Gap in the spin excitations and magnetization curve of the one-dimensional attractive Hubbard model

Thomas B. Bahder
Materials Sciences Laboratory, The Aerospace Corporation, El Segundo, California 90245

Ferenc Woynarovich*
Serin Physics Laboratory, Rutgers University, New Brunswick, New Jersey 08903
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The magnetic properties of a Hubbard chain with on-site attraction are studied as a function of the band filling. Magnetization curves are calculated numerically for several values of the interaction and band filling. An unexpected feature of these curves is that the susceptibility is always finite except for the empty and half-filled band. The gap in the magnetic excitation spectrum is also calculated as a function of the band filling. The numerical results are compared with analytical results, which are obtained for the nearly empty and nearly-half-filled band.

I. INTRODUCTION

For over a decade now there has been continuous interest in quasi-one-dimensional systems.[1–5] The electronic behavior exhibited by these materials is often discussed in terms of the one-dimensional (1D) Hubbard and related models.[6–10] Among these models the 1D Hubbard model plays a special role because it is exactly solvable. Although it is a severe oversimplification of the real systems, it contains much of the physics dealing with the Coulomb interaction. Moreover, because this model is exactly solvable, it can be used to test approximate methods which can treat more realistic models.[11,12] Quantities that are calculated by the approximate methods can be compared with those which are available from the exact solution of this simple, but nontrivial interacting many-body system.

The 1D Hubbard Hamiltonian is given by

$$H=-t\sum_{i=1}^{N}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i\sigma})+U\sum_{i=1}^{N}n_{i\uparrow}n_{i\downarrow}\ , \quad (1)$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (destroys) an electron with spin σ at site i and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. Lieb and Wu have shown that the diagonalization of this Hamiltonian is equivalent to solving a set of nonlinear algebraic equations, which are often called the Lieb-Wu (LW) equations.[13] Most of the theoretical work at zero temperature has been based on the different solutions of the LW equations. The structure of the excitation spectrum has been investigated by Ovchinnikov,[14] Coll,[15] and one of the present authors.[16] The zero-temperature magnetic properties of the model were studied by Takahashi[17] and Shiba.[18] In particular, Takahashi found the magnetization curve for the half-filled band for both positive and negative U. Extending this work, Shiba gave the zero-field magnetic susceptibility for an arbitrary concentration of electrons, but only for positive U.

The aim of the present work is to study the magnetic properties of a Hubbard chain with negative U as a function of band filling. We give the magnetization curves and gap in the magnetic excitation spectrum, calculated by numerical solution of the Lieb-Wu equations for several values of U and band filling. Since the gap is a quantity of special interest, we also derive analytic expressions for it in the cases of low and nearly-half-filled bands. To verify the qualitative features of the magnetization curves, we also analytically calculate the susceptibility near saturation and near the onset of magnetization, the latter only in the large-$|U|$ limit.

The paper is organized as follows: In Sec. II we review the formalism. Section III presents the numerical calculations of the gap and magnetization curves. Section IV is devoted to analytical calculation of the gap for low band filling and close to half-filled band. In Sec. V the susceptibility is calculated analytically near the onset and saturation of magnetization.

II. BASIC FORMALISM

The starting point of our study is given by the LW equations (with $t=1$, which does not restrict their generality)

$$Nk_j=2\pi I_j-\sum_{\alpha=1}^{M}2\arctan\left[\frac{\sin(k_j)-\lambda_\alpha}{U/4}\right], \quad (2)$$

$$\sum_{j=1}^{N_e}2\arctan\left[\frac{\lambda_\alpha-\sin k_j}{U/4}\right]=2\pi J_\alpha+\sum_{\beta=1}^{M}2\arctan\left[\frac{\lambda_\alpha-\lambda_\beta}{U/2}\right]. \quad (3)$$

In these equations N is the number of lattice sites, N_e is the number of electrons, and M is the number of down spins. The variables k_j are the wave numbers of the electrons, while the λ_α's describe the motion of the spins. The integers I_j and J_α are the actual quantum numbers. From any particular solution of this system of equations the wave function can be reconstructed (first article in

