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Excitation spectrum of the one-dimensional Hubbard model*

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We have extended calculations of the zero-temperature excitation spectrum of the one-dimensional Hubbard model to the case where the number of electrons is less than the number of sites in the chain. The results are computed as a function of the ratio U/t, where U represents the on-site Coulomb repulsion and t is the transfer integral, assumed to be nonzero only for nearest neighbors. Exact calculations are made for the energy and momentum of excitations having single-particle character. Unlike the situation for the half-filled band, we find no gap in the excitation spectrum. We have also considered excitations of the spin-wave type. These are shown to vary linearly with momentum for small momentum. The group velocity for small momentum is found to be inversely proportional to the magnetic susceptibility.

I. INTRODUCTION

There has been much interest recently in systems which for some purposes may be considered one dimensional. For example, the system $Cu(NH_3)_4SO_4 \cdot H_2O$ exhibits magnetic properties which are reasonably described by the linear-chain Heisenberg Hamiltonian.[1] Our concern in this work is with the Hubbard model for a linear chain, i.e., a model for interacting itinerant electrons. This model has been used to analyze results of studies of the salt N-methylphenazinium-tetracyanoquinodimethan (NMP-TCNQ).[2] Here the half-filled band is the appropriate model. Other TCNQ salts may be described as more or less than half-filled bands; e.g., in quinolinium-$TCNQ_2$ there presumably exists one electron per two TCNQ molecules and thus a quarter-filled band. It is to these types of materials that we hope the results of this work will prove applicable.

The Hubbard Hamiltonian can be written as[3]

$$H=-\sum_{\substack{i,j\\ \sigma}} t_{ij}C^\dagger_{i\sigma}C_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow} , \tag{1.1}$$

where t_{ij} is the hopping integral, assumed to be nonzero only for (i,j) nearest neighbors. We consider a one-dimensional crystal of N_a lattice sites with a total of $N \leq 2N_a$ electrons. Since the numbers M of spin-down electrons and M' of spin-up electrons are good quantum numbers, we can classify states of the system by, say, the numbers N and M. At zero temperature the model Hamiltonian is characterized by the parameters $u=U/t$, the ratio of the Coulomb interaction energy and the nearest-neighbor hopping integral, and the electron density N/N_a.

Lieb and Wu gave[4] an exact solution for the lowest energy state of the Hubbard model for fixed M/N_a. For the half-filled-band case $[(N/N_a)=1]$ they derived an analytic expression for the ground-state energy as a function of u. Shiba considered the ground-state energy for arbitrary electron density and gave numerical results for various values of u.[5] In addition, he calculated the lowest energy as a function of magnetization and was thereby able to obtain numerical results for the magnetic susceptibility for arbitrary electron density.

For the half-filled band the spectrum of the lowest excitations was considered by Ovchinnikov.[6] He found $S=1$ excitations of spin-wave character having a double periodicity similar to that of the antiferromagnetic chain.[7] He also investigated the spectrum of "quasi-ionic" states, i.e., states of $(N\pm 1)$ electrons with total momentum q. For the case of the half-filled band there is a gap in the spectrum of the quasi-ionic states.

In this work we investigate some of the low-lying excited states of the system for arbitrary electron density. We find excitations of spin-wave character whose group velocity at long wavelengths is inversely proportional to the magnetic susceptibility. For the spectrum of quasi-ionic states we find no gap in the spectrum for $N/N_a<1$. The results are derived for arbitrary $N/N_a<1$ and u. We give numerical results for the quarter-filled band: $N/N_a=\frac{1}{2}$.

II. EQUATIONS DETERMINING DISTRIBUTION FUNCTIONS $\rho(k)$ AND $\sigma(\Lambda)$

For the Hamiltonian of Eq. (1.1) it was shown by Lieb and Wu[4] that the energy and momentum of a system of N electrons, M of which have down spin, is given by

$$E=-2t\sum_{j=1}^{N}\cos k_j , \tag{2.1a}$$

$$p=\sum_{j=1}^{N}k_j . \tag{2.1b}$$

The "momenta" k_j are determined by the equation

$$N_a k_j = 2\pi I_j + \sum_{\beta=1}^{M} \theta(2\sin k_j - 2\Lambda_\beta), \quad j=1,\ldots,N \tag{2.2}$$

where the Λ's are a set of numbers related to the k's by

$$-\sum_{j=1}^{N} \theta(2\Lambda_\alpha - 2\sin k_j) = 2\pi J_\alpha - \sum_{\beta=1}^{M} \theta(\Lambda_\alpha - \Lambda_\beta), \quad \alpha = 1,\ldots,M \tag{2.3}$$

and

$$\theta(x) = -2\tan^{-1}(2x/u) . \tag{2.4}$$

In these equations I_j and J_α are integers (or half-odd integers) which we consider as the quantum numbers describing the state of the system.

From Eqs. (2.2)–(2.4) we see that the momentum p can be conveniently written as

$$p = \frac{2\pi}{N_a}\left(\sum_{j=1}^{N} I_j + \sum_{\alpha=1}^{M} J_\alpha\right) . \tag{2.5}$$

We are interested in solutions to Eqs. (2.2) and (2.3) for real k's and Λ's. It was shown by Ovchinnikov[6] for the half-filled band that there exist singlet ($S=0$) excitations of the system for which some of the k's and Λ's are complex. We hope to return to a study of this case in a future work.

We begin by writing the equations

$$N_a(k_{j+1} - k_j)\left(1 + \cos k_j \frac{1}{N_a}\sum_{\beta=1}^{M} \frac{8u}{u^2 + 16(\sin k_j - \Lambda_\beta)^2}\right) = 2\pi(I_{j+1} - I_j) , \tag{2.6a}$$

$$N_a(\Lambda_{\alpha+1} - \Lambda_\alpha)\left(\frac{1}{N_a}\sum_{j=1}^{N} \frac{8u}{u^2 + 16(\sin k_j - \Lambda_\alpha)} - \frac{1}{N_a}\sum_{\beta=1}^{M} \frac{4u}{u^2 + 4(\Lambda_\alpha - \Lambda_\beta)^2}\right) = 2\pi(J_{\alpha+1} - J_\alpha) , \tag{2.6b}$$

where we have used a Taylor expansion for the function $\theta(x)$, since $(k_{j+1} - k_j) \sim O(1/N_a)$, $(\Lambda_{\alpha+1} - \Lambda_\alpha) \sim O(1/N_a)$, and we are interested eventually in the large-N_a limit.

