Computation of the Optical Conductivity of the t-J Model Using Anyon Techniques

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The zero-temperature optical properties of the t-J Hamiltonian are computed using the formalism of anyon superconductivity. Quantitative agreement is found with exact diagonalization studies.

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The discovery of high-temperature superconductivity has increased interest in model systems of electrons interacting with repulsive forces only. The simplest of these, the t-J Hamiltonian, has received particular attention. The behavior of this system is still controversial in part because conventional many-body techniques do not describe it well. In this Letter we show that the newly developed methods of anyon superconductivity [1-3] may be applied to this problem and yield results in quantitative agreement with exact diagonalization studies.

Our calculations involve the use of the U(1) lattice gauge theory description of this Hamiltonian [4] together with its commensurate flux saddle point [5]. Recently, Rodriguez and Douçot [6] proposed using a simple perturbation expansion of this gauge theory, similar to that successfully applied to the flux-free saddle point [7], as a practical computational technique. However, the particular approach suggested by them, like others using slave-boson techniques, becomes unmanagable at low temperature because of the tendency of the bosons to condense. We shall show that a modification to their scheme eliminates this technical difficulty, leads to charge-2 superfluidity at zero temperature, and agrees with numerical calculations of the optical conductivity of this system based on small clusters.

The t-J Hamiltonian

$$\mathcal{H}_{t\text{-}J}=\sum_{\langle i,j\rangle}\left\{-t\sum_{\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+\frac{J}{2}\mathbf{S}_i\cdot\mathbf{S}_j\right\}, \tag{1}$$

where $\mathbf{S}_i=\frac{1}{2}\boldsymbol{\sigma}_i$, is formally equivalent to the Hamiltonian

$$\mathcal{H}=\mathcal{H}_f+\mathcal{H}_b-\sum_i\phi_i+\sum_{\langle i,j\rangle}\left\{\left[\frac{t^2}{J}-\frac{J}{8}\right]b_i^{\dagger}b_j^{\dagger}b_jb_i+\frac{J}{4}|\chi_{jk}|^2\right\}, \tag{2}$$

with

$$\mathcal{H}_f=-\sum_{\langle i,j\rangle}\sum_{\sigma}\frac{J}{2}\chi_{ij}f_{i\sigma}^{\dagger}f_{j\sigma}+\sum_{i,\sigma}\phi_if_{i\sigma}^{\dagger}f_{i\sigma}, \tag{3}$$

and

$$\mathcal{H}_b=-\sum_{\langle i,j\rangle}t\chi_{ij}e^{iA_{ij}}b_i^{\dagger}b_j+\sum_i(\phi_i+\Phi_i)b_i^{\dagger}b_i, \tag{4}$$

where $b_i^{\dagger}$ and $f_{i\sigma}^{\dagger}$ create a slave boson and fermion of spin σ, respectively, on site i, ϕ_i is a Lagrange multiplier constraining the total number of bosons plus fermions on this site to be 1, and $\chi_{ij}=\chi_{ji}^{\dagger}$ is a Hubbard-Stratonovich variable. $\langle i,j\rangle$ denotes the sum over near-neighbor pairs with each pair counted twice to maintain Hermiticity. We wish to compute the linear response of this system to perturbing electromagnetic potentials $(\varphi,\mathbf{A})$, which couple as

$$\Phi_i=e\varphi(r_i),\quad A_{ij}=\frac{e}{\hbar c}\int_i^j\mathbf{A}\cdot d\mathbf{s}. \tag{5}$$

We follow the usual custom of ignoring magnitude fluctuations and writing $\chi_{ij}=\chi_0\exp(i\theta_{ij})$, where χ_0 is a constant. The Fermi and Bose particle and current densities are given by

$$J_i^{0(f,b)}=\frac{1}{b^2}\frac{\partial\mathcal{H}_{(f,b)}}{\partial\phi_i},\quad J_{ij}^{(f,b)}=\frac{1}{\hbar b}\frac{\partial\mathcal{H}_{(f,b)}}{\partial\theta_{ij}}, \tag{6}$$

