

Nonspherical rigid-muffin-tin calculations of electron-phonon coupling in high- T_c perovskites

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The Hopfield factor (electronic part of the electron-phonon coupling constant) is calculated in the rigid-muffin-tin approximation (RMTA) for several perovskite high- T_c superconductors. Calculations were performed in the conventional "spherical" approximation and take into account the proper local symmetry. It is shown that the layered perovskite crystal symmetry generally favors strong electron-phonon interaction on the copper sites. We also estimate some non-RMTA effects.

I. INTRODUCTION

After it was well established that the isotope effect is comparatively small in the high- T_c superconductors (HTSC),¹ especially in those with $T_c \sim 100$ K (but not^{2,3} in those with $T_c \leq 30$ K), the conventional electron-phonon model fell from favor. However, perovskites are generally known to have relatively strong electron-phonon coupling (EPC). There is experimental and theoretical evidence, some of which is listed below, that EPC is large in the HTSC and possibly plays an important part for superconductivity.

Evidence of the importance of the electron-phonon interaction in HTSC includes the following: (a) the large ratio of $2\Delta/T_c$ (6–10), observed in photoemission, in most tunneling and in some optical experiments,⁴ and the $\sqrt{N(0)}$ scaling of T_c , according to photoemission;⁵ (b) the incompatibility of the observed phonon softening with the weak-coupling pairing;⁶ (c) the anomalously strong changes in the lattice dynamics at the superconducting transition;⁷ (d) the correlations between T_c and small low-temperature lattice distortions in (La,Ba)CuO₄;⁸ (e) the increase of the thermoconductivity below T_c ;⁹ (f) the large EPC, as deduced from the specific-heat measurements;¹⁰ (g) the general agreement between the tunneling spectral function and the phonon density of states;¹¹ (h) the additional weight in the tunneling spectral function in the high-energy (breathing-mode) region;¹¹ (i) the additional (nonphonon?) vibrational mode in the same region found in neutron experiments;¹² (j) the small, but still nonzero, isotope effect¹ for most high- T_c compounds (there is a large isotope effect in the cubic perovskites² and in the low-doped La₂CuO₄-based compounds³); and (k) the independence of the isotope effect on doping for La_{2-x}Sr_xCuO₄ when $x > 0.15$.³

It is worth noting that points (d), (g), and (j) suggest phonon exchange as one of the causes of the superconductivity. Points (a)–(c) are evidence for the strong-coupling regime, and therefore against an exchange of high-energy (electronic) excitations. Points (c), (e), and (f)

indicate that EPC is particularly strong. Points (h), (i), and (k) suggest the existence of a low-energy electronic excitation, strongly coupled with some phonon mode which is responsible for superconductivity [electronic attraction due to an exchange of phonons *plus* that of unrelated electronic excitation would cause a concentration-dependent isotope effect in point (k)].

Independent of whether or not the superconductivity in HTSC is driven by phonons, it is interesting to determine what factors favor EPC in HTSC. Strong EPC in a metal may be caused by different factors. Often it is due to some soft phonons, or to a strong electron-ion interaction (such as is the case when the bonding is to a large extent of ionic character, as occurs in carbides). At present it is not clear if there are soft modes in HTSC. On the other hand, bonding is partially ionic in these compounds. However, this is true independent of crystal structure, and this effect is not directly related to the particular arrangement of atoms. One of the crystal structure related explanations of the strong EPC in the perovskites refers to the Madelung potential. More precisely, it refers to its change with the displacement of ions.^{13–15} Unfortunately, the existing calculations of the EPC are definitely too crude to draw some meaningful conclusions.

Here we shall try to take the first step to the full-scale band-structure-based calculations of the EPC. The aim is to eliminate at least some of the *ad hoc* approximations, such as the so-called spherical (Gaspari-Gyorffy) approximation. We also estimate some non-rigid-muffin-tin corrections. In the following section we review briefly the necessary formulas. In Sec. III three main approximations in the standard technique will be discussed. In the final section we present the results of our calculations and discuss them.

