# Fine structure in the electron density of states, paramagnetic impurities, and anomalous isotope effect for $T_c$ in LSCO:Fe systems

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A superconductor with a sharp peak in the electron density of states and paramagnetic impurities is considered. The values of the critical temperature  $T_c$  and the isotope effect are analyzed as functions of the position of the Fermi level relative to the center of the peak and the impurity concentration. Experimental data on the isotope effect for  $T_c$  in LSCO:Fe systems are analyzed on the basis of the theory developed. © 1995 American Institute of Physics.

## **1. INTRODUCTION**

The question of the isotope shift of the critical superconducting transition temperature  $T_c$  has been discussed regularly in reference to various materials in the literature. The fact is that by definition the isotope effect

$$\alpha = \frac{-\partial \ln T_c}{\partial \ln M}$$

is a differential characteristic. Therefore, its value is more sensitive to features in the spectra of quasiparticles and the spectrum of the attractive interelectronic interaction than are other parameters of superconductors. As a result, the value of  $\alpha$  provides highly significant information.

A recent study of the influence of oxygen isotopic substitution on the superconducting transition temperature  $T_c$  in  $La_{1-y}Sr_yCuO_4$  (LSCO) systems revealed that the partial isotope effect for oxygen is strongly dependent on the concentration y of Sr atoms. Also,  $\alpha$  varies by a factor of approximately 5–10 in the concentration range 0.1 < y < 0.15. For  $y=0.12 \alpha$  is maximal and equal to 0.8-1 (Refs. 1–3).

Several models have been proposed to explain these experiments. They include, first, a model based on the conception of a soft anharmonic mode [which is associated either with low-frequency rotational modes accompanying a structural transition<sup>4</sup> or with the appearance of strong local anharmonicity in vibrations of the apical oxygen atoms (see, for example Ref. 5)]. Second, models with a sharp peak in the electron density of states have been considered. Here it is assumed that doping with Sr alters the number of carriers and simultaneously shifts the Fermi level.<sup>6</sup> For other studies, see the reviews in Refs. 7 and 8.

Subsequently, in Ref. 3 the oxygen isotope effect was also studied in LSCO:Me with an optimum composition with respect to Sr (y=0.15) and with Fe, Co, Ni, and Zn impurities, which replace Cu atoms. The concentration x of the impurities did not exceed several percent. It was discovered that in all cases the values of the critical temperature  $T_c$  decrease significantly, and the corresponding values of  $\alpha$  increase as the defect concentration x increases. These experimental data for LSCO:Me systems, as well as the analogous data for YBCO:Me systems,<sup>9</sup> were attributed in Ref. 10 to the appearance of effective paramagnetic defects in both systems.

The LSCO: Me systems (y=0.15) with different impurities exhibit some significant specific differences along with the general features of the behavior of  $T_c$  and  $\alpha$ . In particular, in the case of M=Zn, Ni, the behavior of  $T_c$  and  $\alpha$  as functions of the concentration x is described according to the Abrikosov-Gor'kov theory<sup>11</sup> (see also Refs. 12 and 13) in the single-parameter approximation. The data for Me=Fe, Co do not fit the simple scheme. We note that in the case of doping with iron atoms the changes in  $\alpha$  are very pronounced: the value of  $\alpha$  varies from 0.1 to 1.3 for x=0.11

The factors causing the differences in the behavior of  $T_c$  and  $\alpha$  in LSCO systems with Fe and Co and with Ni and Zn as impurities have not previously been discussed in the literature. In this paper we propose a model, which makes it possible to qualitatively account for the anomalously large isotope effect in the case of Fe (Co) impurities and the comparatively weak effect in the case of Zn (Ni) impurities. We start out from the phonon mechanism and the ideas in Refs. 6 and 10. More specifically, the existence of a sharp peak in the electron density of states is postulated. (The question of the role of van Hove singularities in one- and twodimensional superconductors and their relationships to the properties of cuprate superconductors were discussed in detail in the review in Ref. 14; see also the recent work in Ref. 15). At the same time, impurities in the copper sites and their local environment are treated as effective paramagnetic defects. (Here we based ourselves on the results in Refs. 16-18, in which the temperature dependence of the susceptibility was measured.) It is also assumed that trivalent Fe impurity atoms, unlike divalent Zn impurity atoms, alter the number of carriers and shift the position of the Fermi level relative to the center of the peak (the valence of Fe was determined in experiments involving measurement of the isomer shift in the Mössbauer spectrum<sup>19</sup>).

