

## Isotope effect on $m^*$ in high- $T_c$ materials due to the breakdown of Migdal's theorem

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**Abstract.** – We show that the inclusion of effects beyond Migdal's limit in the electron-phonon interaction naturally leads to an isotope effect for the effective mass  $m^*$  of the charge carriers even much before reaching the polaron limit. This is the situation already considered in our approach to nonadiabatic superconductivity (*Phys. Rev. Lett.*, **75** (1995) 1158). Such a result provides a scenario different from the polaronic one for the interpretation of the recently observed isotope effect on  $m^*$  in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  and  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (Zhao *et al.*, *Phys. Rev. B*, **51** (1995) 16487 and *Nature*, **385** (1997) 236).

The recent observation of an oxygen-mass-dependent penetration depth  $\lambda(0)$  in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  [1] and in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  [2] has raised the question whether this effect could be attributed to the breakdown of the Migdal approximation [3]. In fact, according to the classical Migdal-Eliashberg theory of superconductivity, the zero-temperature penetration depth in the London limit and in the absence of magnetic impurities [4] is given by

$$\lambda(0) \propto \sqrt{\frac{m^*}{n_s}}, \quad (1)$$

where  $m^*$  is the electronic effective mass and  $n_s$  is the supercarrier density. According to eq. (1), an isotope effect on  $\lambda(0)$  can therefore be induced by an isotope effect on  $m^*$  and/or on  $n_s$ . However, for  $T \ll T_c$ , also assuming an electron-phonon (el-ph) type of pairing, the dependence of  $n_s$  on the ion-mass  $M$  is negligible [5] and a possible isotope-induced dependence of  $n_s$  on the hole concentration has been ruled out [1], [2]. Zhao *et al.*, therefore, concluded that the observed isotope effect on  $\lambda(0)$  can be entirely attributed to an oxygen-mass-dependent  $m^*$ . In this hypothesis and by using eq. (1), the oxygen isotope effect on  $m^*$ ,

$\alpha_{m^*} = -d \ln(m^*)/d \ln(M)$ , has been estimated to be  $\alpha_{m^*} = -0.61 \pm 0.09$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{6.94}$  [1] and  $\alpha_{m^*} \simeq -0.8$  ( $-0.5$ ) for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  for  $x = 0.105$  ( $0.15$ ) [2]. These large negative values of  $\alpha_{m^*}$  cannot be explained by the classical Migdal-Eliashberg (ME) theory of the el-ph interaction, which states that  $\alpha_{m^*} = 0$ . In fact this theory predicts that the electron-mass renormalization factor  $m^*/m = Z_0$  is given by  $Z_0 = 1 + \lambda$ , where  $\lambda$  is the el-ph coupling constant, *i.e.* a quantity independent of the ion-mass  $M$  ( $\lambda$  must not be confused with  $\lambda(0)$ , the penetration depth). This is a consequence of the adiabatic condition  $\lambda \omega_D / (q v_F) \ll 1$ , where  $\omega_D$  is the Debye phonon frequency,  $v_F$  is the Fermi velocity and  $q$  is the momentum transfer in the el-ph scattering. The adiabatic condition permits to neglect the vertex corrections to the el-ph interaction (Migdal approximation) and represents the basis of the formulation of the ME theory. The unusual isotope effect  $\alpha_{m^*}$  observed in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  and in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  could therefore be interpreted as a clear signature of the breakdown of the Migdal approximation.

However, from the quantitative point of view, some care has to be used in estimating  $\alpha_{m^*}$  from the isotope effect of  $\lambda(0)$  via eq. (1), since the latter applies only when the Migdal approximation is a valid assumption. A generalization of eq. (1) beyond Migdal's theorem requires in fact the knowledge of the Eliashberg equations for temperatures below  $T_c$  with the inclusion of the nonadiabatic contributions, *i.e.* a task which even in the perturbative approach presents serious technical difficulties. Nevertheless, the measurements reported in refs. [1], [2] lead to two important consequences. First, the observation of an isotope effect on  $\lambda(0)$  implies a significant role of the el-ph interaction in the high- $T_c$  compounds. Second, as pointed out before, such an el-ph interaction falls outside of the validity of the Migdal approximation. Therefore, the findings of refs. [1], [2] open new perspectives in investigating unusual isotope effects on quantities which, according to the classical (in the sense of ME) theory of the el-ph interaction, should not show isotope effects at all.

