found in [1]. Results obtained from this analytic expression for the renormalization factor compare excellently with exact numerical calculations that were performed for  $\tilde{Z}(0)$  based on the original Eliashberg equations.

The eigenvalue equation for  $T_c$  is then [1]

$$\frac{1}{g} = \frac{1}{\lambda^2} \int_0^\infty d\omega_1 \alpha^2 F(\omega_1) \int_0^\infty d\omega_2 \alpha^2 F(\omega_2) \frac{[P(\omega_1) - P(\omega_2)]}{\omega_2^2 - \omega_1^2}, \quad (2)$$

where  $g = \lambda/\tilde{Z}(0)$  and

$$P(\omega) = \frac{1}{\ln\left(\frac{2W}{t}\right)} \frac{1}{\omega^2} \left[ \ln\left(\frac{1.13\omega}{T_c}\right) \ln\left(\frac{2W}{\sqrt{|t^2 - \omega^2|}}\right) - \frac{1}{2} \ln^2\left(\frac{1.13t}{T_c}\right) + S_t(\omega, T_c) \right],$$

for which we assumed that  $\pi T_c < t$  and  $\pi T_c < \omega$  for any  $\omega$  contained in  $\alpha^2 F(\omega)$ . Similarly [1,26] one has

$$S_t(\omega, T_c) = S_t^\circ(\omega, T_c) + \theta(t - \omega) \Delta S_t(\omega, T_c),$$

where the Heaviside unit step-function  $\theta(t - \omega)$  was introduced to write

$$S_t^\circ(\omega, T_c) = \ln\left(\frac{1.13\omega}{T_c}\right) \ln\left(\frac{1.13\sqrt{|t^2 - \omega^2|}}{T_c}\right) + \delta_1(\omega),$$

$$\Delta S_t(\omega, T_c) = \ln\left(\frac{t}{\omega}\right) \ln\left(\frac{1.13\sqrt{|t^2 - \omega^2|}}{T_c}\right) - \frac{1}{2} \ln^2\left(\frac{1.13\omega}{T_c}\right) + \delta_2(\omega).$$

Two remarks are in order: a)  $\delta_1(\omega)$  and  $\delta_2(\omega)$  do not depend on  $T_c$  – as a result they have no effect on the  $T_c$ -equation functional form, and lead to small corrections to  $T_c$  [1]; and b) due to a specific form for  $S_t(\omega, T_c)$ ,  $T_c$  enters the eigenvalue Eq. (2) only via  $\ln[1.13f(\omega, t)/T_c]$ . Hence, the  $T_c$ -dependence expressed as integrals over  $\omega$  may be factored out since  $\ln[1.13f(\omega, t)/T_c] = \ln(1.13t/T_c) + \ln[f(\omega, t)/t]$ . Then, (2) becomes

$$a(t) \ln^2\left(\frac{1.13t}{T_c}\right) + b(t) \ln\left(\frac{1.13t}{T_c}\right) + c(t) = 0, \quad (3)$$

where the coefficients  $a(t)$ ,  $b(t)$  and  $c(t)$  are functionals of the spectral density of interaction. Their exact expressions, at least for  $t < \omega_{\min}$  and  $t > \omega_{\max}$ , are known [1], e.g.,  $a(t) = 1/2$  or 0 for  $t < \omega_{\min}$  or  $t > \omega_{\max}$ , respectively. In general, they are double integrals over  $\alpha^2 F(\omega)$  and can be determined only if the spectrum  $\alpha^2 F(\omega)$  is specified. However, one can perform in (2) the partial integrations for any  $\alpha^2 F(\omega)$  by introducing the *partial interaction spectra*  $S_1(\omega)$  and  $S_2(\omega)$  split at  $\omega = t$ , and defined as

$$S(\omega) \equiv \alpha^2 F(\omega) = S_1(\omega) \theta(t - \omega) + S_2(\omega) \theta(\omega - t). \quad (4)$$

