# **Transition-temperature features of layered superconductors**

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A model theory for the superconducting transition temperature  $T_c$  is derived that is based on a generalized version of the Eliashberg equations taking into account an energy dependence in the electronic density of states  $N(\epsilon)$ . We treat an electronic structure with characteristic two-dimensional character. An analytical expression for  $T_c$  obtained for intermediate coupling establishes features of the  $T_c$  in the logarithmic van Hove scenario. Results describe the behavior of  $T_c$  vs *x* observed in well-annealed  $\text{La}_{2-x}$ Sr<sub>x</sub>CuO<sub>4</sub> oxides.  $[$ S0163-1829(97)03714-4]

## **INTRODUCTION**

A characteristic feature of nonconventional superconductors is the presence of low-dimensional structural elements such as weakly coupled planes or chains of atoms. Because of this marked anisotropy it is possible that  $N(\epsilon)$ , the electronic density of states (EDOS), in cuprate superconductors, for example, is not smooth but exhibits appreciable variations with energy  $\epsilon$  over a significant scale. In particular, the singularities in a van Hove scenario, necessarily present in periodic potentials, may play an important role.<sup>1-8</sup> Recent experimental,  $9-14$  as well as theoretical results<sup>15–17</sup> in nonconventional superconducting materials suggesting a Fermi level pinned very close to a van Hove saddle point in  $N(\epsilon)$ , raise important questions about the possible role of a nonsmooth EDOS and its subsequent effect on  $T_c$  in these materials.

In conventional superconductivity the  $N(\epsilon)$  is assumed not to vary around the Fermi energy,  $\epsilon_F$ , over the characteristic energy range corresponding to the maximum phonon energy,  $\omega_0$ . The EDOS is then replaced by its value at  $\epsilon_F$ . On the other hand, if  $\epsilon_F$  is located near a singularity any infinitesimal departure of  $\epsilon$  from  $\epsilon_F$  gives rise to sharp variations in  $N(\epsilon)$  that must be taken into account in a consistent theory.

The formalism with nonconstant  $N(\epsilon)$  was initially developed in anticipation of possible applications to ''classical'' high-temperature superconductors such as the *A*15 compounds, and were carried out within the framework of BCS, as well as of Eliashberg theory which has since been extended by many authors.<sup>18–22</sup> With the discovery of high- $T_c$  cuprate superconductors, interest in this area has resurfaced as a possible explanation of the  $T_c$  enhancement observed in the cuprates. Nevertheless, in recent work $^{23}$  within the framework of the Fermi-surface-restricted Eliashberg theory,  $18,24$  it is concluded that a van Hove scenario (VHS) to enhance  $T_c$  operates *only in weak coupling*, and that inclusion of strong coupling deactivates the  $T_c$ -enhancing effects of the VHS. In the pioneering work of Pickett<sup>18</sup> it is argued that for strongly coupled superconductors peaks in the EDOS are quite ineffective in raising  $T_c$ . By assuming that  $\epsilon_F$  lies near the center of a very narrow peak, these authors estimated *a reduction of*  $T_c$  by 15% in *A*15 compounds. However, in more recent studies by Mansor and Carbotte<sup>25</sup> a  $T_c$ greatly enhanced over the value when van Hove singularities are not present is obtained which drops rapidly by shifting  $\epsilon_F$  away from the center of the EDOS peak, as expected. Clearly, additional work is required in order to clarify the situation.

Eliashberg theory determines the critical temperature as a functional of the electron-phonon interaction spectrum,  $\alpha^2 F(\omega)$ , so that obtaining a universal  $T_c$  describing all superconducting materials is, strictly speaking, impossible. Fortunately, however,  $T_c$  depends mainly on the characteristic phonon frequency  $\omega_{ph}$  as well as on the value of the mass renormalization factor  $\lambda$ . This circumstance admits various analytical approaches based on physical assumptions about the actual electron-phonon interaction. Specifically, the familiar expressions for  $T_c$  of McMillan,<sup>26</sup> of Allen and Dynes, $^{27}$  of Leavens and Carbotte, $^{28}$  as well as the more recent formula of Kresin,<sup>29</sup> all follow after making reasonable approximations of the gap function and of the effective electronic mass. These solutions for  $T_c$  succeed in describing the behavior of the exact solution of the ordinary Eliashberg equations for appropriately chosen ranges of the interaction parameter  $\lambda$ . But for modified Eliashberg equations with a nonconstant EDOS analytical solutions for  $T_c$  have not been reported. Results are obtainable either from numerical analyses or for weak coupling,  $\lambda \rightarrow 0$ .<sup>16,17</sup> Meanwhile, a simple analytical representation based on specifically physical assumptions would shed light on the dependence of  $T_c$  on the relevant parameters of the underlying strongly correlated electron-phonon system, and perhaps suggest nontrivial information about such a complex many-particle system.

The purpose of this paper is to present the results of analytic calculations for  $T_c$  for values of  $\lambda$ <1.5 and for

 $\omega_{ph} \geq \pi T_c$ . For such parameter restrictions the method of solving the standard Eliashberg equations was developed in Refs. 30 and 31 (see below) according to which the solution for the gap in the quasiparticle excitation spectrum is represented in a form reflecting features of the  $\alpha^2 F(\omega)$  without specifying its explicit shape. The final expression for the critical temperature follows as the eigenvalue of an integral equation for the gap function and is a functional of  $\alpha^2 F(\omega)$ . Naturally, one looks for a solution of the modified Eliashberg equations by the methods of the usual theory. Since for cuprates one deals with conducting planes, we shall use the general form of  $N(\epsilon)$  which is known for lowdimensional periodic structures.

# **I. BASIC EQUATIONS AND METHOD**

For  $T=T_c$  the Eliashberg equations written in the imaginary-axis representation, valid for general  $N(\epsilon)$ ,<sup>18,22</sup> are

$$
\Delta(i\omega_n)\widetilde{Z}(i\omega_n) = \pi T \sum_{m=-\infty}^{+\infty} \{ \lambda I(m-n) - \mu(\omega_c) \}
$$

$$
\times \frac{\Delta(i\omega_m)}{|\omega_m|} \widetilde{N}(|\widetilde{\omega}_m|), \tag{1}
$$

and

$$
\widetilde{Z}(i\omega_n) = 1 + \frac{\pi T \lambda}{\omega_n} \sum_{m=-\infty}^{+\infty} I(m-n) \operatorname{sgn}(\omega_m) \widetilde{N}(|\widetilde{\omega}_m|), (2)
$$

$$
\widetilde{\omega}_n = \omega_n \widetilde{Z}(i\omega_n),
$$

where  $i\omega_n = i\pi T_c(2n-1)$  are the Matsubara frequencies. Equations  $(1)$  and  $(2)$  determine the critical temperature  $T_c$ resulting from a specific electron-phonon spectral density  $\alpha^2 F(\omega)$  which enters through

$$
I(n-m) = \frac{2}{\lambda} \int_0^\infty \frac{\omega}{\omega^2 + (\omega_n - \omega_m)^2} \alpha^2 F(\omega) d\omega, \qquad (3)
$$

where  $\lambda = 2 \int_0^{\infty} (d\omega/\omega) \alpha^2 F(\omega)$ , and the Coulomb potential  $\mu(\omega_c)$  appropriate to the cutoff  $\omega_c$  in Eq. (1). Finally  $\widetilde{N}(\widetilde{\omega}_n)$  is given by

$$
\widetilde{N}(|\widetilde{\omega}_n|) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon \, \frac{|\widetilde{\omega}_n|}{\epsilon^2 + \widetilde{\omega}_n^2} \frac{N(\epsilon)}{N(\epsilon_F)},\tag{4}
$$

where the energy integral in Eq.  $(4)$  can be performed once the density of states  $N(\epsilon)$  is specified. In the following we assume that the standard electron-phonon spectral density  $\alpha^2 F(\omega)$ , namely wherein all characteristic phonon frequencies  $\omega_{\rm ph}$  are of the same order, and such that the unequalities  $\omega_{ph} \ge \dot{\Delta}(0)$  or  $\omega_{ph} \ge \pi T_c$  hold. Equation (1) can, in principle, then be solved by iteration. For the case of constant  $N(\epsilon)$  the regularization procedure (that is, elimination of the singularity at  $\omega \rightarrow 0$ ) and the iteration solution for the Eliashberg equation at  $T=T_c$  is carried out in the real-axis representation for intermediate coupling ( $\lambda$ <1.5), in Refs. 30 and 31.