We introduce two functions $\rho(k)$ and $\sigma(\Lambda)$ defined at the points k_j and Λ_α, respectively, by

$$\frac{1}{N_a \rho(k_j)} = k_{j+1} - k_j , \tag{2.7a}$$

$$\frac{1}{N_a \sigma(\Lambda_a)} = \Lambda_{\alpha+1} - \Lambda_\alpha . \tag{2.7b}$$

By means of these functions the sums in Eq. (6) may be approximated in the limit of a large system by an integral,

$$\frac{1}{N_a}\sum_{j=1}^{N} f(k_j) \to \int_{-Q}^{Q} \rho(k) f(k)\, dk , \tag{2.8a}$$

$$\frac{1}{N_a}\sum_{\beta=1}^{M} g(\Lambda_\beta) \to \int_{-B}^{B} \sigma(\Lambda) g(\Lambda)\, d\Lambda , \tag{2.8b}$$

where $\rho(k)$ and $\sigma(\Lambda)$ obey the normalization conditions (in the limit N, M, $N_a \to \infty$, N/N_a, M/N fixed)

$$\int_{-Q}^{Q} \rho(k)\, dk = N/N_a , \tag{2.9a}$$

$$\int_{-B}^{B} \sigma(\Lambda)\, d\Lambda = M/N_a . \tag{2.9b}$$

For a large system the meaning of $\rho(k)$ and $\sigma(\Lambda)$ is that $N_a \rho(k)\, dk$ is the number of k's in $(k, k+dk)$; $N_a \sigma(\Lambda)\, d\Lambda$ is the number of Λ's in $(\Lambda, \Lambda + d\Lambda)$. One immediate result of Eqs. (2.8) for a large system is, from Eq. (2.1),

$$E/N_a = -2t \int_{-Q}^{Q} dk \cos k\, \rho(k) .$$

In the following sections we proceed to determine the equations satisfied by $\rho(k)$ and $\sigma(\Lambda)$ for particular choices of I_j, J_α. We repeat results found previously[5] for the ground state, since we will need some of the results for the later investigations. Generally speaking, we will find that the distribution functions determining the energy of various excited states can be written in the form

$$\rho(k) = \rho_0(k) + (1/N_a)\rho_1(k) ,$$

$$\sigma(\Lambda) = \sigma_0(\Lambda) + (1/N_a)\sigma_1(\Lambda) ,$$

where $\rho_0(k)$ and $\sigma_0(\Lambda)$ are the *ground*-state distribution functions. Since we are interested in the excitation energy, i.e., the difference in energies of the excited state and the ground state, we see that the excitation energy is determined by $\rho_1(k)$ and $\sigma_1(\Lambda)$.

III. GROUND STATE

As shown by Lieb and Wu,[4] we take for the ground state

$$I_{j+1} - I_j = 1 , \tag{3.1a}$$

$$J_{\alpha+1} - J_\alpha = 1 . \tag{3.1b}$$

Substituting these expressions into Eqs. (2.6) and changing to a continuous distribution of the numbers k_j and Λ_α, we find the following equations for the distribution functions $\rho(k)$ and $\sigma(\Lambda)$:

$$2\pi\rho_0(k) = 1 + \cos k \int_{-\infty}^{\infty} d\Lambda\, \sigma_0(\Lambda) \frac{8u}{u^2 + 16(\sin k - \Lambda)^2} , \tag{3.2a}$$

$$\int_{-Q_0}^{Q_0} dk\, \rho_0(k) \frac{8u}{u^2 + 16(\sin k - \Lambda)^2} = 2\pi\sigma_0(\Lambda) + \int_{-\infty}^{\infty} d\Lambda'\, \sigma_0(\Lambda') \frac{4u}{u^2 + 4(\Lambda - \Lambda')^2} . \tag{3.2b}$$

We denote the solutions of these equations with a subscript 0. The distribution functions satisfy the subsidiary conditions

$$\int_{-Q_0}^{Q_0} \rho_0(k)\, dk = N/N_a , \tag{3.3a}$$

$$\int_{-\infty}^{\infty} \sigma_0(\Lambda)\, d\Lambda = \tfrac{1}{2}(N/N_a) , \tag{3.3b}$$

i.e., $M/N = \frac{1}{2}$. These equations have been solved previously for the half-filled band by Lieb and Wu[4] and for arbitrary N/N_a by Shiba.[5] We write the solutions here since we will make reference to them later.

By introducing the Fourier transform $\sigma_0(\omega) = \int_{-\infty}^{\infty} \sigma_0(\Lambda) e^{-i\omega\Lambda}\, d\Lambda$ one can show that $\rho_0(k)$ satisfies the following integral equation:

$$\rho_0(k) = \frac{1}{2\pi} + \cos k \int_{-Q_0}^{Q_0} dk'\, R\left(\frac{4}{u}(\sin k - \sin k')\right) \times \rho_0(k') , \tag{3.4}$$

where $R(x)$ is defined as

$$R(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} dy\, \frac{e^{ixy/2}}{1 + e^{|y|}} . \tag{3.5}$$

The solution for $\sigma_0(\Lambda)$ can then be written in terms of $\rho_0(k)$ as

$$\sigma_0(\Lambda) = \frac{1}{u} \int_{-Q_0}^{Q_0} dk\, \rho_0(k)\, \mathrm{sech}\left(\frac{2\pi}{u}(\Lambda - \sin k)\right) . \tag{3.6}$$

For the half-filled band ($N/N_a = 1$; $Q = \pi$) Lieb and Wu[4] found an analytic expression for $\rho_0(k)$. For $N/N_a \neq 1$ one can solve for $\rho_0(k)$ numerically and then use this result in Eq. (3.5) to find $\sigma_0(\Lambda)$.

