Low-temperature conductivity in a narrow half-filled Hubbard chain*

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In this paper, the low-temperature ($k_B T \ll U$) frequency-dependent $\sigma(\omega)$ conductivity in a half-filled Hubbard chain is calculated to the lowest order in the parameter t/U and in closed form to all orders in $t/\omega - U$. Here t is the nearest-neighbor hopping integral and U the intra-atomic Coulomb interaction. The problem is formulated in terms of the number of random walks of an electron and a hole which leave the spin configuration unchanged, at temperatures such that $k_B T \ll t \ll U$ (where k_B is Boltzmann's constant). The conductivity then depends on spin configuration, and for both the antiferromagnetic (AF) ($T = 0$ K) ground state and the equiprobable or random arrangement (R) ($k_B T \gg t^2/U$) an *exact* expression is found. For the partially disordered regime ($T \simeq T_N$) the thermodynamical averaging is expressed in terms of a phenomenological spin-spin correlation length l which interpolates between the AF and R exact limits. This solution is such that for $l = \infty$ the AF line shape is recovered except at the center of the spectrum (i.e., at $\omega = U$), where the absorption always diverges logarithmically. For a ferromagnetic ($l = 0$) arrangement induced by a magnetic field, the absorption then vanishes. The line shapes obtained have sharp edges at $|\omega| = U \pm 4t$ for all temperatures. At the critical value of $4t = U$ the AF ground state is found to undergo a metallic transition. A closed-form analytical expression in terms of the three elliptical integrals is given for the absorption lines. Except for the AF case, which has a square-root edge singularity, the absorption is found to vanish linearly. Finally, a comparison is made with some recent calculations.

I. INTRODUCTION

The behavior of electrons localized in narrow bands has been a matter of considerable recent interest. The works of Hubbard,[1] who succeeded in obtaining successive improved solutions to the problem posed by himself, constitute a breakthrough in this connection. As is known, in such systems the ordinary band theory for the conduction electrons breaks down because of the very strong Coulomb repulsion between the electrons. In the Hubbard model, these are considered to be localized in Wannier cells and only the Coulomb repulsion between electrons on the same lattice site is retained. In this paper, we shall examine this model in an atomic limit in which the transfer energy t is taken as much smaller than the Coulomb repulsion U, and discuss the line shape of the optical absorption due to simultaneous excitation of one carrier and a hole in an otherwise half-filled band chain. This atomic limit of the Hubbard model has been extensively studied. Harris and Lange[2] have shown that the spectral weight function consists of a series of equidistant bands separated in energy by U. Nagaoka and then Sokoloff[3] have formulated this limit of the Hubbard model in terms of the number of possible random walks on a lattice. In particular, Sokoloff[3] considered the thermodynamics and magnetic properties of the infinite-interaction one-dimensional Hubbard model. Brinkman and Rice[4] later used this method to study the mobility of a single hole (or extra carrier) in a half-filled band. Beni, Holstein, and Pincus,[5] and also Klein,[5] essentially reobtained the latter's results for the one-dimensional band case. Here the magnetic properties[6] are largely independent of the model.

Extensive use of this formulation was also made in our previous work.[7]

In the present paper (Sec. II), we reconsider in detail the calculation of the time-dependent velocity-velocity correlation function for the random walks of two impenetrable particles: a doubly occupied site and a hole. At temperatures such that $k_B T \ll t \ll U$ the thermal doubly occupied configurations are negligible and we need consider only the subspace of the 2^N spin states. A doubly occupied site and a hole can then be created by the velocity operator at a certain point, make arbitrary excursions, and be annihilated somewhere else in the chain restoring the initial spin configuration. Lieb and Wu[8] have shown that the exact $T = 0$ K ground state for the half-filled chain is both antiferromagnetic and insulating. Here, it is found that at the critical value of $4t = U$ the system undergoes a metallic transition; we then believe that this should set the radius of convergence of our expansion to the lowest order in t/U.

At temperatures $k_B T \gg t^2/U$ we have averaged over all spin configurations with equal probability. In this case, a logarithmic divergence shows up in the line shape at $\omega = U$. In the critical ordering region $T \simeq T_N$ the antiferromagnetic (AF) and random (R) exact limits are interpolated in terms of an antiferromagnetic spin-spin correlation length of the chain. While we do not make any claims as to the accuracy of this interpolation, we feel that it should at least provide us with a qualitative representation of the line shapes in this more complicated regime. In particular, to the lowest order in t/U the absorption edges turn out to be temperature independent.

In Sec. III, we use two different integral representations of the generating function[9] for the two-particle random walk. We then express in terms of elliptic integrals the line shapes; these are found to be characterized always by two simple curves: an AF circle, to which a parabola is added to account for spin disorder. Finally, in Sec. IV, we compare our well-defined results with some recent calculations.