One of the most unambiguous evidences for the breakdown of the ME theory could be provided by the observation *in the normal state* of an isotope effect on the effective electronic mass  $m^*$ . In principle, isotope-sensitive specific-heat measurements could be able to observe such an effect provided that the electronic contribution to the specific heat can be clearly singled out [6]. With this motivation, we consider in this paper the consequences of the breakdown of Migdal's theorem on  $m^*$  and estimate the coefficient  $\alpha_{m^*}$  of the electron-mass isotope effect. We show that nonzero values of  $\alpha_{m^*}$  in the normal state can be obtained by considering two different regimes of the el-ph coupled system: the polaronic state and the "nonadiabatic regime" as described by the inclusion of the first el-ph vertex correction in the electronic self-energy. We have already studied the latter situation in connection with the superconductive transition [7], [8] and here we show that this theory, which does not imply the crossover towards the polaronic state, naturally leads to an isotope effect for  $m^*$ .

Let us start our discussion with the polaron model. A similar analysis has already been performed in ref. [2] in connection with the experimentally observed isotope effect on the penetration depth  $\lambda(0)$  [1], [2]. For simplicity, we consider the Holstein model [9], where phonons with frequency  $\omega_0$  are locally coupled to electrons through a structureless el-ph coupling  $g$  (small polaron). A polaronic state is characterized by a strong electron-lattice correlation [10] and/or a large effective mass [11]. Within the range of applicability of the Holstein approximation, the effective polaron mass is given as follows:

$$m^* \simeq m \exp \left[ \frac{g^2}{\omega_0^2} \right], \quad (2)$$

where  $m$  is the bare-electron mass. Equation (2) applies to the el-ph system in the antiadiabatic regime  $\omega_0/E_F > 1$ , provided that the quantity  $g^2/\omega_0$  is not too large [11]. Since  $g^2 \propto (M\omega_0)^{-1}$  and  $\omega_0^2 \propto 1/M$ , from eq. (2) we obtain that  $m^* \propto \exp[\sqrt{\gamma M}]$ , where  $\gamma$  is a constant independent

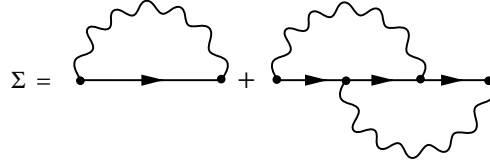


Fig. 1. – Electronic self-energy beyond Migdal's approximation. Solid lines represent electronic Green's functions while the wavy lines are phonon propagators.

of  $M$ . The isotope effect on  $m^*$  is therefore given by

$$\alpha_{m^*} = -\frac{d \ln(m^*)}{d \ln(M)} = -\frac{1}{2} \left( \frac{g^2}{\omega_0^2} \right). \quad (3)$$

The above expression gives a negative value of  $\alpha_{m^*}$  in accordance therefore with the results reported in refs. [1], [2]. We must stress, however, that this result is based on eq. (2), which holds true only as long as  $\omega_0/E_F > 1$ , *i.e.* a rather inadequate limit for  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  and  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  [12]. It is interesting to notice that, at optimal doping, LSCO shows a large negative  $\alpha_{m^*}$  [2] and a negligible isotope coefficient of the critical temperature  $\alpha_{T_c}$  [13]. This behavior is therefore in contrast with the prediction of the bi-polaronic theory of superconductivity which claims that  $\alpha_{m^*} \propto \alpha_{T_c}$ .

Besides the ME and polaronic scenarios, the el-ph coupled system may display also a regime which is beyond Migdal's limit (and therefore beyond ME framework) and well separated from the crossover between the quasi-free electron and the polaronic state. Such a regime, which we call nonadiabatic, is characterized by quasi-free electron states ( $\lambda \lesssim 1$ ) coupled in a nonadiabatic way to the lattice so that the el-ph vertex corrections are relevant. In the nonadiabatic regime, the electronic self-energy  $\Sigma(i\omega_n)$  is given by the graph depicted in fig. 1, where the first vertex correction has been included. The mass renormalization factor  $Z_0 = m^*/m$  is obtained by the  $i\omega_n \rightarrow 0$  limit of  $Z(i\omega_n) = 1 - \Sigma(i\omega_n)/(i\omega_n)$ . The function  $Z(i\omega_n)$  has been obtained in a previous work [8] and its expression is reported below:

$$Z(i\omega_n) = 1 + \frac{\pi T}{\omega_n} \sum_m \frac{\lambda_Z(i\omega_n, i\omega_m; Q_c) \omega_0^2}{(\omega_n - \omega_m)^2 + \omega_0^2} \frac{\omega_m}{|\omega_m|} \frac{2}{\pi} \arctan \left( \frac{E/2}{|\omega_m| Z(i\omega_m)} \right). \quad (4)$$