From Eqs. (3.4)–(3.6) we can gain some insight into the nature of the solutions for $\rho_0(k)$ and $\sigma_0(\Lambda)$. From Eq. (3.4) we see that $\rho_0(k)$ is an even function of k; in addition, using the fact that R is an even function of its argument we see that $\rho_0(k)$ has a maximum at $k = 0$. Physically this is what we expect by looking at the expression for the ground-state energy:

$$E_0 = -2tN_a \int_{-Q_0}^{Q} \rho_0(k) \cos k\, dk . \tag{3.7}$$

From this we see that the energy is minimized if $\rho_0(k)$ is largest for small k.

In Fig. 1 we show numerical results for $\rho_0(k)$ for various values of $u = U/t$ for the quarter-filled band. From this figure we see the effect of increasing u on the ground-state distribution. The resulting effect on the ground-state energy can be seen in the work of Shiba.[5]

From Eq. (3.6) we see that $\sigma_0(\Lambda)$ is an even function of Λ, it has a maximum at $\Lambda = 0$ and decreases exponentially for large Λ.

IV. SPIN-WAVE STATE

This is the state which Lieb and Wu[4] classify as the "hole in the Λ distribution" state. We choose the integers I_j as in the ground state and take

$$J_{\alpha+1} - J_\alpha = 1 + \delta_{\alpha,\alpha_0} . \tag{4.1}$$

Substituting these expressions into Eqs. (2.6) and changing to a continuous distribution for the numbers k_j and Λ_α, we find for the distribution function $\rho(k)$ and $\sigma(\Lambda)$ the equations

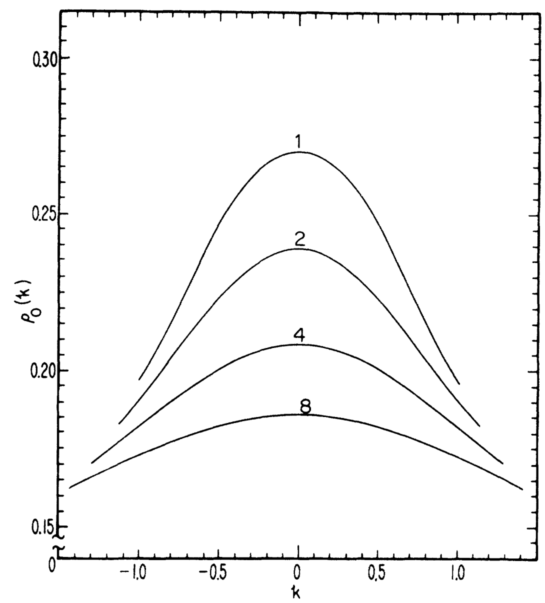

FIG. 1. Ground-state distribution function $\rho_0(k)$ for the quarter-filled band. Individual curves are labeled with the values of $u = U/t$. The cutoff momentum is determined by the normalization condition, $\int_{-Q_0}^{Q_0} \rho_0(k)dk = N/N_a$.

$$2\pi\rho(k) = 1 + \cos k \int_{-\infty}^{\infty} d\Lambda\, \sigma(\Lambda) \frac{8u}{u^2 + 16(\sin k - \Lambda)^2} , \tag{4.2a}$$

$$\int_{-Q}^{Q} dk\, \rho(k) \frac{8u}{u^2 + 16(\sin k - \Lambda)^2} = 2\pi\sigma(\Lambda) + \int_{-\infty}^{\infty} d\Lambda'\, \sigma(\Lambda') \frac{4u}{u^2 + 4(\Lambda - \Lambda')^2} + \frac{2\pi}{N_a}\delta(\Lambda - \Lambda_0) , \tag{4.2b}$$

where Λ_0 is the value of Λ for which $\alpha = \alpha_0$. The limit of the k integration, Q, is in general different from that in the ground state for a given N/N_a. If we denote the corresponding limiting momentum in the ground state by Q_0 then Q will be related to Q_0 by the condition that the ratio N/N_a is fixed. Also note that in Eqs. (4.2) the distribution functions depend explicitly on Λ_0. In general, we would expect the limits of the Λ integration in Eqs. (4.2) to be different from those in the ground state. One can show, using manipulations of the form employed by Shiba,[5] that for purposes of calculating the excitation energy this limit may be taken to be as in the ground state.

Introduce the distribution functions $\rho_1(k)$ and $\sigma_1(\Lambda)$ by

$$\rho(k) = \rho_0(k) + (1/N_a)\rho_1(k) , \tag{4.3a}$$

$$\sigma(\Lambda) = \sigma_0(\Lambda) + (1/N_a)\sigma_1(\Lambda) , \tag{4.3b}$$

where $\rho_0(k)$ and $\sigma_0(\Lambda)$ are the ground-state distribution functions for *fixed* Q. The distribution functions $\rho_1(k)$ and $\sigma_1(\Lambda)$ then satisfy the equations

$$2\pi\rho_1(k)=\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma_1(\Lambda)\frac{8u}{u^2+16(\sin k-\Lambda)^2}\,, \tag{4.4a}$$

$$\int_{-Q}^{Q}dk\,\rho_1(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\delta(\Lambda-\Lambda_0)+2\pi\sigma_1(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\,\sigma_1(\Lambda')\frac{4u}{u^2+4(\Lambda-\Lambda')^2}\,. \tag{4.4b}$$

An integral equation for $\rho_1(k)$ can be obtained by introducing the Fourier transform $\sigma_i(\omega)=\int_{-\infty}^{\infty}d\Lambda\times\sigma_1(\Lambda)e^{-i\omega\Lambda}$. This leads to the equation

$$\rho_1(k)=\frac{-1}{u}\cos k\,\mathrm{sech}\left(\frac{2\pi}{u}(\sin k-\Lambda_0)\right)+\frac{4}{u}\cos k\times\int_{-Q}^{Q}dk'\,R\left(\frac{4}{u}(\sin k-\sin k')\right)\rho_1(k')\,. \tag{4.5}$$

It is useful to note that the inhomogeneous term in the integral equation is the solution for $\rho_1(k)$ for the half-filled band.