Ref. 16), and the energy, momentum, and spin of the system can, respectively, be given as

$$E=-\sum_j 2\cos k_j \ , \tag{4}$$

$$P=\sum_j k_j \ , \tag{5}$$

$$S_z=\tfrac{1}{2}N_e-M \ . \tag{6}$$

Although the LW equations hold regardless of the sign of U, one encounters difficulties in applying these equations directly to chains with on-site attraction, since for the states of interest a macroscopic number ($\sim N$) of k's are complex. However, the electron-hole symmetry provides a way to overcome this inconvenience. Changing only the up-spin electrons into holes is equivalent to changing the on-site attraction into repulsion. (The details of this transformation and its consequences are discussed in the last papers of Ref. 16.) Through this transformation, any eigenstate of a chain with attractive interaction, $U<0$, with N_e electrons and a magnetization S_Z, can be transformed into the eigenstate of a chain with repulsive interaction, $|U|$, with $\overline{N}_e=N-N_e+2M$ electrons with a magnetization $\overline{S}_z=(N-N_e)/2$, and vice versa. The energies of the corresponding states are related by

$$E(N_e,M,-|U|)=-|U|M+E(N-N_e+2M;M;|U|)\ . \tag{7}$$

We need to calculate the lowest-energy states as a function of the band filling $n=N_e/N$ and magnetization $s=N_e/2N-M/N=S_z/N$ for $U<0$. Thus we have to find the lowest-energy states for the interaction $|U|$ with $\overline{N}_e=N(1-2s)$ and $M=N(n/2-s)$. In these states all the k's and λ's are real and in the $N\to\infty$ limit we describe the positions of the k's and λ's by continuous densities $\rho(k)$ and $\sigma(\lambda)$, in the intervals $(-Q,Q)$ and $(-B,B)$, respectively. These densities satisfy the equations[13]

$$2\pi\rho(k)=1+\int_{-B}^{B}2\cos(k)\frac{|U|/4}{(U/4)^2+(\lambda-\sin k)^2}\sigma(\lambda)d\lambda \ , \tag{8}$$

$$\int_{-Q}^{Q}\frac{|U|/2}{(U/4)^2+(\lambda-\sin k)^2}\rho(k)dk=2\pi\sigma(\lambda)+\int_{-B}^{B}\frac{|U|}{(U/2)^2+(\lambda-\lambda')^2}\sigma(\lambda')d\lambda' \ , \tag{9}$$

with the conditions for Q and B

$$\int_{-Q}^{Q}\rho(k)dk=1-2s;\quad \int_{-B}^{B}\sigma(\lambda)d\lambda=\frac{n}{2}-s \ . \tag{10}$$

Due to (4) and (7), the energy can be given as

$$\frac{E}{N}=-|U|\left[\frac{n}{2}-s\right]-2\int_{-Q}^{Q}\cos(k)\rho(k)dk \ . \tag{11}$$

Equations (8)–(11) do not directly describe the states with $U<0$, but rather they describe the states with $|U|$

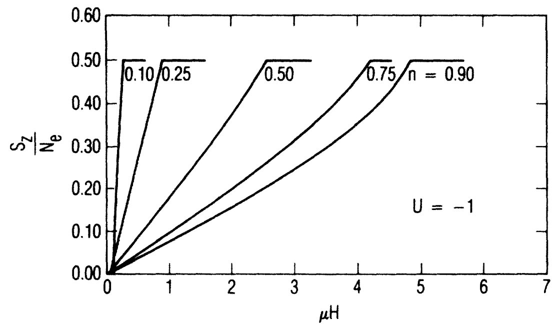

FIG. 1. Magnetization per electron versus magnetization field is shown for several values of band filling for attractive coupling $U=-1$.

from which, by the electron-hole transformation, the states with $-|U|$ can be obtained. Nevertheless, the functions $\rho(k)$ and $\sigma(\lambda)$ can be related to the $U<0$ case. In the states with $U<0$ a part of the particles are in bound pairs with wave numbers $\sin k^{\pm}=\lambda\pm iU/4$ and $\sigma(\lambda)$ describes the distribution of these λ's, while the unbound electrons have wave numbers k distributed in the region $[-(\pi-Q),+(\pi-Q)]$ according to $\overline{\rho}(k)=\rho(\pi-k)$. Performing the substitutions $\overline{\rho}(k)=\rho(\pi-k)$ and $\pi-Q=\overline{Q}$ in Eqs. (8)–(11) leads to the equations presented by Takahashi[17]

$$2\pi\overline{\rho}(k)=1-2\cos(k)\int_{-B}^{B}\frac{|U|/4}{(U/4)^2+(\lambda-\sin k)^2}\sigma(\lambda)d\lambda \ , \tag{12}$$

$$2\pi\sigma(\lambda)+\int_{-B}^{B}2\frac{|U|/2}{(U/2)^2+(\lambda-\lambda')^2}=\mathrm{Re}\left[\frac{2}{[1-(\lambda-iU/4)^2]^{1/2}}\right]-\int_{-\overline{Q}}^{\overline{Q}}\frac{|U|/2}{(U/4)^2+(\lambda-\sin k)^2}\overline{\rho}(k)dk \ , \tag{13}$$

$$\int_{-B}^{B}\sigma(\lambda)d\lambda=\frac{n}{2}-s \ , \tag{14}$$

$$\int_{-\overline{Q}}^{\overline{Q}}\overline{\rho}(k)dk=2s \ , \tag{15}$$

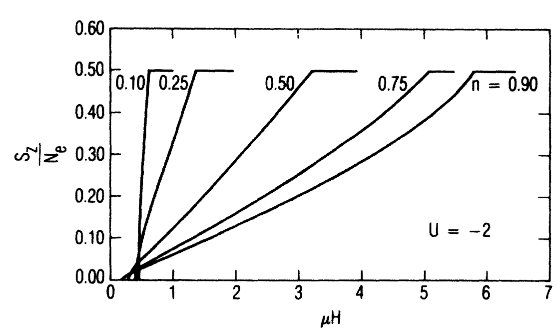

FIG. 2. Same as Fig. 1 but for coupling $U=-2$.