II. VELOCITY-VELOCITY CORRELATION FUNCTION

In this section, we consider in detail the calculation of the time-dependent velocity-velocity correlation function $\phi(\tau)$. This quantity is explicitly[5]

$$\phi(\tau) = \langle v(\tau)\, v(0) + v(0)\, v(\tau)\rangle = \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta\mathcal{H}}\left(e^{i\mathcal{H}\tau}\, v e^{-i\mathcal{H}\tau}\, v + v e^{i\mathcal{H}\tau}\, v e^{-i\mathcal{H}\tau}\right)\right], \tag{2.1}$$

with the Hubbard Hamiltonian $\mathcal{H}$ given by[7]

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij}\, c^{\dagger}_{j\sigma} c_{i\sigma} + \frac{U}{2}\sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma}\,, \tag{2.2}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) creates (destroys) a state of spin σ at site i, and $n_{i\sigma}$ ($\equiv c^{\dagger}_{i\sigma} c_{i\sigma}$) is the number operator. The quantity t_{ij} is the transfer-matrix element between sites i and j and U gives the intra-atomic Coulomb repulsion. We will consider only nearest-neighbor hopping, so that $t_{ij} = t$, if i and j are nearest neighbors and $t_{ij} = 0$, otherwise. The extension of our method to include next-nearest neighbors is very difficult and this matter will not be considered here.

The velocity operator is

$$v = ita \sum_{i,\sigma,\Delta} \Delta c^{\dagger}_{i+\Delta\sigma} c_{i\sigma}\,, \quad \Delta = \pm 1\,, \tag{2.3}$$

where $i+1$ is the lattice site next to i in the field direction, and a is the lattice constant. The partition function Z is

$$Z = \mathrm{Tr}(e^{-\beta\mathcal{H}})\,. \tag{2.4}$$

We will consider only the low-temperature strongly correlated limit of (2.2), such that $k_B T \ll t \ll U$. Because of this, one can restrict the operation of the trace in (2.1) and (2.4) to the 2^N (N being the number of electrons, or sites, in the half-filled chain) spin states without thermal doubly occupied configurations. In this temperature range, (2.2) can be written[10-12] as a Heisenberg spin Hamiltonian with antiferromagnetic constant $J = 2t^2/U$. In one dimension, the ground state of (2.2) is then strictly antiferromagnetic.[8] At the Néel temperature[12] $T_N = zt^2/U$ (z being the coordination number of the lattice, i.e., $z = 2$ for our case) a transition occurs to a paramagnetic or disordered state, so that for $T_N \ll T \ll U/k_B$ the partition function can be written as $Z \simeq 2^N$ since all the spin states are then equiprobable (see Appendix B). For the antiferromagnetic region $T \ll T_N$, we can write $Z \simeq 1$ where only the antiferromagnetic state vector is included in the thermodynamical average. Also, in order to consider a nearly ferromagnetic (F) spin ordering we will assume that an external magnetic field is added to (2.2). Note, however, that such an ordering is inherently unstable because of the antiferromagnetic coupling constant J given by Anderson's[11] kinetic exchange.

Since we consider the limit $t \ll U$, we write the Hubbard Hamiltonian (2.2) as $V + H_0$, where the transfer term [the first term in (2.2)] is treated by a perturbation expansion to all orders. The correlation function $\phi(\tau)$ can then be written[13]

$$\phi(\tau) = Z^{-1}\,\mathrm{Tr}\left[S(\beta, i\tau)\, v(i\tau)\, S(i\tau, 0)\, v + S(\beta + i\tau, 0)\, v(-i\tau)\, S(0, i\tau)\, v\right], \tag{2.5}$$

where the time-ordered development operator is

$$S(x,y) = \sum_{n=0}^{\infty} (-1)^n \int_y^x dx_1 \int_y^{x_1} dx_2 \cdots \int_y^{x_{n-1}} dx_n \left[V(x_1)\, V(x_2) \cdots V(x_n)\right], \tag{2.6}$$

and we have in the interaction representation

$$V(x) = e^{xH_0}\, V e^{-xH_0} \tag{2.7}$$

and the analogous for $v(i\tau)$.

The lowest-order process in t/U that contributes to (2.5) is then[7] that in which a hole and a doubly occupied site are created somewhere in the chain by the velocity operator with a certain probability $p \equiv \exp(-a/l)$, such that

$$2a^2t^2Np = \langle v^2\rangle\,, \tag{2.8}$$

then make arbitrary excursions with the development operator S, without *any* intermediate recombintation, to be finally annihilated by the second velocity operator at some arbitrary point. In this paper only, these processes will be considered. The next order process in t/U, which involves propagation and *one* final recombination by the second development operator S, will be reserved for a future publication.

We remark at this point from (2.8), that in the ground state for the AF ordering $p=1$, while far above the Néel temperature, for the (R) ordering, $p=0.5$. In general, however, (2.8) defines a certain temperature dependence (for $k_BT \ll U$) of the parameter p, where in (2.8) the thermodynamic average is of course taken with respect to the equivalent Heisenberg Hamiltonian[12]

$$\mathcal{H} = \frac{2t^2}{U} \sum_{i>j} \vec{S}_i \cdot \vec{S}_j \,. \tag{2.9}$$

In the present work we introduce this parameter $p(T)$ only to have a simple phenomenological interpolation for the line shapes between the AF and R exact limits. The temperature dependence of $p(T)$ remains to be found. We remark also that if an external magnetic field is added to (2.9) then $p(T,H) < \frac{1}{2}$. For $T=0$ K and a sufficiently strong magnetic field, the ferromagnetic (F) arrangement results with $p=0$.