An integral equation for $\sigma_1(\Lambda)$ can be found by substituting Eq. (4.4a) into Eq. (4.4b):

$$2\pi\sigma_1(\Lambda)=-2\pi\delta(\Lambda-\Lambda_0)-\int_{-\infty}^{\infty}d\Lambda'\,S_Q(\Lambda,\Lambda')\sigma_1(\Lambda')\,, \tag{4.6}$$

where the kernel $S_Q(\Lambda,\Lambda')$ is given by[5]

$$S_Q(\Lambda,\Lambda')=\frac{4u}{u^2+4(\Lambda-\Lambda')^2}-\int_{-Q}^{Q}\frac{dk}{2\pi}\cos k\times\frac{8u}{u^2+16(\sin k-\Lambda)^2}\times\frac{8u}{u^2+16(\sin k-\Lambda')^2}\,. \tag{4.7}$$

We can write the formal solution for $\sigma_1(\Lambda)$ in terms of the resolvent kernel $\mathcal{S}_Q(\Lambda,\Lambda')$ as

$$\sigma_1(\Lambda)=-\delta(\Lambda-\Lambda_0)+\mathcal{S}_Q(\Lambda,\Lambda_0)\,, \tag{4.8}$$

where the resolvent kernel is defined by the equations

$$2\pi\mathcal{S}_Q(\Lambda,\Lambda')=S_Q(\Lambda,\Lambda')-\int_{-\infty}^{\infty}d\Lambda''\,\mathcal{S}_Q(\Lambda,\Lambda'')S_Q(\Lambda'',\Lambda')=S_Q(\Lambda,\Lambda')-\int_{-\infty}^{\infty}d\Lambda''\,S_Q(\Lambda,\Lambda'')\mathcal{S}_Q(\Lambda'',\Lambda')\,. \tag{4.9}$$

The energy of the spin-wave state is given by

$$E=-2tN_a\int_{-Q}^{Q}\rho(k)\cos k\,dk\,, \tag{4.10}$$

or, in terms of $\rho_1(k)$, by

$$E=E_0(Q)-2t\int_{-Q}^{Q}\rho_1(k)\cos k\,dk\,, \tag{4.11}$$

where $E_0(Q)$ is the ground-state energy for *fixed* Q. The excitation energy ϵ is then the difference between this energy and the ground-state energy for a fixed density N/N_a:

$$\epsilon(\Lambda_0)=-2t\int_{-Q}^{Q}\rho_1(k,\Lambda_0)\cos k\,dk+E_0(Q)-E_0(Q_0)\,. \tag{4.12}$$

We have explicitly indicated the dependence on Λ_0 in Eq. (4.12).

To relate Q to Q_0 we use the condition that the density of electrons is fixed; i.e., the distribution function $\rho(k)$ must satisfy the normalization condition

$$\int_{-Q}^{Q}\rho(k)\,dk=\frac{N}{N_a}=\frac{N_0(Q_0)}{N_a} \tag{4.13}$$

or

$$\frac{N_0(Q)}{N_a}+\frac{1}{N_a}\int_{-Q}^{Q}\rho_1(k)\,dk=\frac{N_0(Q_0)}{N_a}\,. \tag{4.14}$$

Equation (4.14) gives us the relation between Q and Q_0. To $O(1/N_a)$ we find

$$Q-Q_0=\left(\frac{1}{N_a}\frac{\partial N_0(Q_0)}{\partial Q_0}\right)^{-1}\left(\frac{-1}{N_a}\int_{-Q_0}^{Q_0}\rho_1(k)\,dk\right)\,. \tag{4.15}$$

In order to calculate the excitation energy correctly we must include all terms of $O(1)$. We can neglect higher-order terms for a large system. Thus for a very large system we find for the excitation energy

$$\epsilon(\Lambda_0)=-2t\int_{-Q_0}^{Q_0}dk\,\rho_1(k,\Lambda_0)\cos k-\mu\int_{-Q_0}^{Q_0}dk\,\rho_1(k,\Lambda_0)\,, \tag{4.16}$$

where we have defined μ as

$$\mu=\left(\frac{1}{N_a}\frac{\partial E_0(Q_0)}{\partial Q_0}\right)\left(\frac{1}{N_a}\frac{\partial N_0(Q_0)}{\partial Q_0}\right)^{-1}\,. \tag{4.17}$$

It is understood that in Eq. (4.16) $\rho_1(k)$ is now to be found as a solution to Eq. (4.5) with $Q=Q_0$.

To complete the calculation of the dispersion relation for the spin-wave state we must find how the momentum is related to the parameter Λ_0. From Eqs. (2.5) and (4.1) it follows that the momentum p is given by

$$p/2\pi=\int_{\Lambda_0}^{\infty}\sigma(\Lambda)\,d\Lambda\,. \tag{4.18}$$

Following the analogous treatment by des Cloizeaux and Pearson,[7] we simplify this equation by replacing $\sigma(\Lambda)$ by $\sigma_0(\Lambda)$. The omitted terms are of order $1/N_a$ and can be neglected. So, combining Eqs. (4.18) and (3.6), we find

$$\frac{p}{2\pi}=\frac{1}{\pi}\int_{-Q_0}^{Q_0}dk\,\rho_0(k)\tan^{-1}\left[\exp\left(-\frac{2\pi}{u}(\Lambda_0-\sin k)\right)\right]\,. \tag{4.19}$$

Equations (4.16) and (4.19) determine the parametric dependence of ϵ on the momentum p.

We can obtain some general properties of the spin-wave dispersion relations by examining the behavior of $\epsilon(\Lambda_0)$ and $p(\Lambda_0)$ as a function of Λ_0. From Eq. (4.5) we see that $\rho_1(-k,-\Lambda_0)=\rho_1(k,\Lambda_0)$.

This implies through Eq. (4.16) that ϵ is an even function of Λ_0. One can also show from Eq. (19), using the fact that $\rho_0(k)=\rho_0(-k)$, that $[p-\frac{1}{2}\pi(N/N_a)]$ is an odd function of Λ_0. This implies that as a function of momentum ϵ is symmetric about $p=\frac{1}{2}\pi\times(N/N_a)$. Further, one can show that as $\Lambda_0\to\infty$ both p and ϵ approach zero. We will show further in Sec. IV A that in the region of small momentum the excitation energy ϵ varies linearly with momentum.