The integrals in (2) then factorize as

$$\langle (\dots) \rangle_{S(\omega)} = \frac{\lambda_1(t)}{\lambda} \langle (\dots) \rangle_{S_1(\omega)} + \frac{\lambda_2(t)}{\lambda} \langle (\dots) \rangle_{S_2(\omega)},$$

via the *partial interaction parameters*

$$\lambda_1(t) = 2 \int_0^t \frac{d\omega}{\omega} S(\omega)$$

and

$$\lambda_2(t) = 2 \int_t^\infty \frac{d\omega}{\omega} S(\omega),$$

where by definition

$$\langle \dots \rangle_{X(\omega)} \equiv \int_0^\infty (d\omega^2/\omega^2) X(\omega) (\dots) / \int_0^\infty (d\omega^2/\omega^2) X(\omega), \quad X = S, S_1 \text{ or } S_2.$$

The spectra  $S_1(\omega)$  and  $S_2(\omega)$  given by (4) lead to physically different channels of charge-carrier Cooper pairings, i.e., to electron-like and hole-like sections simultaneously in different directions of the iso-energy surface  $\epsilon = \epsilon_{\text{VH}}$ . Because  $\epsilon_{\text{F}}$  is shifted from  $\epsilon_{\text{VH}}$  by an amount  $t$ , absorption or emission by an electron of a phonon belonging to the spectrum  $S_1(\omega)$  constrains an electron (hole) to an electron- (hole-) like orbit. Similarly, a phonon of energy  $\omega > t$  [i.e., a phonon from  $S_2(\omega)$ ] may convert an electron into a hole, and vice versa. This is in addition to the conventional channel associated with  $S_1(\omega)$  which does not mix electron- and hole-like excitations.

The coefficients in (3) thus become

$$a(t) = \frac{1}{2} \frac{\lambda_2^2(t)}{\lambda^2} - \frac{1}{\lambda^2} \int_0^t \frac{d\omega_1^2}{\omega_1^2} S(\omega_1) \int_t^\infty \frac{d\omega_2^2}{\omega_2^2} S(\omega_2) \frac{\omega_1^2}{\omega_2^2 - \omega_1^2},$$

$$b(t) = \ln\left(\frac{2W}{t}\right) + \frac{\lambda_2(t)}{\lambda} \ln\left(\frac{\omega_2(t)}{t}\right) - \frac{1}{2} \left( \eta^\circ - \frac{\lambda_1^2(t)}{\lambda^2} \eta(t) \right) + \Delta b(t),$$

$$c(t) = \ln \frac{2W}{t} \left( \ln \frac{\omega_{\text{in}}}{t} - \frac{\eta^\circ}{2} - \frac{1}{g} \right) + \Delta c(t).$$

The *analytic* expressions for  $\Delta b(t)$  and  $\Delta c(t)$ , whose contributions correspondingly to  $b(t)$  and  $c(t)$  are less than 5–10%, will be reported elsewhere. Here,  $\omega_{\text{in}} \equiv \exp\langle \ln \omega \rangle_{S(\omega)}$  is the mean-logarithmic frequency of the total spectrum. The partial frequencies  $\omega_1(t)$  or  $\omega_2(t)$  are given by the expression for  $\omega_{\text{in}}$  but with  $S_1(\omega)$  or  $S_2(\omega)$  instead of  $S(\omega)$ . The quantity  $\eta^\circ$  – as well as  $\omega_{\text{in}}$  – follow from standard Eliashberg theory with constant EDOS [24,25], and is just  $\eta^\circ = \langle \langle \omega^2 / (\omega^2 - \omega'^2) \rangle_{S(\omega')} \rangle_{S(\omega)}$ . The factor  $\eta(t)$  is obtainable by replacing the total  $S(\omega)$  by  $S_1(\omega)$  in  $\eta^\circ$ . The latter quantity, as well as  $\eta(t)$ , are weakly-structure-dependent parameters of the interaction spectrum and thus result in differing asymptotic values of  $T_c$  for small and large  $t$ .

Eq. (3) then leads to the final expression

$$T_c = 1.13t \exp \left[ \frac{b(t) - \sqrt{b^2(t) - 4a(t)c(t)}}{2a(t)} \right], \quad (5)$$

so that  $T_c$  is clearly determined by the filling-parameter-dependent  $a(t)$ ,  $b(t)$  and  $c(t)$  which in turn are functionals of  $S_1(\omega)$  and  $S_2(\omega)$ . It depends principally on *the partial interaction parameters*  $\lambda_1(t)$ ,  $\omega_1(t)$  and  $\lambda_2(t)$ ,  $\omega_2(t)$  connected via the total  $\lambda$  and average frequency  $\omega_{\text{in}}$  through

$$\lambda = \lambda_1(t) + \lambda_2(t), \quad \omega_{\text{in}} = \left[ \omega_1(t) \right]^{\frac{\lambda_1(t)}{\lambda}} \left[ \omega_2(t) \right]^{\frac{\lambda_2(t)}{\lambda}}.$$