Since the second term in (2.5) is the complex conjugate of the first one, we then write

$$\phi(\tau) = 2\,\mathrm{Re}\,\langle v(i\tau)\, S(i\tau, 0)\, v\rangle \,; \tag{2.10}$$

substituting v as given by (2.3) one obtains

$$\phi(\tau) = 4a^2t^2\,\mathrm{Re} \sum_{\substack{i,j\\ \sigma,\sigma'}} \langle c^\dagger_{i-1,\sigma} c_{i\sigma} S'(i\tau,0)\, c^\dagger_{j+1,\sigma'} c_{j\sigma'} - c^\dagger_{i+1,\sigma} c_{i\sigma} S'(i\tau,0)\, c^\dagger_{j+1,\sigma'} c_{j\sigma'}\rangle \,, \tag{2.11}$$

where

$$S'(i\tau,0) = e^{-iH_0\tau} S(i\tau,0)\,.$$

The factor of 2 in (2.11) and (2.8) arises because the doubly occupied site can be created on either side of the hole. We notice that since $S(i\tau,0)$ describes the propagation of two impenetrable particles, the second term in (2.11) does not contribute to $\phi(\tau)$ in our case. In higher dimensions, however, this term may obviously contribute even to the lowest order in t/U. In this respect, the one-dimensional band chain is quite unique and our calculation will be hereafter restricted to it.

We then write

$$\phi(\tau) = 4a^2t^2\,\mathrm{Re} \sum_{i,j,\sigma} \langle c^\dagger_{i-1,\sigma} c_{i\sigma} S'(i\tau,0)\, c^\dagger_{j+1,\sigma} c_{j\sigma}\rangle \,. \tag{2.12}$$

This expression can be easily interpreted, as mentioned above, in the following way: we suppose that the operator $c^\dagger_{j+1,\sigma} c_{j\sigma}$ creates the electron–(i.e., double occupancy) hole pair at some point in the lattice, say $|0,1\rangle$, with probability p. The development operator S', because it contains an arbitrary number of transfer operations, allows the electron-hole pair to move an arbitrary number of steps to some site $|q_1,q_2\rangle$. The second operator, $c^\dagger_{i-1,\sigma} c_{i\sigma}$, then makes somewhere a final recombination, restoring the initial spin configuration. Note that for recombination to be possible, a necessary condition is that $q_2 = q_1+1$. Under these conditions $V(x)$ in the integrals (2.6) is independent of x, and one finds that

$$S(i\tau,0)\,|0,1\rangle = \sum_{n=0}^{\infty} \sum_{q_1,q_2} \frac{(-it\tau)^n}{n!} \times P_n^{(1)}(q_1,q_2)\,|q_1,q_2\rangle \,, \tag{2.13}$$

where $P_n^{(1)}(q_1,q_2)$ is the number of ways two impenetrable particles can walk from, say, $|0,1\rangle$, to a position $|q_1|$ and $|q_2|$ steps away from the origin, after taking a total of n steps. In general, for two such particles starting from, say, $|0,Q\rangle$, one can calculate[14] $P_n^{(Q)}(q_1,q_2)$; when $Q=1$ and $q_2=q_1+1$, one then finds,[7] as shown in our previous work,[7]

$$P_n^{(1)}(q,q+1) = \left(\frac{n!}{[(\frac{1}{2}n)!]^2} - \frac{n!}{[\frac{1}{2}(n+2)]!\,[\frac{1}{2}(n-2)]!}\right) \times \frac{n!}{[\frac{1}{2}(n+2q)]!\,[\frac{1}{2}(n-2q)]!} \,. \tag{2.14}$$

Interestingly enough, one can think of (2.14) as decomposing the correlated motion of the two particles into the independent motion of two fictitious particles: the first factor gives the motion of a particle constrained to a half line,[9] while the second gives that of a free particle in one dimension, that ends up $2q$ steps away from the origin. Recombination on a state $|q,q+1\rangle$ will contribute to (2.12), however, only if there exists an antiferromagnetic domain up to $|q|$ steps away from the creation point. The spin configuration outside this domain is irrelevant insofar as recombination on $|q,q+1\rangle$ is concerned. We will simply assume that the probability of such a domain is given by $p^{|q|}$, with p as given by (2.8). As this obviously does not account for short-range antiferromagnetic spin correlations, it is exact only when $p=0$, 0.5, 1.

Finally from (2.8), (2.12), and (2.13) one finds

$$\phi(\tau) = 4a^2t^2pN\,\mathrm{Re}\left\{e^{-iU\tau} \sum_{n=0}^{\infty} \sum_{q=-\infty}^{+\infty} \frac{(-it\tau)^n}{n!} p^{|q|} \left[\frac{n!}{[\frac{1}{2}(n+2q)]!\,[\frac{1}{2}(n-2q)]!}\right] \left(\frac{n!}{[(\frac{1}{2}n)!]^2} - \frac{n!}{[\frac{1}{2}(n+2)]!\,[\frac{1}{2}(n-2)]!}\right)\right\} , \tag{2.15}$$

where the sum over q can be extended to infinity since the random-walk function (2.14) is null for $|q|>\frac{1}{2}n$, with n even. One can evaluate (2.15) in several different manners, we will present two different ones.