We also note that a situation in which both antiferromagnetic and superconducting properties are displayed in a certain temperature range is realized in systems with heavy fermions. It is assumed that the appearance of heavy fermions can be caused by antiferromagnetic spin fluctuations in the Fermi liquid (see, for example, the review in Ref. 20 and Ref. 21). However, antiferromagnetism and superconductivity also coexist in the case of cuprate superconductors. Therefore, it may be theorized, in principle, that in LSCO systems the van Hove singularity in the density of states of the carriers is caused by spin fluctuations (see the discussion in Refs. 22–24). In such a situation the masking of the fine structure of the density of states by impurities (it is usually very significant; see, for example 25) may be of minor importance.

#### 2. GENERAL RELATIONS

Let us consider the BCS equation for to  $T_c$ 

$$\frac{V_{\rm ph}}{2} \int_{E_F - \omega_D}^{E_F + \omega_D} dz N(z) \quad \frac{\tanh(z/2T_c)}{z} = 1. \tag{1}$$

Here  $V_{\rm ph}$  is the parameter of the attractive interelectronic interaction. (We use a system of units with  $\hbar = k_B = 1$ .) Also, N(z) denotes the electron density of states, which has a fine structure with an energy scale  $\Gamma \leq \omega_D$ .

To be specific, we assume that there is a sharp peak in the density of states  $\tilde{n}_R(\delta)$  with its center at the point  $E=E_R$ . Then

$$N(z) = \frac{N_0}{2} (1 + \tilde{n}_R(z, \delta)),$$
 (2)

where  $N_0/2$  is the value of the density far from the center of the peak (which does not depend on the energy of the "pedestal"),  $\delta = E_F - E_R$  is the position of the Fermi level relative to the center of the peak, and  $z = E - E_R$  is the energy measured relative to the Fermi level.

We represent (1) in the form

$$\frac{V_{\rm ph}}{2} \int_0^{\omega_D} dz N(z+\delta) + N(z-\delta) \frac{\tanh(z/2T_c)}{z} = 1.$$
(3)

We rewrite (3) in another form. We take into account the standard expression for the hyperbolic tangent:

$$\tanh \frac{\pi x}{2} = \frac{4x}{\pi} \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2 + x^2} \, .$$

Then instead of (3) we have

$$2V_{\rm ph}T_c \int_0^{\omega_D} dz [N(z+\delta) + N(z-\delta)] \sum_{k=1}^{\infty} \frac{1}{\omega_k^2 + z^2} = 1,$$
(4)

where

$$\omega_k = \pi T_c(2k-1).$$

We note that the integrand in (4) has the imaginary poles  $\omega_k = \pm iz$ . We qualitatively take into account the influence of paramagnetic impurities. First, the appearance of such impurities with a concentration  $c_s$  results in the appearance of a finite lifetime for the carriers at  $E \approx E_F$ . The resultant renor-

malization of the energy of the carriers reduces to the appearance of an imaginary addition. Here,  $\omega_k \rightarrow \omega_k + \tau_s^{-1}(\omega_k)$ , where <sup>12</sup>

$$\tau_s^{-1} = c_s \frac{7\pi}{24} J^2 S(S+1).$$

Here S is the effective classical spin of the impurity, and J is the exchange integral, which has the dimensions of energy. It is usually several times smaller than the characteristic electron energy  $E_F$ .

