Optical conductivity in the $t$-$J$-Holstein Model

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Using recently developed numerical method we compute charge stiffness and optical conductivity of the $t$-$J$ model coupled to optical phonons. Coherent hole motion is most strongly influenced by the electron-phonon coupling within the physically relevant regime of the exchange interaction. We find unusual non-monotonous dependence of the charge stiffness as a function of the exchange coupling near the crossover to the strong electron-phonon coupling regime. Optical conductivity in this regime shows a two-peak structure. The low-frequency peak represents local magnetic excitation, attached to the hole, while the higher-frequency peak corresponds to the mid infrared band that originates from coupling to spin-wave excitations, broadened and renormalized by phonon excitations. We observe no separate peak at or slightly above the phonon frequency. This finding suggests that the two peak structure seen in recent optical measurements is due to magnetic excitations coupled to lattice degrees of freedom via doped charge carriers.

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I. INTRODUCTION

Despite many years of intensive research of transport properties of a hole doped in an antiferromagnetic background the proper description of this system remains a challenging theoretical problem. The transport of a doped hole leaves in its wake locally distorted, slowly relaxing spin background, leading to the formation of a dressed quasiparticle with an enhanced effective mass and renormalized charge stiffness - a measure of a coherent, free particle like transport. Addition of lattice degrees of freedom to this already elaborate problem reflects the current scientific interest in the field of correlated electron systems.

Long after the pioneering work of Fröhlich$^{13}$, Holstein$^{14}$, and the last term represents the energy of Einstein phonons only at small $J/t \lesssim 0.25$. In this work authors also show that the low-$\omega$ peak is of the magnetic origin while the higher-$\omega$ peak represents the broad polaronic band.

II. MODEL AND NUMERICAL METHOD

The main goal of this work is to investigate in depth optical properties of the $t$-$J$-Holstein model for the case of a single hole in the antiferromagnetic background. We first define the $t$-$J$-Holstein model on a square lattice

$$H = -t \sum_{\langle i,j \rangle, s} \tilde{c}_{i,s}^\dagger \tilde{c}_{j,s} + J \sum_{\langle i,j \rangle} S_i S_j,$$

$$+ g \sum_{i} (1 - n_i) (a_i^+ a_i) + \omega_0 \sum_{i} a_i^+ a_i, \quad (1)$$

where $\tilde{c}_{i,s} = c_{i,s} (1 - n_{i-s})$ is a fermion operator, projected onto a space of no double occupancy, $t$ represents nearest-neighbor overlap integral, the sum $\langle i,j \rangle$ runs over pairs of nearest neighbors, $a_i$ are phonon annihilation operators and $n_i = \sum_s n_{i,s}$. The third term represents EP coupling $g = \sqrt{8 \lambda \omega_0 t}$, where $\lambda$ is the dimensionless EP coupling constant, and the last term represents the energy of Einstein phonons $\omega_0$.

We use recently developed method based on the exact diagonalization within the limited functional space (EDLFS).$^{16,17}$ Since details of the method have been published elsewhere,$^{16,17,18}$ we now briefly discuss only the main...
steps of the method. We first construct the limited functional space by starting from a Néel state with one hole with a given momentum \( \mathbf{k} \) and zero phonon degrees of freedom \( \phi^{(0,0)}_{\mathbf{k}} = c_{\mathbf{k}} \) (Néel: 0), and applying the generator of states \( \{ \phi^{(0,0)}_{\mathbf{k}} \} \rightarrow \{ (H_{\text{kin}} + H^M)N_h \phi^{(0,0)}_{\mathbf{k}} \} \), where \( H_{\text{kin}} \) and \( H^M \) represent the first and the third term respectively of Eq. [1].

This procedure generates exponentially growing basis space of states, consisting of different shapes of strings in the vicinity of the hole with maximum lengths given by \( N_h \) as well as phonon quanta that are as well located in the vicinity of the hole, at a maximal distance \( N_h \). Parameter \( M \) provides generation of additional phonon quanta leading to a maximum number \( N_{ph}^{\text{max}} = MN_h \). Full Hamiltonian given by Eq. [1] is diagonalized within this limited functional space taking into account the translational symmetry while the continued fraction expansion is used to obtain dynamical properties of the model. The method treats spin, charge as well as lattice degrees of freedom on equal footing.