The form of (5) reveals that the contribution of any  $\omega$  to the eigenvalue equation for  $T_c$  depends on the location of  $\epsilon_F$  in  $N(\epsilon)$ . For either small or large  $t \equiv |\epsilon_F - \epsilon_{VH}|$  the form of the three coefficients (3) simplify considerably, and (5) is then expressible in terms of the  $\omega_{ln}$  and  $\lambda$  as

$$T_c^{(1)} = \frac{1.13 \omega_{ln}}{e^{\eta^\circ/2}} \left( \frac{2W}{t} \right) \exp \left( - \sqrt{ \left( \ln \left( \frac{2W}{t} \right) + \frac{1}{g} \right)^2 + \left( \ln \left( \frac{\omega_{ln}}{t} \right) - \frac{\eta^\circ}{2} \right)^2 - \frac{1}{g^2} } \right) \quad (\text{small } t),$$

$$T_c^{(2)} = \frac{1.13 \omega_{ln}}{e^{\eta^\circ/2}} \exp \left( - \frac{1}{g} \right) \quad (\text{large } t),$$

both of which were obtained in [1] and closely resemble those given in the VHS of the BCS theory [8,12]. Note that  $T_c$  also depends on the full electronic bandwidth  $2W$  being a decreasing function of the ratio  $2W/\omega_{ln}$ . As this ratio diverges for fixed  $t$  one obtains the familiar McMillan  $T_c$ -formula [1]. As  $t$  increases, the ‘evolution’ of  $T_c$  (5) from  $T_c^{(1)}$  to  $T_c^{(2)}$  is entirely determined by the behavior of the coefficients (3), with  $a(t)$  the highest-order term of  $\ln(1.13t/T_c)$  being fixed *solely* by the interaction-spectrum parameters. This coefficient changes sign for some  $t$  lying within  $(\omega_{min}, \omega_{max})$ . By contrast,  $b(t)$  and  $c(t)$  being of opposite sign depend mainly on the electronic structure of the system.

To qualitatively understand the effect upon  $T_c$  of any (*non- $\delta$ -function-like*) fine-structure in  $\alpha^2 F(\omega)$  one can model the latter by simple functions reflecting *general* features of some realistic spectrum. Initially  $\alpha^2 F(\omega)$  was modeled by *single peaks* of the form  $S_i(\omega) = A_i \omega^n / [(\omega - \omega_{0i})^2 + B_i^2]$ , with parameters  $A_i$ ,  $B_i$  and  $\omega_{0i}$ , modulating the shapes of  $\alpha^2 F(\omega)$ , and fitted to yield the same  $\omega_{ln}$  and  $\lambda$  for each case ‘ $i$ ’. This guaranteed *nearly* equal values of  $T_c$  for either extreme  $t \ll \omega_{ln}$  or  $t \gg \omega_{ln}$ . Fig. 1 shows that narrowing the spectrum gives slightly higher  $T_c$  in either extreme – a well-known result for constant EDOS [17]. However, the variation of  $T_c$  turns out to be *non-monotonic* in the intermediate region and passes through a *minimum*  $T_c^{min}$ . Fixing  $\lambda$  and  $\omega_{ln}$ ,  $T_c^{min}$  decreases with narrowing  $\alpha^2 F(\omega)$  eventually making superconductivity *disappear altogether* over some interval of intermediate  $t$  values near  $\omega_{ln}$ . Broadening  $\alpha^2 F(\omega)$  leads to  $T_c$  a smoother function of  $t$ , while its minimum shifts towards larger filling-parameter values approaching  $T_c^\circ$ , the value corresponding to constant EDOS, from below. Calculations for a smaller set of  $\nu$  were repeated by fixing  $\omega_{ln}$ , but changing the