II. FORMALISM

The EPC is most completely defined by the Eliashberg spectral function^{16,17}

$$\alpha^2 F(\omega) = \frac{1}{N(0)} \sum_{\substack{\lambda, \lambda', \nu \\ i, j}} \int d\mathbf{k} d\mathbf{k}' \delta(E_{\mathbf{k}\lambda}) \delta(E_{\mathbf{k}'\lambda'}) \frac{(\mathbf{W}_{\mathbf{k}\lambda, \mathbf{k}'\lambda'}^i \mathbf{e}_{\mathbf{k}'-\mathbf{k}, \nu}^i)(\mathbf{W}_{\mathbf{k}'\lambda', \mathbf{k}\lambda}^j \mathbf{e}_{\mathbf{k}-\mathbf{k}', \nu}^j)}{\sqrt{M_i \omega} \sqrt{M_j \omega}} \delta(\omega - \omega_{\mathbf{k}-\mathbf{k}', \nu}), \quad (1)$$

where the matrix element of the electron-ion interaction is

$$\mathbf{W}_{\mathbf{k}'\lambda', \mathbf{k}\lambda}^i = \langle \mathbf{k}\lambda | \delta V(\mathbf{r}) / \delta \mathbf{R}_i | \mathbf{k}'\lambda' \rangle. \quad (2)$$

Several moments of the electronic function are especially important:

$$\lambda = 2M(-1) = 2 \int \alpha^2 F(\omega) \omega^{-1} d\omega, \quad (3)$$

$$\sum_i (\eta_i / M_i) = 2M(1) = 2 \int \alpha^2 F(\omega) \omega d\omega. \quad (4)$$

Many observable quantities are determined by λ , and, to some extent, T_c itself. (η_i / M_i) determines the maximum possible T_c for a given electronic structure and arbitrary phonon spectrum:¹⁶

$$T_c^{\max} \approx 0.18 \left[\sum_i (\eta_i / M_i) \right]^{1/2}. \quad (5)$$

The same quantity defines the renormalization of the average phonon frequency due to the screening by the electrons at the Fermi level:¹⁷

$$\langle \omega^2 \rangle - \langle \omega_0^2 \rangle \sim \sum_i (\eta_i / M_i), \quad (6)$$

where ω_0 refers to the unrenormalized phonon frequencies. η_i , defined by Eq. (4), does not depend directly on the phonon spectra:

$$\eta_i = \frac{1}{N(0)} \sum_{\lambda, \lambda'} \int d\mathbf{k} d\mathbf{k}' \delta(E_{\mathbf{k}\lambda}) \delta(E_{\mathbf{k}'\lambda'}) |\mathbf{W}_{\lambda\mathbf{k}, \lambda'\mathbf{k}'}^i|^2. \quad (7)$$

Very often λ is written in terms of η_i as follows:

$$\lambda = \sum_i \frac{\eta_i}{M_i \langle \omega_i^2 \rangle}, \quad (8)$$

where $1/M_i \langle \omega_i^2 \rangle = D_{ii} = \Phi_{ii}^{-1}$ is the diagonal element of the inverse force constant matrix. Such a factorization may be justified when only local vibrations contribute to λ , which is not always the case. However, even with this assumption one needs to know $\mathbf{W}_{\lambda\mathbf{k}, \lambda'\mathbf{k}'}^i$ to calculate η_i . The usual approximation for it is the so-called rigid-muffin-tin approximation (RMTA),¹⁸ which assumes that the self-consistent potential inside the atomic sphere around a particular ion moves rigidly with its ion. This approximation is difficult to justify. Nevertheless it has been used very widely in the last 15 years. It is empirically established that RMTA works rather well in the transition metals, but not in simple metals. This is understandable, because in the simple metals the potential associated with an ion is more poorly screened and therefore comparatively long range. The total potential near an ion is in fact the sum of its own ion potential and the tails of the potentials from all other ions. In conventional band-structure calculations the zero of potential is chosen to be

equal to the potential between ions, so the depth of the potential well moving with the ion is underestimated. We shall return to this point later.

The RMTA is especially useful when combined with such band-structure calculation techniques as augmented plane wave (APW), Korringa-Kohn-Rostoker (KKR), and linear muffin-tin orbitals (LMTO). In these techniques the potential inside an atomic sphere is assumed spherically symmetric and the wave function inside it is expanded in spherical harmonics. Thus for the states at the Fermi level

$$\Psi_{\mathbf{k}\lambda}(\mathbf{r}) = \sum_{L, i} A_{L, i, \mathbf{k}\lambda} \varphi_{Li}(\mathbf{r}) Y_L(\hat{\mathbf{r}}) \quad (9)$$

with $L = (l, m)$. Then η_i may be written as

$$\eta_i = \frac{2n_i}{N(0)} \sum_{LL_1 L_2 L_3} N_{LL_1}^i(0) \mathbf{V}_{L_1 L_2}^i \mathbf{N}_{L_2 L_3}^i(0) \mathbf{V}_{L_3 L}^i, \quad (10)$$

where N_{LL_1} is the density matrix in the angular representation;

$$N_{LL_1}^i = \sum_{\lambda, \lambda'} \int d\mathbf{k} d\mathbf{k}' \delta(E_{\mathbf{k}\lambda}) A_{L, i, \mathbf{k}\lambda}^* A_{L_1, i, \mathbf{k}\lambda'}, \quad (11)$$

$$\mathbf{V}_{LL_1}^i = \langle Li | \delta V(\mathbf{r}) / \delta \mathbf{R}_i | L_1 i \rangle. \quad (12)$$

