Optical conductivity of a doped Mott insulator: The interplay between correlation and electron-phonon interaction

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The optical conductivity (OC) of cuprates is studied theoretically in the low-density limit of the t-t'-J model taking into account the hole-lattice coupling. By developing a limited phonon basis exact diagonalization method capable of treating the lattice of largest size ever considered (4×4), we are able to discern the fine features of the mid-infrared (MIR) part of the OC revealing a three-peak structure. The two lowest peaks are observed in experiments and the highest one is tacitly resolved in moderately doped cuprates. Comparison of OC with the results of semianalytic approaches and detailed analysis of the calculated isotope effect indicate that the middle-energy MIR peak is of mostly magnetic origin while the lowest MIR band originates from the scattering of holes by phonons.

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I. INTRODUCTION

The way to disclose the nature of the high-temperature superconductors lies on the understanding of the dynamics of the holes doped into a Mott insulator.[1] It is recognized that the dynamics of holes is governed by the interaction with magnetic subsystem as it was proved by the angle-resolved photoemission spectroscopy of underdoped compounds.[2] There is also a growing number of evidences that a considerable coupling to lattice contributes to the properties of the holes too.[3–8] These major interactions are expected to leave fingerprints in the optical conductivity (OC) of cuprates. However, the interpretation of even the basic features of the OC is controversial.

Not to say about fine structure, there is no agreement on the issue of how many peaks are seen in the OC, both theoretically and experimentally. Initially, only the Drude term and mid-infrared (MIR) peak at around 0.5 eV have been considered as contributions coming from the dynamics of charged carriers.[9] Later, improved quality of the samples and experimental techniques gave an indication,[10–14] and finally clearly showed[15] that there is at least one more band ($\mathrm{MIR_{LOW}}$ band) induced by doping in the energy range, $\sim$0.1 eV, which is just above the phonon energy. Moreover, the analysis of the experimental data suggests that also another contribution, peaked at 1.5 eV, should be considered.[11–14] Although there is a temptation to explain this contribution as reminiscent of the charge-transfer peak in the doped system, this third high-energy peak ($\mathrm{MIR_{HIGH}}$ band) is observed in $La_{2-x}Sr_xCuO_4$ at 1.5 eV, which is considerably smaller than the peak energy at 2 eV observed in undoped compound.[11]

Even if the existence of a peak structure is recognized, its nature has been debated. Inability of the prototypical t-J model, where the hole moves in an antiferromagnetic background to explain the experimental structure of OC, attracted a significant interest on this problem. One possible direction consists in considering the Hubbard model with moderate U. The interpretation of the MIR peak, based on a purely electronic effect (associated with the upper/lower Hubbard bands and some in-gap states induced by doping), has been proposed.[16] Recently it was concluded[17] that moderate U can reproduce the OC spectra in $La_{2-x}Sr_xCuO_4$ by $U\cong4$ eV, which is in sharp contrast to the t-J picture in the strong correlation limit. The other possible direction is to consider the additional electron-phonon interaction (EPI), i.e., t-J-Holstein (t-J-H) model, where hole interacts also with dispersionless phonons. The OC of the latter model was calculated by several methods: exact diagonalization (ED) on the small $\sqrt{10}\times\sqrt{10}$ system,[18] self-consistent Born approximation (SCBA) with respect to both phonons and magnons,[19] dynamical mean-field theory (DMFT) for infinite dimensions,[20] diagrammatic Monte Carlo (DMC) with SCBA for magnons,[15] and ED within the limited functional space (EDLFS).[21] The fine structure of the OC in realistic two-dimensional (2D) systems can be studied only by DMC (Refs. 22–25) and EDLFS (Refs. 26–28), whereas the rest of approaches encounter severe problems. DMFT is not able to describe the coherent part of the hole motion and it is not clear whether we can rely on its results for the two-dimensional system. SCBA for phonons is unreliable[29] even for moderate couplings and the spectrum of a rather small $\sqrt{10}\times\sqrt{10}$ in ED is too sparse to see a fine structure.