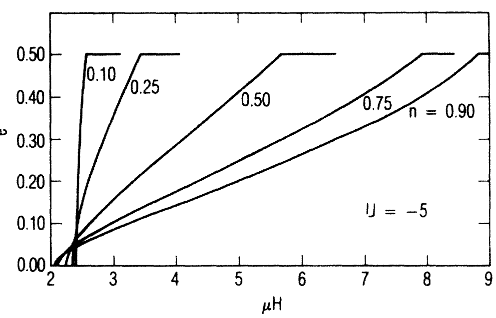

FIG. 3. Same as Fig. 1 but for coupling $U=-5$.

$$\frac{E}{N}=-4\int_{-B}^{B}\mathrm{Re}\left\{\left[1-\left[\lambda-\frac{iU}{4}\right]^2\right]^{1/2}\right\}\sigma(\lambda)d\lambda$$

$$-2\int_{-\bar{Q}}^{\bar{Q}}\cos(k)\bar{\rho}(k)dk\ . \qquad (16)$$

The set (8)—(11) is equivalent to the set (12)—(16). In the numerical calculations the set (12)—(16) was solved, but in the analytical calculations (8)—(11) proved to be more convenient.

III. MAGNETIZATION CURVE AND GAP IN THE SPIN EXCITATIONS

In the presence of a magnetic field H, we add to the Hamiltonian the Zeeman interaction term $-\mu H S_z$, where $\mu=g\mu_B$ with $g\approx 2$ and μ_B is the Bohr magneton. The ground state occurs at a value of $\bar{s}=\langle S_Z\rangle/N_e$ which minimizes

$$\epsilon_H(\bar{s})=\epsilon(\bar{s})-\mu H\bar{s}\ , \qquad (17)$$

where $\epsilon(\bar{s})=E/N_e$, and E/N is given by Eq. (16). The magnetization curve $\bar{s}$ as a function of H is then implicitly given by

$$\frac{\partial\epsilon(\bar{s})}{\partial\bar{s}}=\mu H\ . \qquad (18)$$

Equations (12) and (13) were solved numerically for the functions $\bar{\rho}(k)$ and $\sigma(\lambda)$ with $\bar{Q}$ and B as independent variables. Substitution of $\bar{\rho}(k)$ and $\sigma(\lambda)$ in (14)—(16) gives the energy $\epsilon(\bar{s})$, band filling n, and spin $\bar{s}$ as functions of $\bar{Q}$ and B. To calculate the derivative in Eq. (18) with respect to $\bar{s}$ while holding n constant, a numerical transformation was performed from independent variables $(\bar{Q},B)$ to (n,s), where $s=n\bar{s}$. The Jacobian for this transformation (with $U\leq 0$) was shown to be positive everywhere in the (n,s) plane except for the region $n=1$, which corresponds to $B=\infty$ in Eqs. (12) and (13) (see Ref. 19). Thus, we did not calculate the magnetization curves for $n=1$, the half-filled band case, but they are available in Ref. 17. The calculations were performed on a VAX-11/780 computer equipped with a floating point accelerator. Each magnetization curve required several hours of CPU time to achieve an accuracy of two to six significant figures.

Figures 1, 2, and 3 show the magnetization curves for couplings $U=-1$, -2, and -5, respectively. In each figure, curves are labeled according to band filling n. All three sets of curves share common features. The most apparent difference between them is that for increasing at-

