Optical Conductivity of a t–J Ladder

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The optical conductivity \(\sigma(\omega)\) of a doped two-leg t–J ladder is calculated for an electric field polarized parallel to the legs of the ladder. The conductivity has a Drude weight proportional to the hole doping and an apparent threshold for absorption (a pseudo gap) which may be associated with the energy to break a pair. This pseudogap in \(\sigma(\omega)\) is present even though the pairs have a modified \(d_{x^2-y^2}\)-like wave function because the geometry of the ladder leads to quasi-particle states which probe the gap along an antinode.

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\[
-t \sum_{j,\beta,s} P_G(c_{j,\beta,s}^\dagger c_{j+1,\beta,s} + \text{H.c.}) P_G \\
-t' \sum_{j,s} P_G(c_{1/2,\beta,s}^\dagger c_{2,\beta,s} + \text{H.c.}) P_G
\]

where \(\beta (=1,2)\) labels the two legs of the ladder (oriented along the \(x\)-axis) and \(j\) is a rung index \((j=1,\ldots,L)\). \(S_{j,\beta}\) and \(c_{j,\beta,s}^\dagger\) are electron spin and creation operators and the Gutzwiller projector \(P_G\) excludes configurations with doubly occupied sites. In the materials of interest, the exchange coupling \(J\) along the legs is nearly the same as the exchange coupling \(J'\) across a rung, and similarly the hopping \(t\) along the legs is close to the rung hopping strength \(t'\); therefore, in the following calculations we will work with the isotropic system, \(J = J'\) and \(t = t'\).

For an electric field polarized along the \(x\)-axis (parallel to the legs), the optical conductivity can be expressed as

\[
+\sum_{n(\neq 0)} \frac{\pi}{N} \frac{|\langle \phi_n^M | j_x | \phi_0^M \rangle |^2}{E_n^M - E_0^M} \delta(\omega - E_n^M + E_0^M)
\]

where the final term is usually defined as the regular part of the conductivity \(\langle \sigma^{reg}(\omega) \rangle\). \(D\) is the charge stiffness and \(j_x\) is the paramagnetic current operator

\[
j_x = -it \sum_{j,\beta,s} (c_{j+1,\beta,s}^\dagger c_{j,\beta,s} - c_{j,\beta,s}^\dagger c_{j+1,\beta,s})
\]

where we choose the charge \(e\) to equal unity. \(N = 2L\) is the number of sites and \(M\) is the number of holes in the ladder (assumed to be even throughout). The states \(|\phi_n^M\rangle\) in Eq. 3 are the energy eigenstates of the hamiltonian \(H\) with corresponding energies \(E_n^M\); \(|\phi_0^M\rangle\) is the ground state with energy \(E_0^M\).

The Drude weight \(\sigma_D = 2\pi D\) may be evaluated in two ways. Firstly, as explained in a previous publication, the charge stiffness \(D\) can be calculated by considering the curvature of the ground state energy level \((E_0^M)\) as...
a function of the flux $\Phi$ (in units of the flux quantum $\Phi_0 = h\epsilon/e$) threaded through the two chain system

$$D = \frac{L^2 \partial^2 (E^M / N)}{8\pi^2 \partial \Phi^2}$$

(4)

Secondly, $\sigma_0$ may be calculated using the sum rule

$$\frac{N}{2\pi} \int_{-\infty}^{\infty} \sigma(\omega)d\omega = \frac{1}{2} |\langle \phi_0^M | T_{xx} | \phi_0^M \rangle|$$

(5)

where the Kinetic Energy operator $T_{xx}$ along the chain direction consists of the term proportional to $t$ in the hamiltonian (4). Substituting Eq. 2 into Eq. 5, we have

$$\frac{N\sigma_0}{2\pi} + \sum_{n(\neq 0)}\frac{|\langle \phi_n^M | j_x | \phi_0^M \rangle|^2}{E_n^M - E_0^M} = \frac{1}{2} |\langle \phi_0^M | T_{xx} | \phi_0^M \rangle|$$

(6)

where the second term is equal to $(N/\pi) \int_{-\infty}^{\infty} \sigma^{reg}(\omega)d\omega$.