In the light of the above statement it is extremely alarming that the interpretation of the low-energy peak of OC ($\mathrm{POC_{LOW}}$) in Refs. 15 and 21 is different. In contrast to Ref. 15, where the phononic origin of the $\mathrm{POC_{LOW}}$ was suggested, the magnetic origin of this peak is concluded in Ref. 21. A possible source of error in Ref. 15 might be originated from the SCBA in the magnetic channel or by the linear spin-wave approximation used. Therefore, the convincing evidence for the origin of the POC is an urgent and important issue toward the understanding of the basic interactions governing high-temperature superconductors.

In the present paper we study theoretically the OC of t-t'-J model, including the interaction with two possible dis-

persionless phonons: apical oxygen mode (Holstein model) or in-plane breathing mode. The OC for the two models is directly compared with the experimental observations supporting the vital role of EPI in cuprates. In addition to the inclusion of the realistic next-nearest-neighbor (NNN) hopping t' to reproduce the observed Fermi surfaces in cuprates,[1] we avoid the spin-wave and self-consistent Born approximations for the coupling to the spin system. By developing a limited phonon basis exact diagonalization (LPBED) method, we can calculate the OC of the largest ever considered 4×4 system. Due to the exponential growth in the basis with size of the system, the 4×4 lattice has considerably denser quantum states than the $\sqrt{10}\times\sqrt{10}$ system discussed in Ref. 18 so that it is possible to resolve the fine structure of the OC. We observe, in different ranges of EPI, three peaks in the OC, the highest one being seen because the spin-wave approximation is avoided. Calculating the isotope effect, which induces changes both in phonon frequency and exchange constant J, we show that, in the weak-coupling regime, the low-energy $\mathrm{POC_{LOW}}$ and the middle-energy POC are of phononic and magnetic origin, respectively. Furthermore, in the intermediate-coupling regime the low-energy $\mathrm{POC_{LOW}}$ is still of purely phononic origin, while the middle-energy POC is a mixture of the lattice and magnetic excitations. Finally, comparison with the results of different approximate schemes shows that the highest energy $\mathrm{POC_{HIGH}}$ peak is due to incoherent transitions into the states unaffected by lattice deformation associated with the hole.

II. MODEL

The Hamiltonian for t-t'-J'-Holstein model is a sum of t-t'-J Hamiltonian

$$H_{tt'J} = -t\sum_{i,\delta,\sigma} c^{\dagger}_{i+\delta,\sigma}c_{i,\sigma} - t'\sum_{i,\delta',\sigma} c^{\dagger}_{i+\delta',\sigma}c_{i,\sigma} + \frac{J}{2}\sum_{i,\delta} S_{i+\delta}S_i - \frac{J}{8}\sum_{i,\delta} n_{i+\delta}n_i, \quad (1)$$

EPI Hamiltonian

$$H_{h-ph} = \omega_0 g\sum_i (1-n_i)(a^{\dagger}_i + a_i), \quad (2)$$

and dispersionless phonons Hamiltonian

$$H_{ph} = \omega_0\sum_i a^{\dagger}_i a_i. \quad (3)$$

($a^{\dagger}_i$ is the creation operator of a phonon at site i with frequency ω_0). Here t represents the hopping amplitude of the site i to nearest neighbors $i+\delta$, t' is the diagonal hopping amplitude to next-nearest neighbors $i+\delta'$, J is the exchange constant of the spin-spin interaction, $c_{i,\sigma}$ is the fermionic operator with excluded double occupancy, S_i is the $\frac{1}{2}$-spin operator at site i, and n_i is the site i number operator. We introduce the EPI dimensionless coupling constant, $\lambda = g^2\omega_0/4t$, with the value $\lambda=1$ dividing the weak- and strong-coupling (SC) regimes of the Holstein model in the adiabatic limit. Below we set $\hbar=1$, $t=1$, $J=0.3$, $t'=-0.25$, and $\omega=0.15$, and OC is in units of $2\pi e^2$. The one-hole ground state of the t-J model on 4×4 lattice is sixfold degenerate. This degeneracy between $(\pm\pi/2,\pm\pi/2)$, $(0,\pi)$, and $(\pi,0)$ is partially removed by t' providing a fourfold degenerate ground state at momentum $(\pm\pi/2,\pm\pi/2)$.[30] Hence, one could naively expect that the OC should be sensitive to the value of t'.