In accordance with the foregoing, when  $c_s \neq 0$  Eq. (4) takes on the following form

$$2V_{\rm ph}T_c \int_0^{\omega_D} dz [N(z+\delta) + N(\delta-z)] \\ \times \sum_{k=1}^{\infty} \frac{1}{[\omega_k + \tau_s^{-1}(\omega_k)]^2 + z^2} = 1.$$
(5)

In the absence of a fine structure, in which case  $N(E) = N_0$ , relation (5) becomes the expression previously obtained in Ref. 12.

We neglect the dependence of  $\tau_s^{-1}$  on  $\omega_k$ . Then by means of some simple transformations, instead of (5) we have an equation for  $T_c$  in the form

$$\ln \frac{T_c}{T_c^0} = \Psi\left(\frac{1}{2}\right) - \Psi\left(\frac{1+\rho}{2}\right) + \int_0^{\omega_D} dz n_R(z) \frac{\tanh\left(z/2T_c\right)}{z} + \int_0^{\omega_D} dz n_R(z) \frac{\Phi(\rho, z/\pi T_c)}{z}, \quad \rho = \frac{\tau_s^{-1}}{\pi T_c}.$$
 (6)

Here  $T_c^0$  denotes the critical temperature at  $c_s=0$  and  $\tilde{n}_R=0$ . It is defined by the expression

$$T_c^0 = 1.134\omega_D \exp\left(-\frac{1}{\lambda}\right), \quad \lambda = \frac{N_0 V_{\rm ph}}{2}$$

To make the equations more compact we set

$$n_{R}(z) = \frac{1}{2} (\tilde{n}_{R}(\delta+z) + \tilde{n}_{R}(\delta-z)),$$

$$\Phi\left(\rho, \frac{z}{\pi T_{c}}\right) = \frac{2}{\pi} \operatorname{Im}\left[\Upsilon\left(\frac{1+\rho+iz/\pi T_{c}}{2}\right) - \Upsilon\left(\frac{1+iz/\pi T_{c}}{2}\right)\right],$$

where  $\Upsilon$  is the digamma function.

We note that separate terms in (6) describe the influence of paramagnetic impurities and the sharp peak, as well as their combined action, on  $T_c$ . The situation in which  $\tau_s^{-1} = \tau_s^{-1}(\omega_k)$  holds is discussed in the appendix.

The isotope shift  $\alpha$  is defined as

$$\alpha = -\frac{\partial \ln T_c}{\partial \ln M} = -\frac{M}{T_c} \frac{\partial \omega_D}{\partial M} \frac{\partial T_c}{\partial \omega_D}$$

In the situation under consideration we find

$$\alpha = \alpha_0 \frac{1 + \tanh\left(\omega_D/2T_c\right) n_R(\omega_D) + \Phi(\rho, (\omega_D/\pi T_c)) n_R(\omega_D)}{1 + \int_0^{\omega_D} \frac{dz}{2T_c} \frac{n_R(z)}{\cosh^2(z/2T_c)} - \rho \Upsilon_{\rho}' \left(\frac{1+\rho}{2}\right) - \int_0^{\omega_D} \frac{dz}{z} T_c \frac{\partial}{\partial T_c} \Phi(\rho, z/\pi T_c)},$$
(7)

where

$$\alpha_0 = -\frac{\partial \ln T_c^0}{\partial \ln M} \,.$$

We note that when  $\rho \rightarrow 0$ , the expressions for  $T_c$  (6) and  $\alpha$  (7) actually coincide with the expressions previously obtained in Refs. 6 and 26. In another limiting case, in which  $n_r \rightarrow 0$ , they coincide with the results in Ref. 10 (see also Refs. 12 and 13). Using (6), we obtain an equation for the extrema values of  $T_c$  with respect to  $\delta$  at arbitrary values of  $c_s$ . We have

$$\frac{\partial T_c(\rho,\delta)}{\partial \delta} = T_c \frac{F_1(\rho,\delta)}{F_2(\rho,\delta)}, \qquad (8)$$