We define OC per doped hole as

\[
\sigma(\omega) = \frac{i}{\omega} \langle \tau - \chi(\omega) \rangle
\]

\[
\chi(\omega) = i \int_0^\infty e^{\omega t} \langle [j(t), j(0)] \rangle \, dt
\]

where \( \tau = \sum_{i,j,s} t_{ij} (\mathbf{R}_i \otimes \mathbf{R}_j) \mathbf{e}_s^i \mathbf{e}_s^j \) represents the stress tensor, \( j = i \sum_{i,j,s} t_{ij} \mathbf{R}_j \mathbf{e}_s^j \) is the current operator, \( t_{ij} = -t \) for next nearest neighbors only and zero otherwise, and \( \mathbf{R}_i = \mathbf{R}_j - \mathbf{R}_i \). We also note that in the case of next-neighbour tight binding models, \( \langle \tau \rangle \) is related to the kinetic energy, \( \langle \tau_{\mu,\mu} \rangle = -\langle H_{\text{kin}} \rangle / 2 \).

III. CHARGE STIFFNESS AND SUM-RULES

Charge stiffness per doped hole can be on a square lattice for the \( t-J \)-Holstein model computed via its spectral representation:

\[
D_{\mu,\mu} = \frac{1}{4} \langle H_{\text{kin}} \rangle + \sum_n \frac{\langle j_{\mu} | n \rangle \langle n | j_{\mu} \rangle}{(E_0 - E_n)} \tag{4}
\]

\[
D_{\mu,\mu} = S^{\text{tot}}_{\mu,\mu} - S_{\mu,\mu}^{\text{reg}} \tag{5}
\]

where \( S^{\text{tot}} \) represents normalized optical sum-rule \( \int_0^\infty \sigma_{\mu,\mu}^{\text{tot}}(\omega) \, d\omega = 2\pi S^{\text{tot}} \), while \( S_{\mu,\mu}^{\text{reg}} \) is defined by \( \int_0^\infty \sigma_{\mu,\mu}^{\text{reg}}(\omega) \, d\omega = \pi S_{\mu,\mu}^{\text{reg}} \) and \( \sigma(\omega) \) represents the real part of the optical conductivity tensor in Eq. [2]. We have computed \( D_{\mu,\mu} \) in the single-hole ground-state, \( \mathbf{k} = (\pm \pi/2, \pm \pi/2) \). It is well known that the dispersion \( E(\mathbf{k}) \) is highly anisotropic around its single-hole minimum, which is in turn reflected in the anisotropy of the effective mass tensor. It is thus instructive to compute tensors representing the charge stiffness as well as the OC in the direction of their eigen-axis, i.e. along the nodal \( ((\pi/2, \pi/2) \rightarrow (0, 0)) \) direction that gives \( D_{\parallel,\parallel} \sigma_{\parallel}(\omega) \), and along the anti-nodal \( ((\pi/2, \pi/2) \rightarrow (\pi, 0)) \) direction that leads to \( D_{\perp,\perp} \) and \( \sigma_{\perp}(\omega) \).