III. LIMITED PHONON BASIS EXACT DIAGONALIZATION METHOD

The LPBED method is based on the modified Lanczos algorithm,[31] where magnetic degrees of freedom are treated exactly whereas the phonon variables are efficiently limited to a set, which, as it is shown below, gives much better results than both the momentum average (MA) approximation[32] and SCBA. We use the translational symmetry associated to periodic boundary conditions, requiring that the states have a definite momentum, and work in the one-hole subspace with $\Sigma_i S^z_i = \frac{1}{2}$. Each basis vector is a linear superposition with appropriate phases of the 16 translational copies (hole, spin, and lattice configurations are together rigidly translated) of a state having the hole fixed at site i_0 and spin flips and phonon quanta located around it. All the 6435 spin configurations of the 4×4 lattice are included.

The real bottleneck comes from Hilbert space required by the phonon's basis that is not limited. For instance, if we distribute $M=15$ phonon states in all possible ways,[18] the size of the system is strongly limited $(\sqrt{10}\times\sqrt{10})$. To circumvent this difficulty, LPBED keeps only two groups of phonon states. In the first group there are lattice configurations involving only *single-site* deformations, all the others being undeformed

$$|ph\rangle^{(n)}_j = (a^{\dagger}_j)^n|0\rangle_j[\sqrt{n!}]^{-1}\prod_{i\neq j}|0\rangle_i. \quad (4)$$

Here $j=1,\ldots N$ denotes the lattice sites, $|0\rangle_i$ is the i-site phonon vacuum state, and all possible $n=0,1,\ldots M$ values are limited by $M=20$, which is shown to be enough for convergence even in the strong-coupling regime.[18] In particular, if the deformations were present only on the site where the hole is located, the exact antiadiabatic limit is recovered. The inclusion in the basis of states containing lattice deformations on sites different from the hole position allows us to describe scattering processes between the hole and local phonons and then introduces a reasonable description of adiabatic processes in the strong-coupling limit. On the other hand, only the scattering processes with one phonon in q space are exactly treated. In any case, it has been shown[33] that restriction to such basis makes the method equivalent to the MA approximation,[32] where the Green's function is obtained by summing all diagrams, but with each diagram averaged over the momenta of its free propagators. This is already a reasonable approximation, which satisfies exactly the first six spectral weight sum rules for the Lehmann spectral function.[32] From the above discussion it is clear that the MA approximation works well when the problem is dominated by strong or very weak deformations. However, it is

well known that in the intermediate regime and for strong adiabaticity the system is characterized by not very localized deformations. In the language of the ordinary diagrammatic expansion this can be viewed as the need for vertex renormalizations that are not correctly taken into account in the MA approach. Furthermore, it is worthy to note that the MA approach contains correctly the simpler SCBA approximation only at the lowest order in g^2 expansion. To improve the MA scheme in the weak and intermediate-coupling limit within the adiabatic regime, LPBED method includes additional phonon states with up to three $(n_1+n_2+n_3 \leq 3)$ phonons on *different lattice* sites

$$|ph\rangle_{j_1,j_2,j_3}^{(n_1,n_2,n_3)} = \prod_{h=1}^{3} (a_{j_h}^{\dagger})^{n_h} [\sqrt{n_h!}]^{-1} |0\rangle_{j_h} \prod_{i \neq j_1,j_2,j_3} |0\rangle_i. \quad (5)$$

This three-phonon basis is able to recover the SCBA contribution (up to three phonons) and it goes beyond including all other processes of the same order, which are not present in the SCBA approach.[34] In this way the scattering processes between the hole and the lattice up to three phonons in q space are exactly treated so that the weak-coupling limit is optimally described. The restriction to three phonons, due to computational limitation, is not very serious and it has been tested successfully in the simpler Holstein model. Hence, LPBED approach is better than MA and SCBA methods and the only domain where it can fail is the case when there is a strong nonlocal deformation. However, strong deformations are realized only in the strong-coupling regime, where deformation in the case of local Holstein interaction is essentially restricted to the hole position. It is worth noticing that our approach, which is able to improve MA, is somehow related to that introduced in Ref. 35, with the advantage that in LPBED method it is possible to calculate not only the self-energy of the quasiparticle but any correlation function. Our computational scheme can also be extended in a systematic way without increasing the complexity of the numerical code. Summarizing, the above method is able to treat correctly strong- and weak-coupling limits for any value of the adiabatic ratio and allows a reasonable interpolation in the intermediate-coupling regime.