Let us define the function

$$
\phi(i\omega_n) = \frac{\Delta(i\omega_n)\widetilde{Z}(i\omega_n)}{\Delta(0)\widetilde{Z}(0)},
$$
\n(5)

where  $\Delta(0)$  and  $\tilde{Z}(0)$  are understood in the limit of  $\omega \rightarrow 0$ . Then Eq.  $(1)$  can be rewritten as

$$
\phi(i\omega_n) = \phi^o(i\omega_n) + \pi T \lambda \sum_{m=-\infty}^{+\infty} [I(n,m) - I(n,0)I(0,m)]
$$

$$
\times \frac{1}{|\omega_m|} \frac{\phi(i\omega_m)}{\tilde{Z}(i\omega_m)} \tilde{N}(|\tilde{\omega}_m|), \tag{6}
$$

where in the last expression the identity  $\phi(0)=1$  was used, namely,

$$
\pi T \sum_{m=-\infty}^{+\infty} {\{\lambda I(0,m) - \mu(\omega_c)\}} \frac{1}{|\omega_m|} \frac{\phi(i\omega_m)}{\widetilde{Z}(i\omega_m)} \widetilde{N}(|\widetilde{\omega}_m|) = 1,
$$
\n(7)

and the functions,  $\phi^{\circ}(i\omega)$  and  $\kappa$  are introduced

$$
\phi^{o}(i\omega_{n}) = I(n,0) + \kappa[I(n,0)-1],
$$
\n(8)

$$
\kappa = \mu(\omega_c) \pi T \sum_{m=-\infty}^{+\infty} \frac{1}{|\omega_m|} \frac{\phi(i\omega_m)}{\widetilde{Z}(i\omega_m)} \widetilde{N}(|\widetilde{\omega}_m|). \tag{9}
$$

Note, however, that  $\kappa$  does not depend on frequency but only on temperature. By definition  $I(0,0)=1$ . Moreover, for values *n*→ $\infty$  (and also for *m*→ $\infty$ ) the function *I*( $\omega_n$ , $\omega_m$ ) goes to zero. The latter circumstance ensures a vanishing kernel in Eq. (6) for small and large  $\omega_n$ . Therefore, for small and large values of  $\omega_n$  the free term  $\phi^o(i\omega_n)$  is equivalent to an exact solution of Eq. (6)  $\phi(i\omega_n)$ . Because of the factor  $|\omega_m|$  in the denominator in Eq. (7) as well as the rapid decrease of  $I(\omega_n, \omega_m)$  with increasing  $\omega_n$ , it is not difficult to see that low frequencies  $\omega_n$  dominate in Eq. (7), which in turn is an eigenvalue equation. But for such frequencies the difference between  $\phi^o(i\omega_n)$  and the exact solution  $\phi(i\omega_n)$ is negligible. That is why using  $\phi^o(i\omega_n)$  instead of  $\phi(i\omega)$  in Eq.  $(7)$  leads to an equation for determining  $T_c$  whose solution differs negligibly from the exact eigenvalue of Eq.  $(6)$ . It is also of interest that the analytical continuation of the free term  $\phi^{\circ}(i\omega_n)$  on the real axis  $\omega$  has the characteristic features at  $\omega_i < \omega_0$ , repeating the features of  $\alpha^2 F(\omega)$  (which stem from the interaction of electrons with individual groups of phonons with frequency  $\omega_i$ ), while at  $\omega \geq \omega_0$  its behavior is determined by the Coulomb interaction. Note that  $\omega_0$  is just max $\{\omega_i\}$ . Following the results of Refs. 30,31 we construct an iteration series for Eq.  $(6)$  by starting from the trial function  $\phi^o(i\omega_n)$  expressed in terms of  $I(n,0)$  and with  $\kappa$  as the zero-order approximation. The kernel of Eq.  $(6)$  possesses no singularities so that the iteration procedure converges rapidly. Subsequent iteration corrections are small and do not significantly affect the accuracy of results obtained by using  $\phi^{\circ}(\omega_n)$ . In this scheme Eq. (7) is effectively clearly an eigenvalue equation.

As to the renormalization factor for the electronic mass Eq.  $(2)$ , it is convenient to write it as

$$
\widetilde{Z}(i\omega_n) = 1 + 2 \int_0^{\infty} d\omega^2 S(\omega) \sum_{m=0}^{\infty} \frac{\pi T_c}{\omega_m} \frac{\widetilde{N}(|\widetilde{\omega}_m|)}{\omega^2 + \omega_n^2 + \omega_m^2} \times \sum_{p=0}^{\infty} \left( \frac{2\omega_n \omega_m}{\omega^2 + \omega_n^2 + \omega_m^2} \right)^{2p} . \tag{10}
$$

In the above equation and from now on the electron-phonon interaction spectrum  $\alpha^2 F(\omega)$  will be denoted as  $S(\omega)$ . Expression  $(10)$  differs from the standard one only by the factor  $N(\tilde{\omega}_m)$ . The convergence of the sum over *p* in Eq. (10) is sufficiently rapid. Specifically, for the case of a constant EDOS only the first term needed being retained. Further-EDOS only the first term needed being retained. Furthermore, the variation of  $\tilde{Z}(i\omega_n)$  with *n* is not large, so that in more, the variation of  $Z(i\omega_n)$  with *n* is not large, so that in the integrals  $\tilde{Z}(i\omega_n)$  can be replaced by a constant value at the integrals  $Z(i\omega_n)$  can be replaced by a constant value at  $n = 1.^{32}$  In determining  $\tilde{Z}(i\omega_n)$  and  $T_c$  we use for  $\tilde{N}(\tilde{\omega}_m)$  the value  $\tilde{\omega}_n = \omega_n Z(0)$ , where  $Z(0) = 1 + \lambda$  is a renormalization factor corresponding to  $N(\epsilon)$ =const.