The procedure followed to calculate the dispersion relation is to solve Eq. (4.5) for $\rho_1(k)$ numerically. The value of μ is also determined numerically in the manner demonstrated by Shiba.[5] Then the excitation energy and the momentum [using numerical results for $\rho_0(k)$] are calculated as a function of Λ_0. These results for various values of U/t are shown in Fig. 2 for $N/N_a=\frac{1}{2}$.

A. Spin-wave velocity

We would like to examine the dispersion relation for small values of the momentum. From Eq. (4.19) we see that small momentum corresponds to large values of the parameter Λ_0. Thus for large Λ_0

$$p/2\pi\to(1/\pi)e^{(-2\pi/u)\Lambda_0}\int_{-Q_0}^{Q_0}dk\,\rho_0(k)e^{(2\pi/u)\sin k}\ . \qquad (4.20)$$

One can show that $1/2\pi\int_{-Q_0}^{Q_0}\rho_0(k)e^{(2\pi/u)\sin k}=I_{Q_0}^{(0)}(u)$, where the function $I_{Q_0}^{(n)}(u)$ were introduced by Shiba in the calculation of the magnetic susceptibility.[5] Thus for small momentum

$$p/2\pi=2e^{(-2\pi/u)\Lambda_0}I_{Q_0}^{(0)}(u)\ . \qquad (4.21)$$

From Eq. (4.5) we see that for large Λ_0, $\rho_1(k)$ has the asymptotic form

$$\rho_1(k)=(-2/u)\cos k\,e^{(-2\pi/u)\Lambda_0}\psi(k)\ , \qquad (4.22)$$

where $\psi(k)$ has been introduced by Shiba[5] and, as shown there, satisfies the equation

$$\psi(k)=e^{(2\pi/u)\sin k}+\int_{-Q_0}^{Q_0}dk'\cos k'\times\left[\frac{4}{u}R\left(\frac{4}{u}(\sin k-\sin k')\right)\right]\psi(k')\ . \qquad (4.23)$$

The functions $I_{Q_0}^{(n)}(u)$ are written in terms of $\psi(k)$ as

$$I_{Q_0}^{(n)}(u)=\int_{-Q_0}^{Q_0}\frac{dk}{2\pi}\cos^n k\,\psi(k)\ . \qquad (4.24)$$

Therefore for large Λ_0, $\epsilon(\Lambda_0)$ has the form

$$\epsilon(\Lambda_0)\to\frac{4t}{u}2\pi\left(I_{Q_0}^{(2)}(u)+\frac{u}{2t}I_{Q_0}^{(1)}(u)\right)e^{(-2\pi/u)\Lambda_0}\ . \qquad (4.25)$$

Thus, if we define the velocity v_s as $\lim_{p\to 0}[\epsilon(p)/p]$, we have

$$v_s=\pi\frac{4t^2}{u}\left(\frac{I_Q^{(2)}(u)}{I_Q^{(0)}(u)}+\frac{\mu}{2t}\frac{I_Q^{(1)}(u)}{I_Q^{(0)}(u)}\right)\ . \qquad (4.26)$$

Comparing this result with the work of Shiba[5] we see that v_s is inversely proportional to the magnetic suceptibility:

$$v_s=\frac{2t}{\pi}\left(\frac{\chi}{N_a\mu_B^2}\right)^{-1}\ . \qquad (4.27)$$

This relationship was pointed out by Takahashi[8] for the case of the half-filled band. We see that the relationship is valid for arbitrary electron density.

B. Atomic limit of spin-wave frequency

As $U/t\to\infty$ we may approximate the distribution function $\rho_1(k)$ by

$$\rho_1(k)\underset{u\to\infty}{\longrightarrow}-\frac{1}{u}\cos k\,\mathrm{sech}\left(\frac{2\pi}{u}\Lambda_0\right)\ . \qquad (4.28)$$

Then for large u

$$\epsilon(\Lambda_0)\underset{u\to\infty}{\longrightarrow}\frac{2t}{u}\mathrm{sech}\left(\frac{2\pi}{u}\Lambda_0\right)\left(\int_{-Q_0}^{Q_0}\cos^2 k\,dk+\frac{\mu}{2t}\int_{-Q_0}^{Q_0}dk\cos k\right)\ . \qquad (4.29)$$

For large u the momentum p assumes the simple form

$$p(\Lambda_0)=\frac{N}{N_a}\sin^{-1}\left(\mathrm{sech}\,\frac{2\pi}{u}\Lambda_0\right)\ . \qquad (4.30)$$

Therefore in the large-u limit

$$\epsilon(p)=\pi\frac{4t^2}{U}\left(\int_{-Q}^{Q}\frac{dk}{2\pi}\cos^2 k+\frac{\mu}{2t}\int_{-Q}^{Q}\frac{dk}{2\pi}\cos k\right)\times\sin\frac{p}{\rho}, \qquad (4.31)$$

where $\rho=N/N_a$ is the electron density. For $u\to\infty$ we have $Q_0\to\pi(N/N_a)$ and $\mu/2t\to-\cos\pi(N/N_a)$. So to first order in t/U we have for the dispersion relation

$$\epsilon(p)=\frac{\pi}{2}\left(\frac{4t^2}{U}\right)\rho\left(1-\frac{\sin 2\pi\rho}{2\pi\rho}\right)\sin\left(\frac{p}{\rho}\right)\ . \qquad (4.32)$$

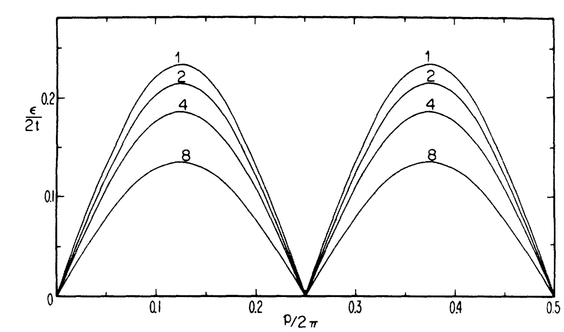

FIG. 2. Spin-wave energy for the quarter-filled band. Individual curves are labeled with the value of $u=U/t$.