In RMTA, only dipole transitions are possible, i.e., $l = l_3 \pm 1$ and $l_1 = l_2 \pm 1$. Selection rules for $N_{LL_1}^i$ are defined by the crystal symmetry; if it were spherical, then only diagonal elements in (11) would be nonzero and Eq. (10) would have the especially simple form¹⁸

$$\eta_i = \sum_l (l+1) N_l^i N_{l+1}^i (\omega_l^i)^2 \quad (13)$$

with

$$\omega_l^i = \int \varphi_l^i(r) \varphi_{l+1}^i(r) [dV(r)/dr] r^2 dr.$$

It can be shown that in case of cubic symmetry Eq. (13) is exact up to $l=2$, for which no f electrons are taken into account. Unfortunately, the most important contribution to η in d metals comes from the df transitions. Additional terms appear in (10) in comparison with (13), which are fortuitously small in cubic transition metals.

In the past most numerical estimations of the EPC, including those for high- T_c compounds, were made according to this formalism, which is based on the three assumptions described above: factorization (8); spherical selection rules for $N_{LL_1}^i(0)$, and the RMTA. We discuss in the next section the validity of these assumptions and possible ways to avoid them.

III. DISCUSSION OF THE APPROXIMATIONS

A. Local-vibrations approximation

As we mentioned above, factorization (8) is justified only when local ion vibrations contribute in the EPC. Otherwise, instead of (8) we should write¹⁴

$$\lambda = \sum_{i,j} \eta_{ij} \Phi_{ij}^{-1}, \quad (14)$$

where η_{ij} is defined as in (7) but with the matrix elements W on different sites. For simple metals, the factorization (8) was shown to be rather poor.¹⁹ On the other hand, calculations of the EPC in transition metals using Eq. (14) indicate²⁰ that the inclusion of the nearest neighbors in Eq. (14) is usually sufficient, and that for most metals even Eq. (9) is a reasonable approximation (10–30% error). It has not been checked, however, whether this works for many atoms per cell. There are calculations²¹ of the off-site density matrix $N_{LL'}^{ij}$ for $\text{YBa}_2\text{Cu}_3\text{O}_7$. There are some elements, for instance between two chain oxygens, which are comparable with the diagonal components, which is an indication of the relative importance of the nondiagonal terms in (14). It is worth noting that calculations according to Eq. (14) are in principle feasible for HTSC, at least for La_2CuO_4 .

B. The RMTA

This approximation is very difficult to avoid. The direct way would be to give finite displacements to each atom and to find the difference between the self-consistent crystal potentials in order to calculate the integrals (2). This demands extremely accurate full-potential band-structure calculations, which seems impossible for such complicated compounds. Another approach would be to improve the RMTA by including some correction to it. We know of one attempt of this kind,^{13,14} where the change of the spherically symmetrized MT potential was taken into account self-consistently. For $\text{YBa}_2\text{Cu}_3\text{O}_7$ (but not for La_2CuO_4) the effect was considerable, but in the same paper it was shown that allowance for intersite screening (taken into account) diminishes the calculated effect drastically. It seems very likely that allowance for the intra-atomic screening (in other words, non-MT effects in screening) will considerably decrease the contribution in question. Another way to account for the non-RMTA corrections is to include additional shift of the MT zero, as has been done before for simple metals.^{22,23} This we did in our calculations for La_2CuO_4 , as will be discussed in the last section.

C. Spherical selection rules

In the framework of the RMTA Eq. (10) may be rewritten as

$$\eta_i = \frac{2n_i}{N(0)} \sum_{l,l'} w_l^i w_{l'}^i \sum_{m,m',\mu,\nu} [N_{LL'}^i g_{\Lambda',1\mu}^{L'} N_{\Lambda'L}^i g_{\Lambda,1\mu}^L + (-1)^\nu N_{\mathcal{L}L'}^i g_{\Lambda',1\mu}^{L'} N_{\Lambda'L}^i g_{\mathcal{L},1(-\mu)}^L] \delta_{\mu\nu}. \quad (15)$$

Here $\Lambda' = (l'+1, m' - \mu)$, $\Lambda = (l+1, m - \nu)$, $\mathcal{L} = (l+1, m + \nu)$, and g are Gaunt coefficients. In case of spherical symmetry the first term reduces to the Gaspari-Gyorffy formula (13) and the second one vanishes identically. Calculations using (15) are not much more complicated than in the spherical approximation and were actually done in this paper.