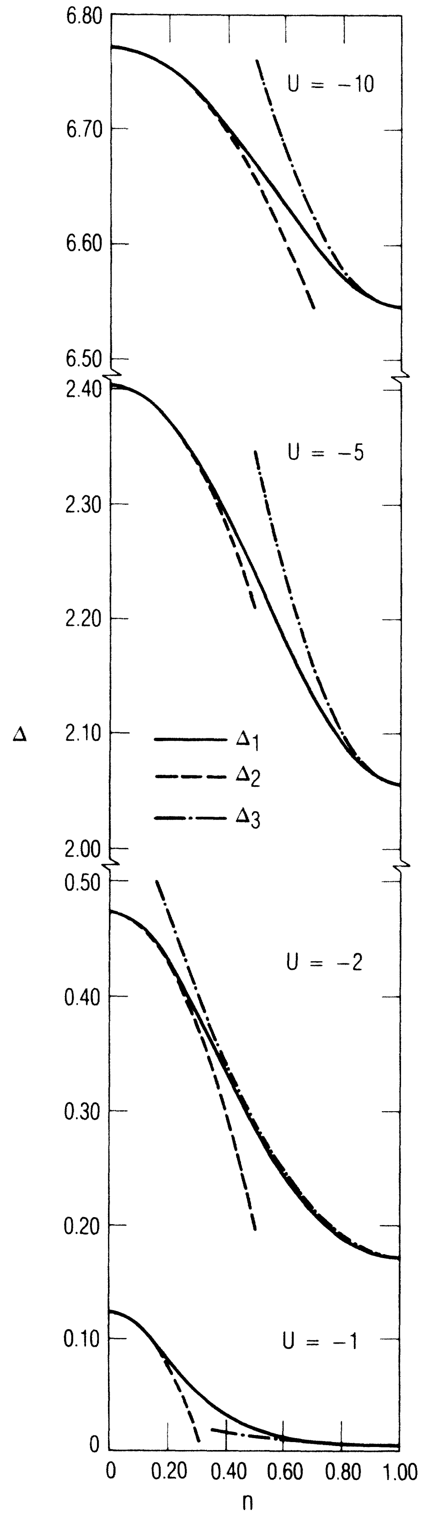

FIG. 4. The gap in the spin-excitation spectrum is shown versus band filling for several values of coupling U. The curves labeled Δ_1 are the numerical results while Δ_2 and Δ_3 are the analytical results given in Eqs. (43) and (28), respectively.

traction, the onset of magnetization occurs at higher values of critical field H_c and the difference $H_s - H_c$, where H_s is the saturation field, becomes larger. This is an obvious consequence of the competition between the magnetic field, which favors alignment of the spins parallel to the field, and the attractive interaction, which attempts to keep the electrons in singlet bound pairs.

In the limit of low electron density, the magnetization curves for all U approach step functions. In this limit the bound pairs are independent of one another and as the field H approaches its critical value from below, all the pairs break up simultaneously.

For increasing electron density, the magnetization begins at lower values of magnetic fields and the curves are all less steep with increasing n. The decrease in the critical field with increased band filling shows that the effective coupling strength of the bound pairs decreases with increasing electron density. The increasing overlap of the bound pairs leads to a weaker coupling between the electrons. Although in the formalism of Bethe ansatz, the Fermi velocity does not play a role, and the coupling constant, U/v_F, used in other methods can not be singled out (except in the limit $U \to 0$, $n \to 0$, U/n finite), apparently it controls the qualitative behavior of the system.

The field at which the onset of magnetization occurs is the critical field H_c and μH_c is also the gap $\Delta(n,U)$ in the spin-excitation spectrum. The gap is plotted as a function of band filling for $U=-1$, -2, -5, and -10 in Fig. 4. In some sense, the size of the gap is a measure of the strength of the effective interaction between the electrons. For any coupling, the gap is largest in the limit of zero band filling and decreases monotonically as $n=1$ is approached. The variation in the gap, defined to be

$$\delta\Delta(U) = \Delta(n \to 0^+, U) - \Delta(n \to 1^-, U) , \quad (19)$$

is a measure of the dependence of the effective interaction on band filling. Figure 5 shows this dependence is strongest near $U \cong -3.5$.

The slope of the magnetization curves is sensitive to the rate at which the bound-pair coupling changes with the relative number of bound-electron pairs and unbound electrons. This behavior stands in contrast to that of the critical field, H_c, which is sensitive to the bound-pair coupling itself. The slope of the magnetization curves is also affected by the width of the band available for unbound electrons above the continuum of bound pairs and the way the shape and width of this band changes with the relative number of bound pairs and unbound electrons.

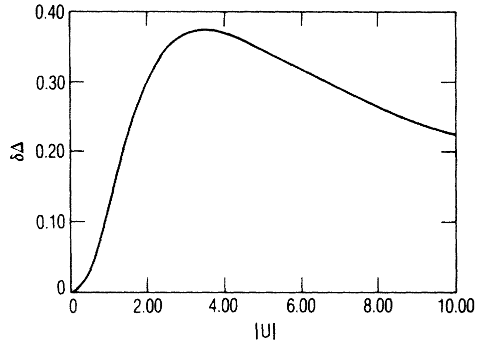

FIG. 5. The variation in the gap (i.e., the gap at zero band filling minus the gap at half-filled band) is plotted versus the magnitude of the coupling $|U|$.