At $T=0$ the OC at nonzero frequency is calculated using the Kubo expression of the OC in terms of the current-current correlation function

$$\sigma_{xx}(\omega) = -(N\omega)^{-1} \Im[\Pi(\omega + i\eta) + \Pi(-\omega - i\eta)], \quad (6)$$

with

$$\Pi(\omega + i\eta) = \langle \psi_0 | j_x (\omega + i\eta - H + E_0)^{-1} j_x | \psi_0 \rangle. \quad (7)$$

Here $|\psi_0\rangle$ is the ground state $[\vec{k}=(\frac{\pi}{2},\frac{\pi}{2})]$ with energy E_0, N indicates the number of lattice sites, η is the broadening factor that shifts the poles of $\sigma_{xx}(\omega)$ in the complex plane by replacing the δ functions by Lorentzians, and

$$j_x = iet \sum_{i,\delta,\sigma} c_{i+\delta,\sigma}^{\dagger} c_{i,\sigma} (\vec{\delta})_x + iet' \sum_{i,\delta',\sigma} c_{i+\delta',\sigma}^{\dagger} c_{i,\sigma} (\vec{\delta}')_x. \quad (8)$$

It is also worth noticing that the electronic operators in the t-t'-J model are the projected ones in the space without doubly occupied sites. In calculating any physical observables, one needs to transform the operator of such an observable by the same canonical transformation as the t-t'-J model is transformed from the t-t'-Hubbard one.[36] Such procedure has not been used in the present work, where we have adopted the standard form of the current operator used in the literature. To the best of our knowledge, even in the simplest t-t'-J model the modifications on the OC induced by these terms of the t/U order have not been studied. The main structure of the OC in this model at an energy on the order of $2J$ is expected to be sufficiently robust with respect to this energy scale that, on the other hand, could introduce other small satellite structures at lower and/or higher energies. When the EPI is introduced in the model, the low structure in the OC, due to the coupling with bosonic lattice excitations, could interfere with that produced by the electron correlations giving rise to a more complicated absorption in the low-infrared energy range. However, it is necessary to perform further studies in this direction to extract the exact physical features due to these contributions.

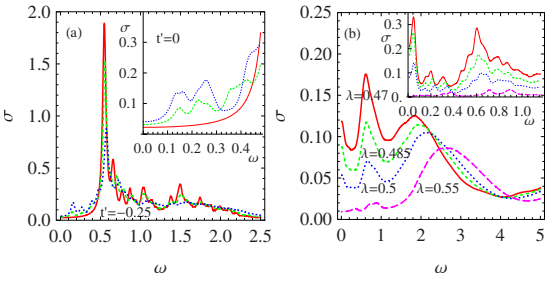

FIG. 1. (Color online) (a) OC in weak-coupling regime ($\eta=0.025$) for $t'=-0.25$ and (inset) for $t'=0$ ($\lambda=0$ (solid line, red), $\lambda=0.1$ (dashed line, green), and $\lambda=0.3$ (dotted line, blue). (b) OC at $t'=-0.25$ from intermediate to SC regime with the broadening factor $\eta=0.1$ and (inset) $\eta=0.025$.

IV. RESULTS AND DISCUSSION

In this section we present numeric studies of the OC and reveal the nature of different peaks appearing in the optical response. First, we apply LPBED method and show data for OC from the weak- to strong-coupling regime. Second, we compare numeric results obtained by LPBED method with various semianalytic strong-coupling approaches. Third, we study the effect of the isotope substitution on the peaks in OC.