In Fig. [II(a)] we present the charge stiffness vs. \( J/t \) for various values of EP coupling strength. To obtain accurate results in the strong EP coupling (SC) limit, we had to rely on only \( N_{ph} = 9786 \) different combinations of spin-flip states, while the total number of states, including phonon degrees of freedom, was \( N_{ph} = 9 \times 10^6 \). To test the quality of \( \lambda = 0 \) results, we show with the dashed line \( D_{\parallel} \) computed with zero phonon degrees of freedom using \( N_{ph} = 5 \times 10^6 \). Agreement with the \( \lambda = 0 \) case, obtained with \( N_{ph} = 9786 \) is rather surprising, given the fact that results were computed using Hilbert spaces that differ nearly three orders of magnitude. This fast convergence is in contrast to calculations on finite-size clusters where due to the existence of persistent currents \( D \) varies rather uncontrollably between different system sizes.
At the onset of the SC regime, be isotropic in the SC regime, distribution at the SC regime, Refs.\textsuperscript{16,23}. We now make some general comments about the effect of the EP interaction on the correlated system at the onset of the SC regime, i.e. at $\lambda \sim 0.25$, EP coupling is most effective in the physically relevant $J/t \sim 0.3 - 0.4$ regime, where there is a strong competition between kinetic energy and magnetic excitations. The critical $\lambda_c$ as well reaches its minimum around $J/t \sim 0.3$ as shown in Ref.\textsuperscript{16}. At larger $J/t \sim 1$ EP coupling becomes again less effective due to more coherent quasiparticle motion as reflected in the enhanced charge stiffness, quasiparticle weight, as well as the bandwidth\textsuperscript{16,17}.

The optical sum-rule $S_{\text{tot}}$, presented in Fig.\textsuperscript{1}(b), as well decreases with increasing $\lambda$. It however remains finite even deep in the SC regime where $D_\parallel \sim 0$ since $S_{\text{tot}}$ includes both coherent as well as incoherent transport. The latter remains finite due to processes, where the hole hops back and forth between neighboring sites while leaving lattice deformation unchanged. Despite charge localization we thus expect nonzero optical response $\sigma(\omega)$ even deep in the SC regime, with its spectral weight shifted towards larger $\omega$ and zero contribution at $\omega = 0$. Due to localization we also expect OC to be isotropic in the SC regime, i.e. $\sigma_\parallel(\omega) \approx \sigma_\perp(\omega)$.

In the insets of Fig.\textsuperscript{2} we show $S_{\text{reg}}^{\text{rep}}$ and $S_{\text{reg}}^{\text{FR}}$ representing the integrated regular part of the OC. $S_{\text{reg}}^{\text{FR}}$ steeply decreases with increasing $J/t$ due to the simultaneous increase of coherent transport, captured by $D_\parallel$, as well as due to decrease of $S_{\text{tot}}$, see also Eq.\textsuperscript{5}. We observe, that EP coupling have little effect on $S_{\text{reg}}^{\text{FR}}$ for $J/t \lesssim 0.4$, since its value is rather independent on $\lambda$ except deep in the SC regime, i.e. at $\lambda \sim 0.3$ in this particular case. Due to small values of $D_\perp$ we find $S_{\text{reg}}^{\text{FR}} \sim S_{\text{tot}}$, see Figs.\textsuperscript{1} and \textsuperscript{2}.

In Fig.\textsuperscript{2} we present the average of the square of the electrical current defining the following sum-rule $\int_0^\infty \omega \sigma_{\mu,\nu}(\omega) d\omega = \pi (j_{\mu,\nu}^2)$, that furthermore represents the fluctuation of the current operator. In the ground state there is no persistent currents that usually appear on finite-size clusters, since our method is defined on an infinite lattice. This enables more reliable calculation of the charge stiffness. At $\lambda = 0$ ($j_{\parallel}^2$) in Fig.\textsuperscript{2}(a) and ($j_{\perp}^2$) in Fig.\textsuperscript{2}(b) display rather distinctive $J/t$ dependence. While ($j_{\parallel}^2$) shows weak non-monotonous dependence on $J/t$, ($j_{\perp}^2$) shows a substantial increase. With increasing $\lambda$ current fluctuations as well increase in both directions even though the increase is more pronounced in the case of ($j_{\perp}^2$). In the SC regime we obtain ($j_{\parallel}^2$) $\sim$ ($j_{\perp}^2$) as a consequence of localization due to lattice degrees of freedom.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{(Color online) a) Expectation value of the square of the electrical current along the nodal direction ($j_{\parallel}^2$) ($S_{\text{reg}}^{\text{rep}}$ in the inset), b) expectation value of the square of the electrical current along the anti-nodal direction ($j_{\perp}^2$) ($S_{\text{reg}}^{\text{FR}}$ in the inset) vs. $J/t$ at $\omega_0/t = 0.1$ (full lines) and $\omega_0/t = 0.3$ (dashed lines).}
\end{figure}