At the onset of magnetization, $H=H_c$, and near saturation, $H=H_s$, the susceptibility diverges both for $n \to 0$ and $n \to 1$, but is finite for all intermediate n, see Figs. 1, 2, and 3 and Sec. V. The behavior of the susceptibility at low electron density ($n \to 0$) is well understood on the basis of independence of bound pairs and that the unbound electrons, produced by breaking bound pairs, occupy the almost flat bottom of the band. The divergences at $n=1$ near H_c and H_s are known from the work of Takahashi.[17] The fact that the susceptibility at H_c diverges when $n \to 1$ suggests that for $n=1$ and $s \cong 0$, the binding energy of bound pairs does not depend on the relative number of bound pairs and unbound electrons. The divergence of the susceptibility at $n=1$ as $H \to H_s$ can be understood as follows: as $s \to n/2$ there is a small number of bound pairs which become independent and the unbound electrons, produced by breaking these pairs, occupy the flat top of the band.

IV. ANALYTIC CALCULATIONS FOR THE GAP

In the ground state there is zero magnetization, so $s=0$ and $Q=\pi$, as can be seen by integrating Eq. (8) over the interval $(-\pi,\pi)$. The gap is the minimum energy needed to turn up one spin. It can be calculated by setting $s=1/N$, which corresponds to

$$Q = \pi - 1/[N\rho(k)] .$$

For this value of Q, Eqs. (8) and (10) can be eliminated from the set (8)–(11), which leads to

$$\frac{1}{\pi}\int_{-\pi}^{\pi} \frac{|U|/4}{(U/4)^2+(\lambda-\sin k)^2}dk - \frac{1}{N}\frac{U}{(U/4)^2+\lambda^2} = 2\pi\sigma(\lambda) + \int_{-B}^{B} \frac{|U|}{(U/2)^2+(\lambda-\lambda')^2}\sigma(\lambda')d\lambda' , \quad (20)$$

$$\int_{-B}^{B} \sigma(\lambda)d\lambda = \frac{n}{2} - \frac{1}{N} , \quad (21)$$

$$\frac{E}{N} = -\frac{n|U|}{2} + \frac{|U|-4}{N} - \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \int_{-B}^{B} \cos^2(k)\frac{|U|}{(U/4)^2+(\lambda-\sin k)^2}\sigma(\lambda)d\lambda . \quad (22)$$

After solving Eqs. (20) and (21), the ground-state energy will be given by terms of the order of unity while the gap will be given by the coefficient of the $1/N$ term in (22). No method is known by which Eqs. (20) and (21) can be solved in closed form for all values of n, but in the limiting cases $1-n \ll 1$ and $n \ll 1$, approximate methods yield results of sufficient accuracy.

A. $(1-n) \ll 1$

Since $B=\infty$ corresponds to $n=1$, we expect B to be large. In this case we use a form of Eqs. (20)–(22) in which the λ integrals are over the region $(-\infty, B)$ and (B,∞). This form can be found by straightforward algebraic manipulation involving a Fourier transformation of Eq. (20):

$$\int_{-\pi}^{\pi} \sigma_0(\lambda-\sin k)dk - \frac{4\pi}{N}\sigma_0(\lambda) = 2\pi\sigma(\lambda) - \int_B^{\infty} [K(\lambda-\lambda')+K(\lambda+\lambda')]\sigma(\lambda')d\lambda' , \quad (23)$$

$$\int_B^{\infty} \sigma(\lambda)d\lambda = \tfrac{1}{2}(1-n) , \quad (24)$$

$$\frac{E}{N} = -\frac{n\,|U|}{2} + \frac{|U|-4}{N} + \frac{1}{2\pi N}\int_{-\pi}^{\pi} \cos^2(k)K(\sin k)dk$$
$$- \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} 2\cos^2(k)K(\sin k - \sin k')dk\,dk' + \int_{-\pi}^{\pi} 4\cos^2 k \int_B^{\infty} \sigma_0(\lambda-\sin k)\sigma(\lambda)d\lambda\, dk , \quad (25)$$

where

$$\sigma_0(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{i\omega\lambda}}{2\cosh(\omega U/4)}d\lambda, \quad K(\lambda) = \int_{-\pi}^{\pi} \frac{e^{-|\omega|\,|U|/4}}{2\cosh(\omega U/4)}e^{i\omega\lambda}d\omega . \quad (26)$$