where

$$F_{1}(\rho,\delta) = \int_{0}^{\omega_{D}} \frac{dz}{z} \frac{\partial n_{R}(z)}{\partial \delta} \tanh \frac{z}{2T_{c}}$$
$$-\rho \Upsilon_{\rho}' \left(\frac{1+\rho}{2}\right) \frac{\partial \tilde{n}_{R}(0)}{\partial \delta} \frac{1}{1+\tilde{n}_{R}(0)}$$
$$+ \int_{0}^{\omega_{D}} \frac{dz}{z} \frac{\partial}{\partial \delta} \left[ \Phi \left(\rho, \frac{z}{\pi T_{c}}\right) n_{R}(z) \right], \qquad (9a)$$

$$F_{2}(\rho, \delta) = 1 - \rho \Upsilon_{\rho}' \left( \frac{1+\rho}{2} \right) + \int_{0}^{\omega_{D}} \frac{dz}{2T_{c}} \frac{n_{R}(z)}{\cosh^{2}(z/2T_{c})} + \int_{0}^{\omega_{D}} \frac{dz}{z} n_{R}(z) T_{c} \frac{\partial}{\partial T_{c}} \Phi\left(\rho, \frac{z}{\pi T_{c}}\right).$$
(9b)

In order to obtain accurate results for  $T_c$  and  $\alpha$ , a numerical solution should be found for the system of Eliashberg integral equations in the form

$$\begin{split} \tilde{\Delta}_{n} &= \pi T_{c} \sum_{m=-N}^{N} \left( \lambda(n-m) - \mu_{*} \right) \frac{\tilde{\Delta}_{m}}{|\omega_{m}|} \tilde{N}(\tilde{\omega}_{m}) \\ &- \pi t_{s} \tilde{N}(\tilde{\omega}_{n}) \frac{\tilde{\Delta}_{n}}{\tilde{\omega}_{n}}, \\ \tilde{\omega}_{n} &= \omega_{n} + \pi T_{c} \sum_{m=-N}^{N} \lambda(n-m) \tilde{N}(\tilde{\omega}_{m}) \operatorname{Sgn}(\omega_{m}) \\ &+ \pi t_{s} \tilde{N}(\tilde{\omega}_{n}) \operatorname{Sgn}(\tilde{\omega}_{n}), \end{split}$$
(10)

(see Ref. 27, as well as Refs. 28–33). Here  $\tilde{\Delta}_n$  and  $\tilde{\omega}_n$  are, by definition, the order and renormalization parameters of the electron mass;

$$\lambda(m) = 2 \int_0^\infty d\Omega \, \frac{F(\Omega)}{\Omega^2 + \omega_m^2} \, ,$$

where  $F(\Omega)$  is the spectral function of the electron-phonon interaction,  $\mu_*$  is the Coulomb pseudopotential, and  $t_s = 1/(\pi \tau_s)$ . The notation  $\tilde{N}(\tilde{\omega}_m)$  represents the following quantity

$$\tilde{N}(\tilde{\omega}_m) = \frac{\tilde{\omega}_m}{\pi} \int_{-\infty}^{\infty} dE \ \frac{N(E)}{N(E_F)} \frac{1}{E^2 + \tilde{\omega}_m^2}$$

We note that the possibility of using Eqs. (10) was discussed very recently in the literature.<sup>34-36</sup> The essential point of the discussion was that the averaging over the impurity configurations has actually been performed in these equations for the microscopic characteristics  $\tilde{\Delta}_n$  and  $\tilde{\omega}_n$ . From a rigorous standpoint, such averaging should have been performed using some analytical expression for the macroscopic "selfaveraged" parameter  $T_c$ . In the present work we are actually doing just that, since the entire treatment is based on the use of the equation for  $T_c$  in form (6).