Figure 3: (Color online) $\sigma_\parallel$ in a), b), and c), and $\sigma_\perp$ in d), e), and f) for three different values of $J/t$ as indicated in the figures for the $t$-$J$ model for a single doped hole at $\lambda = 0$ and $k = (\pi/2, \pi/2)$. Hilbert space with no phonon degrees of freedom and $N_{\text{tot}} = 5 \times 10^6$ was used in all cases except in b) and e) where for comparison we in addition present calculations with $N_{\text{tot}} = 9786$. In a), b), and d) we also show $\sigma_{xx} = (\sigma_\parallel + \sigma_\perp)/2$ (turquoise circle) and $\sigma_{zz} = (\sigma_\parallel - \sigma_\perp)/2$ (gray circle). Arrows in a) and b) indicate positions of lowest-energy peaks, $\omega_i$. Dashed lines in c) and f) are given by $\sigma_{\mu,\nu}(\omega) = \pi/(\omega + \omega_i)$. Insert in c) represents scaling of $\omega_{\text{ini}}$ vs. $J/t$. In this and in the subsequent figures, the Drude peak is not shown. Artificial broadening $\epsilon = 0.1t$ was used. Dashed areas in c) and f) define small frequency regimes $(\omega/t \lesssim 0.2)$ where at $J/t = 0.05$ EDLFS does not lead accurate results due to the vicinity of the Nagoka regime.
IV. DYNAMIC PROPERTIES

Turning to dynamic properties we first establish numerical efficiency of our method by presenting optical properties of the $t$-$J$ model. In Fig. 4 we display different components of the conductivity tensor $\sigma_{\mu,\nu}(\omega)$ in the single-hole minimum $k = (\pi/2, \pi/2)$, computed using EDLFS. At physically relevant value $J/t = 0.4$ we reproduce well known features, characteristic of $\sigma_{xx}(\omega)$: a) in the regime $1.6J \lesssim \omega \lesssim 2t$ we find peaks forming a rather broad band, appearing within the well known mid-infrared (MIR) frequency regime, separated from the Drude peak (not shown) by a gap of the order of $J$ and b) there is a broad featureless tail, extending to large frequencies, $\omega \gtrsim 7t$. MIR peaks for $J/t \gtrsim 0.2$ scale with the exchange coupling $(J/t)^6$, where $\eta \sim 1$. We stress that such scaling is consistent with local magnetic excitations as well as spin waves. Obtained scaling is however not consistent with the string picture where $\eta = 2/3$ (see also Ref. 24).

At $J/t = 0.4$ as well as at $J/t = 1$, the lowest peak appears at $J/t \sim 1.6$. Location of the lowest-frequency peak (indicated by arrows in Figs. 3a and b) is surprisingly close to the location of the peak in OC of the $t$-$J_z$ model in the limit $J_z/t \to \infty$, given by $\sigma(\omega) \sim \sqrt{J}\delta(\omega - \frac{2}{3}J_z)$. In this trivial case the peak appears at the frequency that corresponds to the energy (measured from the Néel state) of a single spin-flip, attached to the hole, created as the hole hops one lattice site from its origin in the undisturbed Néel background. It is somewhat surprising that such a naive interpretation seems to survive even in the (spin) isotropic $t$-$J$ model and at rather small value of $J/t = 0.4$. The scaling of the position of the low-frequency peak closely follows the following expression $\omega_1 = 1.62(J/t)^{1/3}$, indicated by a dashed line, connecting the circles shown the insert of Fig. 3c. Our results of OC qualitatively agree with those, obtained on small lattice systems.