where b denotes the bond length. We confine our attention to the commensurate flux saddle point, which is characterized (in Landau gauge) by the time-independent values $\phi_i^0=0$ and $\theta_{ij}^0=\pi(p/q)(x_j-x_i)(y_i+y_j)/b^2$, where p and q are integers related to δ, the number of holes per site, by $\delta=1-2p/q$. Substitution of these for ϕ_i and θ_{ij} in Eqs. (2)-(4) and (6) defines the "unperturbed" Hamiltonian $\mathcal{H}^0$ and paramagnetic current operators $j_{ij}^{\mu(f,b)}$. Our convention for lattice Fourier transforms is

$$J_{\mathbf{q}}^{0(f,b)}=b^2\sum_iJ_i^{0(f,b)}e^{-i\mathbf{q}\cdot\mathbf{r}_i},\qquad J_{\mathbf{q}}^{(f,b)}=b^2\sum_{i,j}J_{ij}^{(f,b)}e^{-i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{r}_j)/2}, \tag{7}$$

and

$$a_{\mathbf{q}}^0=\frac{1}{N}\sum_i\phi_ie^{-i\mathbf{q}\cdot\mathbf{r}_i},\qquad a_{\mathbf{q}}=\frac{1}{N}\frac{\hbar}{b}\sum_{i,j}(\theta_{ij}-\theta_{ij}^0)e^{-i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{r}_j)/2}. \tag{8}$$

The value of χ_0 we assume satisfies

$$JN\chi_0^2=-\langle0|\mathcal{H}_f^0|0\rangle-\langle0|\mathcal{H}_b^0|0\rangle, \tag{9}$$

where $|0\rangle$ denotes the unperturbed ground state and N is the number of sites. This is *twice* the value obtained by minimizing the Hamiltonian of Eq. (2) with respect to χ_0. This factor of 2 has been discussed previously in the context of Gutzwiller projection studies [8] and has been checked by us three ways: The value of $\chi_0=0.96$ for $\delta=0$ gives a "boson" bandwidth of $4\sqrt{2}\chi_0 t=5.4t$, which agrees with the $\sim 6t$ found numerically [9] for the spectral function bandwidth in the limit of $J\to 0$ and $\delta\to 0$. The near-neighbor "boson" hopping matrix element $\chi_0 t=0.96t$ agrees with the $\sim 0.9t$ found in variational studies [10] of the "holon" hopping matrix element. Finally, the average energy $\chi_0^2 J=0.92J$ of a "Fermi" excitation of $\mathcal{H}_f^0$ agrees with the value $\frac{3}{2}NJ\delta h_G(1)\cong 0.9J$ found variationally [11] for the energy to create a "spinon." This factor of 2 becomes unreliable for $\delta>0$ and has been approximated in previous work [8] by $2/(1+\delta)$. Our work ignores such corrections and thus overestimates χ_0 at large δ.

Let us first consider the Fermi part of the problem, which has no low-temperature instability. Diagonalization of the one-particle Hamiltonian $\mathcal{H}_f^0$ is straightforward and results in q distinct bands [12] characterized by the energy scale $J/2$. The unperturbed Fermi polarizability,

$$Nb^2\Pi_f^{\mu\nu}=\frac{i}{h}\int_{-\infty}^{\infty}\langle 0|T[j_{\mathbf{q}}^{\mu,f}(t)j_{-\mathbf{q}}^{\nu,f}(0)]|0\rangle^0 e^{-i\omega t-\eta|t|}dt+\frac{1}{2}\left(\frac{b}{\hbar}\right)^2(1-\delta^{\mu 0})\delta^{\mu\nu}\langle 0|\mathcal{H}_f^0|0\rangle\,, \tag{10}$$

is obtained from this band structure by occupying the lower p bands with two spin species and computing the zero-temperature dielectric response of the system as though it were a semiconductor. There is characteristically a large energy gap between the pth band and the $(p+1)$st and a quantized Hall conductance of

$$\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\frac{i}{\omega}\Pi_f^{xy}=\frac{2}{h}\,, \tag{11}$$

for any value of p and q [1,2]. Π_f defines the dynamics of the gauge field in the limit that the bosons are held fixed. The gauge propagator is given to one-loop order by