### 3. MODEL AND DISCUSSION OF RESULTS

As was noted, the present work assumes that the density of states N(z) has a fine structure in the form of a symmetric peak. We chose the corresponding parameter  $\tilde{n}_R(z)$ , first, in the same form as in Ref. 26:

$$\tilde{n}_{R}(z) = f \exp\left(-\eta \frac{|z-\delta|}{\omega_{D}}\right), \qquad (11)$$

where  $\eta$  is a parameter which amounts to several units and  $f \approx 1$  characterizes the intensity of the peak. In addition, we also represented  $\tilde{n}_R(z)$  in the form of a Lorentzian peak:

$$\tilde{n}_R(z) = \frac{f}{\pi} \frac{\Gamma \omega_D}{(z-\delta)^2 + \Gamma^2} .$$
(12)

This was done to show that the results are not qualitatively dependent on the specific form of the fine structure. The fact is that the width  $\Gamma \leq \omega_D$  of the peak is not of fundamental significance. If  $\Gamma \ll \omega_D$  holds,  $T_c$  is weakly dependent on  $\omega$  (see, for example, Ref. 25). In such a situation the influence of the sharp peak on the isotope effect is masked.

In the present work we assume that the peak shape defined by (11) and (12) remains unchanged when the atomic composition is varied and when impurities are added. At the same time, it is assumed that the number of carriers varies in response to doping by heterovalent impurities. As a result, the Fermi level "moves" relative to the center of the peak  $E_F$ . Figure 1 shows plots of N(z) for  $\eta=4$  and f=1 in the case of the representation (11), as well as for  $\Gamma/\omega_D=0.25$ and f=1/3 in the case (12). Using the relations obtained above, we determined how  $T_c$  and  $\alpha$  depend on the position of the Fermi level relative to the sharp peak in the density of states for different concentrations of paramagnetic impurities. It was assumed in the calculations that  $\lambda=0.4$  and  $\omega_D=240$  K. The main results are presented in Fig. 2.

Let us first consider the situation for the case  $c_s = 0$ . Curves *l* in Fig. 2 are plots of  $T_c(\delta)$  and  $\alpha(\delta)$ . As is seen at once, the values of  $T_c$  are largest when  $E_F = E_R$ . Also, the value of  $T_c$  depends on  $N(E_F)$ , but it is not determined by it alone. The closeness of  $E_F$  to  $E_R$  in the integral sense is more important. As for  $\alpha$ , it has a minimum at  $E_R = E_F$ . The value of  $\alpha$  reaches its maximum for  $|E_F - E_R|/\omega_D \approx 1$ . The dependence of  $\alpha$  on  $\delta$  is described approximately by the equation

$$\alpha(\delta) = \alpha_0 \frac{1 + (\pi/2)n_R(\delta, \omega_D)}{1 + n_R(\delta, 0)} \,.$$



FIG. 1. Energy dependence of the fine structure of the density of states  $\tilde{n}_R(z)$  (11) and (12) for f=1, h=4 (curve 1) and f=1/3,  $\Gamma/\omega_D=1/4$  (curve 2).

Thus, the isotope effect is sensitive to the fine structure of the electronic spectrum, i.e., to the derivative  $\partial N/\partial E$ .

Let us discuss the general case in which we have  $c_s \neq 0$  and  $n_R \neq 0$ . In this case the curves appearing in Figs. 2a and 2b make it possible to understand the main features of the behavior of  $T_c$  and  $\alpha$ . Figures 2c and 2d illustrate the variation of the picture as a function of the intensity of the sharp peak in  $n_R(z)$ . Let us analyze the plots presented in Fig. 2. It is seen at once that the situation is not described in the single-parameter approximation when  $|\delta| \leq \omega_D$ . First, we turn our attention here to the drastic asymmetry of the values of  $T_c$  and  $\alpha$  in cases in which the superconductor is doped by impurities which can shift the position of the Fermi level (in the model adopted these impurity atoms simultaneously serve as paramagnetic defects). Moreover, if the Fermi level moves on the energy scale from the center of the peak to its periphery as a result of doping,  $T_c$  drops sharply, and  $\alpha$ increases just as sharply. Conversely, in the limit  $\delta \rightarrow 0$  the variation of  $T_c$  and  $\alpha$  is comparatively weak (compare  $T_c$ and  $\alpha$  in Figs 2a and 2b at points A and B and at points A' and B'). We note that the last term in expression (6) for  $T_c$  plays a minor role when  $|\delta| \ge \omega_D/2$ . The corresponding value of the isotope effect  $\alpha$  is given approximately by the formula