### **II. THE MODEL**

We retain only nearest-neighbor terms in the dispersion relation

$$
\epsilon(k) = -2B[\cos(k_x a) + \cos(k_y a)] + 4B. \tag{11}
$$

The EDOS per spin associated with the plane band Eq.  $(11)$ is given for  $\epsilon < 4B$  by<sup>33</sup>

$$
N(\epsilon) = \frac{4N}{\pi^2} \frac{1}{4B - \epsilon} K \left( \frac{\epsilon}{8B - \epsilon} \right),\tag{12}
$$

where *K* is an elliptic integral<sup>34</sup> and *N* is the number of atoms per unit two-dimensional lattice cell. In the vicinity of the middle of the band  $\epsilon \sim 4B$ ,  $N(\epsilon)$  is well approximated by

$$
N(\epsilon) = N_0 \ln \left( \frac{2W}{|\epsilon - 4B|} \right). \tag{13}
$$

In expression (13)  $N_0 = N/2\pi^2 B$  where  $W = 8B$  is the full bandwidth. Let us define the filling factor  $s=4B-\epsilon_F$  which describes the position of  $\epsilon_F$  with respect to the saddle point in *N*( $\epsilon$ ). As usual, put  $\epsilon \rightarrow \epsilon - \epsilon_F$ . We then have

$$
N(\epsilon) = N_0 \ln \frac{2W}{|\epsilon - s|}.
$$
 (14)

Since the variation of the EDOS is important only near  $\epsilon_F$ , one may represent  $N(\epsilon)$  over the entire energy range as

$$
N(\epsilon) = N_0[1 + \delta n(\epsilon)],\tag{15}
$$

where the background value  $N_0$  is chosen so as to yield the critical temperature  $T_c^{(0)}$ . This corresponds to the case of  $N(\epsilon)$  = const, and the function  $\delta n(\epsilon)$  (whose implicit form is postulated according to the physical situation) modulates the variation of  $N(\epsilon)$  near  $\epsilon_F$ . By definition,  $\delta n(\epsilon)$  goes to zero over a characteristic energy scale describing the damping of the rapidly varying portion of  $N(\epsilon)$ . If the EDOS is modeled, for example, by a Lorentzian factor of width *a* and superimposed on a background  $N_0$ , then  $\delta n(\epsilon)$  vanishes for energies of the order of *a*. But for a logarithmic variation of  $\delta n(\epsilon)$ , if we wish to represent a varying EDOS in the form  $(15)$  one must utilize some prefactor for  $\delta n(\epsilon)$  in order to suppress the logarithm at large energies ( $\delta n \rightarrow 0$  only at  $\epsilon \rightarrow \infty$ ). Including an energy-dependent damping factor (as done, for example, in Ref. 25) only causes additional difficulties in the analytic calculations due to the additional complication of an explicit form of  $N(\tilde{\omega}_n)$ . These difficulties are avoidable by employing the direct definition (4) for  $N(\tilde{\omega}_n)$  since as emphasized in Ref. 4, Eq.  $(13)$  is a very good approximation to Eq. (12). Specifically, the values of  $N(\epsilon_F)$  (as well as magnitudes of EDOS integrated over the entire range of  $\epsilon$ ), calculated, respectively, by using Eq.  $(13)$  as well as the exact expression  $(12)$ , differed only slightly from each other. Therefore one can approximate the exact EDOS  $(12)$  by the simple form (13) over the entire range of  $\epsilon$ —and this guarantees analytic results. Inserting expression (13) for  $N(\epsilon)$ into Eq.  $(4)$  immediately leads to

$$
\widetilde{N}(\widetilde{\omega}_n) = \frac{1}{N(s)} \ln \frac{2W}{\sqrt{s^2 + |\widetilde{\omega}_n^2|}},\tag{16}
$$

where  $N(s) = \ln(2W/s)$ . It should be noted that the EDOS at  $\epsilon_F$  is given by

$$
N(\epsilon_F) = N_0 \ln \frac{2W}{s},\tag{17}
$$

and depends on the filling factor *s*. To obtain a physical value for  $N(\epsilon_F)$  at  $s \rightarrow 0$  we must include, e.g., the transition matrix elements for charge carriers between conducting layers. Henceforth we deal only with the case of  $s \geq \pi T_c$  rather than  $s=0$ .

## **III. SUPERCONDUCTING TRANSITION TEMPERATURE**

At temperatures near  $T_c$  the electron mass renormaliza-At temperatures near  $I_c$  the electron mass renormalization factor  $\widetilde{Z}(\omega_n)$  does not involve the gap function  $\Delta(\omega_n)$ so that it may calculated independently. Due to rapid convergence of the sum over  $p$  in Eq.  $(10)$  one can accurately gence of the sum<br>represent  $\widetilde{Z}(\omega_n)$  as

$$
\widetilde{Z}(\omega_n) = 1 + \int_0^\infty d\omega^2 S(\omega)
$$
\n
$$
\times \left\{ \frac{1}{\omega^2 + \omega_n^2} + \frac{1}{\ln(2W/s)} \frac{1}{[s/Z(0)]^2 - \omega^2 - \omega_n^2} \right\}
$$
\n
$$
\times \left[ \frac{s^2}{\omega^2 + \omega_n^2} \frac{\ln Z(0)}{Z^2(0)} + \ln \frac{\sqrt{\omega^2 + \omega_n^2}}{s} \right] \right\}.
$$
\n(18)

In Eq.  $(18)$  we have neglected terms proportional to In Eq. (18) we have neglected terms proportional to  $(\pi T_c)^2 / \bar{\omega}_{ph}^2$ . Expression (18) differs from the analogous result for  $Z(\omega_n)$  corresponding to constant EDOS only by the second term in the curly brackets. As a rule, because of the small variation with  $\omega_n$ , the  $Z(\omega_n)$  can be replaced by its constant value at  $n=1$  which thus allows analytic calculation  $(see, for example in Ref. 32).$  It is not difficult to realize that such is the case here; namely, as  $\omega_n$  increases up to the such is the case here; namely, as  $\omega_n$  increases up to the maximum phonon frequency  $\omega_0$ ,  $\tilde{Z}(\omega_n)$  changes only by a few percent. Therefore, to the same accuracy as in the usual

$$
\widetilde{Z}(0) = Z(0)[1 + \nu \rho(s)],\tag{19}
$$

where  $\nu = \lambda/(1+\lambda)$  and  $Z(0) = 1+\lambda$  is the renormalization factor corresponding to constant EDOS;  $\rho(s)$  is given by

$$
\rho(s) = \frac{1}{\ln(2W/s)} \frac{\int_0^\infty d\omega^2 S(\omega) [1/(t^2 - \omega^2)][(t^2/\omega^2)\ln Z(0) + \ln(\omega/s)]}{\int_0^\infty (d\omega^2/\omega^2) S(\omega)}, \quad t = s/Z(0). \tag{20}
$$

Consider the eigenvalue equation  $(7)$  where we put Consider the eigenvalue equation (*i*) where we put  $\phi(i\omega_n) = \phi^o(i\omega_n)$ . Substituting  $\widetilde{Z}(0)$  for  $\widetilde{Z}(\omega_m)$  Eq. (7) can be rewritten as

$$
\frac{1}{g} = I_1 - \frac{\kappa^o}{1 + \kappa^o} I_2,\tag{21}
$$

where the following notation was used:

$$
g = \frac{\lambda}{\tilde{Z}(0)},\tag{22}
$$

$$
I_1 = \frac{1}{\lambda^2} \int_0^\infty d\omega_1^2 S(\omega_1)
$$
  
 
$$
\times \int_0^\infty d\omega_2^2 S(\omega_2) \frac{1}{\omega_2^2 - \omega_1^2} [P(\omega_1) - P(\omega_2)], \quad (23)
$$

$$
I_2 = \frac{1}{\lambda} \int_0^\infty d\omega^2 S(\omega) P(\omega), \tag{24}
$$

$$
P(\omega) = \sum_{m=0}^{\infty} \frac{2\pi T_c}{|\omega_m|} \frac{1}{\omega^2 + \omega_m^2} \widetilde{N}(|\widetilde{\omega}_m|),
$$
 (25)

$$
\kappa^{o} = \mu_{\star} I_{2}, \quad \mu_{\star} = \frac{\mu(\omega_{c})/Z(0)}{1 + [\mu(\omega_{c})/Z(0)]\ln(2W/\omega_{\text{ph}})}.
$$
\n(26)