$$\mathcal{D}_f^{\mu\nu}=\left\{\frac{i}{h}\int_{-\infty}^{\infty}\langle 0|T[a_{\mathbf{q}}^{\mu}(t)a_{-\mathbf{q}}^{\nu}(0)]|0\rangle^f e^{-i\omega t-\eta|t|}dt\right\}\Bigg|_{\text{bosons fixed}}\cong-\lim_{\alpha\to\infty}\frac{1}{Nb^2}\{(\Pi_f+\Pi_{\text{gf}})^{-1}\}^{\mu\nu}\,, \tag{12}$$

where $\Pi_{\text{gf}}^{\mu\nu}=\alpha\delta^{\mu 0}\delta^{\nu 0}$ is a gauge-fixing term [13]. Evaluating Eq. (12) in the $(\mathbf{q},\omega)\to 0$ limit, we find that $\mathcal{D}_f^{\mu\nu}=ih/(2\omega)\epsilon^{0\mu\nu}$ exactly. This is the radiation gauge ($\phi=0$) version of the propagator assumed in previous studies of the $\frac{1}{2}$-fractional-statistics gas [14].

Let us now proceed with the full calculation. Since gauge fluctuations formally prevent the "bosons" from condensing by transmuting them to particles obeying $\frac{1}{2}$ fractional statistics, we shall follow precedent and stabilize the perturbation theory by transforming the bosons to their Fermi representation [14]. The transformed Bose degrees of freedom consist of spinless fermions described by the Hamiltonian of Eq. (4) with the commutation relations of b_i and $b_i^\dagger$ replaced with anticommutation relations. They interact with a fictitious gauge field described by the (radiation gauge) propagator $\mathcal{D}_{\text{C-S}}^{\mu\nu}=-ih/(\omega)\times\epsilon^{0\mu\nu}$. This gauge field is not to be confused with that described by Eq. (12), and, in particular, does not couple to the Fermi particles of Eq. (3). The latter is important because the Hartree graphs involving this field no longer sum to zero, but effectively reverse the sign of the excess magnetic field seen by the spinless particles. The "unperturbed" polarizability of these particles is thus the transpose $\bar{\Pi}_b^T$. $\bar{\Pi}_b$ is the polarizability obtained by occupying the lowest $q-2p$ bands of the one-particle Hamiltonian $\mathcal{H}_b^0$, which is identical to $\mathcal{H}_f^0$ except for substitution of the energy scale t for $J/2$, with spinless fermions. The band filling is unambiguous, as in the case of Π_f, because of the distinct energy gap between bands $q-2p$ and $q-2p+1$. The Hall conductance of $\bar{\Pi}_b$ is minus that of Π_f [2]. Thus evaluating $\mathcal{K}$, the response of the system to externally applied electromagnetic potentials, in the random phase approximation [14], we obtain

$$\mathcal{K}\cong e^2\bar{\Pi}_b^T+\bar{\Pi}_b^T(\mathcal{D}_f+\mathcal{D}_{\text{C-S}})\mathcal{K}=e^2\lim_{\alpha\to 0}[(\bar{\Pi}_b^T+\Pi_{\text{gf}})^{-1}+(\Pi_f+\Pi_{\text{gf}})^{-1}+(\Pi_{\text{C-S}}+\Pi_{\text{gf}})^{-1}]^{-1}\,, \tag{13}$$

where

$$\Pi_{\text{C-S}}=\frac{1}{h}\begin{pmatrix}0 & -2i\sin(q_y b/2)/b & 2i\sin(q_x b/2)/b\\ 2i\sin(q_y b/2)/b & 0 & i\omega\\ -2i\sin(q_x b/2)/b & -i\omega & 0\end{pmatrix} \tag{14}$$

is a lattice Chern-Simons term. Note that the double lattice periodicity of this expression follows from the definitions in Eqs. (7) and (8). We ignore the interaction term in Eq. (2), which is appropriate in the limit of small δ. The symmetry of Eq. (13) shows that the approximations involved in Eqs. (12) and (13) are consistent, and that the reasoning works equally well with the roles of "Bose" and "Fermi" reversed. The expression is similar to that of Ioffe and Larkin [4].