FIG. 2. Behavior of  $T_c/T_c^0$  and  $\alpha/\alpha_0$  as a function of the values of  $\delta$  and  $c_s/c_s^*$  ( $c_s^*$  is the critical concentration at which  $T_c$  vanishes) when f=1,  $\eta=4$  (a, b) and f=1/3,  $\Gamma/\omega_D=1/4$  (c, d):1)  $c_s/c_s^*=0$ ; 2)  $c_s/c_s^*=0.245$ ; 3)  $c_s/c_s^*=0.490$ ; 4)  $c_s/c_s^*=0.735$ .

$$\alpha(\rho,\delta) \approx \alpha_0 \frac{1 + (\pi/2)n_R(\delta,\omega_D)}{1 + n_R(\delta,0) - \rho \Upsilon'_{\rho} \left(\frac{1+\rho}{2}\right)}$$

Hence it also follows that the presence of a sharp peak in the spectrum can significantly enhance the effect caused by the paramagnetic impurities.

A few words regarding the specific behavior of  $T_c$  (and  $\alpha$ ) as  $\delta \rightarrow 0$  are in order. In the situation in which the singularity in the spectrum is described by a Lorentzian peak, the extremum point for  $T_c$  is described approximately, according to (8)–(9), by the relations

$$\frac{\partial I_c}{\partial \delta} \approx -\delta Z,$$

$$Z = \ln \frac{\beta \omega_D}{2T_c} - \frac{1}{2} \left( \ln (1+\beta^2) + \frac{1}{1+\beta^2} \right) - \left( 1 - \frac{\beta^4}{(1+\beta^2)^2} \right)$$

$$-\rho \Upsilon'_{\rho} \left( \frac{1+\rho}{2} \right) \frac{\beta}{1+\beta'},$$

where  $\beta = \Gamma / \omega_D$ .

Thus, if the peak is not excessively sharp, i.e., if  $\beta \approx 1$  holds, we have Z > 0. Then  $T_c$  passes through a maximum at  $\delta \approx 0$ . However, if the peak is very sharp, then Z < 0 holds, and  $T_c$  passes through a minimum at  $\delta \approx 0$ . We note that the presence of paramagnetic defects decreases Z and promotes the appearance of singularities in  $T_c(\delta)$ .

The results obtained can be used to qualitatively explain the experimental results obtained in Ref. 3. We recall that in an LSCO system whose composition is optimized with respect to strontium the Fermi level lies close to the center of the peak in the density of states. When a portion of the copper atoms are replaced by isovalent zinc impurity atoms the position of this level should not vary. In such a situation the experimental data for  $T_c$  and  $\alpha$  should be described approximately using the single-parameter version of the theory when only the concentration of the paramagnetic defects varies. At the same time, if copper atoms are replaced by trivalent iron impurity atoms, the Fermi level shifts to the left on the energy scale. Then the electron density of the system is close to the density of the undoped compound LSCO (y=0.12). As follows from our results, in this case the experiment is not described in the single-parameter model. The effect of the paramagnetic impurities is greatly enhanced due to the fine structure of the density of states. Precisely these differences in the behavior of  $T_c$  and  $\alpha$  for LSCO:Zn and LSCO:Fe systems are illustrated in Figs. 2a and 2b and in Figs. 2c, and 2d, respectively. In the case of Zn, as the concentration of paramagnetic defects increases, these parameters vary in the direction  $A \rightarrow B$ . At the same time, for an iron impurity the variation of  $T_c$  and  $\alpha$  as  $c_s$  increases follows the line joining points A and A'.

We note that the curves presented in Fig. 2 for LSCO:Fe systems are, in fact, not symmetric relative to the point  $E_R = E_F$ . The fact is that in compounds which are Sr-overdoped, the magnetic properties vary significantly, and the spin correlations are suppressed to a considerable extent (see, for example, Refs. 17 and 18). In such a situation,

therefore, in LSCO: Me systems with y > 0.15 the variation of  $T_c$  and  $\alpha$  as functions of the concentration, which is determined by the fine structure of the density of states and simultaneously by the effect of the paramagnetic impurities, should be greatly weakened. This assertion was recently confirmed by experimental data.