Note that for $\rho=1$ this agrees with result of des Cloizeaux and Pearson[7] for the Heisenberg antiferromagnetic chain if we identify $J=4t^2/U$.

V. HOLE STATE

For this state, which is classified by Lieb and Wu[4] as the "hole in the k distribution" state we choose the integers J_α as in the ground state and take

$$I_{j+1}-I_j=1+\delta_{j,n}\ . \tag{5.1}$$

With these expressions for the integers J_α and I_j, and proceeding to a continuous distribution for the numbers k_j and Λ_α, we find the equations

$$2\pi\rho(k)=\frac{-2\pi}{N_a}\,\delta(k-k_0)+1+\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma(\Lambda)\times\frac{8u}{u^2+16(\sin k-\Lambda)^2}\,, \tag{5.2a}$$

$$\int_{-Q}^{Q}dk\,\rho(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\sigma(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\,\sigma(\Lambda')\frac{4u}{u^2+4(\Lambda-\Lambda')^2}\,, \tag{5.2b}$$

where k_0 is the value of k for which $j=n$ and $|k_0|\leq Q_0$ will be determined from the ground-state distribution.

We again introduce distribution functions $\rho_1(k)$ and $\sigma_1(\Lambda)$ defined by Eqs. (4.3) and find that these distribution functions satisfy the equations

$$2\pi\rho_1(k)=-2\pi\delta(k-k_0)+\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma_1(\Lambda)\times\frac{8u}{u^2+16(\sin k-\Lambda)^2}\,, \tag{5.3a}$$

$$\int_{-Q}^{Q}dk\,\rho_1(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\sigma_1(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\,\sigma_1(\Lambda')\frac{4u}{u^2+4(\Lambda-\Lambda')^2}\,. \tag{5.3b}$$

We isolate the δ-function term in the equation for the distribution function by writing

$$\rho_1(k)=-\delta(k-k_0)+\rho_1'(k)\ . \tag{5.4}$$

Then the equations determining the distribution functions are given by

$$2\pi\rho_1'(k)=\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma_1(\Lambda)\,\frac{8u}{u^2+16(\sin k-\Lambda)^2}\,, \tag{5.5a}$$

$$\int_{-Q}^{Q}dk\,\rho_1'(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\sigma_1(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\,\sigma_1(\Lambda')\frac{4u}{u^2+4(\Lambda-\Lambda')^2}+\frac{8u}{u^2+16(\sin k_0-\Lambda)^2}\,. \tag{5.5b}$$

We construct an integral equation for $\rho_1'(k)$ by introducing the Fourier transform of $\sigma_1(\Lambda)$, as we did in Sec. IV. We find

$$\rho_1'(k)=-\frac{4}{u}\cos k\,R\left(\frac{4}{u}(\sin k-\sin k_0)\right)+\frac{4}{u}\cos k\times\int_{-Q}^{Q}dk'\,R\left(\frac{4}{u}\,(\sin k-\sin k')\right)\rho_1'(k')\ . \tag{5.6}$$

The energy of the hole state relative to the ground state is found to be

$$\epsilon=2t\cos k_0-2t\int_{-Q}^{Q}\rho_1'(k)\cos k\,dk+E_0(Q)-E_0(Q_0)\ , \tag{5.7}$$

where again Q_0 is the limiting momentum for the ground-state distribution for a fixed electron density N/N_a and $E_0(Q)$ is the ground-state energy for fixed Q.

Q is determined in terms of Q_0 by the requirement that the distribution functions $\rho(k)$ describe the same electron density as the ground-state distribution function. Using this requirement and keeping all terms in ϵ of first order we find for the excitation energy the result

$$\epsilon(k_0)=2t\cos k_0-2t\int_{-Q_0}^{Q_0}\rho_1'(k)\cos k\,dk+\mu\left(1-\int_{-Q_0}^{Q_0}dk\,\rho_1'(k)\right)\ , \tag{5.8}$$

where μ is as defined in Eq. (4.17). Again it is understood that the distribution function $\rho_1'(k)$ in Eq. (5.8) is a solution to Eq. (5.6) with $Q=Q_0$ there.

The momentum is related to the parameter k_0 by the equation

$$\frac{p}{2\pi}=\int_{k_0}^{Q_0}\rho(k)\,dk\simeq\int_{k_0}^{Q_0}\rho_0(k)\,dk\ , \tag{5.9}$$

where we may, with sufficient accuracy in the limit of a large system, treat the approximation in Eq. (5.9) as an equality.

After some manipulation we can write an expression for p in terms of $\rho_0(k)$ as

$$\frac{p}{2\pi}=\frac{1}{2}\frac{N}{N_a}-\frac{k_0}{2\pi}-\int_{-Q_0}^{Q_0}dk\,\rho_0(k)\times F\left(\frac{4}{u}\,(\sin k_0-\sin k)\right)\ . \tag{5.10}$$

where $F(x)$ is defined in terms of $R(x)$ as

$$F(x)=\int^{x}dx'\,R(x')\ . \tag{5.11}$$

From Eqs. (5.8) and (5.10) we can examine some general features of the dispersion relation. From Eq. (5.6) we see that $\rho_1'(-k,-k_0)=\rho_1'(k,k_0)$. This implies through Eq. (5.8) that ϵ is an even function of k_0. From Eq. (5.10), using the fact that $F(x)$ is an odd function of its argument, we find that $p-\pi(N/N_a)$ is an odd function of k_0. This implies that as a function of momentum ϵ is symmetric about $p=\pi N/N_a$.