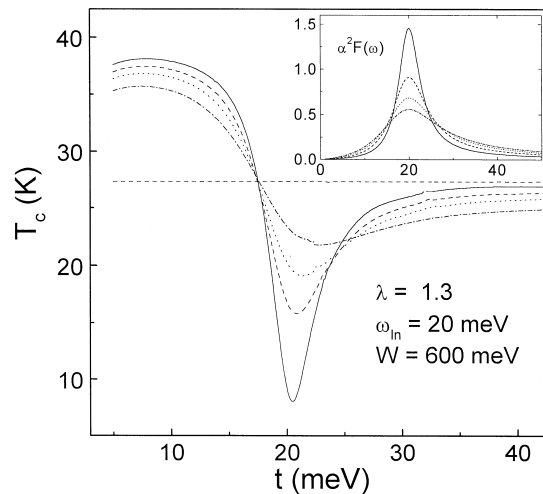


Fig. 1.  $T_c$  vs  $t$  for different shape-types of  $\alpha^2 F(\omega)$ ; single-peak results shown in inset. The set of parameters  $(A, B, \omega_0)$  were chosen (in meV) as: (0.65, 3, 19.8) full curve; (1.12, 5, 19.4) dashed; (1.62, 7, 18.9) dotted; and (2.2, 9, 18.2) dot-dashed. All parameter sets yield the same  $\lambda$  and  $\omega_{ln}$ . Horizontal dashed-line is  $T_c^\circ$  as defined in text.

height of the (single-peak) curve in  $\alpha^2 F(\omega)$  so as to ensure different  $\lambda$ 's. The  $T_c$ -enhancing effect of the VHS over that of constant EDOS increased significantly by *decreasing*  $\lambda$  [1,27], but the characteristic non-monotonic behavior of  $T_c$  vs  $t$  *remained unchanged*. Because the iterative solution of (1) is 'exact' for small  $\nu$ , we conclude that this non-trivial variation of  $T_c$  is an *inherent* property of *real* superconductors, i.e., systems with varying  $N(\epsilon)$ .

Next,  $\alpha^2 F(\omega)$  was put in the form of two superposed peaks, motivated by the fact that  $T_c$  itself depends critically on the details of variation of  $a(t)$  (5) which in turn is quite sensitive to the structure in  $\alpha^2 F(\omega)$ . The strongest variation in  $T_c$  then occurs near the characteristic peaks of  $\alpha^2 F(\omega)$ , while far from these peaks  $T_c$  changes slightly [1]. Thus, for the two-peak-structured  $\alpha^2 F(\omega)$  we expect a 'ladder-like' behavior in the evolution of  $T_c$  between the two extremes  $t < \omega_{\min}$  and  $t > \omega_{\max}$ , the exact nature of which is then dictated by the details of  $\alpha^2 F(\omega)$ . In fact, when the peaks in  $\alpha^2 F(\omega)$  are narrowed, thus rendering sharper individual peaks, for  $t$  varying over the considerable part of the interval  $(\omega_{\min}, \omega_{\max})$  the magnitude of  $T_c$  is more concentrated near two different but nearly constant values  $T_{c1}$  and  $T_{c2}$ . The width over which  $T_c$  changes from  $T_{c1}$  to  $T_{c2}$  is given by the width of the low-frequency part of  $\alpha^2 F(\omega)$ , but the magnitude of  $T_{c1} - T_{c2}$  is fixed by the interaction parameters  $\lambda^{(1)}$  and  $\lambda^{(2)}$  associated with each peak, Fig. 2. As in the case of a single peak, Fig. 1,  $T_c$  passes through a minimum  $T_c^{\min}$  and at  $t \gg \omega_{\ln}$  approaches  $T_c^{\circ}$ . Decreasing  $\lambda$  does not eliminate the non-monotonic behavior of the evolution of  $T_c$  between the extremes  $t \ll \omega_{\ln}$  and  $t \gg \omega_{\ln}$ . The reason for the slight  $T_c$ -reduction at very small shifts in Figs. 1 and 2 is discussed in [1], as well in pioneering work by Pickett [16]. BCS-like theories predict maximum  $T_c$  when  $\epsilon_F$  and  $\epsilon_{VH}$  coincide; however, additional work is needed when  $t \leq \pi T_c$ . Also, one finds that non-zero values of  $\mu_*$  drastically decrease  $T_c$  for large  $t$  [1], but as shown in [12] for small  $t$  (viz., in the high-temperature region) the influence of  $\mu_*$  is significantly reduced.