III. INTEGRAL REPRESENTATIONS

One can write an integral representation[9] for the factor in large square brackets in (2.15) as

$$\Theta_n(p)\equiv\sum_{q=-\infty}^{+\infty}p^{|q|}\frac{n!}{[\frac{1}{2}(n+2q)]!\,[\frac{1}{2}(n-2q)]!}=\frac{1}{2\pi i}\oint\frac{dz}{z^{n+1}}\left[\frac{1}{(1-4z^2)^{1/2}}\sum_{q=-\infty}^{+\infty}p^{|q|}\left(\frac{1-(1-4z^2)^{1/2}}{2z}\right)^{2|q|}\right],\tag{3.1}$$

where the counterclockwise contour need only enclose the origin with $|z|<\frac{1}{2}$. Note that the factor in large square brackets is nonanalytic only on the real axis for $|z|\geq\frac{1}{2}$; we use this property to transform (3.1) into a real integral. We obtain first by summing the geometric series in q, that

$$\Theta_n(p)=\frac{1}{2\pi i}\oint\frac{dz}{z^{n+1}}\frac{1}{(1-4z^2)^{1/2}}\left(\frac{4z^2+p[1-(1-4z^2)^{1/2}]^2}{4z^2-p[1-(1-4z^2)^{1/2}]^2}\right).\tag{3.2}$$

Note also that the geometric series converges for all values of z, since the equation $[1-(1-4z^2)^{1/2}]^2p=4z^2$ has no solution for $p<1$, even when $p\to1$. One now follows a standard procedure[7] and deforms the contour in (3.2) to reduce the integration to a real integral. One finds

$$\Theta_n(p)=\frac{1}{2\pi i}(2i)\,2\int_{1/2}^{\infty}\frac{dz}{z^{n+1}}\operatorname{Im}\left[\frac{1}{(1-4z^2)^{1/2}}\left(\frac{4z^2+p[1-(1-4z^2)^{1/2}]^2}{4z^2-p[1-(1-4z^2)^{1/2}]^2}\right)\right]\tag{3.3}$$

for n even, and zero otherwise. To find the imaginary part in (3.3) one must calculate the real part of the factor in large parentheses. One finds after some algebra

$$\operatorname{Re}\frac{4z^2+p[1-(1-4z^2)^{1/2}]^2}{4z^2-p[1-(1-4z^2)^{1/2}]^2}=\frac{z^2(1-p^2)}{z^2(1+p)^2-p},\tag{3.4}$$

so that

$$\Theta_n(p)=\frac{2}{\pi}\int_{1/2}^{\infty}\frac{dz}{z^{n+1}}\frac{1}{(4z^2-1)^{1/2}}\left(\frac{z^2(1-p^2)}{z^2(1+p)^2-p}\right).\tag{3.5}$$

In Appendix A, we show that for $p=1$, (3.5) reduces to $\Theta_n(p=1)=2^n$, in agreement with (3.1). Substituting (3.5) into (2.15), one obtains

$$\phi(\tau)=4a^2t^2pN\operatorname{Re}\left[e^{-iU\tau}\sum_{n=0}^{\infty}(-it\tau)^n\Theta_n(p)\left(\frac{1}{[(\frac{1}{2}n)!]^2}-\frac{1}{[\frac{1}{2}(n+2)]!\,[\frac{1}{2}(n-2)]!}\right)\right].\tag{3.6}$$

Then using the series expansion of the Bessel functions,[15] namely,

$$\sum_{n=0}^{\infty}\frac{\lambda^n}{[\frac{1}{2}(n+\alpha)]!\,[\frac{1}{2}(n-\alpha)]!}=i^{|\alpha|}J_{|\alpha|}(2i\lambda),\tag{3.7}$$

where J_α is the Bessel function of order α, one obtains with $\lambda=-it\tau/z$, and interchanging integration with summation

$$\phi(\tau)=4a^2t^2pN\operatorname{Re}\left[e^{-iU\tau}\frac{2}{\pi}\int_{1/2}^{\infty}\frac{dz}{z}\frac{1}{(4z^2-1)^{1/2}}\left(\frac{z^2(1-p^2)}{z^2(1+p)^2-p}\right)[J_0(2i\lambda)+J_2(2i\lambda)]\right],\tag{3.8}$$

but since

$$J_0(2i\lambda)+J_2(2i\lambda)=(-i/\lambda)J_1(2i\lambda),\tag{3.9}$$

one obtains finally for $\phi(\tau)$, the following representation:

$$\phi(\tau)=4a^2t^2pN\left[\frac{\cos U\tau}{t\tau}\frac{2}{\pi}\int_{1/2}^{\infty}\frac{dz}{(4z^2-1)^{1/2}}J_1\left(\frac{2t\tau}{z}\right)\left(\frac{z^2(1-p^2)}{z^2(1+p)^2-p}\right)\right].\tag{3.10}$$

