Effects of nonmagnetic impurities on optical conductivity in strongly correlated systems

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Abstract

Effects of nonmagnetic impurities on optical conductivity in the systems of antiferromagnetically correlated electrons are examined based on the Lanczos exact diagonalization scheme. As a result of resonant scattering a low-frequency peak in the optical conductivity is predicted to occur in the presence of the nonmagnetic impurities, which is consistent with the observed normal-state optical conductivity of YBa$_2$(Cu$_{1-x}$Zn$_x$)$_3$O$_{7-\delta}$. In addition, a relatively high and broad peak is found to occur at a high frequency region as a consequence of the Heisenberg interaction between electrons, in agreement with observation in the peak position.

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I. INTRODUCTION

Optical spectroscopy is an important tool in probing electronic states of strongly correlated systems including high-$T_c$ cuprates. Infrared properties of optical conductivity for YBa$_2$Cu$_3$O$_{7-\delta}$ crystals have been intensively investigated to explore the low-energy dynamics of charge carriers. Optical conductivity of La$_{2-x}$Sr$_x$CuO$_4$ for several doping rates between $x = 0$ and $x = 0.34$ at room temperature exhibited the appearance of mid-infrared band near 0.5 eV with the increase of hole doping concentration. The mid-infrared band was also observed for nonstoichiometric cuprates of Nd$_2$CuO$_{4-y}$ and La$_2$CuO$_{4+y}$ with some vacancies on oxygen sites. Exact diagonalization calculations on small clusters verified the existence of the mid-infrared band upon doping holes away from half filling.

Nonmagnetic impurities embedded in the high-$T_c$ cuprates have been used to investigate transport and magnetic properties of the cuprates. A small amount of Zn substituted for Cu is known to appreciably reduce the superconducting transition temperature. Magnetic susceptibility data for La$_{1.85}$Sr$_{0.15}$Cu$_{1-x}$Zn$_x$O$_4$ and NMR data for YBa$_2$(Cu$_{1-x}$Zn$_x$)$_3$O$_{7-\delta}$ provided evidences that Zn induces magnetic moments in the CuO$_2$ plane. However, not much attention has been paid to the effect of nonmagnetic impurities on optical conductivity of the cuprates. In the present paper we report an exact diagonalization study of optical conductivity when a nonmagnetic impurity is introduced into the systems of antiferromagnetically correlated electrons.

II. OPTICAL CONDUCTIVITY

We consider the following model Hamiltonian for the study of optical conductivity in strongly correlated electron systems,

$$H = -t \sum_{\langle ij \rangle \sigma} \langle \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} \rangle + \text{H.c.} + J \sum_{\langle ij \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) + V_{\text{imp}} \sum_{\ell} (1 - n_{\ell}) .$$

Here $\tilde{c}_{i\sigma}$ is the electron annihilation operator at site $i$ with no double occupancy. $\mathbf{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \sigma_{\alpha\beta} c_{i\beta}$ is the electron spin operator and $n_i = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator. $t$ is the
hopping energy and $J$, the Heisenberg exchange energy. The prime in $\sum'_{ij}$ denotes the sum over the nearest neighbor links $\langle ij \rangle$ only between copper sites, thus excluding the impurity site.\[12\]

Nonmagnetic impurities Zn substituted for Cu atoms have closed-shell configuration of Zn$^{2+}$ ($3d^{10}$) and are inert to electron hopping. The one-body Coulomb potential of the impurity, $V_{\text{imp}}$, represents a repulsive interaction as a result of a positive charge (Zn$^{2+}$ ion) of the nonmagnetic impurity interacting with a doped charge carrier (hole). $\sum_\ell$ is the sum over the nearest neighbor links with the impurity site.

The optical conductivity is obtained from\[4\]

$$\sigma(\omega) = -\frac{1}{\omega \pi} \text{Im} \left\langle \psi_0 \left| j_x \frac{1}{\omega - H + E_0 + i\epsilon} j_x \right| \psi_0 \right\rangle , \quad (2)$$

where $j_x$ is the current operator in the $x$-direction,

$$j_x = it \sum_{i,\sigma} (c_{i+x\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i+x\sigma}) \quad (3)$$

and $|\psi_0\rangle$ is the ground state of energy $E_0$. For the study of optical conductivity in the presence of impurity for a hole-doped system we introduce a nonmagnetic impurity atom and one mobile hole into the systems of $4 \times 4$ and $\sqrt{20} \times \sqrt{20}$ square lattices with periodic boundary conditions, in order to allow Lanczos exact diagonalization calculations.

