Finite-size effects on the optical conductivity of a half-filled Hubbard ring

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We use the Bethe-ansatz equations to calculate the total and zero-frequency spectral weight in the optical conductivity of the half-filled one-dimensional Hubbard model as a function of the lattice size L and the on-site repulsion U. The zero-frequency spectral weight πD scales as $L^{1/2}\exp(-L/\xi)$ as $L\rightarrow\infty$. Near $U=0$, ξ varies as the inverse of the Lieb-Wu charge gap. In the strongly correlated regime ($U\gg t$), $\xi^{-1}=\ln(U/t)-1.48$. D is negative when L is a multiple of 4, corresponding to a negative inductance. We give a physical explanation of our results in terms of a simple model of ring exchange. The finite-size corrections to the total spectral weight scale as L^{-2}. We discuss the implications of our results for exact diagonalization calculations of the optical conductivity.

The optical conductivity of strongly correlated electron systems has recently been of interest both experimentally and theoretically. Experiments on high-T_c superconductors[1] and on quasi-one-dimensional organic conductors[2] show large deviations from the predictions of band theory, and various attempts have been made to reproduce these results theoretically, including exact diagonalization of model Hamiltonians on small lattices.[3,4] However, the small system sizes and the lack of theoretical analysis of finite-size corrections make interpretation of these results uncertain. In this paper we report calculations of the system size dependence of the zero-frequency spectral weight and the total spectral weight in the optical conductivity of the one-dimensional (1D) Hubbard model with periodic boundary conditions and a mean density of one electron per site. A succeeding paper will present results at different electron concentrations. These results are of fundamental interest because the scaling with system size of the zero-frequency spectral weight yields the localization length of the Mott insulating phase of the 1D Hubbard model.

We study the Hubbard Hamiltonian,

$$H=T+U\sum_{i=1}^{L}n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where T is the kinetic energy operator, to be defined below, and the lattice spacing is unity. A calculation of the optical conductivity $\sigma(\omega)$ of (1) would in general require a knowledge of its entire spectrum. However, an argument due to Kohn[5,6] allows one to extract some information about $\sigma(\omega)$ from ground-state properties alone. Let us thread the system with a (dimensionless) flux ϕ, which we represent by a vector potential $A=(\hbar c/e)\phi/L$. The kinetic energy operator becomes

$$T(\phi)=-t\sum_{i,\sigma}(e^{i\phi/L}c^{\dagger}_{i+1\sigma}c_{i\sigma}+\text{H.c.})\ , \tag{2}$$

where the sum runs from $i=1$ to L and $c_{L+1\sigma}\equiv c_{1\sigma}$ (periodic boundary conditions). Below we will take $t=1$ unless explicitly stated. The ground state carries no current at $\phi=0$, so its energy shift is second order in ϕ, and may be characterized by the charge stiffness,

$$D=\frac{1}{2}\frac{d^2(E_0/L)}{d(\phi/L)^2}\bigg|_{\phi=0}\ . \tag{3}$$

Kohn showed that the real part, $\sigma_r(\omega)$, of the optical conductivity may be written[5-7]

$$\sigma_r(\omega)=\frac{2\pi e^2}{\hbar^2}D\delta(\omega)+\text{regular terms}\ . \tag{4}$$

The total spectral weight is[3,6,7]

$$\int_0^{\infty}\sigma_r(\omega)d\omega=-\frac{\pi e^2}{2\hbar^2}\left\langle\frac{T(0)}{L}\right\rangle\ , \tag{5}$$

where $\langle\ \rangle$ denotes the expectation value in the ground state.

Both D and $\langle T\rangle$, as ground-state properties, may be calculated from the Bethe-ansatz for (1). The Bethe-ansatz equations for (1) with arbitrary ϕ were derived by Shastry and Sutherland, and are[6]

$$Lk_n=2\pi I_n+\phi+2\sum_{j=1}^{M}\tan^{-1}[4(\Lambda_j-\sin k_n)/U]\ , \tag{6}$$

$$2\sum_{n=1}^{N}\tan^{-1}[4(\Lambda_j-\sin k_n)/U]=2\pi J_j+2\sum_{\substack{i=1\\(i\neq j)}}^{M}\tan^{-1}[2(\Lambda_j-\Lambda_i)/U]\ , \tag{7}$$

where N is the number of electrons and M the number with spin up. We wish to consider the ground state at half filling ($N=L$). In addition we will consider only even L, so that the ground state is a singlet ($M=L/2$), and nondegenerate. The quantum numbers are then

$$J_j=\{-(M-1)/2,-(M-3)/2,\ldots,(M-1)/2\}\ ,$$

$$I_n=\begin{cases}\{-(L-1)/2,-(L-3)/2,\ldots,(L-1)/2\} & \text{if } L \pmod 4 \neq 2\ ,\\ \{-L/2+1,-L/2+2,\ldots,L/2\} & \text{if } L \pmod 4 = 0\ .\end{cases}$$