## 4. CONCLUSIONS

A model for explaining the anomalous isotope effect for  $T_c$  observed in LSCO:Fe (Ref. 3) has been proposed in this paper. The model was based on the phonon mechanism of superconductivity and the idea that the density of states of the carriers has a fine structure. The existence of this fine structure was attributed to a specific property of the Fermi liquid: the quasi-two-dimensional character of the spectrum of the carriers. It was assumed that the van Hove singularities in the density of states of the carriers are enhanced by spin fluctuations. Then it was postulated that the presence of Fe and Zn impurity atoms in the copper sublattice results in local decompensation of the spatially compensated magnetic moment of the matrix and the appearance of effective paramagnetic point defects. Finally, it was assumed that trivalent Fe impurity atoms alter the number of carriers and shift the Fermi level and that a situation characteristic of undoped LSCO is realized. As for Zn impurity atoms, they act as isoelectronic defects. It has been shown that in such a model the fine structure of the spectrum of carriers significantly enhances the effect of the paramagnetic impurities on the isotope shift of  $T_c$ .

We thank V. I. Ozhogin, N. A. Babushkina, and A. V. Inyushkin for their interest in this work. This research was performed as part of Project No. 93090 of the Russian High- $T_c$  Superconductivity Program with financial support from the International Science Foundation under grant No. N93000 and also from the International Science Foundation and the Fund of the Russian Government under grant No. N93300.

#### APPENDIX A

We consider the equation for  $T_c$  in the form

$$4\lambda T_c \int_0^{\omega_D} dz [1 + n_R(z)] \sum_{k=1}^{\infty} \frac{1}{[\omega_k + \tau_s^{-1}(\omega_k)]^2 + z^2} = 1,$$
(A1)

where the reciprocal of the relaxation time of the carriers is defined as

$$\tau_s^{-1}(\omega_k) = \tau_s^{-1} \frac{N(E_F + \omega_k)}{N(E_F)}.$$

After some transformations, Eq. (A1) can be brought into a form similar to (6). We then have

$$\ln \frac{T_c}{T_c^0} = \Phi_1(\rho) + \int_0^{\omega_D} \frac{dz}{z} \tanh \frac{z}{2T_c} n_R(z) + \int_0^{\omega_D} \frac{dz}{z} n_R(z) \Phi_2\left(\rho, \frac{z}{\pi T_k}\right).$$
(A2)

Here we have written

$$\Phi_{1}(\rho) = \sum_{k=0}^{\infty} \left( \frac{1}{k + \frac{1}{2} + \frac{1}{2}\rho(k)} - \frac{1}{k + \frac{1}{2}} \right),$$
$$\rho(k) = \rho \frac{N(E_{F} + \omega_{k})}{N(E_{F})}.$$

 $\overline{N(E_F)}$ 

$$\Phi_2(\rho,2u) = \frac{2}{\pi} \sum_{k=0}^{\infty} \left[ \frac{u}{\left[k + \frac{1}{2} + \frac{1}{2}\rho(k)\right]^2 + u^2} - \frac{u}{\left(k + \frac{1}{2}\right)^2 + u^2} \right]$$

The corresponding expression for the isotope effect has the form

$$\alpha = \alpha_0 \frac{1 + \tanh(\omega_D/2T_c)n_R(\omega_D) + \Phi_2(\rho,\omega_D/\pi T_c)n_R(\omega_D)}{1 + \int_0^{\omega_D} \frac{dz}{2T_c}n_R(z)\frac{1}{\cosh^2(z/2T_c)} - T_c\frac{\partial}{\partial T_c}\Phi_1(\rho) - \int_0^{\omega_D} \frac{dz}{z}T_c\frac{\partial}{\partial T_c}\Phi_2(\rho,z/\pi T_c)}.$$
(A3)

When relations (A2) and (A3) are used instead of (6) and (9) for  $T_c$  and  $\alpha$ , the main results obtained above remain unchanged.

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- Translated by P. Shelnitz