A. Numeric results from the weak- to strong-coupling regime

For $\lambda=0$ we duly observe the well-known POC in the t-J model at the energy $2J$: the presence of t' has little influence on the main feature of OC of t-t'-J model [Fig. 1(a)]. At weak EPI, in agreement with Ref. 15, we detect $\mathrm{POC_{LOW}}$ just above the phonon frequency. We stress that the existence of $\mathrm{POC_{LOW}}$ is not related to t' hopping term, since the $\mathrm{POC_{LOW}}$ is also observed in the t-J-H model [inset in Fig. 1(a)]. This low-energy peak appears only at nonzero EPI and persists up to the strong-coupling regime [inset in Fig. 1(b)]. By increasing λ, the POC peak, which is around $2J$ at $\lambda=0$, shifts to higher energies and its weight is gradually transferred to the

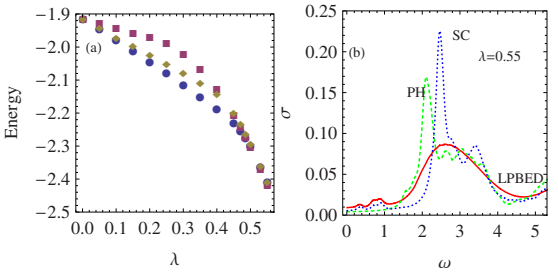

FIG. 2. (Color online) (a) Binding energy obtained within LPBED method (circles), MA method (diamonds), and SC scheme (squares). (b) OC in the SC regime (η=0.1).

high-energy POC_{HIGH} above $\omega \geq 2t$. Hence, the EPI changes the spectrum of the t-J model: OC exhibits three peaks. The nature of these peaks is either unknown or under dispute (cf. Refs. 15 and 21). In the following we present several results unambiguously revealing genesis of these peaks in the weak- and strong-coupling regimes.

B. Comparison with the strong-coupling approach

To study the origin of the three peaks for large EPI, we introduce strong-coupling adiabatic approach, in which wave function is factorized into a product of normalized variational functions $|\psi(\mathbf{r})\rangle$ and $|\phi(\mathbf{R})\rangle$ depending on electron $\mathbf{r}$ and phonon $\mathbf{R}$ coordinates, respectively. The factorization becomes exact in the fully adiabatic regime. The variational problem with respect to $|\phi\rangle$ leads to a coherent state with parameters depending on the site hole density that has to be fixed in a self-consistent way. The expectation value of the Hamiltonian on the above-determined state $|\phi\rangle$ provides a Hamiltonian, H_{el}, depending only on the electronic degrees of freedom, that describes the t-t'-J model in a potential well. A self-consistent procedure allows us to determine the electron wave function and consequently the phonon wave function. In Fig. 2(a) we compared results of SC approach for ground-state energies of t-t'-J model with data obtained by LPBED method. For λ above the critical $\lambda_c \approx 0.5$ the results of SC, MA, and LPBED approaches are in good agreement and, thus, the system is in the strong-coupling regime. In the SC limit, according to Franck-Condon principle, the lattice is frozen in the ground state during the hole optical excitations and the OC can be calculated considering excitations of the hole in the static potential well formed by the lattice deformation. Comparison of SC result for OC with that obtained by LPBED for λ=0.55 [Fig. 2(b)] shows that SC approach reproduces all three peaks. We note that in the SC approach both initial and final electronic states are calculated in the lattice potential associated with the ground-state wave function of the hole. On the other hand, if one assumes that the hole in the final state releases the deformation, we obtain another curve for OC with only the high-energy POC_{HIGH}. Such an approach is often called "photoemission" (PH) process because the lattice deformation is only present in one of the counterparts of the states linked by the current operator. Comparing results from LPBED, SC, and PH approaches we conclude that POC_{LOW} and POC in the strong-coupling regime represents hole transitions between states

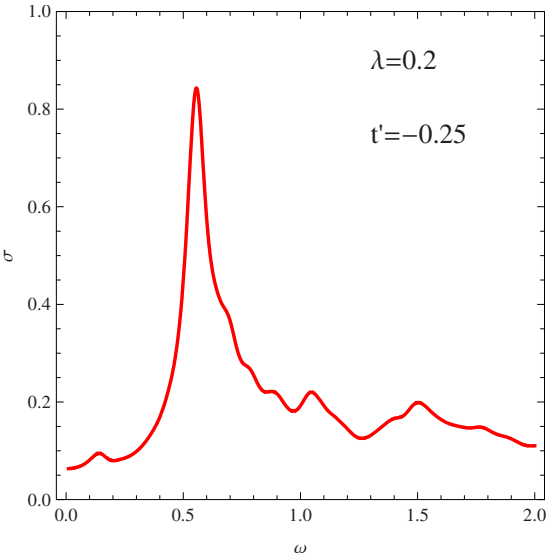

FIG. 3. (Color online) OC in the weak-coupling regime (η =0.05) for the breathing mode.

within the self-consistent potential well generated by the phonons. In contrary, POC_{HIGH} is associated with transitions into states, which are intact by the EPI-driven lattice deformation. Here we note that the association of the theoretical POC_{HIGH} with experimental MIR_{HIGH} band should be done with some care, since the energies involved are close to the limit of applicability of the t-J model, where one is required to use methods, which can handle the initial irreducible three-band Hubbard model.[37] We stress that the above-discussed scenario is valid also in the simpler t-J-Holstein model.