In Fig. 3 we plot $N \times \sigma^{reg}(\omega)$ for the ladder system with various values of the ratio $J/t$: The results were obtained using the Lanczos approach and data from both the $2 \times 5$ and $2 \times 10$ system are shown. In order to obtain the absolute ground state of the system, we have chosen boundary conditions to form a closed shell in the non-interacting Fermi sea (obtained by turning off the interactions $J$ and $J'$): specifically this corresponds to anti-periodic boundary conditions for $n < 0.5$ and periodic boundary conditions for $n > 0.5$. We have also considered the parity of the states under a reflection in the symmetry axis of the ladder along the direction of the chains (even $(R_x = 1)$ or odd $(R_x = -1)$).

In Fig. 4 we plot the Drude weight $\sigma_0$ as a function of electron density for various values of the ratio $J/t$: we note that both of the methods above were used (Eqs. 4 and 5), and the results were in excellent agreement. In Fig. 4 we plot the integrated finite frequency conductivity $2 \sigma_0 \int_{0}^{\infty} d\omega \sigma^{reg}(\omega)$ as a function of electron density for various values of the ratio $J/t$; this quantity can be directly related to $\sigma_0$ and to times the kinetic energy per site through the sum rule (Eqs. 5 and 6).

There are several important features of Figs. 1 and 2 we should mention. We have checked that as the system size is increased, the ratio of weight at finite frequency to the total conductivity remains effectively constant; the difference in the number of delta peaks as the system size is changed is merely a finite size effect. We have also checked that the moments of the finite frequency distribution are effectively unchanged with increasing system size. A ‘pseudogap’ appears in the optical conductivity, below which there appears to be no weight; we discuss this feature in some detail below; note that as the ratio $J/t$ is increased, the ‘pseudogap’ increases. Secondly, as can be seen by comparing Figs. 3 and 4, the weight of the conductivity at finite frequency is extremely small as compared to that at zero frequency (the Drude weight). This behaviour is reminiscent of the one-dimensional $t$–$J$ model and in contrast to the larger finite frequency weight found in the two-dimensional system.

The Drude weight is proportional to the hole-doping at low doping levels, and at low densities is effectively independent of $J$ as we would expect for a spin-charge separated state. Note however, that the small finite frequency absorption has a larger magnitude together with a larger and opposite $J$ dependence for $n > 0.5$. These differences might be related to the nature of the ground state, a Tomonaga Luttinger liquid at low electron density and a Luther-Emery like liquid with a spin gap at small hole density.

In picturing the intermediate states which enter Eq. 2 for the conductivity, it is convenient to consider the limit in which the rung exchange $J'$ is large compared to both $J$ and the hopping $t (= t')$. In this case, when two holes are doped into the antiferromagnetic ladder they will go onto the same rung in order to minimize the number of broken singlet rung bonds. The binding energy of this state is approximately $J' - 2t - 2t'$, reflecting $J'$ the energy required to break another rung singlet minus the kinetic energy gain for two separate holes. In the limit of large $J'$, the doped system can therefore be thought of in terms of hole pairs moving on a lattice of rung singlets with an effective pair transfer matrix element of order $-2t^2/J'$. The fact that only one pair of holes can occupy a given rung leads to a low-energy description in terms of hardcore charge $2e$ bosons.

The coherent propagation of pairs leads to a finite Drude weight. In addition, when $\omega$ exceeds an energy of the order of the pair binding energy $E_B$, it is possible for the system to absorb a photon and excite a state containing two quasi-particles (each with charge $e$ and spin $1/2$). The two quasi-particle state which enters Eq. 2 for $\sigma(\omega)$ has $S = 0$ and a center of mass momentum equal to zero. There is in fact a continuum of two quasi-particle scattering states above the threshold energy for breaking a pair in the infinite ladder. As discussed by Tsunetsugu et al., a similar two quasi-particle state with $S = 1$ determines the spin gap in the doped two-leg ladder. An estimate of the pair binding energy can be obtained by considering the ground state energy of a system with an even number of holes $M$ and the corresponding energy if a hole with a momentum $k$ along the chains is either added or removed. Such excitations are infact the quantities we would expect to measure in the spectral functions, $A(k, \omega) = \sum_n |\langle \phi_n^{M-1} | c_{k,s} | \phi_0^M \rangle|^2 \delta(\omega - E_n^{M-1} + E_0^M)$ and $A(k, \omega) = \sum_n |\langle \phi_n^{M+1} | c_{k,s} | \phi_0^M \rangle|^2 \delta(\omega + E_n^{M+1} - E_0^M)$ where the first expression relates to the addition of an electron and the second relates to the addition of a hole. Indeed, sharp features in the spectral function should appear at energies $\epsilon_{k,R_x}^\pm = \pm(E_0^M - E_0^{M\pm1})(k, R_x)$ where we can obtain two different values depending whether we look at bonding or antibonding excitations $(R_x = \pm1)$.