Note that the weak Coulomb pseudopotential  $\mu_{\star}$  Eq. (26) differs from the analogous Tolmachev<sup>35</sup> or Anderson and Morel<sup>36</sup> results by a factor  $Z(0)$  in both denominator and numerator. Putting  $N(\vert \tilde{\omega}_m \vert)$  as given by Eq. (16) into  $P(\omega)$  Eq. (25) one can perform the summation over *m*, the result being easily expressed in terms of combinations of digamma functions  $\Psi[1/2 \pm i(x/2\pi T_c)]^{20,34}$ , where  $x = s/Z(0)$  or  $\omega$ . For  $\pi T_c \ll \omega_{ph}$  we obtain

$$
P(\omega) = \frac{1}{N(s)} \frac{1}{\omega^2} \left( \ln \frac{1.13\omega}{T_c} \ln \frac{2W}{\sqrt{t^2 - \omega^2}} - \frac{1}{2} \ln^2 \frac{1.13\omega}{T_c} + S_t(\omega, T_c) \right),\tag{27}
$$

where in the last equation we have set  $t = s/Z(0)$  and

$$
S_t(\omega, T_c) = \frac{1}{2} \int \frac{dt^2}{t^2 - \omega^2} \ln \frac{1.13t}{T_c}.
$$

The integral  $S_t(\omega, T_c)$  cannot be expressed in terms of elementary functions; but depending on the value of  $s = tZ(0)$  it can be written as a sum of leading terms  $S_i^o(\omega, T_c)$  plus correction terms  $\delta_i(\omega)$ ; that is

$$
S_t(\omega, T_c) = S_i^o(\omega, T_c) + \delta_i(\omega). \tag{28}
$$

In the last equation the index *i* is 1 or 2 and labels the different domains in which the filling parameter *s* takes on values corresponding to  $t<\omega$  (*i*=1) and  $t>\omega$  (*i*=2), respectively (see Appendix A). It turns out that the explicit formula for  $S_t(\omega, T_c)$  is a piecewise-continuous function of the filling parameter  $s = tZ(0)$ , and in passing through the point  $s^* = \omega Z(0)$  the functional dependence of  $S_t(\omega, T_c)$  on *s* changes. In the meantime, it is noteworthy that the discontinuous character of  $S_t(\omega, T_c)$  is an intrinsic property of the logarithmic VHS. Simple inspection convinces one that the situation does not change when other models such as the two-square well<sup>27</sup> or two-step<sup>28</sup> models are used for the gap function  $\phi(\omega)$  in the eigenvalue equation (21) instead of  $\phi^o(\omega)$  Eq. (8). It should also be noted that our representation (28) for  $S_t(\omega, T_c)$  is not an expansion in the interaction parameter  $\lambda$ . We retain all terms  $\delta_i(\omega)$  considering them as small corrections of  $S_i^o(\omega, T_c)$ . Taking into account the specific expressions for  $S_t(\omega, T_c)$  in Eqs. (21)–(27) finally gives an eigenvalue equation from which  $T_c$  is ultimately determined. The final form of  $T_c$  depends on the relative positions of the filling parameter *s* with respect to the peaks in  $S(\omega)$ . One obtains the following distinct cases.

#### A. Case of small separations,  $s < \omega Z(0)$

Here we assume that all phonon frequencies  $\omega_{ph}$  represented in the spectral density of interaction  $S(\omega)$  satisfy the condition  $t<\omega$ . This is the most important case since the Fermi energy lies in a region where the EDOS exhibits a pronounced structure in energy. For simplicity we use the weak Coulomb pseudopotential (26)  $\mu_{\star}=0$ . Using the implicit expressions for  $S_1(\omega, T_c)$  (Appendix A) in Eqs. (21)–  $(27)$ , the eigenvalue equation  $(21)$  becomes quadratic in  $ln(1.13t/T_c)$  (Appendix B); from this the final result for  $T_c$  is just

$$
T_c = 1.13 \Omega \exp(-D),\tag{29}
$$

$$
\Omega = 2\,We^{-\,\eta^o/2} \bigg(\frac{\overline{\omega}_{\text{ph}}}{t}\bigg),\tag{30}
$$

$$
D = \sqrt{\left[\ln\left(\frac{2W}{t}\right) + \frac{1}{g}\right]^2 + \left[\ln\left(\frac{\overline{\omega}_{ph}}{t}\right) - \frac{\eta^o}{2}\right]^2 - \frac{1}{g^2} - \frac{2\ln Z(0)}{g} - 2\,\overline{\delta}}.\tag{31}
$$

In expressions  $(29)$ – $(31)$  for  $T_c$  we set

$$
\overline{\omega}_{\text{ph}} = \exp(\ln \omega)_{S(\omega)}, \quad \frac{1}{g} = \frac{1}{\nu} + \rho(s), \quad t = \frac{s}{Z(0)}, \quad (32)
$$

$$
\eta^o = \left\langle \left\langle \frac{\omega^2}{\omega^2 - \omega_1^2} \ln \frac{\omega_1^2}{\omega^2} \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega)} \sim 1,
$$
 (33)

$$
\overline{\delta} = \left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left( \frac{1}{\omega_1^2} \delta_1(\omega_1, t) - \frac{1}{\omega_2^2} \delta_1(\omega_2, t) \right) \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega_2)},
$$
\n(34)

where the factors  $\rho(s)$  and  $\delta_1(\omega,t)$  are determined correspondingly, by Eqs.  $(20)$  and  $(28)$ ; the symbol  $\langle (\dots) \rangle$ should be understood as

$$
\langle (\ldots) \rangle = \frac{\int_0^\infty (d\omega^2/\omega^2) S(\omega) (\ldots)}{\int_0^\infty (d\omega^2/\omega^2) S(\omega)}.
$$
 (35)

This expression for  $T_c$  closely resembles that obtained in the van Hove scenario within the framework of BCS theory by Tsuei *et al.*<sup>6</sup> Physically, however, formulas  $(29)–(31)$  are much richer since they differ from the well-known result which is an exponential factor *D* premultipied by  $\Omega$ . The  $\Omega$  includes the full bandwidth 2*W* as well as the characteristic phonon energy  $\bar{\omega}_{ph}$ . In addition  $\Omega$  depends on the filling factor *s* as well as on the mass renormalization factor *Z*(0). The exponential factor *D* also involves characteristic parameters which in turn depend upon electronic, phononic and electron-phonon properties. Formula (29) also has another very interesting feature. To illustrate this, in accordance with the ordinary Eliashberg theory [when  $N(\epsilon)$ =const] let us assume that  $2W/\bar{\omega}_{ph} \ge 1$ . For not very small values of  $\lambda$  (approximately, for  $\lambda > 0.5$ ) one can then neglect all terms in the exponential factor  $D$  Eq.  $(31)$  except the first. Thus, expression  $(29)$  for  $T_c$  takes the form

$$
T_c = \frac{\overline{\omega}_{\text{ph}}}{1.45} \exp\left(-\frac{1+\lambda}{\lambda}(1+\rho)\right), \quad \rho \sim 10^{-2}
$$

which is precisely the familiar McMillan formula<sup>37</sup> with zero Coulomb pseudopotential.