In particular for $p=1$, we get the following results:

$$\phi_{\rm AF}(\tau)=(4a^2t^2N/t\tau)(2/\pi)(\cos U\tau)(\pi/4)\,\delta(z-\tfrac{1}{2})J_1(2t\tau/z)\tag{3.11}$$

$$=(2a^2tN/\tau)(\cos U\tau)J_1(4t\tau).\tag{3.12}$$

This is then the correlation function of a propagating particle and hole that move in opposite directions.[7]

In general, from (3.10) one can easily find the real part of the conductivity as given by the symmetrized

Kubo[16] formula

$$\sigma_R(\omega) = \frac{e^2 \tanh(\frac{1}{2}\beta\omega)}{2\Omega\omega} \int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau}\, \phi(\tau)\,, \tag{3.13}$$

where e, Ω, ω are the electronic charge, the volume of the system and the external frequency, respectively. Inserting (3.10) into (3.13) and interchanging the order of integrations, one obtains

$$\phi(\omega) \equiv \int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau}\phi(\tau)$$

$$= 4a^2tpN\left(\frac{2}{\pi}\right)\int_{1/2}^{\infty} \frac{dz}{(4z^2-1)^{1/2}}\left(\frac{z^2(1-p^2)}{z^2(1+p)^2-p}\right)\int_0^{\infty}\frac{d\alpha}{\alpha}J_1(\alpha)\left[\cos\left((\omega-U)\frac{\alpha z}{2t}\right)+\cos\left((\omega+U)\frac{\alpha z}{2t}\right)\right] \tag{3.14}$$

$$= \frac{4a^2tpN}{\pi}\int_{k'}^{1}\frac{dz}{(z^2-k'^2)^{1/2}}\left(\frac{z^2(1-p^2)}{z^2(1+p)^2-4pk'^2}\right)(1-z^2)^{1/2} + (k' \to k'^*)\,, \tag{3.15}$$

where $k' = |(\omega-U)/4t| \leq 1$ [Eq. (3.15)], and we have used[15]

$$\int_0^{\infty}\frac{d\alpha}{\alpha}J_1(\alpha)\cos(2k'z\alpha) = (1-4k'^2z^2)^{1/2} \tag{3.16}$$

for $2k'z \leq 1$, and zero otherwise. The second term in (3.15) is obtained from the first upon interchange of k' by $k'^* = |(\omega+U)/4t|$, so that one has $\phi(\omega) = \phi(-\omega)$.

From (3.13) and (3.15) one sees that for $4t/U<1$ one has $\sigma(0)=0$, while at $T=0$ K, $\sigma(0)=\infty$ for $4t/U=1$. The insulator to metal transition found here by *extrapolation* corresponds to the point at which the upper and lower Hubbard[1] pseudobands would first touch each other as t is turned on. This is then also similar to an analogous transition found by Bari[17] for the classical (infinite spin) limit of (2.2). In our case, however, there should be no transition, as Lieb and Wu[8] have shown the ground state of (2.2) to be always insulating for $U\neq 0$. To the extent that (3.15) is exact only to the lowest order in $t/U \ll 1$ we think that higher-order terms ought to remove this divergence.

From (3.15), one can calculate $\phi(\omega)$ numerically for any value of $p(T,H)$; we remark, however, that because of the peculiar manner the integrand behaves for $p\to 1$, it is convenient to undo the singular character of the integral in this region. This can be easily accomplished with the introduction of Heuman's lambda function.[18] It is straightforward, though rather lengthy, to show that (3.15) can be written

$$\phi(\omega) = (4a^2tpN/\pi)\left[(1-k'^2\sin^2\beta)\cos\beta\, K(k) + \tfrac{1}{2}\pi\sin\beta\,(1-k'^2\sin^2\beta)^{1/2}\Lambda_0(\beta,k) - \cos\beta\; E(k)\right] + (k'\to k'^*)\,, \tag{3.17}$$

where[18] $k=(1-k'^2)^{1/2}$, $p=\tan^2(\frac{1}{2}\beta)$ with $0\leq\beta\leq\frac{1}{2}\pi$, and $K(k), E(k)$ are, respectively, the complete elliptic integrals of the first and second kind; finally, $\Lambda_0(\beta,k)$ is Heuman's lambda function.[18]

For the AF case, one has $\Lambda_0(\frac{1}{2}\pi,k)=1$ from Legendre's relation,[18] so that

$$\phi_{AF}(\omega) = (4a^2tN/\pi)(\tfrac{1}{2}\pi)(1-k'^2)^{1/2}. \tag{3.18}$$

For the ferromagnetic case, $p\to 0$, one has

$$\lim_{p\to 0}\frac{\phi_F(\omega)}{p} = \frac{4a^2tN}{\pi}\left[K(k)-E(k)\right]. \tag{3.19}$$

In general, one has $0\leq\Lambda_0(\beta,k)\leq 1$ and (3.17) expresses in a remarkable manner the line shapes in terms of a *circle* of radius $k'\sin\beta$ and of a corresponding *parabola*. From (3.18) one can associate the circle with the perfectly ordered AF configuration, while the parabola (being out of phase with it) can be associated with the randomized spin configuration.