For L a multiple of 4 there is an ambiguity in the choice of $\{I_n\}$. We could also choose $I_n=\{-L/2,\ldots,L/2-1\}$, which is another representation of the same state. From (6), (7), and the definition of the Bethe-ansatz wave function it follows that the total momentum is $P_{\rm tot}=\sum_{n=1}^{L}k_n=\phi+(2\pi/L)\sum_{n=1}^{L}I_n$. This reduces to $P_{\rm tot}=\phi$ unless L a multiple of 4, in which case $P_{\rm tot}=\phi\pm\pi$, according to the choice made for $\{I_n\}$. The ground-state momentum of a half-filled Hubbard ring whose length is a multiple of 4 is thus minimized at a flux of π (half a flux quantum). This rather peculiar property is related to the negative charge stiffness discussed below.

The ground-state energy of the system is expressed in terms of the momenta $\{k_n\}$ as $E_0(\phi)=-2\sum_n \cos k_n(\phi)$. $E_0(\phi)$ is a periodic function of ϕ with period 2π. We find that $E_0(\phi)$ is a minimum at $\phi=\pi$ when L is a multiple of 4, and at $\phi=0$ otherwise. Substituting the expression for $E_0(\phi)$ into (3), we obtain

$$D=L\sum_n\left[\cos k_n\left[\frac{dk_n}{d\phi}\right]^2+\sin k_n\frac{d^2k_n}{d\phi^2}\right]\ , \tag{8}$$

where all quantities are evaluated at $\phi=0$. By taking ϕ derivatives of the Bethe-ansatz equations (6) and (7) one can obtain linear matrix equations for $\{dk_n/d\phi\}$ and $\{d^2k_n/d\phi^2\}$, with coefficients that are functions of U, L, $\{k_n(0)\}$, and $\{\Lambda_j(0)\}$. We solved (6) and (7) numerically for $\{k_n(0)\}$ and $\{\Lambda_j(0)\}$, then inverted the equations for $\{dk_n/d\phi\}$ and $\{d^2k_n/d\phi^2\}$ numerically to calculate the charge stiffness from (8). We find that D has the asymptotic form

$$D(L,U)\sim-(-1)^{L/2}L^{\eta}\exp[-L/\xi(U)]\quad\text{as } L\to\infty \tag{9}$$

with $\eta\sim0.5$. This behavior is displayed in Fig. 1. We interpret $\xi(U)$ as the localization length of the Mott insulating phase of the 1D Hubbard model.[5] The localization length exceeds our system size ($L\sim100$) for $U<2$. However, for $U<2$ the regime $\xi\gg L\gg1$ is accessible, and we have determined that $D(L,U)$ is essentially independent of L in this regime, except that D is large and negative when L is a multiple of 4, and of order unity and positive otherwise. The L independence of D in this regime is expected from the intuitive argument that the system is metallic on scales small compared with ξ.

The asymptotic form of the charge stiffness can be obtained analytically in the large-U limit using the Poisson summation formula and the observation that the Λ_j and the density of k points are U independent to $O(U^{1-L})$, and we find

$$D(L,U)\sim-(-1)^{L/2}L^{1/2}\left[\frac{4.38}{U}\right]^{L-1}\quad\text{as } L\to\infty\ , \tag{10}$$

which implies $\xi^{-1}=\ln(U/t)-1.48$. The localization length begins to deviate significantly from its large-U form when it exceeds the lattice spacing, and it diverges at the critical point $U=0$. In the critical regime where $\xi\gg1$ we believe ξ to scale as the inverse of the Lieb-Wu charge gap, defined by[8,9]

$$\Delta=\frac{16t^2}{U}\int_1^{\infty}\frac{(y^2-1)^{1/2}dy}{\sinh(2\pi ty/U)}\ .$$

This behavior is displayed in Fig. 2.