One can also show that $-[\rho_1'(k, Q_0)+\rho_1'(-k, Q_0)]$ satisfies the same equation as $[1/\rho_0(Q_0)]\partial\rho_0(k)/\partial Q_0$. This implies that we can write

$$\frac{\mu}{2t}=-\left(\frac{\cos Q_0-\int_{-Q_0}^{Q_0}dk\cos k\rho_1'(k, Q_0)}{1-\int_{-Q_0}^{Q_0}dk\,\rho_1'(k, Q_0)}\right). \quad (5.12)$$

From this relation and Eq. (5.8) it is evident that

$$\epsilon(k_0)\xrightarrow[k_0\to\pm Q_0]{}0 .$$

One can also show by integrating Eq. (3.2a) that p vanishes in the same limit.

The dispersion curves are found as a function of U/t by solving Eq. (6) for $\rho_1'(k)$ numerically and using numerical results for $\rho_0(k)$.

VI. PARTICLE STATE

Here we have in mind removing an electron from the highest occupied momentum in the ground state Q_0 and placing it in a momentum state $k_0>Q_0$. We choose the integers J_α as in the ground state. The numbers I_j are chosen as follows:

$$I_{j+1}-I_j=1,\quad j=1,\ldots, N-2 \quad (6.1a)$$

$$I_N-I_{N-1}\gg 1 . \quad (6.1b)$$

So we find from Eqs. (2.6)

$$2\pi\rho(k_j)=1+\cos k_j\sum_{\beta=1}^{m}\frac{8u}{u^2+16(\sin k_j-\Lambda_\beta)^2}, \quad j=1,\ldots,N-2 \quad (6.2)$$

$$\frac{1}{N_a}\sum_{j=1}^{N}\frac{8u}{u^2+16(\sin k_j-\Lambda_\beta)^2}=2\pi\sigma(\Lambda_\alpha)+\frac{1}{N_a}\sum_{\beta=1}^{m}\frac{4u}{u^2+4(\Lambda_\alpha-\Lambda_\alpha)^2} . \quad (6.3)$$

Separating from Eq. (6.3) the term with $k_N=k_0$ and proceeding to the limit of a large system, we find for the distribution function $\rho(k)$ and $\sigma(\Lambda)$ the equations

$$2\pi\rho(k)=1+\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma(\Lambda)\frac{8u}{u^2+16(\sin k-\Lambda)^2}, \quad (6.4a)$$

$$\int_{-Q}^{Q}dk\,\rho(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\sigma(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\,\sigma(\Lambda')\frac{4u}{u^2+4(\Lambda-\Lambda')^2}-\frac{1}{N_a}\times\frac{8u}{u^2+16(\sin k_0-\Lambda)^2} . \quad (6.4b)$$

It must be recognized that in Eqs. (6.4) $\rho(k)$ is the distribution function for $N-1$ electrons; i.e., it satisfies the normalization condition

$$\int_{-Q}^{Q}dk\,\rho(k)=\frac{N-1}{N_a} . \quad (6.5)$$

We introduce the distribution functions $\rho_1(k)$ and $\sigma_1(\Lambda)$ defined by Eq. (4.3). These distribution functions satisfy the equations

$$2\pi\rho_1(k)=\cos k\int_{-\infty}^{\infty}d\Lambda\,\sigma_1(\Lambda)\frac{8u}{u^2+16(\sin k-\Lambda)^2}, \quad (6.6a)$$

$$\int_{-Q}^{Q}dk\,\rho_1(k)\frac{8u}{u^2+16(\sin k-\Lambda)^2}=2\pi\sigma_1(\Lambda)+\int_{-\infty}^{\infty}d\Lambda'\frac{\sigma_1(\Lambda')4u}{u^2+4(\Lambda-\Lambda')^2}-\frac{8u}{u^2+16(\sin k_0-\Lambda)^2} . \quad (6.6b)$$

We find an integral equation for $\rho_1(k)$ alone by again introducing the Fourier transform of $\sigma_1(\Lambda)$:

$$\rho_1(k)=\frac{4}{u}\cos k\,R\left(\frac{4}{u}(\sin k-\sin k_0)\right)+\frac{4}{u}\cos k\times\int_{-Q}^{Q}dk'R\left(\frac{4}{u}(\sin k-\sin k')\right)\rho_1(k') . \quad (6.7)$$

Notice the similarity between the equation and Eq. (5.6). The differences are that here $|k_0|\geq Q_0$ and the inhomogeneous term has the opposite sign.

The energy of the particle state relative to that of the ground state is given by

$$\epsilon=-2t\cos k_0-2t\int_{-Q}^{Q}\cos k\rho_1(k)\,dk+E_0(Q)-E_0(Q_0) . \quad (6.8)$$

If we relate Q to Q_0 by the condition that the density of electrons is fixed, we find

$$\epsilon(k_0)=-2t\cos k_0-2t\int_{-Q_0}^{Q_0}dk\cos k\rho_1(k, k_0)-\mu\left(1+\int_{-Q_0}^{Q_0}dk\rho_1(k, k_0)\right) . \quad (6.9)$$

By manipulations similar to those mentioned in Sec. V we can show that

$$\mu=-2t\left(\frac{\cos Q_0+\int_{-Q_0}^{Q_0}dk\cos k\rho_1(k, Q_0)}{1+\int_{-Q_0}^{Q_0}dk\,\rho_1(k, Q_0)}\right). \quad (6.10)$$

From this relation it is evident that $\epsilon(k_0)\to 0$ as $k_0\to Q_0$.

The momentum of the particle state is related to the parameter k_0 by the equation

$$\frac{p}{2\pi}=\int_{Q_0}^{k_0}\rho_0(k)\,dk,\quad k_0\geq Q_0 . \quad (6.11)$$

We can rewrite this in terms of the function F [Eq. (5.11)] as

$$\frac{p}{2\pi}=\frac{-1}{2}\frac{N}{N_a}+\frac{k_0}{2\pi}+\int_{-Q_0}^{Q_0}dk\,\rho_0(k)F\left(\frac{4}{u}(\sin k_0-\sin k)\right) . \quad (6.12)$$

From Eqs. (6.9) and (6.12) we can examine the general properties of ϵ as a function of momentum. Since $\rho_1(k, k_0)=\rho_1(-k, -k_0)$ we see that $\epsilon(k_0)$ is an even function of k_0. Likewise, we see from (6.12) that $p+\pi(N/N_a)$ is an odd function of k_0. This implies that as a function of momentum $\epsilon(p)$ is symmetric about $\pm\pi N/N_a$.