When conductivity tensor $\sigma(\omega)$ is computed in its eigen directions, distinct (incoherent) finite-$\omega$ peaks are obtained in the case of $\sigma_1(\omega)$ and $\sigma_{\perp}(\omega)$, as best seen at $J/t = 1$ and $J/t = 0.4$. For comparison we present in Figs. 3(a), 3(b), and 3(c) the case of $\sigma_{\perp}(\omega)$ as well as $\sigma_{\parallel}(\omega)$. The reason is, that the ground state at $\mathbf{k} = (\pi/2, \pi/2)$ or $\mathbf{Q}_x$ point belongs to an irreducible representation $\Sigma_1$ of the small group of $k$, i.e. $C_2$. Current operators $j_\parallel$ and $j_{\perp}$, defining $\sigma_1(\omega)$ and $\sigma_{\perp}(\omega)$ through Eqs. 2 and 3 transform as distinct irreducible representations $\Sigma_1$ and $\Sigma_2$. Selection rules allow only transitions into states that transform according to a direct product of irreducible representations of the group $C_2$. Since $j_\parallel$ does not transform according to irreducible representations of $C_2$, the above mentioned selection rules do not apply.

In Figs. 3(b) and (c) we present as well results, computed on a much smaller set of states, i.e. with $N_{st} = 9786$. Apart for a small shift of one of the MIR peaks at larger $\omega$, the agreement with results, obtained with more than three orders of magnitude larger systems ($N_{st} = 5 \times 10^6$) underlines the efficiency of our method. Obtaining relevant results for the pure $t$-$J$ model at moderate number of states is of crucial importance for successful implementation of additional lattice degrees of freedom. Last, we present in Figs. 3(c) and (f) results at small $J/t = 0.05$. Dashed lines represent known analytical estimate $\sigma(\omega) = \pi/(\omega z)$, where $z = 4$, Ref. 24. This result is characteristic for systems with a nearly constant density of states and diffusive hole motion where current operators $\sigma_{\parallel}(\omega)$ are arbitrary, yet chosen identical in a) and b); a different scale was used for c), nevertheless identical among different plots in c). Artificial broadening was set to $\epsilon/t = 0.05$.

Figure 4: (Color online) $\sigma_{xx}$ for $\omega_0/t = 0.3$ in a), $\omega_0/t = 0.1$ in b) and c) at $J/t = 0.3$, and at $k = (\pi/2, \pi/2)$. Total number of functions was $N_{st} = 9 \times 10^6$. Up to 56 phonon quanta was used to obtain accurate results for $\lambda \gtrsim 0.2$. Arrows in b) indicate $\omega_{11} = 16\lambda t$ where $t = 0.45t$. Units of $\omega$ are arbitrary, yet chosen identical in a) and b); a different scale was used for c), nevertheless identical among different plots in c). Artificial broadening was set to $\epsilon/t = 0.05$.
separate peak at or slightly above the phonon frequency. This is more clearly seen in Fig. 4(c) where $\sigma_{xx}(\omega)$ is shown in an expanded frequency range. This result is consistent with DMFT calculations of Ref. 15. Nevertheless, we find quantitative agreement at $\lambda \sim 0.24$ with measurements on $(\text{Eu}_{1-x}\text{Ca}_x)\text{Ba}_2\text{Cu}_3\text{O}_6$ in the low hole-doping regime published in Ref. 13. In our calculation $\lambda \sim 0.24$ represents the maximum EP coupling constant where the low-$\omega$ peak, located at $\omega \sim 1.56J \sim 187 \text{ meV}$ (choosing $t = 400 \text{ meV}$ and $J/t = 0.3$), is just barely visible. This peak is, as discussed above, due to the local magnetic excitation and remains separated from the continuum forming the rest of the MIR band. Experimental value of the corresponding peak is $\omega_{\text{exp}} = 174 \text{ meV}$.12. The higher $\omega -$ peak at $\omega_1 \sim 1.4t = 560 \text{ meV}$ (experimental value is $\omega_{\text{exp}} = 590 \text{ meV}$) corresponds to MIR band, slightly broadened and renormalized by phonon excitations. This part of OC is in agreement with calculations in Ref. 13.