Here,  $\omega_n$  and  $\omega_m$  are fermionic Matsubara frequencies and  $\lambda_Z(i\omega_n, i\omega_m; Q_c)$  is the frequency-dependent el-ph coupling resulting from the inclusion of the first vertex correction function  $P_V(i\omega_n, i\omega_m; Q_c)$  into the electronic self-energy:

$$\lambda_Z(i\omega_n, i\omega_m; Q_c) = \lambda [1 + \lambda P_V(i\omega_n, i\omega_m; Q_c)]. \quad (5)$$

The explicit expression of the vertex function  $P_V$  has already been presented in ref. [8] for the three-dimensional case and in ref. [14] for the two-dimensional one. The dimensionless parameter  $Q_c = q_c/(2k_F)$ , where  $q_c$  is a cut-off over the momentum transfer  $q$  and  $k_F$  is the Fermi wave number, follows from the model we use for the el-ph coupling function  $g^2(Q) = (g^2/Q_c^2)\theta(Q_c - Q)$ , where  $Q = q/(2k_F)$  and  $\theta$  is the Heaviside function. The aim of this model is to simulate the effect of strong electronic correlations on the el-ph matrix element. In fact, according to different theoretical approaches, the tendency of the electronic correlation [15] and the weak screening [16] is to suppress the scattering processes with large momentum transfer and, at the same time, to enhance the small  $Q = q/(2k_F)$  scatterings.

The calculated  $Z(i\omega)$  is shown in fig. 2 as a function of  $\omega/\omega_0$  for  $\omega_0/E_F = 0.2$ ,  $\lambda = 1.0$ . When the vertex correction is not included (dashed line),  $Z(i\omega)$  takes the maximum value

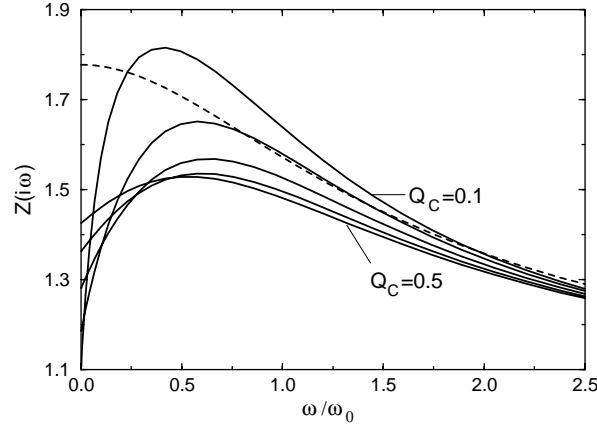


Fig. 2. – Renormalization function  $Z(i\omega)$  for  $\omega_0/E_F = 0.2$  and  $\lambda = 1$ . Solid lines: case with vertex correction for  $Q_c = 0.1, 0.2, \dots, 0.5$ . Dashed line: case without vertex correction.

$Z_{\max}$  at  $\omega = 0$ . The deviation from the adiabatic limit ( $\lim_{\omega_0/E_F \rightarrow 0} Z_{\max} = 1 + \lambda$ ) is due only to the finiteness of the electronic band [8]. When the vertex correction is included (solid lines) the maximum of  $Z(i\omega)$  is shifted towards higher values of the frequency  $\omega$ . For fixed values of  $\omega_0/E_F$  and  $\lambda$ , the position and the amplitude of  $Z_{\max}$  depend on the cut-off parameter  $Q_c$ . Moreover, the value of  $Z(i\omega)$  at  $\omega = 0$  is considerably lowered by the presence of the vertex correction. This feature can be understood by considering that at  $\omega = 0$  the electron-mass renormalization factor  $Z_0$  is mostly modified by the static limit of the vertex function,  $P_V(i\omega_n, i\omega_m \rightarrow i\omega_n; Q_c)$ , which is found to be negative [8]. This can be recovered also by the following analytic expression valid for  $\omega_0/E_F \rightarrow 0$  and  $\omega_0/(Q_c^2 E_F)$  small:

$$Z_0 \simeq 1 + \lambda - \lambda^2 \frac{\pi}{4} \left( \frac{\omega_0}{Q_c^2 E_F} \right), \quad (6)$$

where the contribution of the negative static limit is given by the third term of the right-hand side. Note instead that for the superconducting transition the situation is rather different, since the range of the relevant frequencies is of the order of  $\omega_0$ . In such a region of frequencies the vertex function shows a complex behavior that can lead to an amplification or a suppression of  $T_c$  depending on the value of the parameter  $Q_c$  [7], [8]. This different role of the nonadiabatic contribution in  $Z_0$  and  $T_c$  reflects the fact that the inclusion of the vertex corrections cannot be merely interpreted as a simple renormalization of the el-ph coupling.

We show in fig. 3 the calculated coefficient of  $\alpha_{m^*}$  as a function of the adiabatic parameter  $\omega_0/E_F$  for  $\lambda = 1$  and different values of  $Q_c$ .  $\alpha_{m^*}$  takes negative values regardless of the absence (dashed line) or the presence (solid lines) of the vertex correction. The presence of a nonzero  $\alpha_{m^*}$  for the case without vertex correction has to be ascribed only to finite-band effects, which give rather small absolute values of the isotope coefficient. The inclusion of the vertex correction amplifies the nonadiabatic effects and leads to more negative values of  $\alpha_{m^*}$  with respect to the case without vertex correction. This can be also inferred from eq. (6) which gives

$$\alpha_{m^*} \simeq -\frac{1}{2} \frac{\lambda^2 \pi}{Z_0} \left( \frac{\omega_0}{Q_c^2 E_F} \right), \quad (7)$$

where the finite-band effects have been neglected ( $\omega_0/E_F \ll 1$ ) and the vertex correction is

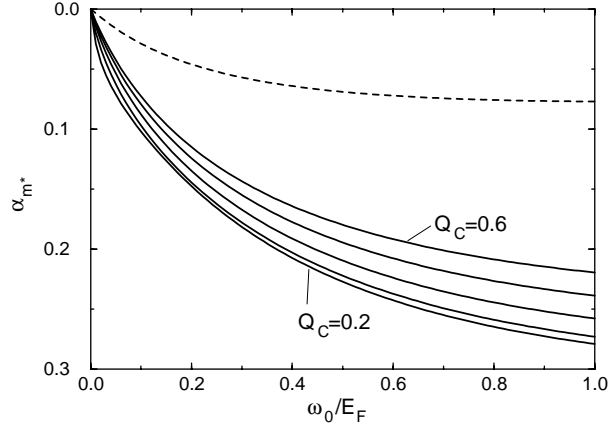


Fig. 3. – Coefficient  $\alpha_{m^*}$  of the isotope effect of the effective electronic mass calculated for  $\lambda = 1$ . Solid lines: case with vertex correction for  $Q_c = 0.2, 0.3, \dots, 0.6$ . Dashed line: case without vertex correction.

evaluated only up to the linear term  $\omega_0/(Q_c^2 E_F)$ . Note that in fig. 3  $\alpha_{m^*}$  does not show in the whole region of  $\omega_0/E_F$  a crucial dependence on  $Q_c$  as instead is observed for the superconducting transition temperature  $T_c$  [7], [8]. As a consequence, the isotope effects on  $T_c$  and  $m^*$  are not proportional as in the bi-polaron theory of superconductivity and in principle it is possible to have a negligible  $\alpha_{T_c}$  and at the same time an appreciably nonzero  $\alpha_{m^*}$ .