From (3.17) one obtains the edge derivative as

$$\left|\frac{\partial\phi(\omega)}{\partial k'}\right|_{k'=1} = \frac{4a^2tpN}{\pi}\left(\frac{\pi}{2}\right)\sec\beta \tag{3.20}$$

and except for the AF case with a square-root edge singularity, the spectrum is seen to rise linearly. Also, from (3.17) one easily obtains

$$\phi(\omega\to U) = (4a^2tpN/\pi) \times\left[(\cos\beta)\ln(4/k')_{k'\to 0} + \beta\sin\beta - \cos\beta\right] \tag{3.21}$$

from the corresponding values[18] of the elliptic integrals. Since $\cos\beta=(1-p)/(1+p)$ from (3.17) one recovers the AF spectrum (3.18) except at $\omega=U$. One may speculate here as to whether the inclusion in (2.16) of short range AF correlations would provide a smooth transition from (3.17) to (3.18) at the center of the spectrum, where the logarithmic divergence occurs.

Let us turn now to the generating function[9] $G^{(1)}(\omega)$ for the two-particle random walk. One has as definition

$$|\omega-U|G^{(1)}(\omega) = \sum_{n=0}^{\infty}\left(\frac{t}{\omega-U}\right)^n\sum_q p^{|q|}P_n^{(1)}(q,q+1)\,, \tag{3.22}$$

where $P_n^{(1)}(q, q+1)$ is given by (2.15). Then for $\omega \geq 0$ (see Appendix B), we obtain $\phi(\omega)$ from

$$\phi(\omega) = 4a^2t^2pN \,\mathrm{Im}\, G^{(1)}(\omega - i\delta) . \tag{3.23}$$

Note that this follows from (2.15), since one has

$$\frac{1}{2}\int_{-\infty}^{+\infty} d\tau\, (-i\tau)^n e^{i(\omega-U)\tau} = n!\, \mathrm{Im}\left(\frac{1}{\omega - U - i\delta}\right)^{n+1} , \tag{3.24}$$

and in (3.23) the analytical continuation of $G^{(1)}(\omega)$, as defined by the series expansion (3.22), is of course understood. According to (2.14) one can then write

$$P_n^{(1)}(q, q+1) = \frac{1}{2\pi i}\oint \frac{dz'}{z'^{n+1}}\left(\frac{2}{1+(1-4z'^2)^{1/2}}\right)\frac{n!}{[\frac{1}{2}(n+2q)]!\,[\frac{1}{2}(n-2q)]!} , \tag{3.25}$$

where only the walks on a half line are written in integral representation.[9] Inserting (3.25) into (3.22), one can easily evaluate the sums over n and q in terms of (3.1). One has

$$|\omega - U| G^{(1)}(\omega) = \frac{1}{2\pi i}(2i)\int_{1/2}^{\infty}\frac{dz'}{z'}\mathrm{Im}\left(\frac{4}{1+(1-4z'^2)^{1/2}}\right)\frac{1}{(1-4z^2)^{1/2}}\sum_{q=-\infty}^{+\infty} p^{|q|}\left(\frac{1-(1-4z^2)^{1/2}}{2z}\right)^{2|q|} , \tag{3.26}$$

where $z = t/(\omega - U)z'$; or finally

$$G^{(1)}(\omega) = \frac{1}{\pi t}\int_1^{\infty}\frac{dz}{z^2}\frac{(z^2-1)^{1/2}}{(k'^2z^2-1)^{1/2}}\left(\frac{1+p[zk'-(z^2k'^2-1)^{1/2}]^2}{1-p[zk'-(z^2k'^2-1)^{1/2}]^2}\right) . \tag{3.27}$$

From the above and using (3.23) one finds of course (3.15). For both the AF and F cases, (3.27) is particularly interesting. When $p = 1$ one sees that from (3.22) one obtains only the quantity $\sum_q P_n^{(1)}(q, q+1)$ as a generalized "moment" in the expansion of $G^{(1)}(\omega)$. In this case, $G_{\mathrm{AF}}^{(1)}(\omega)$ becomes a renormalized one-particle Green's function corresponding to walks on a half line,[9] namely,

$$G_{\mathrm{AF}}^{(1)}(\omega) = (2t)^{-1}\,[k' + (k'^2 - 1)^{1/2}]^{-1} . \tag{3.28}$$

For the F case, only the walks that return to the origin (i.e., $q = 0$) matter; hence for $p = 0$ one finds

$$G_F^{(1)}(\omega) = \frac{1}{\pi t}\int_1^{\infty}\frac{dz}{z^2}\frac{(z^2-1)^{1/2}}{(k'^2z^2-1)^{1/2}} \tag{3.29}$$

$$= \frac{k'}{\pi t}\left[E\left(\frac{1}{k'}\right) - \left(1 - \frac{1}{k'^2}\right)K\left(\frac{1}{k'}\right)\right] . \tag{3.30}$$

The analytical continuation of (3.22) and (3.30) for $k' \leq 1$ can be expressed as[18]

$$G_F^{(1)}(\omega) = \frac{1}{\pi t}\{E(k') + i[K(k) - E(k)]\} , \tag{3.31}$$

from which (3.19) follows.

IV. SUMMARY AND CONCLUSION

As we have seen, the low-temperature ($k_BT \ll U$) conductivity line shape of the strongly correlated half-filled Hubbard chain, can be obtained exactly to all orders in $t/\omega - U$, for the antiferromagnetic ground state, and also for the random ($k_BT \gg t^2/U$) spin arrangement. This, to our knowledge, is quite remarkable, as it implies that a line shape of absorption (or emission) in a many-body problem has been calculated exactly to a well-defined order of accuracy, i.e., to lowest order in t/U.