#### **B.** Case of large separations,  $s > \omega Z(0)$

Let us consider values of the filling parameter *s* for which the condition  $t > \omega$  is satisfied for all characteristic frequencies of  $S(\omega)$ . In analogy with the case of  $s \leq \omega Z(0)$  we obtain (see Appendix  $C$ )

$$
T_c(s) = 1.13 \Omega(s) \exp\left(-\frac{A(s)}{g(s) - \mu_\star}\right),\tag{36}
$$

where in Eq.  $(36)$  one introduces the notation

$$
\Omega(s) = \overline{\omega}_{ph} \exp(\gamma(s) + \delta(s)),
$$
  
\n
$$
A(s) = \frac{N(s)}{N(t)} = 1 - \frac{\ln Z(0)}{N(t)},
$$
\n(37)

$$
g(s) = \frac{\nu}{1 + \nu E(s)}, \quad E(s) = \rho(s) + \eta(s) + \delta'(s). \quad (38)
$$

In expression (36) for  $T_c$  the factor  $g(s)$  Eq. (38) plays the role of an effective interaction parameter, the Coulomb pseudopotential  $\mu_{\star}$  being given by Eq. (26). Specific expressions for  $\rho(s)$  Eq. (20),  $\gamma(s)$ ,  $\eta(s)$ , and  $\delta(s)$  in Eq. (36) are then determined by the shape of interaction spectrum  $S(\omega)$ , namely,

$$
\gamma(s) = -\frac{1}{2N(t)} \left\langle \ln \frac{\omega}{t} \ln \left( 1 - \frac{\omega^2}{t^2} \right) \right\rangle_{S(\omega)},
$$
  

$$
\delta(s) = \frac{1}{N(t)} \left\langle \delta_2(\omega, t) \right\rangle_{S(\omega)},
$$
 (39)

$$
\eta(s) = \frac{1}{2N(s)} \left\{ N(t) \eta^o + \frac{1}{2} \left\langle \left\langle \frac{\omega^2 + \omega_1^2}{\omega^2 - \omega_1^2} \left[ \ln \frac{\omega_1}{t} \ln \left( 1 - \frac{\omega_1^2}{t^2} \right) \right] - \ln \frac{\omega}{t} \ln \left( 1 - \frac{\omega^2}{t^2} \right) \right] \right\}_{S(\omega_1)} \right\},
$$
\n(40)

$$
\delta'(s) = \frac{1}{2N(s)} \left\langle \left\langle \frac{\omega^2 + \omega_1^2}{\omega^2 - \omega_1^2} \left[ \delta_2(\omega, t) - \delta_2(\omega_1, t) \right] \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega)}
$$
\n(41)

In the above formulas  $N(t) = \ln(2W/t)$ ,  $N(s) = \ln(2W/s)$ ;  $\delta_2(\omega,t)$ ,  $\overline{\omega}_{\text{ph}}$ , and  $\eta^{\circ}$  are given correspondingly, by Eqs.  $(28)$ ,  $(32)$ , and  $(33)$ .

According to Eq.  $(17)$  the values of parameters  $A(s)$  Eq.  $(37)$ ,  $\gamma(s)$  Eq.  $(39)$ , and  $\eta(s)$  Eq.  $(40)$  depend on the magnitude of  $N(\epsilon_F)$ . For a large shift *s* of  $\epsilon_F$  from the saddle point the function  $(17)$  is slowly varying. Therefore, in agreement with the physical situation, far from the peak in EDOS we can suppress the logarithmic variation of the  $N(\epsilon_F)$  that enters expressions (37)–(40) and take it as constant for large energy values  $s^{25}$  Fixing  $N(\epsilon_F)$  at the interdomain boundary  $s^*$  we set

$$
N(t) = \ln \frac{2W}{\overline{\omega}_{\text{ph}}}.
$$

If the interaction spectrum  $S(\omega)$  is a  $\delta$  function centered about some average frequency  $\omega_{\rm ph}$ , and in addition if  $\mu^*$ =0, then a little algebra leads to the following expression for  $T_c$ :

$$
T_c = \frac{\omega_{\text{ph}}}{1.45} \exp\bigg(-\frac{1}{\nu} + R(s)\bigg),\tag{42}
$$

where

$$
R(s) = \frac{1}{\ln(2W/\omega_{\rm ph})} \left[ \frac{\ln Z(0)}{\lambda} - \frac{1}{2} \ln \frac{\omega_{\rm ph}}{t} \ln \left( 1 - \frac{\omega_{\rm ph}^2}{t^2} \right) - \frac{3}{2} \frac{\omega_{\rm ph}^2}{t^2 - \omega_{\rm ph}^2} \ln \frac{\omega_{\rm ph}}{t} - \frac{1}{4} \sum_{k=1}^{\infty} \frac{1}{k^2} \left( \frac{\omega_{\rm ph}^2}{t^2} \right)^k \right].
$$

It is not difficult to see that formula Eq.  $(36)$  for  $T_c$  has the correct asymptotic "behavior," namely, if  $2W/\overline{\omega}_{ph} \rightarrow \infty$ then Eq.  $(36)$  assumes the form

$$
T_c^o = 1.13 \overline{\omega}_{\text{ph}} \exp\left(-\frac{1}{g^o - \mu_\star}\right), \quad g^o = \frac{\nu}{1 + (1/2) \eta^o \nu}.
$$
\n(43)

Expression  $(43)$  is well known from the theory<sup>38</sup> with constant EDOS for intermediate coupling. In particular, this expression turns out to be extremely useful in understanding the differences in partial isotope shift factors  $\alpha_i = (m_i/T_c) dT_c / dm_i$  in compounds arising from the dissimilar variation in the interaction spectrum  $\alpha^2 F(\omega)$  under substitutions of *i* type of atoms by different isotopes. On the basis of formula  $(43)$  it was shown,<sup>39,40</sup> though the critical temperature itself is a weak function of the shape of  $\alpha^2 F(\omega)$  ( $T_c$  is determined mainly by average phonon frequency  $\bar{\omega}$ , interaction parameter  $\lambda$  as well as weak Coulomb pseudopotential  $\mu_{\star}$ ) the differential parameters, such as, e.g., the partial isotope shift factor and the pressure variation of  $T_c$  may be very sensitive to changes in the interaction spectrum.

It should be stressed that formulas  $(29)–(31)$  and  $(36)–$  $(38)$  for  $T_c$  were obtained solely within the framework of Eliashberg theory. That is, we deal with the *real parameters* of the electron-phonon system, which has a specific *microscopic origin*. Again, the final expressions for  $T_c$  include parameters of electronic, phononic, and electron-phonon origin. Moreover, the results for  $T_c$  are obtained as a functional of the interaction spectrum  $\alpha^2 F(\omega)$ . In arriving at final formulas  $(29)–(31)$  and  $(36)–(38)$  one need not specify the shape of  $\alpha^2 F(\omega)$ , by which one understands *any spectrum* including spectra associated with *monoatomic* or with *compound* superconductors (see Refs. 39 and 40).

## **IV. DISCUSSION OF RESULTS**

Consider now the expression for the critical temperature  $T_c$  for various parameter values of the model adopted above. We are interested in cases when the Fermi level is either near or far from the saddle point in the EDOS. Physically, we expect higher values of  $T_c$  for small *s*. The shift of  $\epsilon_F$  from the middle of the conduction band may be considered as comparatively small in the domains labeled by  $i=1$  in Eq. (28), since in these cases the distance between  $\epsilon_F$  and the EDOS peak is of the order of the phonon frequency  $\bar{\omega}_{\text{ph}}$ which is the characteristic energy scale important for superconductivity. By contrast, when  $\epsilon_F$  is off the saddle point, we can expect a secondary  $T_c$ -enhancing effect due to the peak structure in the EDOS and we recover a result for  $T_c$  values consistent with those from ordinary Eliashberg theory [namely,  $N(\epsilon)$ =const, comparatively small values of  $T_c$ ]. A significant separation of  $\epsilon_F$  from the middle of the conduction band occurs when  $s > \bar{\omega}_{ph}Z(0)$  (in the domain labeled with  $i=2$ ). It should be emphasized, that the width of the segment of the filling parameter values where we expect higher values of  $T_c$  implicitly depends on the interaction parameter  $\lambda$ . Actually, the energy dependence in  $N(\epsilon)$  is incorporated into Eliashberg theory by introducing an additional factor  $N(\vert \tilde{\omega}_m \vert)$  Eq. (4) into the sums of the ordinary equations. The factor  $N(\vert \tilde{\omega}_m \vert)$  is determined not by "bare" Matsubara frequencies  $\omega_m$  but rather by the renormalized ones  $\tilde{\omega}_m$  Eq. (2). The final expressions for  $T_c$  Eqs. (29)–(31) and  $(36)–(38)$  are obtained after a preliminary summation in eigenvalue equation (21) over discrete  $\tilde{\omega}_m$ , which in turn depend on the value of the factor  $Z(\omega_m)$ . Because of the summation in Eq.  $(21)$  the superconducting critical temperature,  $T_c$ , depends on the filling parameter *s* by means of the ratio  $t = s/Z(0)$ . Separation into domains where one expects, respectively, large and moderate values of  $T_c$  occurs at respectively, large and moderate values of  $T_c$  occurs at  $t^* = \overline{\omega}_{ph}$ . Thus, the width of the segment of the filling parameter values, where a higher  $T_c$  is expected, depends on *Z*(0).