IV. CALCULATIONAL TECHNIQUE

We used in this work a standard linear muffin-tin orbitals method²⁴ for the band-structure calculations. Scalar relativistic terms were included as well as the combined corrections. During the self-consistency iterations the semicore states were treated as soft-core levels (which is a poor approximation for the total-energy calculations but is quite sufficient when one is interested in the states at the Fermi level). In order to have the representation (9) valid at the Fermi level in the LMTO we always chose the expansion energies $E_\nu = E_F$. As the main contribution in η comes from the d - f transitions on the copper sites and from the p - d transitions on the oxygen sites, we were to include the Cu_f and O_d orbitals. However, in

this case the Hamiltonian matrix becomes too large. Also it turns out that for Cu_f and O_d orbitals $E_\nu = E_F$ is not a good energy about which to linearize (spurious “ghost bands” appear in some cases). We avoided this problem by using the method of folding down of the higher partial waves,²⁴ restoring them in the wave functions afterwards. This corresponds to taking into account the higher angular momenta in the tails, but not in the heads of the MT orbitals. As was pointed out by Andersen,²⁴ this saves computational time (Hamiltonian matrix dimension is defined by heads only) and avoids the problem with the linearization of the “down-folded orbitals.” All integrations in the Brillouin zone were performed by the linear tetrahedron method using approximately 100 k points in the irreducible Brillouin zone edge.

V. NUMERICAL RESULTS

A. Nonspherical RMTA calculations

In Table I we show the results of our calculations of η using Eqs. (13) and (15).²⁵ To give a guide to the magni-

TABLE I. The largest atomic components of the Hopfield parameter η (10^{-3} Ry/ a_0^2).

	Spherical approximation Eq. (13)	Nonspherical Eq. (15)
La ₂ CuO ₄ , total	46.5	55.5
Cu	10.0	32.2
2O(1)	28.1	20.3
YBa ₂ Cu ₃ O ₇ , total	27.2	34.4
Cu(1)	2.09	4.66
2Cu(2)	7.62	16.7
O(1)	3.43	3.48
2O(2)	6.10	4.32
2O(3)	5.82	3.84
2O(4)	1.94	1.23
KBaBi ₂ O ₆ , total	25.4	31.8
2Bi	3.42	3.43
O(1)	5.87	11.7
O(2)	2.71	1.36
4O(3)	13.2	15.3
Bi ₂ Sr ₂ CaCu ₂ O ₈ , total	37.6	66.1
2Cu	12.1	42.7
4O(1)	25.0	23.0
Tl ₂ Ba ₂ CaCu ₂ O ₈ , total	28.3	46.0
2Cu	9.16	30.2
4O(1)	19.0	15.8

tude of the effect we note that assuming all force constants equal, corresponding to ≈ 400 K for oxygen's vibrations (the mode which has the strongest coupling with the electrons in Raman experiments), $\lambda \approx (10.6a_0^2/\text{Ry}) \times \eta$. We shall not discuss in detail the results of Gaspari-Gyorffy-type calculations as they are discussed in literature,^{15,26} and our data agree well with those published. Instead we pay attention to the effect of including proper local symmetry. In all investigated HTSC, including those not listed in the table, the difference between the first term in (15) and Eq. (13) is positive, i.e., the lowering of the symmetry increases the EPC. The second term in (15) has different signs in different cases. It is particularly large (and positive) on Cu in Cu-O planes, where the first term is also large. As a result, the relative weight of Cu in the total η increases several times—the ratio $\eta_{\text{Cu}}/\eta_{\text{O}}$ becomes 1.5–2 while in the spherical approximation it was $\frac{1}{2}-\frac{1}{3}$. This means that the widespread opinion that the electron-phonon contribution in the HTSC is mainly due to the oxygen vibrations^{27,28} is contradictory to the RMTA calculation.

It is not unexpected that the large increase of the EPC after including proper symmetry is found just on copper sites. Indeed, the error of the spherical approximation is greater when higher angular momenta are taken into account, and on Cu the main contribution comes from the d - f scattering. An analysis shows that the change of η_{Cu} is due to the change of this leading term, which is proportional to $N_{dd}V_{df}N_{ff}V_{df}$. The p - d - f term, nonexistent in spherical approximation at all, is also considerable.