Equation (23) is very similar to an integral equation which arose in the treatment of the Heisenberg model.[20] Following the method used there,[20] one obtains the energy as a power series in $(1-n)$, which, up to second order is

$$\frac{E}{N} = \frac{E_0}{N} + \frac{\Delta}{N} , \quad (27)$$

$$\frac{E_0}{N} = -\frac{|U|}{2} - \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} 2\cos^2 k K(\sin k - \sin k')dk\,dk' + \frac{|U|}{2}(1-n) + \frac{\pi}{2}\frac{I_1(2\pi/|U|)}{I_0(2\pi/|U|)}(1-n)^2 ,$$

$$\Delta = |U| - 4 + \frac{2}{\pi}\int_{-\pi}^{\pi} \cos^2 k K(\sin k)dk + (1-n)^2\pi\frac{I_1(2\pi/|U|)}{I_0(2\pi/|U|)^2} , \quad (28)$$

where $I_0(x)$ and $I_1(x)$ are the Bessel functions of imaginary argument. The neglected terms are of the order of $(1-n)^4$. However, the validity of (27) and (28) is not only limited by $1-n \ll 1$, but also the procedure applied, which converges only if

$$(1-n) < \frac{4}{\pi e} I_0\left[\frac{2\pi}{|U|}\right] e^{-(2\pi/|U|)} \simeq \frac{2}{e}\frac{\sqrt{|U|}}{\pi^2} . \quad (29)$$

B. $n \ll 1$

In this case, according to (21), B is expected to be small. Iterating Eq. (20) should be a convergent process, increasing the accuracy by one power of $(n-1/N)$ with each step of iteration. To obtain results correct up to second order, however, there is a simpler method. In Eqs. (20)–(22) separating the terms $1/N$ from those characteristic of the ground state, leads to the set of equations

$$f_1(\lambda) = 2\pi\sigma_0(\lambda) + \int_{-B_0}^{B_0} \frac{|U|}{(U/2)^2-(\lambda-\lambda')^2}\sigma_0(\lambda')d\lambda' , \quad (30)$$

$$\int_{-B_0}^{B_0} \sigma_0(\lambda)d\lambda = \frac{n}{2} , \quad (31)$$

$$\frac{E_0}{N} = \int_{-B_0}^{B_0} f_2(\lambda)\sigma_0(\lambda)d\lambda - \frac{|U|}{2}n , \quad (32)$$

and

$$-\frac{|U|}{(U/4)^2+\lambda^2} - z\left[\frac{|U|}{(U/2)^2+(\lambda-B_0)^2} + \frac{|U|}{(U/2)^2+(\lambda+B_0)^2}\right] = 2\pi\delta(\lambda) + \int_{-B_0}^{B_0} \frac{|U|/2}{(U/2)^2+(\lambda-\lambda')^2}\delta(\lambda')d\lambda' , \quad (33)$$

$$\int_{-B_0}^{B_0} \delta(\lambda)d\lambda = -1-2z , \quad (34)$$

$$\Delta = |U| - 4 - \int_{-B_0}^{B_0} f_2(\lambda)\delta(\lambda)d\lambda - 2zf_2(B_0) , \quad (35)$$

where

$$f_1(\lambda) = \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{|U|/4}{(U/4)^2+(\lambda-\sin k)^2}dk ,$$
$$f_2(\lambda) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \cos^2 k \frac{|U|}{(U/4)^2+(\lambda-\sin k)^2}dk , \quad (36)$$

and

$$\delta(\lambda)=[\sigma(\lambda)-\sigma_0(\lambda)]/N, \quad z=\frac{B-B_0}{N}\sigma_0(B) . \tag{37}$$

Using the equality

$$\int_{-B}^{B} f(\lambda)\sigma(\lambda)d\lambda=f(\lambda^*)\int_{-B}^{B}\sigma(\lambda)d\lambda, \quad -B<\lambda^*<B \tag{38}$$

one finds that

$$\frac{E_0}{N}=-|U|\frac{n}{2}-f_2(0)n+O(B_0^2 n) , \tag{39}$$

$$\Delta=|U|-4+f_2(0)-\frac{B_0^2}{2}f_2''(0)+O(B_0^3) . \tag{40}$$

B_0 linear in n is given by (30) and (31) as

$$B_0 \cong \pi n/2f_1(0) . \tag{41}$$

Finally, after evaluating $f_1(0)$, $f_2(0)$, and $f''(0)$ one obtains

$$\frac{E_0}{N}=\left[\frac{|U|}{2}-(U^2+16)^{1/2}\right]n \tag{42}$$

and

$$\Delta=[(U^2+16)^{1/2}-4]-\left[1+\left[\frac{U}{4}\right]^2\right]^{-1/2}\frac{(\pi n)^2}{8} . \tag{43}$$

Previously, Krivnov and Ovchinnikov have calculated the gap on the basis of the LW equations by calculating the quasi-ionic excitation spectrum.[21] Larkin and Sak have prescribed a formula for the gap by solving the renormalization-group equations.[22] For the case $(1-n)\ll 1$ and $n\to 0$, $|U|\to 0$, with $n/|U|$ $=$constant, our result, given in Eq. (28), agrees with that of Refs. 21 and 22. For the case $n \ll 1$, our result in Eq. (43) holds for any $U<0$. In this limit $n\to 0$, $|U|\to 0$ with $n/|U|\ll 1$, Eq. (43) does not reproduce the earlier results. According to Ref. 21, there is no quadratic term in the gap. Our result cannot be compared with that of Ref. 22, since that result is valid only in the weak coupling limit, $|U|/n \ll 1$, which cannot be obtained from our formula.