Note that in the derivation of formulas for  $T_c$  Eqs. (29)–  $(31)$  we have used the digamma function representation<sup>20</sup>

$$
\Psi(X) = \ln |X| - \frac{1}{2X} - \frac{1}{12X^2} + \cdots,
$$

which is valid for  $|X| > 1$  (here  $X = 1/2 - s/2\pi T_c$ ). Therefore, for very small separation *s* of the Fermi level from the saddle point, when the application of the above-mentioned formula is invalid, our result for  $T_c$  is not correct and the range of values of *s*, where the final expression for  $T_c$  Eqs. (29)–(31) is applicable, must be restricted from below, say at  $\overline{\omega}_{ph}/2$ . Here, it was assumed that  $\omega_{ph} \geq 2 \pi T_c$ , which is the case for La-Sr-Cu-O (LSCO) superconductors. Experimentally, LSCO electrons interact mainly with the O and Cu atoms in the conducting planes for which  $\omega_{ph} \sim 300$  K and  $T_c \sim 40$  K. Thus, if  $s > \omega_{ph}/2$  then the condition  $s > 2\pi T_c$  holds.



FIG. 1.  $T_c/T_c^o$  vs  $\lambda$ , for  $(2W/\omega_{ph})=200$  (solid line) and 40 (dashed line), the so-called "high-temperature region."

Next we analyze the  $T_c$  formulas. Direct inspection of  $T_c$  Eqs.  $(29)$ – $(31)$  allows one to conclude that for values of the filling parameter *s* such that  $\overline{\omega}_{ph}/2 < s < \overline{\omega}_{ph}Z(0)$ , the transition temperature  $T_c$  exceeds the value  $T_c^o$  corresponding to constant  $N(\epsilon)$ . However, enhancement of  $T_c$  will depend on the value of the interaction parameter. The relative enhancement of  $T_c$  is more noticeable for small  $\lambda$ , viz., as seen from Fig. 1 where  $T_c/T_c^o$  versus  $\lambda$  appears. For  $\lambda$  = 0.3 the critical temperature increases nearly four times, while for  $\lambda = 1.5$  the increase in  $T_c$  is only about 50%. Actually, in the modified Eliashberg theory for  $T_c$  the factor  $N(\tilde{\omega}_n)$  Eq. (4) describes the broadening in the EDOS peak structure. Washing out of the EDOS peaks due to this broadening is more pronounced for large  $\lambda$ . Therefore, for strongly coupled superconductors a sharp structure in  $N(\epsilon)$  is less effective for  $T_c$  enhancement than for weakly coupled ones.

Figure 2 shows plots of  $T_c$  as a function of  $s$  ( $s \leq s^*$ ), for Figure 2 shows plots of  $T_c$  as a function of  $S(S \leq S)$ , for different values of  $2W/\bar{\omega}_{ph}$ . The magnitude of  $T_c^o$  is indi-



FIG. 2.  $T_c$  as a function of  $t/\bar{\omega}_{ph}$  (high-temperature region). Curves correspond to  $2W/\omega_{ph} = 200$  and 40. Here  $\lambda = 1.2$ ,  $\omega_{ph}$  = 20 meV. The horizontal dotted line is  $T_c^o$ .



FIG. 3.  $T_c$  as function of  $t/\omega_{ph}$  for large separation of  $\epsilon_F$  from the saddle point.  $2W/\omega_{ph}$ =200 (solid line) and 100 (dashed line). Dotted and dash-dotted lines at bottom correspond, respectively, to cases  $2W/\omega_{ph} \rightarrow \infty$  and constant EDOS. Here  $\lambda = 1.2$ ,  $\omega_{ph} = 20$ meV.

cated by the horizontal line at the bottom. This figure clearly illustrates the considerably higher  $T_c$  compared with  $T_c^o$ throughout the entire range of variation of *s* from  $\overline{\omega}_{ph}/2$  to  $\overline{\omega}_{ph}Z(0)$ . Henceforth, this domain will be referred to as the ''high-temperature region.'' Significantly, however, in this region  $T_c$  is nonmonotonic in the filling parameter *s*. As *s* decreases from  $\bar{\omega}_{ph}Z(0)$ ,  $T_c$  increases initially and then reaches a maximum value at some s'. Further decrease of *s*, namely, further increasing  $N(\epsilon_F)$  through the saddle point, produces a gradual decrease of  $T_c$ , in agreement with the Pickett result<sup>18</sup> for *A*15 compounds. The reason for the reduction of  $T_c$  for small separation *s* of  $\epsilon_F$  from the middle of the conducting band can be understood if we recall the substantial decrease of the factor  $N(\tilde{\omega}_n)$  Eq. (16) produced by decreasing *s*. Because  $N(\tilde{\omega}_n)$  is proportional to  $1/N(\epsilon_F)$ which vanishes rapidly as  $\epsilon_F$  varies up to the saddle point, we have a reduction of  $T_c$  for small  $s$  instead of its expected increase. Another remarkable feature of  $T_c$  is that the strongest variation in  $T_c$  does not occur in our so-called hightemperature region. Namely,  $\Delta T_c / T_c$  is of order 0.1, where  $\Delta T_c$  is the total change in  $T_c$  as *s* varies from  $\bar{\omega}_{\text{ph}}/2$  to  $\overline{\omega}_{\rm ph}Z(0)$ . We again stress that the width of the "hightemperature region'' thus defined depends on the value of the interaction parameter: large values of  $\lambda$  correspond to a broader such region.