It is interesting to compare our results to those obtained by solving (1) in the Hartree-Fock (HF) approximation. This approximation incorrectly predicts long-range magnetic order at $T=0$, but correctly gives a charge gap. In the limit $U\gg t$ we find $D\sim-t(-1)^{L/2}L^{1/2}(2t/U)^{L-1}$. The factor of 2 is replaced by 4.38 in the Bethe-ansatz result. In the limit $U\ll t$ and $L\to\infty$ the HF approximation yields $D\sim-(-1)^{L/2}(L/\xi)^{1/2}\exp(-L/\xi)$, with $\xi\Delta_{\rm MF}=4t$ and $\Delta_{\rm MF}$ the mean-field charge gap. The mean-field value of $\xi\Delta$ is indicated by an arrow on the inset to Fig. 2, and agrees with the apparent $U\to0$ limit of the Bethe-ansatz results. The HF result for $\xi\gg L\gg1$ is $D\sim t$ when L is not a multiple of 4, in agreement with the exact result, and $D\sim-\xi/L$ when L is a multiple of 4. The exact result has a much weaker L dependence when L is a multiple of 4 and $\xi\gg L\gg1$, but the HF calculation correctly predicts that D diverges as $U\to0$ in this regime and that this divergence is cut off when $L\sim\xi$.

In the regime of strong correlations $U\gg t$, collective

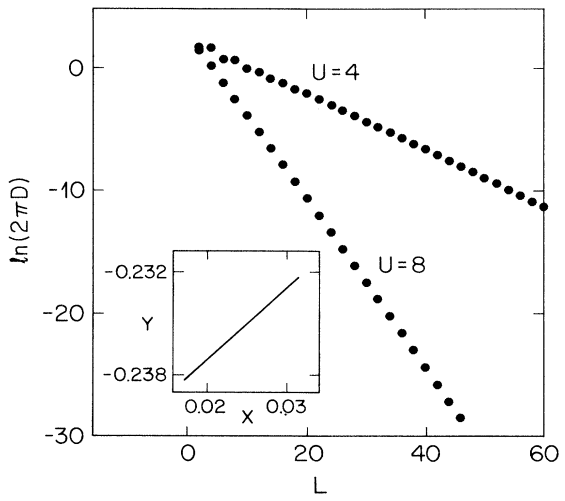

FIG. 1. $\ln|2\pi D|$ as a function of system size for $U=4$ (upper curve) and $U=8$ (lower curve). πD is the dc spectral weight in units where $e=\hbar=1$. Inset: A plot of $y=\ln[D(L)/D(40)]/(L-40)$ vs $x=\ln[L/40]/(L-40)$ for $L=42$–100 and $U=4$, displaying the asymptotic form $y=-\xi^{-1}+\eta x$. Here $x=4.06$ and $\eta=0.45$.

motions of the electrons give the dominant contribution to D, and their effect may be understood in terms of a Brillouin-Wigner perturbation expansion in t/U. Let us split the kinetic energy operator (2) into a left moving term V and a right moving term $V^\dagger$:

$$T(\phi)=-t(e^{i\phi/L}V^\dagger+e^{-i\phi/L}V) \quad \text{with } V^\dagger=\sum_{i,\sigma} c^\dagger_{i+1\sigma}c_{i\sigma} .$$

The lowest order term in t/U which gives a flux-dependent shift to the ground-state energy of a ring of length L is

$$\Delta E_0(\phi)=-\frac{t^L}{U^{L-1}}\left[e^{i\phi}\sum_{\psi_1,\psi_2,\cdots,\psi_{L-1}}\frac{\langle 0|V^\dagger|\psi_{L-1}\rangle\langle\psi_{L-1}|V^\dagger|\psi_{L-2}\rangle\cdots\langle\psi_1|V^\dagger|0\rangle}{d_{\psi_{L-1}}d_{\psi_{L-2}}\cdots d_{\psi_1}}+\text{H.c.}\right], \tag{11}$$

where $d_{\psi_i}>0$ is the number of doubly occupied sites in the intermediate state $|\psi_i\rangle$, and $|0\rangle=\lim_{U\to\infty}|0\rangle_U$, $|0\rangle_U$ being the ground state of (1). This energy shift is the result of the ring exchange processes which transport one unit of charge around the ring in the minimum number of steps, L. The charge stiffness for a ring of length L, to leading order in t/U, is $D_L=(L/2)d^2[\Delta E_0(\phi)]/d\phi^2|_{\phi=0}$. This expression may be evaluated directly for small L, and we obtain $D_2=8t^2/U$, $D_4=-144t^4/U^3$, in agreement with our numerical results. From Eq. (11), one sees that $D(L+1)/D(L)\equiv\exp(-1/\xi)\sim t/U$, so $\xi^{-1}\sim\ln(U/t)$.