In Fig. 1(a) the predicted optical conductivity is shown for various values of $J$ and $V_{\text{imp}} = 0$ on $4 \times 4$ square lattice. A Drude peak is seen to appear in the zero-frequency limit $\omega \to 0$ for all chosen values of $J$. For $J = 0.1t$ a broad Drude peak is predicted with no special feature, as is shown in Fig. 1(a1). As the Heisenberg interaction strength $J$ increases further, interestingly enough, an additional small peak (denoted as $E_B$ and indicated by an upward arrow in the figure) is predicted to occur at a low frequency, as is shown in Figs. 1(a2)–(a4). In addition a large peak (denoted as $E_J$ and indicated by an downward arrow) is seen to appear at a higher frequency. This peak becomes increasingly separated from both the Drude peak and the small peak with the increase of $J$. The larger peak at a higher frequency may be directly associated with the Heisenberg exchange correlation, but not with the nonmagnetic impurity.
For further study of the low energy peak, we choose $t \simeq 0.44$ eV for the hopping energy and $J \simeq 0.128$ eV for the Heisenberg exchange energy (i.e., $J \simeq 0.3t$) obtained from a local-density-functional study. Similar features without the disappearance of the low energy peaks appear for the larger cluster of $\sqrt{20} \times \sqrt{20}$ size as is shown in Fig. 1(b). The presence of the low energy peak $E_B$ may not be subject to the finite size effect, although quantitative differences may exist.

In Fig. 2(a1) the predicted optical conductivity is shown for $J = 0.3t$ and $V_{\text{imp}} = 0$. The low-energy peak occurred at $E_B \sim 0.16t$. As the strength of the impurity potential $V_{\text{imp}}$ increases, the intensity of the predicted peak becomes larger and its position is seen to shift to a higher frequency value of $E_B \sim 0.20t$. This feature is shown in Figs. 2(a2)–(a4). For comparison the optical conductivity in the absence of impurity is displayed in Fig. 2(a5). In the absence of impurity the low energy peak disappeared, while the position of the high energy peak $E_J$ remained unchanged at the same value of $J = 0.3t$, as is shown in Fig. 2(a4) and Fig. 2(a5). The occurrence of the new small peak at a low-frequency region is attributed to the presence of the nonmagnetic impurity in the systems of antiferromagnetically correlated electrons, while the large peak at a high-frequency region is contributed by the Heisenberg interaction between electrons. Recent experimental data of optical conductivity for YBa$_2$(Cu$_{1-x}$Zn$_x$)$_3$O$_{7-\delta}$ crystals exhibited a similar trend (see the two figures in the second row of Fig. 2 in Ref. 11). The observed optical conductivity for 4% Zn-doped samples measured at room temperature showed a small hump near 750 cm$^{-1}$. For the choice of $t \simeq 0.44$ eV [Ref. 13] the predicted peak position at $E_B \sim 0.2t$ corresponds to the wave number of 710 cm$^{-1}$, which is consistent with the measurement. Based on the conjecture of Poilblanc et al., this small low energy peak may be the reflection of forming a quasi-bound state as a result of resonant scattering with the nonmagnetic impurity.

As mentioned above, the large peak which occurred at $E_J \sim 0.54t$ [Fig. 2(a5)] with $J = 0.3t$ is attributed to the Heisenberg interaction between electrons. This can be clearly understood from Fig. 2(a6): in the absence of impurity the peak position is shifted to a higher frequency, $E_J \sim 1.1t$ for an increased value of $J$, say, $J = 0.6t$. Experimental studies
of cuprate materials revealed that broad bands associated with the Heisenberg interaction appear near 0.2 eV (see Fig. 3 in Ref. 5). Our predicted value of $E_J \sim 0.54t \approx 0.24$ eV is in good agreement with the experimental observation.