Figure 4 shows a comparison of the gap given by the analytical results in Eqs. (28) and (43), with the gap calculated from the numerical solution of Eqs. (12)–(16). This figure shows very good agreement between the numerical and analytical results, within the range of validity of the latter.

V. SUSCEPTIBILITY NEAR ONSET AND THE SATURATION OF MAGNETIZATION

As already indicated, the magnetization curves for less than half-filled bands, $n<1$, are qualitatively different from those for half-filled bands, $n=1$, which were found by Takahashi.[17] While for $n=1$, all curves start, and terminate with infinite slopes, for $n<1$ this behavior is not seen. The following calculations confirm, that the infinite susceptibility at the onset and saturation of magnetization is really only a characteristic of the $n\to 0$ and $n\to 1$ limits.

To see the behavior at the onset of magnetization, we solve the LW equations directly for a strong on-site repulsion $|U|\gg 1$, and applying (4) and (7), we calculate the energy and magnetization for $U \ll 1$.

In Eqs. (2) and (3) in the large-U limit, all λ are proportional to $|U|$, thus Eqs. (2) and (3) for symmetrical k and λ distributions to leading order in $1/|U|$ become

$$k_j=2\pi\frac{I_j}{N}-\frac{\sin k_j}{|U|}\frac{1}{N}\sum_{\alpha=1}^{\overline{M}}\frac{2}{1-(4\lambda_\alpha/U)^2} , \tag{44}$$

$$2\overline{N}_e\arctan\left[\frac{4\lambda_\alpha}{|U|}\right]=2\pi J_\alpha+\sum_{\alpha=1}^{\overline{M}}2\arctan\left[\frac{\lambda_\alpha-\lambda_\beta}{|U|/2}\right] . \tag{45}$$

The solution of (44) to leading order in $1/|U|$ is

$$k_j=2\pi I_j-\frac{\sin\left[2\pi\frac{I_j}{N}\right]}{|U|}\frac{1}{N}\sum_{\alpha=1}^{\overline{M}}\frac{2}{1+(4\lambda_\alpha/U)^2} . \tag{46}$$

Equation (45) is the Bethe ansatz equation for an isotropic Heisenberg chain of $\overline{N}_e=N(1-2s)$ spins with total magnetization $\overline{S}_z=\frac{1}{2}(\overline{N}_e-2\overline{M})=(1-n)N/2$. According to (4), (7), and (46) the energy is

$$\frac{E}{N}=-|U|\overline{M}-\sum_{j=-\overline{N}_e/2}^{\overline{N}_e/2}2\cos\left[\frac{2\pi j}{N}\right]-\frac{1}{N}\sum_\alpha\frac{2}{1+4(\lambda_\alpha/U)^2}\frac{4}{|U|}\sum_j\sin^2\left[\frac{2\pi j}{N}\right]$$
$$=-|U|\left[\frac{n}{2}-s\right]-\frac{2}{\pi}\sin(2\pi s)+\frac{2}{|U|}(1-2s)\epsilon_H\left[\frac{1-n}{2(1-2s)}\right]\left[1-2s+\frac{\sin 4\pi s}{2\pi}\right] , \tag{47}$$

where $\epsilon_H(x)$ is the energy per spin in a Heisenberg chain with magnetization per spin equal to x. This expression for the energy leads to a magnetization per site, just above the onset given by

$$\overline{s}=\frac{|U|}{4}\frac{1}{n(1-n)^2\epsilon''\left[\frac{1-n}{2}\right]}\mu(H-H_c) , \tag{48}$$

with

$$\mu H_c = |U| - 4 + \frac{4}{|U|}\left[\frac{1-n}{2}\epsilon'_H\left[\frac{1-n}{2}\right] - \epsilon_H\left[\frac{1-n}{2}\right]\right] . \quad (49)$$

Equation (48) clearly shows that the magnetization starts with a finite slope provided $n \neq 0$ and $n \neq 1$. This result is strictly valid for large $|U|$ only, but it indicates that the finite susceptibility at the onset of magnetization is a property of the empty and half-filled band for any finite $U<0$. Equation (48) also shows that the susceptibility should diverge for any band filling as $|U| \to \infty$. This is a tendency which can also be seen in Figs. 1–3. In several other Bethe ansatz models where there is a gap in the magnetic spectrum (Gross-Neveu[23] or the J-V model[24,25]), the magnetization was found to start with infinite slope. Our result shows that this is not a common feature of all Bethe ansatz systems.