As mentioned above, the charge stiffness of a half-filled Hubbard ring of length L is negative if L is a multiple of 4, and positive otherwise. The sign of the stiffness in the large-U limit results from the fact that the lowest-order ring exchange processes contributing to D connect the ground state to itself, translated by one lattice constant, so that the momentum of the ground state at $\phi=0$ determines the sign of D:

$$\text{sign}(D_L)=\exp(iP_0)=\exp[i\pi(L/2+1)] . \tag{12}$$

This may be seen explicitly from (11) if we make the approximation that $d_i=1\forall i$, i.e., we consider only the lowest-energy intermediate states contributing to (11). In this case we can further simplify to $D_L=(Lt^L/U^{L-1})\langle 0|V_{\text{eff}}|0\rangle$, where the operator $V_{\text{eff}}=P_0V^\dagger P_1V^\dagger P_1\cdots P_1V^\dagger P_0$, and P_n projects onto the subspace with n doubly occupied sites. The operator V_{eff} describes the Aharonov-Bohm effect of a doubly occupied site and a hole created by the first $V^\dagger$, which propagate around the ring in opposite directions, then recombine, encircling the flux ϕ. We can express V_{eff} in closed form as

$$V_{\text{eff}}=\hat{\tau}_{\text{cyclic}}\sum_n\sum_{\nu=0}^{L-2}\binom{L-2}{\nu}q_{n+\nu}\cdots q_{n+1}q_n ,$$

where $q_n\equiv\frac{1}{2}(1-\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_{n+1})$ is the singlet projection operator and $\hat{\tau}_{\text{cyclic}}$ is the unit lattice translation operator, whose ground-state eigenvalue is $\exp\{iP_0\}$. The result (12) then follows from the fact that $\langle 0|q_{n+\nu}\cdots q_n|0\rangle\geq 0$, which may be proven as follows. We first make the unitary transformation $S=\prod_{n\in\text{odd}}\sigma^z_n$. The transformed ground state $S|0\rangle$ can be written in the standard σ^z basis as a sum over configurations with the same sign (this is the familiar Marshall nodeless property[10]. Under S, the projection operator q_n turns into an operator with non-negative diagonal matrix elements and positive off-diagonal elements in the σ^z basis. A string of q's clearly has the same property, and hence the result quoted above follows.

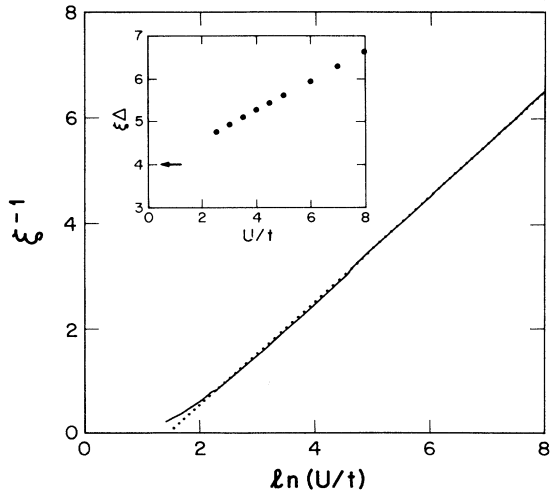

FIG. 2. The inverse of the localization length, ξ, vs $\ln(U/t)$. The analytic result $\xi^{-1}=\ln(U/t)-1.48$ for $U\gg t$ is shown as a dashed line. Note that $\xi\to\infty$ as $U\to 0$. Inset: $\xi\Delta$ vs U/t, where Δ is the Lieb-Wu charge gap. $\xi\Delta$ appears to approach the mean-field result $\xi\Delta/t=4$ (indicated by an arrow) as $U\to 0$.