In Fig. 1 we compare the $\mathbf{q}=0$ optical conductivity,

$$\sigma_{xx} = \mathrm{Re}\left[\frac{i}{\omega}\mathcal{K}_{xx}\right], \qquad (15)$$

calculated from Eq. (13) for the case of $p/q=19/41$ and $J/t=0.4$ with that computed by Moreo and Dagotto [15,16] using Lanczos diagonalization for a single hole on a 4×4 lattice. Both calculations have been artificially broadened for clarity. There is agreement in the overall shape, energy scale, and absolute magnitude of the two calculations. The peak at $\omega=0$ in our calculation is infinitely narrow and is the oscillator associated with the Meissner effect. A feature similar to this, although not necessarily narrow, is implicit in the Lanczos calculation. The f-sum rule,

$$\int_0^\infty \sigma_{xx}(\omega)d\omega = \frac{\pi}{2}\lim_{\omega\to\infty}\mathcal{K}_{yy}(\omega) = \frac{\pi}{2}\left(\frac{e}{\hbar}\right)^2\frac{\langle T\rangle}{2N}, \qquad (16)$$

where $\langle T\rangle$ denotes the expected ground-state kinetic energy, is only 40% exhausted by the finite-frequency conductivity [17]. The remainder defines the strength of the missing "Drude" peak. Our value for this same fraction is 40%. The broad continuum near $\hbar\omega=t$, which has also been seen in a Schwinger boson study [18], may be understood as a spin-wave shakeoff. Its position and shape are relatively insensitive to δ but change radically in the limit of large t.

Using the f-sum rule to define $\langle T\rangle$ we obtain

$$\langle T\rangle = [\langle 0|\mathcal{H}_b^0|0\rangle^{-1} + \langle 0|\mathcal{H}_f^0|0\rangle^{-1}]^{-1}. \qquad (17)$$

In Fig. 2 we compare this value with the Lanczos kinetic energy [16] and with the "flux" energy obtained by Liang and Trivedi [19], which is equivalent to a variational study of the $\frac{1}{2}$-fractional-statistics gas using specific multiholon wave functions [2]. All three curves satisfy $\langle T\rangle = 2.5Nt\delta$ for small δ, and thus correspond to the same kinetic energy per hole. When δ is arbitrarily small, $\langle T\rangle$ is dominated by $\langle 0|\mathcal{H}_b^0|0\rangle$, and thus reflects the variational energy of an isolated holon. The linearity of $\langle T\rangle$ over the entire range of δ shown in Fig. 2 indicates that this is true even when δ is large. This result is important because the decrease in $\langle T\rangle$ due to the presence of $\langle 0|\mathcal{H}_f^0|0\rangle^{-1}$ in Eq. (17) just compensates the increase in χ_0 required by Eq. (9). Figure 1, for example, is computed using $\chi_0=1.43$. The cancellation of these two effects causes $\langle T\rangle$ to reflect the value of $\langle 0|\mathcal{H}_b^0|0\rangle$ evaluated *using the $\delta=0$ value of* χ_0. This is consistent with previous variational work on the properties of holons at finite δ [2], and also with the work of Liang and Trivedi [19]. We also note that Eq. (17) evaluated with the χ_0 of Eq. (9) yields a J-independent $\langle T\rangle$, which is consistent with the minimal J dependence of the Lanczos results for $\langle T\rangle$ [16].

Superconductivity is indicated in our calculation by the zero width of the Drude oscillator in Fig. 1 and a nonzero Meissner kernel $\mathcal{K}_{yy}(\omega)$ at $\omega=0$. The ratio $\mathcal{K}_{yy}(0)/\mathcal{K}_{yy}(\infty)=0.6$, which is determined primarily by the oscillators in $\hbar\omega=t$ continuum, is consistent with the 40% Drude fraction found in σ_{xx}.