III. CONCLUSION

We have investigated the effect of nonmagnetic impurities on the optical conductivity in the systems of antiferromagnetically correlated electrons by using the Lanczos exact diagonalization scheme. It is found that a low-frequency peak in the optical conductivity appears near 710 cm$^{-1}$ in the presence of nonmagnetic impurities, in good agreement with experimental results. The predicted low-frequency peak in optical conductivity may be due to the resonant scattering of hole with the nonmagnetic impurity by allowing a possibility of forming a quasi-bound state. In addition, a relatively high and broad peak is found to occur at a high frequency region as a consequence of the Heisenberg interaction between electrons, in general agreement with observation in the peak position.
REFERENCES

1. T. Timusk, S. L. Herr, K. Kamarás, C. D. Porter, D. B. Tanner, D. A. Bonn, J. D. Garrett, C. V. Stager, J. E. Greedan, and M. Reedyk, Phys. Rev. B 38, 6683 (1988).

2. S. L. Cooper, G. A. Thomas, J. Orenstein, D. H. Rapkine, M. Capizzi, T. Timusk, A. J. Millis, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. B 40, 11358 (1989).

3. J. Orenstein, G. A. Thomas, A. J. Millis, S. L. Cooper, D. H. Rapkine, T. Timusk, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. B 42, 6342 (1990).

4. S. Uchida, T. Ido, H. Takagi, T. Arima, Y. Tokura, and S. Tajima, Phys. Rev. B 43, 7942 (1991).

5. G. A. Thomas, D. H. Rapkine, S. L. Cooper, S.-W. Cheong, A. S. Cooper, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. B 45, 2474 (1992).

6. A. Moreo and E. Dagotto, Phys. Rev. B 42, 4786 (1990).

7. E. Dagotto, A. Moreo, F. Ortolani, J. Riera, and D. J. Scalapino, Phys. Rev. B 45, 10107 (1992).

8. E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).

9. G. Xiao, M. Z. Cieplak, J. Q. Xiao, and C. L. Chien, Phys. Rev. B 42, 8752 (1990).

10. H. Alloul, P. Mendels, H. Casalta, J. F. Marucco, and J. Arabski, Phy. Rev. Lett. 67, 3140 (1991).

11. N. L. Wang, S. Tajima, A. I. Rykov, and K. Tomimoto, Phys. Rev. B 57, R11 081 (1998).

12. D. Poilblanc, D. J. Scalapino, and W. Hanke, Phy. Rev. Lett. 72, 884 (1994).

13. M. S. Hybertsen, E. B. Stechel, M. Schluter, and D. R. Jennison, Phys. Rev. B 41, 11 068 (1990).
FIGURE CAPTIONS

FIG. 1 Optical conductivity versus frequency for various values of $J$ and $V_{\text{imp}} = 0$. Clusters of size (a) $4 \times 4$ and (b) $\sqrt{20} \times \sqrt{20}$ with one doped hole in the presence of a single nonmagnetic impurity atom are considered. The $\delta$-functions are given with the width, $\epsilon = 0.05t$. $E_B$ indicates a low-energy peak owing to the presence of a nonmagnetic impurity with a positive charge and $E_J$, a peak associated with Heisenberg exchange interaction.

FIG. 2 Optical conductivity versus frequency for $J = 0.3t$ and various values of $V_{\text{imp}}$. Clusters of size (a) $4 \times 4$ and (b) $\sqrt{20} \times \sqrt{20}$ with one doped hole in the presence of one nonmagnetic impurity are considered. The $\delta$-functions are given with the width, $\epsilon = 0.05t$. $E_B$ indicates a low-energy peak owing to the impurity and $E_J$ is associated with Heisenberg exchange correlation.
FIGURES

N=16 J=0.1t (a1)
V_{imp}=0

J=0.2t (a2)
V_{imp}=0

J=0.3t (a3)
V_{imp}=0

J=0.4t (a4)
V_{imp}=0

\( \sigma(\omega) \)

\( \omega/t \)

FIG. 1.
FIG. 1.
FIG. 2.
FIG. 2.