In order to consider in more detail the quasi-particle excitations we define (the average) chemical potential as $\mu = 1/2(E_0^{M+1} - E_0^{M-1})$ where $E_R^\nu$ relates now to the absolute ground state energy for $P$ holes irrespective of the
quantum numbers $k$ and $R_x$. In Fig. 3 we show the dispersions $e_{n \sigma}^{kR_z} - \mu$ for the $2 \times 10$ ladder at $n = 0.8$ and $J/t = 1.0$ with positive energies corresponding to the case of adding an electron to the 4 hole ground state and negative energies corresponding to adding a hole to the 4 hole case. A finite gap separating the electron and hole quasi particle spectra can be clearly seen on the figure both for the bonding or antibonding sectors. Indeed, these gaps are related to the binding energies of a pair,

$$E_B(R_x) = E_0^{M-1}(R_x) + E_0^{M+1}(R_x) - 2E_0^M,$$

i.e. the energy required to create an electron-hole excitation with $R_x = \pm 1$. These two processes correspond in Fig. 3 to transitions involving the smallest energy excitations as indicated by the arrows.

Since these transitions conserve momentum (not quite exactly for $R_x = -1$) they can be considered as ‘vertical’ optical transitions and should be seen in the optical absorption (3). In Fig. 3 we compare the binding energies, the pseudogap obtained from the optical conductivity data and the two spin gaps (corresponding to bonding and anti-bonding spin excitations) at $n = 0.8$ (i.e $N_h = 4$) for various ratios of the parameter $J/t$ in the $2 \times 10$ ladder. As expected the threshold for absorption is of the order of the pair binding energy and also provides a measure of the spin gap in the $R_x = 1$ spin excitation spectrum. This adds credit to our picture of the pseudogap being a threshold for unbinding pairs. It is interesting to note that other lower energy gapped spin excitations exist (with $R_x = -1$) which probably do not involve pair breaking.

In conclusion, we find that $\sigma(\omega)$ for the two leg ladder has a Drude contribution consistent with a coherent pair motion and an absorption onset which we associate with the creation of two quasi-particles. It is interesting to note that for the ladder there is a pseudo-gap in $\sigma(\omega)$ even though the pairs have a $d_{x^2-y^2}$-like wavefunction. Basically, one is confined by the geometry to probe the gap along the antinode so that $\sigma(\omega)$ has a finite threshold.

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FIG. 1. $N \times \sigma^{reg}(\omega)$ for $2 \times 5$ and $2 \times 10$ ladders at electron density $n = 0.8$. The different plots correspond to a) $J/t = 0.5$ b) $J/t = 1.0$ c) $J/t = 1.5$.

FIG. 2. a) The Drude weight $\sigma_0$, and b) The sum of the finite frequency conductivity $2 \int_0^\omega \sigma(\omega)$, versus electron density for various values of $J/t$. These two quantities are related by the sum rule (see text).

FIG. 3. Energy dispersion for the $2 \times 10$ ladder system ($J/t = 1.0$) with 3 holes (upper curves) and 5 holes (lower curves); the results for both $R_x = 1$ and $R_x = -1$ are shown. Momentum is in units of $\pi$. The arrows represent the energy required to create an electron-hole excitation with either $R_x = \pm 1$ (see text).

FIG. 4. A comparison of the the binding energy, the pseudogap (obtained from the optical conductivity data) and the spin gaps. These quantities are defined in the text.