The negative charge stiffness for half-filled Hubbard rings of length $4n$ may also be understood in the small-U limit on the basis of first-order degenerate perturbation theory in U.[11] The noninteracting system with a multiple of 4 particles has a level crossing at $\phi=0$, owing to the fact that the states of momentum $\pm\pi$ are distinct but degenerate states for free particles, corresponding to a filled Fermi sea of momentum zero plus a single pair of electrons either in the state $k=\pi/2$ or $k=-\pi/2$. Any small perturbation lifts the degeneracy and gives $E_0(\phi)$ a negative curvature at $\phi=0$. Physically, a negative charge stiffness corresponds to a negative inductance, or orbital paramagnetism. This effect was observed many years ago in NMR spectra of [16]annulene and [24]annulene,[12] larger analogs of benzene. Orbital paramagnetism is a generic feature of half-filled single-band $4n$ electron systems, and arises in a noninteracting dimerized model[13] as well as in a dimerized Hubbard model.[14] The related issue of whether $E_0(\phi)$ has a minimum at $\phi=0$ or at $\phi=\pi$ was first discussed in a slightly different context by Byers and Yang.[15]

We have also evaluated the ground-state expectation value of the kinetic energy as a function of U and L, which gives the total spectral weight in the optical conductivity through (5), by numerically differentiating the ground-state energy: $\langle T\rangle = E_0 - U dE_0/dU$. Figure 3 shows the finite frequency spectral weight $F = -(\pi/2L)\langle T\rangle - \pi D$ (in units where $e = \hbar = 1$) as a function of L for $U = 4$. F deviates by more than 20% from its large-L value for $L \leq 3\xi$, the finite-size corrections to F being significantly larger than those to the total spectral weight. We note that recent literature contains many reports of calculations of $\sigma(\omega)$ for the two-dimensional Hubbard model on finite clusters of linear dimension $L \sim 3$ lattice sites.[4] Although the extent to which our results extrapolate to two dimensions is not clear, they suggest that even if exact diagonalization calculations give reasonable values for $\int_0^\infty \sigma_r(\omega)d\omega$, the detailed form of $\sigma(\omega)$ may be subject to severe finite-size corrections, for $U < 15$.

The inset to Fig. 3 displays the deviation of $\langle T\rangle$ from its infinite-size limit on a log-log plot for $U = 10$. The value in the thermodynamic limit was obtained by differentiating Lieb and Wu's expression for $E_0(U)$,[8] and performing the resulting integration numerically. As is clear from the figure, the behavior for large L is

$$\left| \left\langle \frac{T}{L} \right\rangle - \lim_{L\to\infty} \left\langle \frac{T}{L} \right\rangle \right| \propto L^{-2} , \tag{13}$$

consistent with the system size dependence of the total ground-state energy obtained by Woynarovich and Eckle.[16]

In conclusion, we have calculated the system size dependence of the dc conductivity and the total spectral weight in the optical conductivity of the Mott insulating phase of the 1D Hubbard model. The spectral weight πD in the dc conductivity was found to decay as $L^{1/2}\exp(-L/\xi)$. The localization length ξ was found to vary as the inverse of the Lieb-Wu charge gap Δ when $\Delta < t$, and as the inverse of the logarithm of the on-site repulsion U when $U \gg t$. D is negative for rings with $4n$ electrons, indicating orbital paramagnetism. The finite-size corrections to the total spectral weight scale as L^{-2} for $L \gg \xi$ and are large for $L \leq 3\xi$. The finite-size corrections to the spectral weight at $\omega > 0$ are roughly twice as large and decay more slowly with system size. This suggests that the detailed form of the conductivity as a function of frequency obtained from exact diagonalization may be modified by finite-size effects even if the total spectral weight so obtained is near its thermodynamic limit.

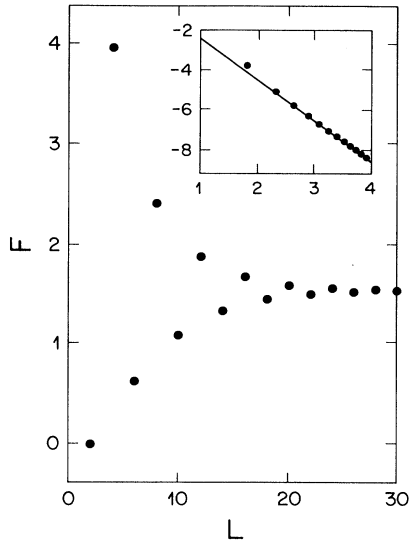

FIG. 3. Finite frequency spectral weight $F = -(\pi/2L)\langle T\rangle - \pi D$ as a function of system size for $U = 4$. Inset: Finite-size corrections to the total spectral weight displayed on a log-log plot for $U = 10$, showing L^{-2} behavior.

Note added. During the preparation of this manuscript we received an unpublished report of work by R. M. Fye, M. J. Martins, D. J. Scalapino, J. Wagner, and W. Hanke, which represents results of a similar study for various electron concentrations including one electron per site. In the half-filled case they assert that the large-L behavior of D is purely exponential and they do not discuss the large-U limit.

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