We also investigated some cubic BaBiO₃-derived perovskites. There, the changes are less significant, due

to the higher symmetry. However, doubling the cubic unit cell for KBaBi₂O₆, so that K and Ba layers alternate, lowers the symmetry and this yields a $\approx 100\%$ increase of η on the O(1) site, where O(1) belong to K-O layers (see Table I).

Another point from our calculations relates to the decomposition of η according to Descartes indices. In fact Eq. (15) may be rewritten as

$$\eta_i = \sum_{\mu,\nu} \eta_{\mu\nu}^i \delta_{\mu\nu} = \sum_{\mu} \eta_{\mu}^i,$$

where $\eta_{x(y,z)}$ characterize coupling with the vibrations of the i th ion in the $x(y,z)$ direction. It turns out that for oxygen the coupling is particularly strong for the vibrations along the Cu—O or Bi—O bonds, as for instance in the breathing mode. However, breathing modes have rather high frequencies in these compounds. So the main contribution to the EPC should come not from them, but from the modes where the oxygen atoms around a copper atom have antiphase oscillations, such as quadrupolar mode.

B. Non-RMTA corrections due to the long-range tails of the potential

It is known that in simple metals RMTA considerably underestimates EPC. On the other hand, pseudopotential calculations give quite reasonable results in this case. The explanation is very simple: In simple metals, in contrast to the transition metals, screening is comparatively weak and the potential associated with a particular atom has a considerable tail outside its MT (or atomic) sphere.

When the atom is displaced, only a part of its potential is displaced in RMTA, namely that inside the MT sphere. This results in the underestimation of the RMTA matrix elements in Eq. (10). The simplest way to correct for this effect is to add a constant potential *inside* the MT sphere, as was done in Refs. 22, 23, and others.

There are different prescriptions for choosing this constant potential ΔV_{MTZ} . In this work we used the following two: The first is based on the Friedel sum rule and gives $\Delta V_{MTZ} = 1/N(0)$. The second makes use of the Thomas-Fermi description of screening to estimate ΔV_{MTZ} : $\Delta V_{MTZ}^i = 7.5 \exp(-q_{TF} S_i) / S_i$, where S_i is the i th atomic sphere radius. To estimate the possible effect of such a correction on the EPC in HTSC, we applied these two prescriptions to La_2CuO_4 , and found that the effect was rather small. We also tried to estimate the possible correction to V_{MTZ} due to the finite charge of the atomic sphere: $\Delta V_{MTZ} = Q_i / S_i$, with the same result. It seems that the most important correction to the RMTA is due to the nonsphericity of the potential inside the atomic sphere, but this effect has still to be estimated.

VI. CONCLUSIONS

To conclude, we have carried out the first calculations of the electronic part of the electron-phonon coupling constant (Hopfield factor) in the framework of the rigid-muffin-tin approximation, but without any additional ap-

proximations. The effect of taking the proper perovskite symmetry of the wave functions into account is, first, some increase in the electron-phonon coupling and, second, a redistribution of the partial components of the electron-phonon interaction, so that the Cu vibrations play a larger part than the O vibrations. We also argue that going beyond the rigid-muffin-tin approximation does not change this characteristic strongly, as long as the crystal potential is assumed spherically symmetric. This means that unless one includes nonspherical terms in the potential the calculated coupling is still quite small, taking into account the experimental factors^{2,3,8-11} discussed in the Introduction. One may expect, however, considerable changes in full-potential calculations, including nonlocal terms in the Hopfield factor η . Moreover, it is still possible that there are only a few particular phonon modes which are strongly interacting with electrons and account for some or all experimental facts mentioned above. *Average* EPI, reflected in the Hopfield factor, may nevertheless be quite small.

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²⁵It should be mentioned that the result for 123 compound depends strongly on the position of the Fermi level with respect to the quasi-one-dimensional Cu—O $pd-\pi$ bands, which is in turn very sensitive to the details of calculations. For instance, in some full-potential calculations (Ref. 15) these bands partially cross the Fermi level, while in others (Ref. 28) they lie below it, as in our calculations. Such crossing leads to an increase of the density of states and of the partial contribution of Ba and especially of O(4) atoms in the EP interaction in comparison with our calculations. This effect is even stronger when the Fermi level is displaced some 0.05 eV further down. Such a strong sensitivity to the energy scale of ≈ 500 K is not due to the RMTA and signalizes possible strong nonadiabatic effects.

²⁶One of the consequences of this fact is that analysis of the isotope-effect measurements are usually done in terms of the "fraction of the isotope effect to the ideal one," the ideal isotope effect being calculated with the complete neglect of possible Cu contribution to the electron-phonon interaction.

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