Next we calculate the magnetization curve near saturation. Close to saturation $s \lesssim n/2$, the parameter $\nu = n/2 - s$ is small, and, B is again a small parameter, similar to the calculation of the gap for $n \ll 1$, but now we do not have the convenience of Q being near to π. After eliminating Eq. (8) from the set (8)–(11) we have

$$\frac{1}{\pi}\int_{-Q}^{Q}\frac{|U|/4}{(U/4)^2+(\lambda-\sin k)^2}dk = 2\pi\sigma(\lambda) + \int_{-B}^{B}\frac{|U|}{(U/2)^2+(\lambda-\lambda')^2}\sigma(\lambda')\alpha\lambda' - \int_{-\sin Q}^{\sin Q}\frac{|U|/4}{(U/4)^2+(\lambda-x)^2}\frac{|U|}{(U/4)^2+(\lambda'-x)^2}\sigma(\lambda')d\lambda' , \quad (50)$$

$$\frac{Q}{\pi} + \frac{1}{2\pi}\int_{-B}^{B}\left[2\arctan\left[\frac{\lambda+\sin Q}{|U|/4}\right] - 2\arctan\left[\frac{\lambda-\sin Q}{|U|/4}\right]\right]\sigma(\lambda)d\lambda = (1-n) + 2\nu , \quad (51)$$

$$\int_{-B}^{B}\sigma(\lambda)d\lambda = \nu , \quad (52)$$

and

$$\frac{E}{N} = -|U|\nu - \frac{|U|}{2\pi}\int_{-B}^{B}d\lambda\int_{-Q}^{Q}dk\frac{\cos^2 k}{(U/4)^2+(\lambda-\sin k)^2}\sigma(\lambda) - \frac{2}{\pi}\sin Q . \quad (53)$$

When this system of equations is treated by the same method as the equations for the gap Δ with $U \ll 1$, it yields

$$\frac{E}{N} = -|U|\nu - \nu\frac{|U|}{2\pi}\int_{-Q}^{Q}\frac{\cos^2 k}{(U/4)^2+\sin^2 k}dk - \frac{2}{\pi}\sin Q + O(\nu^3) , \quad (54)$$

$$\frac{Q}{\pi} + \frac{2}{\pi}\nu\arctan\left[\frac{\sin Q}{|U|/4}\right] + O(\nu^3) = 1 - n + 2\nu . \quad (55)$$

After solving Eq. (55) for Q up to quadratic terms in ν, and calculating the energy, by Eq. (54), we get a magnetization per electron of

$$\bar{s} = \frac{s}{n} = \frac{1}{2} + \frac{\mu(H - H_S)}{\frac{2}{\pi}n\sin(\pi n)\left[2\pi - 2\arctan\left[\frac{\sin(\pi n)}{|U|/4}\right]\right]} , \quad (56)$$

where the field at which saturation occurs is given by

$$\mu H_S = \mu H_S^{>} = \frac{2}{\pi}\cos(\pi n)\left[2\pi - 2\arctan\left[\frac{\sin(\pi n)}{|U|/4}\right]\right] - \frac{|U|}{\pi}\left[\frac{(U^2+16)^{1/2}}{|U|}\arctan\left[\frac{(U^2+16)^{1/2}}{|U|}\tan(\pi\rho)\right] - \pi\rho\right] \text{ if } n > \tfrac{1}{2} , \quad (57)$$

$$\mu H_S = \mu H_S^{<} = \mu H_S^{>} + (U^2+16)^{1/2} \text{ if } n < \tfrac{1}{2} . \quad (58)$$

Equation (56) confirms that the susceptibility at saturation should be infinite for $n=1$ (and $n \to 0$), but it is finite for $0<n<1$. The value of the critical field H_S given by (57) and (58) agrees with the values obtained numerically to within four significant figures.

VI. SUMMARY

In the present work, we have calculated the magnetization curves for a Hubbard chain with on-site attraction, for several values of the band filling at different values of attraction (see Figs. 1–3), by solving numerically the Lieb-Wu equations. The curves are found to share common features except that the range in magnetic field between the onset of magnetization H_c and saturation H_s increases with increasing attraction. A new feature of the less than half-filled band is that the magnetization curves start and terminate with finite susceptibility, unlike the magnetization curves found by Takahashi for the half-filled band. This property of the magnetization curves is verified by analytic calculations.

We also calculated the gap in the magnetic excitation spectrum numerically as a function of the band filling, and by approximate analytical methods, for the case of close to empty and close to half-filled band. Comparison of the numerical and analytical results (Fig. 4) shows good agreement in the range of validity of the analytical expressions.

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*Permanent address: Central Research Institute for Physics, H-1525 Budapest, POB 49, Hungary.

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