C. Breathing mode

The t-t'-J-Holstein model is a simplified model frequently used in literature to capture the essential physical features of cuprates. However, more realistic electron-phonon couplings have been suggested to play an important role for a quantitative agreement between calculations and experiments.[3] Among these ones the electron-phonon interaction arising from the in-plane breathing motion of an O(2) oxygen is believed to be the most relevant.[38] In Figs. 3 and 4, we show the OC for the EPI related to the in-plane breathing motion

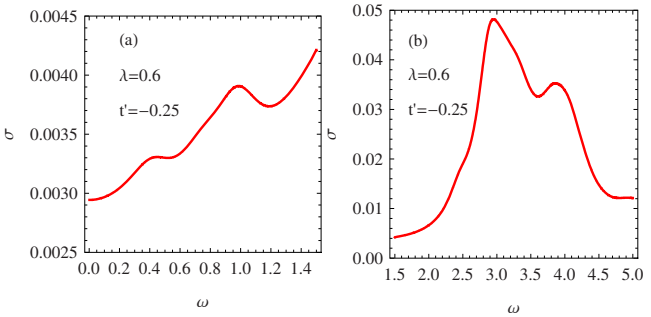

FIG. 4. (Color online) OC in the SC regime (η=0.2) for the breathing mode in the (a) low and (b) high-energy range.

$$H_{h-ph} = \omega_0 g \sqrt{2} \sum_i (1 - n_i) \left[a_i^\dagger + a_i - \frac{1}{4} \sum_\delta (a_{i+\delta}^\dagger + a_{i+\delta}) \right]. \tag{9}$$

The strength of EPI is characterized by dimensionless coupling constant $\lambda = \Sigma_{\vec{q}} M_q^2 / 4\omega_0 t$, where $M_q = \sqrt{2} g \omega_0 [\sin^2(q_x/2) + \sin^2(q_y/2)] / \sqrt{N}$ is the Fourier transform of the hole-phonon coupling. As in the case of Holstein EPI, the inclusion of the scattering processes between the hole and the lattice up to three phonons in the q space allows us to treat correctly, also for this model, the weak-coupling limit (see Fig. 3). On the other hand, in the strong-coupling regime the introduced local basis is too poor for this nonlocal interaction. In order to circumvent this limitation we performed the calculations in the adiabatic regime, where we can use the above-discussed approach whose implementation is independent of the specific form of hole-phonon coupling (see Fig. 4). The plots in Figs. 3 and 4 show that the presence of a three-peak structure in the OC is recovered showing that it is robust with respect to the specific characteristics of the hole-phonon interaction. We stress that, by assuming $t = 0.4$ eV and strong EPI ($\lambda = 0.6$), the three calculated peaks are located at energies approximately (0.15, 0.45, and 1.4 eV) that are in very good agreement with those experimentally observed in the underdoped phase. Finally it is worth noticing that the maximum intensity of the high-energy peak [Fig. 4(b)] is around ten times larger than that associated to the two low-energy structure. Also this feature reproduces the experimental results (see, for example, Ref. 10).

D. Isotope effect

Another way to establish the nature of the peaks of OC is to study the changes in OC with small variations in the phonon frequency ω_0 and/or exchange constant J. Such study does not serve solely as Gedanken experiment but establishes how the spectra will be altered by the isotope substitution (IS). First of all, changes in the oxygen from ^{16}O to ^{18}O induce modifications in the values of coupling constant g and phonon frequency ω_0. Phonon frequency $\omega_0 = \sqrt{k/M}$ is expressed in terms of k, which is the restoring force for length unit of the local oscillators, and M, which is the mass of oxygen atoms surrounding the Cu ion in the CuO_2 plain. IS changes the values of ω_0 and g to $\omega_0^* = \omega_0 \sqrt{M/M^*}$ and $g^* = g(M^*/M)^{1/4}$ with the value of λ being independent of isotope. In particular, the relative shift in ω_0 is about 6%. The second possible effect of IS is the decrease in the antiferromagnetic exchange constant J in compounds with the apical oxygen,[39,40] driven by its vibrations out-of-plane. With the IS the value of J is reduced by about 1% and in the following we assume $\Delta J/J = -0.01$.