The dispersion curves are found as a function of U/t by solving numerically Eq. (6.7) for $\rho_1(k)$ and using numerical results for $\rho_0(k)$.

VII. PARTICLE-HOLE EXCITATIONS

We can combine the results of Secs. V and VI to calculate the energy and momentum of those states which arise by removing one electron from a momentum level k_0 occupied in the ground state and placing it in a momentum level p_0 not occupied in the ground state. The energy and momentum of this state, denoted by $\epsilon(k_0,p_0)$ and $p(k_0,p_0)$, respectively, will depend parametrically on the quantities k_0 and p_0, the momenta of the "hole" and the "electron," respectively. The energy $\epsilon(k_0,p_0)$ is defined as

$$\epsilon(k_0,p_0)=[E(N+1,p_0)-E_0(N)]-[E_0(N)-E(N-1,k_0)]\ . \qquad (7.1)$$

In Eq. (7.1) $E_0(N)$ is the ground-state energy for N particles, $E(N+1,p_0)$ is the energy of that state which arises by adding one electron with momentum p_0 to the ground state of N electrons, and $E(N-1,k_0)$ is the energy of that state which arises by removing an electron with momentum k_0 from the ground state of N electrons. As k_0 (or p_0) $\to Q_0$, $[E_0(N)-E(N-1,k_0)]$ $\{[E(N+1,p_0)-E_0(N)]\}$ $\to\mu_-$ (μ_+). The parameters μ_+ and μ_- were introduced by Lieb and Wu.[4] The explicit expression for $\epsilon(k_0,p_0)$ is

$$\epsilon(k_0,p_0)=2t\cos k_0-2t\cos p_0-\mu\int_{-Q_0}^{Q_0}[\rho_h(k,k_0)+\rho_p(k,p_0)]\,dk-2t\int_{-Q_0}^{Q_0}[\rho_h(k,k_0)+\rho_p(k,p_0)]\cos k\,dk\ , \qquad (7.2)$$

where $\rho_h(k,k_0)$ and $\rho_p(k,p_0)$ satisfy Eqs. (5.6) and (6.7), respectively. The quantity μ is defined in Eq. (4.17).

We have calculated the energy $\epsilon(k_0,p_0)$ and momentum $p(k_0,p_0)$ by using numerical results for the distribution functions ρ_n and ρ_p. We then find a band of states for the "particle-hole" excitations. We show in Fig. 3 results for the quarter-filled band for various values of U/t.

VIII. SUMMARY AND CONCLUSIONS

Using the formalism of Lieb and Wu[4] we have been able to write down the integral equations determining the dispersion relation for excitations having either single-particle or spin-wave character. We have restricted attention in this investigation to a class of states in which the parameters k_j and Λ_α of Eqs. (2.2) and (2.3) are real. This is an extension of the work of Ovchinnikov[8] to the situation in which the number of electrons is less than the number of sites in the chain. The results are found as numerical solutions to a set of coupled integral equations. Analytic results are given for some limiting cases.

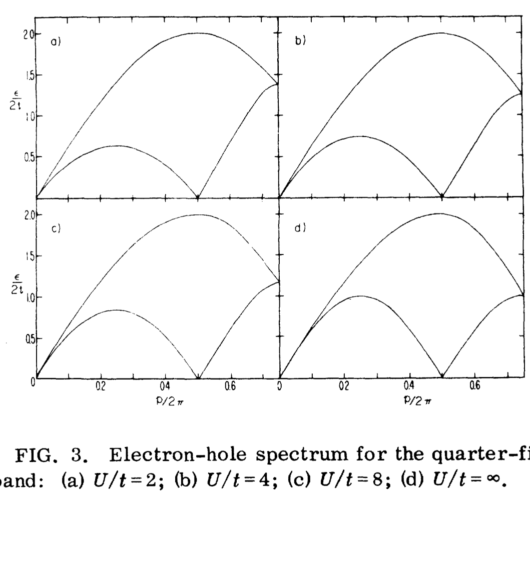

FIG. 3. Electron-hole spectrum for the quarter-filled band: (a) $U/t=2$; (b) $U/t=4$; (c) $U/t=8$; (d) $U/t=\infty$.

For the case of the single-particle excitations we have been able to demonstrate that there is no gap in the spectrum for $N/N_a<1$, unlike the result for the half-filled band $(N/N_a=1)$. Thus, according to the criterion of Lieb and Wu,[4] the system has the properties of a conductor regardless of the magnitude of U/t. As a consequence one would expect a linear term $(\sim\gamma T)$ in the specific heat from thermal excitation of these modes. We have graphically displayed the shape of the single-particle band for $N/N_a<1$, and the numerical results indicate that the shape is relatively insensitive to the magnitude of U/t, at least if $U/t\geqslant 1$.

Several interesting features emerge from the investigation of the excitations of the spin-wave type. We find that the period of the spin-wave excitation energy is incommensurate with the periodicity of the lattice unless N_a/N equals an integer. For small momentum the energy varies linearly with momentum. This is the type of behavior one associates with antiferromagnetic systems. Therefore one expects[2] a linear contribution $(\sim\alpha_M T)$ to the low-temperature specific heat from thermal excitation of these modes. This contribution may be difficult to isolate experimentally from the contribution expected from the single-particle excitations. It has also been shown that the slope of the spin-wave dispersion curve for small momentum is a measure of the inverse of the static magnetic susceptibility. This relationship, first noted for the half-filled band by Takahashi,[8] is seen to be valid for arbitrary electron density.

In attempting to apply the results of these calculations to the interpretation of the experimental results one is beset by at least two difficulties. First, one has only partial knowledge of the spectrum of low-lying states. Assuredly there are other modes, not enumerated, which need to be considered. In fact, Ovchinnikov[6] showed that for the half-filled band there exist spin-wave bound states which certainly contribute to the low-temperature thermodynamic properties of the system. Second, as emphasized in Ref. 2, there is the uncertainty of the contribution of each mode to the thermodynamic properties; i.e., we don't know the spectral weight function.

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