Figure 3 displays plots of  $T_c$  vs  $s$  for large separations  $s$  $(s > s^*)$ . As seen from Figs. 2 and 3, both drawn for the  $\delta$ -like interaction spectrum and for the same values of  $\lambda$  and  $2W/\omega_{\rm ph}$ , for a value of  $\overline{\omega}_{\rm ph}Z(0)$  for the filling parameter *s*,  $T_c$  drops discontinuously toward the  $T_c^o$  lying a little higher than  $T_c^o$ . The difference  $T_c - T_c^o$  tends to zero for significant values of the ratio  $2W/\bar{\omega}_{ph}$ , in accordance with the constant EDOS case. In fact, variation of the functional form of  $T_c(t)$  by increasing the filling parameter [that is, transfer of expressions  $(29)$ – $(31)$  for  $T_c$  to formulas of the form  $(36)–(41)$ ] takes place over the full "width" of the spectral density  $S(\omega)$ . The Eliashberg function  $S(\omega)$  consists of several narrow peaks at certain  $\{\omega_i\}$  ( $i=1,2,\dots$ ) arising from the interaction of electrons with individual groups of phonons with frequencies  $\omega_i$ .<sup>32</sup> The  $\delta$ -like structure of  $S(\omega)$  leads to a discontinuity of  $T_c$  as a function of  $s = tZ(0)$ . Note that the magnitude of  $T_c - T_c^o$  at large *s* (Fig. 3) is associated with the factor  $ln Z(0)$  in the expression for  $T_c$  [Eq. (42)] arising from using renormalized frequencies  $\tilde{\omega}_n = \omega_n \tilde{Z}(0)$  in the broadening factor  $\tilde{N}(\tilde{\omega}_n)$  Eq. (4). Using in our  $T_c$  calculations the "bare" Matsubara frequencies  $\omega_n$ , instead of  $\tilde{\omega}_n$ , then beginning approximately from  $(t/\overline{\omega}_{ph}) = 2$  the critical temperature  $T_c$  approaches  $T_c^o$ . The qualitative picture shown in Fig. 2 does not change on substitution of  $\omega_n$  for the renormalized  $\tilde{\omega}_n$ , but the  $\lambda$  dependence of  $T_c$  (Fig. 1) steepens, and for  $\lambda = 1.5$  we have only  $\sim$  25% of the  $T_c$  enhancement. It is easy to understand that representing the spectral function  $S(\omega)$  as a sum of several  $\delta$ -like peaks, that is, allowing for simultaneous contribution of frequencies from two different domains with  $t < \omega$  and with  $t > \omega$  to the integrals (23) and (24), does not alter the discontinuous character of  $T_c$  nor its asymptotic behavior at large values of  $s$ . Therefore, *discontinuity of*  $T_c$  *as a function of the filling parameter is an intrinsic feature of quasi-twodimensional superconductivity.* Taking into account the finite widths of the peaks in  $S(\omega)$ , as well as the transition matrix elements for electrons between adjacent conducting layers will "spoil" this ideal discontinuous picture in the  $T_c$  behavior and smooth out the transition from the high-temperature region to a region where  $T_c$  is moderate. We believe that, physically, the discontinuous nature of  $T_c$  as a function of the distance between  $\epsilon_F$  and saddle point in  $N(\epsilon)$  is a result of the *short-range character in the energy space* of the indirect electron-electron interaction via phonons. The mathematical origin of this discontinuity is hidden in the nonanalytic behavior of the integral (28). In energy space this interaction is spread over a region  $\omega_0$  around the Fermi surface. Let us assume that the singularity in EDOS is located at exactly a distance  $\omega_0$  from  $\epsilon_F$ . Then any small increase of *s* will remove the singularity from the energy shell  $\epsilon_F - \omega_0 \leq \epsilon \leq \epsilon_F + \omega_0$  and lead to exclusion of the contribution to  $T_c$  due to the singularity in  $N(\epsilon)$ . Namely, the latter contribution is responsible for the discontinuous nature of  $T_c$  .

It is not difficult to see that  $(\delta T_c / \delta W)$  < 0 everywhere. Thus, decreasing  $2W/\bar{\omega}_{ph}$  always results in a slight increase in  $T_c$ , the influence of bandwidth on  $T_c$  becoming more significant for relatively smaller ratios of  $2W/\bar{\omega}_{ph}$ .

In Fig. 4 the influence of the correction terms  $\delta_i(\omega, s)$  on *T<sub>c</sub>* is exhibited, the dashed curve corresponding to a plot of  $T_c$  including correction terms in expressions  $(29)$ – $(31)$  and  $(36)$ – $(38)$ . The full curve is the same plot but without the  $\delta_i(\omega, s)$ . Evidently, over the entire range of variation of the filling parameter, taking these correction terms  $\delta_i(\omega, s)$  into account leads to small changes in the magnitude of  $T_c$ .

Our results may be useful in understanding the experimental data of Ref. 41 where it was established that the phase diagram of well-annealed  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  oxides differs sharply from that held by conventional wisdom. The concentration dependence of  $T_c$  in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  does not follow the commonly assumed ''inverted-parabola'' behavior; rather it remains in the 35–40 K range for



FIG. 4.  $T_c$  as function of  $t/\omega_{ph}$ . Dashed curve is plot of  $T_c$ when correction terms discussed in text are included. Full curve is same plot but without  $\delta_i(\omega, s)$ . 2*W*/ $\omega_{ph}$ =200;  $\lambda$  and  $\omega$  are as in Figs. 2 and 3.

 $x=0.14-0.21$ . At  $x_{cr}$   $\sim$  0.21 – 0.22,  $T_c$  drops discontinuously to zero. If one assumes that critical doping  $x_{cr}$  corresponds to filling parameter  $s^* = \omega_{ph} Z(0)$  in our consideration, then one can explain  $T_c$  as nearly constant over the concentration range  $x=0.14-0.21$ , and one can understand its discontinuity as well. It has also been found $41$  that at a concentration where *Tc* experiences an abrupt decrease, a second-order structural transition takes place from a low-temperature orthorhombic phase to a high-temperature tetragonal phase. Such drastic changes in the material at nearly the same concentration  $x_{cr}$ may, in principle, have an identical origin. Thus, it would be extremely interesting to investigate this phase transition in layered systems by assuming a van Hove scenario.

To conclude, an analytic expression is obtained for the superconducting critical temperature  $T_c$  in the logarithmic van Hove scenario (VHS) within the framework of the modified Eliashberg equations allowing for sharp variations in the electronic density of states. The behavior of  $T_c$  as a function of the Fermi energy shift from the van Hove saddle point is analyzed, and we identify the region of the filling parameter values where the effectiveness of VHS in enhancing  $T_c$  is most appreciable. The dependence of  $T_c$  enhancing on the value of interaction parameter  $\lambda$  in VHS is thus established. It is shown that though an increasing  $T_c$  is more effective for weak coupling, nevertheless, for intermediate coupling the critical temperature is still considerably higher than  $T_c^o$ , corresponding to a constant EDOS. Based on the existence of low-dimensional structural elements such as planes, a possible explanation is suggested for a curious discontinuous change in transition temperature observed experimentally in  $La_{2-x}Sr_xCuO_4$  oxides.

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# **APPENDIX A**

To obtain concrete expressions for  $S_t(\omega, T_c)$  Eq. (28) integral tables $34$  give

$$
S_1(\omega, T_c) = \ln \frac{1.13 \omega / T_c}{\ln} \frac{1.13 \sqrt{\omega^2 - t^2}}{T_c} + \delta_1(\omega, t), \quad t < \omega;
$$
\n(A1)

$$
S_2(\omega, T_c) = \ln \frac{1.13t}{T_c} \ln \frac{1.13\sqrt{t^2 - \omega^2}}{T_c} - \frac{1}{2} \ln^2 \frac{1.13t}{T_c} + \delta_2(\omega, t),
$$

 $t > \omega,$  (A2)

where

$$
\delta_1(\omega) = -\frac{1}{4} \sum_{k=1}^{\infty} \frac{1}{k^2} \left( \frac{\omega^2 - t^2}{\omega^2} \right)^k, \quad t < \omega,
$$

$$
\delta_2(\omega) = -\frac{1}{4} \sum_{k=1}^{\infty} \frac{1}{k^2} \left( \frac{\omega^2}{t^2} \right)^k, \quad t > \omega.
$$

If the Eliashberg function  $S(\omega)$  is located in the interval  $(\omega_{\min}, \omega_{\max})$  then, depending on the relation  $t < \omega_{\min}$  or  $t > \omega_{\text{max}}$ , the integrals (23) and (24) are determined correspondingly by Eq. (A1) or (A2). The use of  $S_1(\omega, T_c)$  or  $S_2(\omega, T_c)$ , for Eqs. (21)–(27), results in expressions for  $T_c$ which have different functional forms (see below).