Our explanation of the experimetal results relies on the conjecture that lightly doped $(\text{Eu}_{1-x}\text{Ca}_x)\text{Ba}_2\text{Cu}_3\text{O}_6$ compound lies in the crossover from from weak to strong coupling electron-phonon regime where physical properties (quasiparticle weight, charge stiffness and dynamic properties) are extremely sensitive to small changes of $\lambda$. This is evident from Fig. 4 and from results, published in Ref. 13. MIR peak in OC is at $\lambda = 0$ centered around $\omega_1 = 2J = 240 \text{ meV}$. This value corresponds to the peak of the magnon density of states, it however underestimates the position of the main peak, seen in the experiment of Ref. 13. Increasing $\lambda$ beyond the weak coupling regime $\lambda > \lambda_c$, the center of MIR peaks starts moving towards higher frequencies and broadens as it transforms into a wide polaron band, thus approaching the experimental value. Simultaneously the peak due to the local magnetic excitation at $\omega_1$ as well broadens and disappears above $\lambda \gtrsim 0.24$.

The lack of a peak at $\omega \sim \omega_0$ in OC can be explained in simple terms in the large-$J/t$ limit of the simplified $t$-$J$-Holstein model. Starting from a hole in the Néel background, the lowest energy contribution to $\sigma_{xx}(\omega)$ comes from the hop of the hole to the neighboring site. This move generates a single spin-flip with the energy $E_1 = 3J_z/2$ above the ground state. The contribution to OC that would include a single phonon excitation would thus be located at $\omega \gtrsim 3J_z/2 + \omega_0$.

In order to explore the interplay of magnetic and polaronic degrees of freedom in the structure of $\sigma_{xx}(\omega)$ in more detail, we present in Figs. 5(a) and (b) comparison of optical spectra at fixed $\lambda = 0.3$ and different values of the exchange interaction $J/t$. Decreasing $J/t$ leads to a shift of the broad polaronic peak towards smaller values of $\omega$. At smaller $\omega_0/t = 0.1$ more pronounced structure abruptly appears at low $\omega/t \lesssim 0.5$ at small $J/t = 0.05$, Fig. 5(a). At larger value of $\omega_0/t = 0.3$, Fig. 5(b), a shoulder starts appearing at $J/t = 0.3$ in the low-$\omega$ regime that corresponds to the onset of the respective magnetic peaks (as indicated by arrows in Fig. 5(c)) of the pure $t$-$J$ model. Below $J/t \lesssim 0.2$ well formed peaks emerge being clearly of the magnetic origin. The disentanglement of lattice degrees of freedom, clearly seen in Fig. 5(b), is consistent with DMFT calculations.

V. SUMMARY

In summary, we have explored effects of magnetic as well as lattice degrees of freedom on optical properties of the $t$-$J$-Holstein model. EDLFS captures well optical properties of a single hole in the $t$-$J$-Holstein model in the range of physically relevant parameters of the model since it treats spin and lattice degrees of freedom on equal footing. Competition between kinetic energy and spin degrees of freedom strongly influences the coherent hole motion as measured by charge stiffness near the crossover to SC polaron regime. In the adiabatic regime increasing EP coupling leads to the shift of the OC spectra towards higher frequencies and broadening of peaks that in the pure $t$-$J$ model originate in magnetic excitations. As an important as well as unusual finding we report a lack of a peak in the OC spectra at or slightly above the phonon frequency that we attribute to the inherently strong correlations that are present in the $t$-$J$ model. This finding suggests that the two peak structure seen in recent optical measurements is entirely due to magnetic excitations. Based on our calculations, the two peak structure can be explained with the observation of local magnetic excitations, created by the hole motion at lower frequencies and the contribution of spin waves, coupled via doped hole to lattice degrees of freedom at higher frequencies.

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24. String states represent excited states of a particle (hole) in the linear potential created by the overturned spins left in the wake of a mobile hole as it propagates through an ordered Néel background. Since spin fluctuation arising from the off-diagonal part of the exchange interaction keep erasing the trace of overturned spins, string states, in reality, represent only a naive and approximate physical picture of excited states of the hole doped in the antiferromagnetic background. The physical realization of the string picture emerges as scaling of excited state energies with $J/t$ as $\Delta E \sim (J/t)^{\eta}$ where $\eta \sim 2/3$.
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