Calculations based on partial moment expansions, as well as decoupling schemes[19,20] sometimes lead to incorrect predictions. In particular, it has recently been pointed out by Lawson and Smith[21] that Kubo's[19] use of Hubbard's decoupling[1] is in error to the extent that it leads to a spurious dc conductivity. Also, as Lyo[22] has recently shown, Kubo's[19] calculation of the optical conductivity would be asymptotically correct only for the almost empty band. As we have already remarked,[7] it is then not surprising that even his[19] optical line shapes should also differ from what is found here.

On the other hand from (3.17) and Appendix C, for $t \to 0$, it follows that the optical conductivity (for $k_BT \ll U$) is given by

$$\lim_{t\to 0}\sigma(\omega) = \frac{2\pi e^2a^2t^2pN}{U\Omega} \times [\delta(\omega - U) + \delta(\omega + U)] . \tag{4.1}$$

In this case the strength of the antiferromagnetic coupling constant, t^2/U, vanishes, and the spin states become degenerate. As seen from (2.8), however, if $k_BT \ll t^2/U$ then $p = 1$, while for $T \gg T_N$, $p = 0.5$. As emphasized by Bari and Kaplan[23] it is then only to this latter temperature range that their calculation[23] applies; otherwise the limit (4.1) is clearly undefined.

As follows from (3.17) for both the AF and R

cases the absorption edges are at $\omega = U \pm 4t$; this seems to be a feature of our calculation, and, while it is not claimed that the true line shapes (even to this order in t/U) interpolate according to (3.17), it is plausible, nevertheless, to conjecture that the *absorption edges* are indeed temperature independent as predicted by (3.17).

As concerns Eq. (2.14) we should say that although it is presented within the context of random walk theory, and this may be thought of as more of a "mean-field theory," it is, as shown in our previous work[7], rigorously exact. As already stated, our calculation is then *exact* to lowest order in the parameter t/U for the AF, F, and R cases considered.

Also, we must remark that a greatly simplifying characteristic of the one-dimensional band case presented in this paper lies on the fact that motion of the electron (i.e., double occupancy) and hole does not introduce disorder into the spin configuration of the chain. In fact, as we have seen, recombination of the electron-hole pair can occur on all states of the form $|q, q+1\rangle$ (irrespective of the previous motion) restoring the initial antiferromagnetic spin ordering in the chain. Furthermore, if the configuration is initially random, recombination at a certain site does not contribute only if there is a break in the antiferromagnetic ordering *between* the point of creation of the electron-hole excitation and the given site.

Finally, when $4t = U$ the density of states obtained in (3.23) from the generalized two-particle Green's function $G^{(1)}(\omega)$ extends down to $\omega = 0$. Because of this the dc conductivity behaves as $1/\sqrt{\omega}$ or $\sqrt{\omega}/T$ for $T \to 0$. It has been asked[24] whether a finite bandwidth could possible give rise to a nonzero dc conductivity under these conditions. It is possible, however, that $t/U < \frac{1}{4}$ may indeed be the region of convergence of our expansion (in powers of t/U), and that consequently the transition found here simply arises as a consequence of extrapolating an approximate result outside of its range of validity. To the extent that Lieb and Wu[8] have shown the exact ground state to be insulating (for $U \neq 0$), one should think that this is indeed the case.

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APPENDIX A

We show that one has $\Theta_n(1) = 2^n$ from (3.5). To show this we prove that

$$\lim_{p\to 1} \frac{1}{(4z^2-1)^{1/2}} \frac{z^2(1-p^2)}{z^2(1+p)^2 - p} = \tfrac{1}{4}\pi\delta(z - \tfrac{1}{2}) \qquad \text{(A1)}$$

for $z \geq \frac{1}{2}$. One has

$$\lim_{p\to 1} \lim_{z\to 1/2} \frac{1}{(4z^2-1)^{1/2}} \frac{z^2(1-p^2)}{z^2(1+p)^2 - p} = \lim_{p\to 1} \frac{1-p^2}{(1-p)^2} \lim_{z\to 1/2} \frac{1}{(4z^2-1)^{1/2}} = \infty, \qquad \text{(A2)}$$

and also

$$\lim_{p\to 1} \int_{1/2} \frac{dz}{(4z^2-1)^{1/2}} \frac{z^2(1-p^2)}{z^2(1+p)^2 - p} = \frac{1}{2} \lim_{p\to 1} \int_1 \frac{1}{(z-1)^{1/2}} \frac{1-p^2}{z(1+p) - 2\sqrt{p}} \times \lim_{z\to 1} \frac{z^2}{(z+1)^{1/2}[z(1+p)+2\sqrt{p}]}$$
$$= \lim_{z\to 1} \lim_{p\to 1} \frac{(1-p^2)}{[(1+p)(1-\sqrt{p})^2]^{1/2}} \times \tan^{-1}\left(\frac{(1+p)(z-1)^{1/2}}{[(1+p)(1-\sqrt{p})^2]^{1/2}}\right) \frac{1}{4\sqrt{2}} = \frac{\pi}{4}, \qquad \text{(A3)}$$

which ends the proof.