The result reported in fig. 3 have been obtained by considering a structureless electronic density of states (DOS) and are therefore relevant for three-dimensional systems like the fullerene and the BaBiO<sub>3</sub> compounds. However, photoemission measurements have given evidence for flat electronic bands close to the Fermi level for a large class of cuprates [17], opening the possibility that van Hove singularities (vHs) in the DOS could lead to important effects on both the normal and the superconducting phases [18]. As discussed in ref. [14], the presence of a vHs near the Fermi level represents an intrinsic nonadiabatic situation, where Migdal's theorem is not valid even if  $\omega_0/E_F \ll 1$ . It is natural therefore to investigate the effect on  $\alpha_{m^*}$  of the vertex correction calculated by using a vHs in the DOS. Here we anticipate some preliminary results valid for  $\omega_0/E_F \ll 1$  obtained by using the following DOS:

$$N(\epsilon) = -N_0 \ln \left| \frac{2\epsilon}{E} \right|, \quad (8)$$

where  $-E/2 \leq \epsilon \leq +E/2$  and  $N_0 = N/E$  corresponds to a constant DOS with  $N$  electronic states. In this model, the vHs is located at the Fermi energy  $E_F = E/2$ . By making use of eq. (8), we have found that for  $\lambda_0 = 1$  and  $\omega_0/E_F = 0.05$ , the isotope coefficient  $\alpha_{m^*}$  is  $-0.29$  ( $-0.6$ ) for  $Q_c = 0.4$  ( $0.2$ ). Therefore, the combined effect of the vHs and the vertex correction leads to a magnification of the values of  $\alpha_{m^*}$ , in better agreement with the experimental ones.

In summary, we have discussed the effect of different el-ph regimes on the effective electronic mass  $m^*$ . The main result is that the possibility of having nonzero values of  $\alpha_{m^*}$  cannot be associated exclusively to the presence of polaronic charge carriers. We have shown, in fact, that a negative isotope  $m^*$  coefficient can be obtained by taking into account the first el-ph vertex correction beyond Migdal's limit. The latter result appears to be of particular interest in view of the fact that in the nonadiabatic theory of superconductivity the breakdown of Migdal's theorem can lead to a strong enhancement of  $T_c$  and various other effects [7], [8], [14].

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## REFERENCES

- [1] ZHAO G. M. and MORRIS D. E., *Phys. Rev. B*, **51** (1995) 16487.
- [2] ZHAO G. M., HUNT M. B., KELLER H. and MÜLLER K. A., *Nature*, **385** (1997) 236.
- [3] MIGDAL A. B., *Sov. Phys. JETP*, **7** (1958) 996.
- [4] BILL A., KRESIN V. Z. and WOLF S. A., cond-mat/9801186 Preprint (1998).
- [5] ABRIKOSOV A. A., GORKOV L. P. and DZYALOSHINSKI I. E., *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs) 1963.
- [6] LORAM J. W. *et al.*, *Physica C*, **235-240** (1994) 134.
- [7] GRIMALDI C., PIETRONERO L. and STRÄSSLER S., *Phys. Rev. Lett.*, **75** (1995) 1158.
- [8] PIETRONERO L., STRÄSSLER S. and GRIMALDI C., *Phys. Rev. B*, **52** (1995) 1995; GRIMALDI C., PIETRONERO L. and STRÄSSLER S., *Phys. Rev. B*, **52** (1995) 10530.
- [9] HOLSTEIN T., *Ann. Phys. (N.Y.)*, **8** (1959) 343.
- [10] CAPONE M., STEPHAN W. and GRILLI M., *Phys. Rev. B*, **56** (1997) 4484.
- [11] CIUCHI S., DE PASQUALE F., FRATINI S. and FEINBERG D., *Phys. Rev. B*, **56** (1997) 4494.
- [12] PLAKIDA N. M., *High-Temperature Superconductivity*, (Springer, Berlin) 1995.
- [13] FRANCK J. P. *et al.*, *Phys. Rev. Lett.*, **71** (1991) 283.
- [14] CAPPELLUTI E. and PIETRONERO L., *Phys. Rev. B*, **53** (1996) 932; *Europhys. Lett.*, **36** (1996) 619.
- [15] ZEYHER R. and KULIC M., *Phys. Rev. B*, **53** (1996) 2850; GRILLI M. and CASTELLANI C., *Phys. Rev. B*, **50** (1994) 16880.
- [16] WEGER M., PETER M. and PITAEVSKII L. P., *Z. Phys. B*, **101** (1996) 573.
- [17] For an extensive review see: SHEN Z. X. and DESSAU D. S., *Phys. Rep.*, **253** (1995) 1, and references therein.
- [18] LABBE J. and BOK J., *Europhys. Lett.*, **3** (1987) 1225; NEWNS D. M. *et al.*, *Comm. Condens. Matter Phys.*, **15** (1992) 273; ABRIKOSOV A. A., *Physica C*, **244** (1995) 243.