In Fig. 5 we present the changes in OC induced both by changes in the in-plane oxygen mass and exchange constant J. The contribution of these changes is well distinct with only one exception. In the weak-coupling regime [Figs. 5(a) and 5(b)] POC at frequencies around $2J$ is shifted down by about 1% indicating the clear magnetic origin of this peak in the weak-coupling regime. In contrast, POC_{LOW}, with

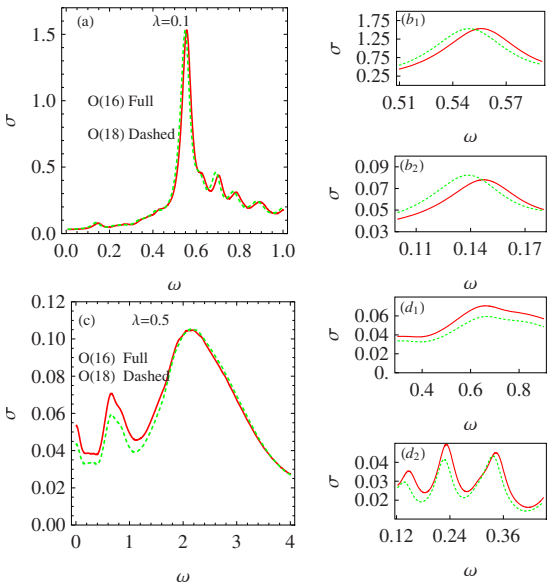

FIG. 5. (Color online) Effect of the O IS on OC in the weak- [(a), (b_1), and (b_2)], and the intermediate-coupling regime [(c), (d_1), and (d_2)].

frequency around ω_0, is shifted down about 6% [Fig. 5(b)], that is just the softening of ω_0 induced by IS. Thus, we get one more confirmation of the phononic origin of theoretical POC_{LOW} and experimental MIR_{LOW} band, in agreement with Ref. 15.

One gets the same conclusion about POC_{LOW} from the IS in the intermediate coupling regime [Figs. 5(c) and 5(d)]. Indeed the POC_{LOW} is shifted down by 6% again. On the contrary, behavior of the middle-energy POC differs from that in the weak-coupling regime since it reduces its intensity and almost does not move with the IS. It is known that the middle-energy POC increases by increasing λ/λ_c.[15] Moreover, λ_c decreases by decreasing ω_0.[41] Thus, the decrease in ω_0 increases the energy of POC. In contrary, decrease in J tends to soften the POC. Hence, joint influence of both effects leaves the peak at the same position. To confirm this conclusion we repeated the calculations setting to zero the change in J and found (not shown) the increase in POC energy. Hence, we conclude that in the intermediate-coupling regime the middle POC is of mixed origin.

V. CONCLUSIONS

In conclusion, we developed a method capable of studying the fine structure of the optical conductivity of the t-t'-J-Holstein model and found that the influence of the diagonal hopping t on it is surprisingly little. We revealed a three-peak structure of the optical conductivity and established the origin of these peaks in the whole range of hole-phonon couplings. The lowest peak is of phononic origin for the whole range of parameters. The middle peak, known for a long time as mid-infrared band, is of purely magnetic origin at weak phonon coupling but develops mixed magnetic and lattice nature at the intermediate strength of EPI. We have shown that this scenario is robust with respect to the

specific form of the EPI. We also predicted the influence of the isotope substitution on the optical conductivity whose fine details depend on whether or not the material contains apical oxygen. Our prediction for isotope substitution effect could be compared with experiment after the problem of residual ^{16}O in the matrix of ^{18}O, strongly influencing low-energy part of optical conductivity,[42] will be solved.

ACKNOWLEDGMENTS

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