APPENDIX B

In this Appendix we show (3.23) in the text. Following Brinkman and Rice[4] we can write for $\omega \geq 0$,

$$\sigma_R(\omega) = \frac{e^2}{Z\Omega} \int\int \frac{d\epsilon d\epsilon'}{4\pi} \delta(\omega + \epsilon' - \epsilon) \times \frac{e^{-\beta\epsilon'} - e^{-\beta\epsilon}}{\epsilon' - \epsilon} F(\epsilon', \epsilon), \qquad \text{(B1)}$$

where

$$F(\epsilon', \epsilon) = \mathfrak{F}(\epsilon' + i\delta, \epsilon + i\delta) + \mathfrak{F}(\epsilon' - i\delta, \epsilon - i\delta) - \mathfrak{F}(\epsilon' + i\delta, \epsilon - i\delta) - \mathfrak{F}(\epsilon' - i\delta, \epsilon + i\delta) \qquad \text{(B2)}$$

and

$$\mathfrak{F}(\epsilon', \epsilon) = \mathrm{Tr}\left(\frac{1}{\epsilon' - \mathcal{H}} v \frac{1}{\epsilon - \mathcal{H}} v\right). \qquad \text{(B3)}$$

But to our order of accuracy we can write (B3) as

$$\mathfrak{F}(\epsilon', \epsilon) = \cong (1/\epsilon') \mathrm{Tr}\{v[1/(\epsilon - \mathcal{H})]v\}, \qquad \text{(B4)}$$

whereupon using (B2) and substituting in (B1) one finds

$$\sigma_R(\omega) = \frac{-e^2}{\Omega}\int\int d\epsilon\, d\epsilon'\, \delta(\omega+\epsilon'-\epsilon) \times\left(\frac{e^{-\beta\epsilon'}-e^{-\beta\epsilon}}{\epsilon'-\epsilon}\right)\delta(\epsilon')(2a^2t^2pN) \times \mathrm{Im}G^{(1)}(\epsilon - i\delta), \quad \text{(B5)}$$

or finally

$$\sigma_R(\omega) = \frac{2e^2a^2t^2pN}{\Omega}\,\frac{1-e^{-\beta\omega}}{\omega}\,\mathrm{Im}G^{(1)}(\omega - i\delta), \quad \text{(B6)}$$

where we must remark that to obtain (B5) we have written in the partition function

$$Z = \frac{1}{\pi}\int d\epsilon\, e^{-\beta\epsilon}\,\mathrm{Im\,Tr}\left(\frac{1}{\epsilon - \mathcal{H} - i\delta}\right) \quad \text{(B7)}$$

that

$$\mathrm{Im}\left(\frac{1}{\epsilon - \mathcal{H} - i\delta}\right) \cong \pi\delta(\epsilon),$$

so that $Z \cong 1$ for $T \ll T_N$ and $Z \cong 2^N$ for $T \gg T_N$, to the lowest order in t/U.

APPENDIX C

In this Appendix we show that (3.17) satisfies the general condition

$$\frac{1}{\pi}\int_0^\infty \phi(\omega)\, d\omega = \phi(\tau=0) = 2\langle v^2\rangle, \quad \text{(C1)}$$

where $\langle v^2\rangle = 2a^2t^2Np$. To show this one proves that

$$\frac{\partial}{\partial\beta}\int_0^1 I(k';\beta)\, dk' = 0, \quad \text{(C2)}$$

where

$$\phi(\omega) \equiv (4a^2tpN/\pi)I(k';\beta) \quad \text{for } \omega > 0.$$

In fact,

$$\frac{\partial}{\partial\beta}\int_0^1 I(k';\beta)dk' \quad \text{(C3)}$$

$$= \frac{\pi^2}{8}\left[-\sin\beta(1-\tfrac{1}{2}\sin^2\beta) - \cos^2\beta\sin\beta\right] + \frac{\pi}{2}\frac{\partial}{\partial\beta}\int_0^\beta d\theta\cos^2\theta\;\Lambda_0\!\left(\beta, \left[1-\left(\frac{\sin\theta}{\sin\beta}\right)^2\right]^{1/2}\right).$$

Upon substitution of the derivatives of $\Lambda_0(\beta, k)$ by their values[18] and use of $\Lambda_0(\beta, 0) = \sin\beta$, one finds for (C3),

$$\frac{\partial}{\partial\beta}\int_0^1 I(k';\beta)dk' = \frac{\pi}{2}\sin\beta\cos^2\beta \times\left(1 - \frac{2}{\pi}\int_0^1 \frac{dk'}{k^2}[K(k) - E(k)]\right) = 0. \quad \text{(C4)}$$

But then with $\beta = \frac{1}{2}\pi$, one finally obtains

$$\frac{1}{\pi}\int_0^\infty \frac{\phi(\omega)d\omega}{p} = \frac{4a^2tN}{\pi^2}(8t) \times\int_0^1 I\left(k';\, \frac{\pi}{2}\right)dk' = 4a^2t^2N. \quad \text{(C5)}$$

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