A clue in understanding the origin of this nontrivial  $T_c$  behavior as a function of  $t$  follows by proposing a Fourier transform  $V(\omega)$  for the indirect pairwise boson-mediated interaction potential that is a complicated function and *changes sign* for some frequencies – thus resulting in a *depairing effect* for the Cooper pairs. In BCS-like theories this interaction potential is mimicked by a negative constant or zero depending on whether  $\omega$  is or is not, respectively, in the interval  $(-\omega_{\max}, \omega_{\max})$ . The reason for the depairing component of  $V(\omega)$  is clarified by considering physically-different pairing channels  $S_1(\omega)$  and  $S_2(\omega)$  in (4), as discussed above, and by assuming for the moment that there is only an  $S_1(\omega)$ -type channel (different from zero provided  $\omega \leq t$ ).

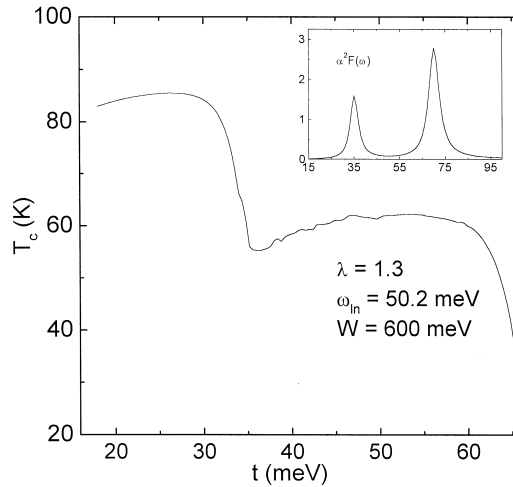


Fig. 2.  $T_c$  vs  $t$  for a two-peak-structured  $\alpha^2 F(\omega)$ . Inset figure is for  $\alpha^2 F(\omega) = A_1 \omega^n / [(\omega - \omega_{01})^2 + B_1^2] + A_2 \omega^n / [(\omega - \omega_{02})^2 + B_2^2]$  with  $A_1 = 0.2$ ,  $B_1 = 2.1$ ,  $\omega_{01} = 35$  meV and  $A_2 = 0.31$ ,  $B_2 = 2.8$ ,  $\omega_{02} = 70$  meV.

Then, by applying BCS-theory it is easy to find a repulsive contribution to the total  $V(\omega)$  originating from the exchange of two electrons via phonons of frequencies  $\omega > t$ .

The following argument may shed additional light into the origin of the non-monotonic  $T_c$  vs  $t$ -behavior. Since the EDOS varies sharply (even infinitely so at distances of order  $t = |\epsilon_F - \epsilon_{VH}|$  from  $\epsilon_F$ ) pairing due to an individual boson of energy close to  $t$  is much stronger than that due to phonons with energies differing significantly from  $t$ , there being a large number of final states for electrons to be scattered into via phonons of energy  $\sim t$ . In other words, due to the logarithmic  $N(\epsilon)$  the main contribution in the basic equations to the gap energy (which is proportional to  $T_c$ ) comes from phonons with energies concentrated near  $t$ . On the other hand, as shown by several studies in conventional superconductors, e.g., [14], the gap function is roughly slowly-varying for frequencies less than  $\omega_{max}$ , *decreases rapidly* near the upper edge of the phonon spectrum, and changes sign near  $\omega_{max}$ . In fact, in many analytic studies of conventional superconductors, the gap function is simulated by single- or two-step shapes. Assuming now a very narrow electron-phonon interaction spectrum ‘located’ near some  $\omega_0$  (i.e., a spectrum for which  $\omega_{max} \sim \omega_0$ ) and placing  $t$  near  $\omega_{max}$  where the magnitude of the gap is significantly reduced, a reduction in  $T_c$  ensues.