# **APPENDIX B**

Substitution of  $S_1(\omega, T_c)$  (Appendix A) into Eq. (27) after rearrangement gives

$$
P(\omega) = \frac{1}{N(s)} \frac{1}{\omega^2} \left( \frac{1}{2} L^2 + L \ln \frac{2W\omega}{t^2} + \ln \frac{\omega}{t} \ln \frac{2W}{t} + \delta_1(\omega, t) \right),
$$

where  $L=\ln(1.13t/T_c)$ ;  $\delta_i(\omega,t)$  for  $i=1$  is given by Eq.  $(A1)$ . From definitions  $(23)$  and  $(35)$  we have

$$
I_1 = \left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left[ P(\omega_1) - P(\omega_2) \right] \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega_2)}
$$

Using in the last equality the relations

$$
\left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left( \frac{1}{\omega_1^2} \frac{2W\omega_1}{t^2} - \frac{1}{\omega_2^2} \frac{2W\omega_2}{t^2} \right) \right\rangle_{S(\omega)} \right\rangle_{S(\omega)}
$$
  
\n
$$
= \ln \frac{2W\overline{\omega}}{t^2} - \frac{1}{2} \eta^o,
$$
  
\n
$$
\left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left( \frac{1}{\omega_1^2} \frac{\omega_1}{t} - \frac{1}{\omega_2^2} \frac{\omega_2}{t} \right) \right\rangle \right\rangle = \ln \frac{\overline{\omega}}{t} - \frac{1}{2} \eta^o,
$$

where the factors  $\bar{\omega}$  and  $\eta^o$  in the above expressions are given by Eqs.  $(31)$  and  $(33)$ , and inserting a zero Coulomb pseudopotential  $\mu^*=0$  into the eigenvalue equation (21) we arrive at

$$
L^{2} + 2L\left(\ln\frac{2W\overline{\omega}}{t^{2}} - \frac{\eta^{o}}{2}\right)
$$
  
+ 2\ln\frac{2W}{t}\left(\ln\frac{\overline{\omega}}{t} - \frac{\eta^{o}}{2}\right) + 2\overline{\delta} = \frac{2N(s)}{g}. (B1)

.

The solution for *L* of the last equation gives

$$
L_{\pm} = -\left(\ln\frac{2W\overline{\omega}}{t^2} - \frac{\eta^o}{2}\right) \pm \sqrt{\left(\ln\frac{2W\overline{\omega}}{t^2} - \frac{\eta^o}{2}\right)^2 - 2\ln\frac{2W}{t}\left(\ln\frac{\overline{\omega}}{t} - \frac{\eta^o}{2}\right) + \frac{2N(s)}{g} - 2\overline{\delta}}.
$$

 $\overline{\phantom{a}}$ 

Taking into account in  $L_{\pm}$  the identity

$$
N(s) = \ln \frac{2W}{t} + \ln \frac{t}{s},
$$

we get, after simple algebra,

$$
L = -\left(\ln\frac{2W\overline{\omega}}{t^2} - \frac{\eta^o}{2}\right) + \sqrt{\left(\ln\frac{2W}{t} + \frac{1}{g}\right)^2 + \left(\ln\frac{\overline{\omega}}{t} - \frac{\eta o}{2}\right)^2 - \frac{1}{g^2} - \frac{2\ln Z(0)}{g} - 2\,\overline{\delta},}
$$

which is the physically possible solution  $L_{+}$  of equation (B1). One finally obtains the expression for  $T_c$  in Eqs. (29)–  $(31).$ 

## **APPENDIX C**

Let us rewrite the eigenvalue equation  $(21)$  for  $T_c$  in the form

$$
\frac{\widetilde{Z}(0)}{\lambda} - (I_1 - I_2) = \frac{I_2}{1 + \mu_{\star} I_2}.
$$
 (C1)

In the denominator Eq. (26) was used, and  $\widetilde{Z}(0)$  is given by Eq.  $(20)$ . Recalling Eqs.  $(23)$  and  $(24)$  the concrete expression for  $S_2(\omega, T_c)$  Eq. (A2) gives

.

,

$$
I_1 = \frac{1}{N(s)} (L + \eta_1 + \overline{\delta}_2), \tag{C2}
$$

$$
I_2 = \frac{1}{N(s)} (L + \eta_2 + \overline{\delta}_2'),
$$
 (C3)

where the following notation was introduced:

$$
L = \ln \frac{1.13t}{T_c} \ln \frac{2W}{t},
$$
\n
$$
\eta_1 = \left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left( \frac{1}{\omega_1^2} \ln \frac{\omega_1}{t} \ln \frac{2W}{\sqrt{t^2 - \omega_1^2}} \right) - \frac{1}{\omega_2^2} \ln \frac{\omega_2}{t} \ln \frac{2W}{\sqrt{t^2 - \omega_2^2}} \right\rangle \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega_2)},
$$
\n
$$
\eta_2 = \left\langle \ln \frac{\omega_1}{t} \ln \frac{2W}{\sqrt{t^2 - \omega^2}} \right\rangle_{S(\omega)}
$$
\n
$$
\overline{\delta}_2 = \left\langle \left\langle \frac{\omega_1^2 \omega_2^2}{\omega_2^2 - \omega_1^2} \left( \frac{1}{\omega_1^2} \delta_2(\omega_1) - \frac{1}{\omega_2^2} \delta_2(\omega_2) \right) \right\rangle_{S(\omega_1)} \right\rangle_{S(\omega_2)}
$$
\n
$$
\overline{\delta}_3' = \left\langle \delta_2(\omega, t) \right\rangle_{S(\omega)}.
$$

$$
\delta_2' = \langle \delta_2(\omega, t) \rangle_{S(\omega)}.
$$

The left-hand side of Eq.  $(C1)$  does not depend on  $T_c$  and is denoted by  $1/g(s)$ . Then from Eq. (C1) we have  $I_2 = 1/g - \mu_{\star}$  which in conjunction with Eq. (C3) leads to the final expressions  $(36)$ – $(38)$  for  $T_c$ .

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# **APPENDIX D**

In this appendix we derive formulas for parameters appearing in the final expressions  $(29)–(31)$  and  $(36)–(38)$  for  $T_c$ , assuming that the interaction spectrum  $S(\omega)$  has a  $\delta$ -like shape:

$$
\overline{\omega}_{ph} = \omega_{ph}, \quad \eta^o = 1,
$$
  

$$
\overline{\delta}(s) = \frac{1}{8} \left[ \frac{t^2}{\omega_{ph}^2 - t^2} \ln \frac{\omega_{ph}^2}{t^2} - \sum_{k=1}^{\infty} \frac{1}{k^2} \left( \frac{\omega_{ph}^2 - t^2}{\omega_{ph}^2} \right)^k \right],
$$
  

$$
\rho(s) = \frac{1}{N(s)} \left( \ln Z(0) + \frac{\omega_{ph}^2}{t^2 - \omega_{ph}^2} \ln \frac{\omega_{ph}}{t} \right),
$$
  

$$
\gamma(s) = -\frac{1}{2N(t)} \ln \frac{\omega_{ph}}{t} \ln \left( 1 - \frac{\omega_{ph}^2}{t^2} \right),
$$
  

$$
\eta(s) = \frac{1}{2} \frac{N(t)}{N(s)} - \frac{1}{4N(s)} \left\{ \ln \left( 1 - \frac{\omega_{ph}^2}{t^2} \right) - \frac{2\omega_{ph}^2}{t^2 - \omega_{ph}^2} \ln \frac{\omega_{ph}}{t} \right\},
$$
  

$$
\delta(s) = -\frac{1}{4N(t)} \sum_{k=1}^{\infty} \frac{1}{k^2} \left( \frac{\omega_{ph}^2}{t^2} \right)^k,
$$
  

$$
\delta'(s) = -\frac{1}{4N(s)} \ln \left( 1 - \frac{\omega_{ph}^2}{t^2} \right)^k,
$$

where  $N(t) = \ln(2W/t)$  and  $N(s) = \ln(2W/s)$ .

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