Our calculation has several significant failures which we attribute to its crudeness. Approximately 5% of the oscillator strength of Fig. 1 is contained in a peak near $\hbar\omega=7t$, which correspond to no distinct feature in the Lanczos result. $\bar{\Pi}_b$ and Π_f possess energy gaps of $0.40t$ and $0.37t$, respectively, which are 10 times larger than the "gap" features seen in experiment and inconsistent with numerical studies of the t-J model. The structure in $\bar{\Pi}_b$ and Π_f at these energies does not produce structure in $\mathcal{K}$ and is invisible in Fig. 1. The sharp resonances in Fig. 1, such as that at $0.6t$, are similar to those found in RPA studies of the fractional-statistics gas [14] and are artifacts that disappear at higher orders in perturbation theory. The splitting near $\hbar\omega=t$ may also be an artifact, although this is not clear. It should be remarked that the large-energy structure of the electron spectral function

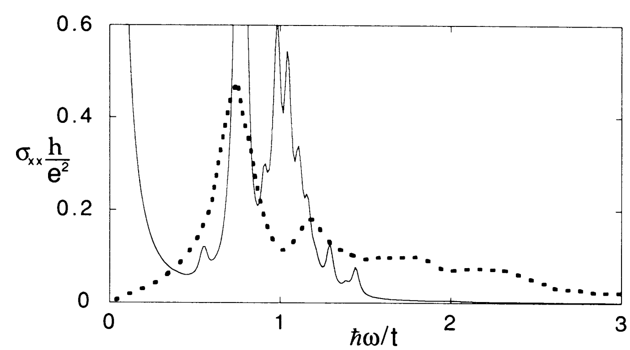

FIG. 1. Optical conductivity σ_{xx} calculated using Eq. (15) (solid line) vs the Lanczos result of Ref. [15] (dashed line). $J/t=0.4$ for both.

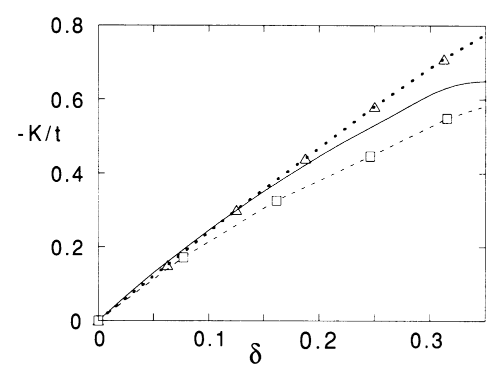

FIG. 2. Total kinetic energy per site calculated using Eq. (17) (solid line) and variationally by Liang and Trivedi [19] (squares) vs the Lanczos result of Ref. [16] (triangles). Note that only the Lanczos result depends on J/t and that this dependence is weak. The value assumed is 0.4.

calculated using this formalism [20] agrees roughly with the large-energy structure found in exact diagonalization studies. The Hall conductivity $\sigma_{xy}(\omega)$ is large ($\sim 0.2e^2/h$) at frequencies ω for which $\sigma_{xx}(\omega)$ is large, and is nonzero at $\omega=0$. This behavior, which is similar to that predicted by Wen and Zee [21], is inconsistent with the Lanczos results and with experimental searches for optical activity in high-T_c materials. σ_{xy} has been found in studies of the fractional-statistics gas [14] to be particularly sensitive to Feynman graphs omitted from this calculation.

The gauge propagator at small **q** and ω is effectively the sum of a piece that mediates fractional statistics and a piece that behaves like that of ordinary electromagnetism, including a propagating "photon" and a $1/q^2$ "Coulomb" interaction. Both of these have been seen in studies of the fractional-statistics gas [14]. The "photon" is equivalent to the Goldstone mode of the superfluid and describes ordinary compressional sound. The "Coulomb" interaction corresponds to the Magnus force between vortices, to which the f and b particles are equivalent in anyon superconductivity. Because the "photon" has no energy gap, the fractional statistics it mediates is due *not* to a Chern-Simons term in its effective Lagrangian, but to a relevant term of order q^3, as was predicted by Wiegmann [22]. Inclusion of the divergent "Coulomb" interaction in exchange and ladder graphs has little effect at zero temperature but drastically changes the finite-temperature behavior of $\mathcal{H}$. Both the $1/q^2$ divergence and the infinite lifetime of the "photon" are signatures of superconductivity.

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