To conclude, the behavior of  $T_c$  as a function of  $t$  depicted in special cases in Figs. 1 and 2 is useful in interpreting observations in several oxide superconductors. In  $\text{Bi}_2\text{Sr}_2\text{Cu}_1\text{O}_x$  ( $T_c \approx 10\text{K}$ ) [28] and  $\text{Sr}_2\text{RuO}_4$  ( $T_c \approx 0.1\text{K}$ ) [29,30]  $T_c$  is *unexpectedly* small in spite of  $\epsilon_{VH}$  lying very close to  $\epsilon_F$ . Assuming that the shift of  $\epsilon_F$  from  $\epsilon_{VH}$  in these compounds corresponds to values of  $t$  such that  $T_c$  falls near its minimum value (see, e.g., Fig. 1) then Eq. (5) adequately describes experiment. Moreover, for a two-peak-shaped  $\alpha^2F(\omega)$ , assuming an inter-electron (or -hole) interaction via bosons from the higher-frequency parts of  $\alpha^2F(\omega)$  to be significant, the two-plateau structure, Fig. 2, for  $T_c$  is obtained which is well-established in empirical  $T_c$  vs  $x$  curves for  $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ . Finally, the origin of so-called anomalous isotope effects in high- $T_c$ -materials might be clarified, given the novel element that the partial  $\lambda_1(t)$  and  $\lambda_2(t)$  *depend* on the ionic mass (unlike the total  $\lambda$  in the harmonic approximation) and thus lead to non-vanishing terms in the isotopic-shift factor, as will be examined in detail elsewhere.

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## References

- [1] T.A. Mamedov, M. de Llano, T. Firat, Phys. Rev. B 55 (1997) 9077.
- [2] J.E. Hirsch, D.J. Scalapino, Phys. Rev. Lett. 56 (1986) 2732.
- [3] I.E. Dzyaloshinskii, Zh. Exp. Teor. Fiz. 93 (1987) 1487.
- [4] J. Labbé, J. Bok, Europhys. Lett. 3 (1987) 1225.
- [5] J. Friedel, J. Phys. 48 (1987) 1787.
- [6] R. Combescot, J. Labbe, Phys. Rev. B 38 (1988) 262.
- [7] R.S. Markievic, J. of Phys. Chem. Sol. 58 (1997) 1179.
- [8] C.C. Tsuei, Phys. Rev. Lett. 65 (1990) 2724.
- [9] D.M. Newns, Phys. Rev. Lett. 69 (1992) 1264.
- [10] P.C. Pattnaik, Phys. Rev. B 45 (1992) 5714.
- [11] A.A. Abrikosov, Physica C 222 (1994) 191; C 233 (1994) 102; C 244 (1995) 361.
- [12] J. Bok, Physica C 209 (1993) 107; J. Bok, J. Bouvier, Physica C 244 (1995) 357; 249 (1995) 117; 274 (1997) 1.
- [13] J.P. Carbotte, F. Marsiglio, in: A. Narlikar (Ed.), Studies of High Temperature Superconductors, vol. 1, Nova, 1989, p. 64.
- [14] J.P. Carbotte, Rev. Mod. Phys. 62 (1990) 1027.

- [15] D. Allender, J. Bray, J. Bardeen, *Phys. Rev. B* 7 (1973) 1020.
- [16] W.E. Pickett, *Phys. Rev. B* 21 (1980) 3897.
- [17] P.B. Allen, B. Mitrovic, in: H. Ehrenreich, D. Turnbull (Eds.), *Solid State Physics*, vol. 37, Academic, NY, 1982, p. 1.
- [18] B. Mitrovic, J.P. Carbotte, *Can. J. Phys.* 61 (1983) 784.
- [19] J.P. Carbotte, E.J. Nicol, *Physica C* 185–190 (1991) 162.
- [20] M.D. Whitemore, J.P. Hare, L.B. Knee, *Phys. Rev. B* 26 (1982) 3733.
- [21] A.P. Zhernov, T.A. Mamedov, *Supercond. SPCT* 3 (1990) 23.
- [22] J.W. Garland, *Phys. Rev.* 153 (1973) 460.
- [23] D.N. Zubarev, *Usp. Fiz. Nauk.* 71 (1960) 71.
- [24] E.G. Maximov, *Problems of High- $T_c$ -Superconductivity*, Nauka, Moscow, 1977.
- [25] A.P. Zhernov, Y.A. Malov, *Fiz. Tverd. Tela (Leningrad)* 19 (1977) 2096.
- [26] I.S. Gradshteyn, I.M. Ryzhik, *Tables of Integrals, Series and Products*, Academic, NY, 1980.
- [27] R.J. Radtke, S. Ullah, K. Levin, M.R. Norman, *Phys. Rev. B* 46 (1992) 11975.
- [28] D.M. King, *Phys. Rev. Lett.* 73 (1994) 3298.
- [29] T. Yokoya, *Phys. Rev. Lett.* 76 (1996) 3009.
- [30] D.H. Lu, *Phys. Rev. Lett.* 76 (1996) 4845.