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LETTER TO THE EDITOR

Finite-size corrections for the low lying states of a half-filled Hubbard chain

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Abstract. The finite-size corrections to the ground state and the energy of the low magnetisation ($S \ll N$) states as a function of the size N are calculated analytically for the one-dimensional half-filled Hubbard model with on-site repulsion ($U > 0$). It is found that the contribution of the charge degrees of freedom is negligible, while the contribution of the spin degrees is the same as that in the one-dimensional isotropic Heisenberg model. The analytical results are compared to numerical ones obtained for the chain lengths up to $N = 512$.

As is well known, several strictly one-dimensional quantum systems are in critical phases at zero temperature. These systems—similarly to those higher-dimensional ones which exhibit real phase transitions at finite temperatures—are believed to form universality classes. Within these classes the microscopic details do not play an important role, and the critical exponents are common. Due to recent developments in studying conformal invariance (Cardy 1984, 1986a, b, Blöte *et al* 1986, Affleck 1986)—a symmetry widely accepted to be present in critical systems—it is known that the dependence of the ground-state energy and low lying part of the spectrum on the size of these systems is also universal:

$$E_0 = AL - \pi c/6L \qquad E_n - E_0 = 2\pi x_n/L \tag{1}$$

where the E_n are the energy eigenvalues, x_n are the scaling dimensions of the scaling operators and L is the size of the system. The conformal anomaly number c classifies the system. Systems for which c and x_n coincide are expected to show identical critical behaviour.

In the present letter we report on analytical and numerical studies on the one-dimensional half-filled Hubbard model with on-site repulsion, which is known to be critical. We have calculated analytically the finite-size corrections to the ground-state energy and the size dependence of the mass gap. We have found that both quantities follow the rule (1) with $c = 1$ and $x_S = S^2/2$, just as the one-dimensional isotropic Heisenberg chain does (Avdeev and Dörfel 1986, Hamer 1985, 1986, Woynarovich and Eckle 1987). It is also found that the next corrections are also the same in the two models. The one-dimensional Hubbard model exhibits two kinds of excitations, one connected with the charge, the other with the spin degrees of freedom (Woynarovich 1982a, b, 1983). The latter ones are gapless, and in the infinite repulsion limit they

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coincide with the excitations of the isotropic antiferromagnetic Heisenberg chain. Thus the critical behaviour should coincide in that limit. Since $c=1$ would allow for a coupling dependence of the critical behaviour (as in the anisotropic Heisenberg model) it is remarkable that the spin part of the Hubbard model shows the same critical behaviour as the isotropic Heisenberg model for all non-zero values of the on-site repulsion.

The one-dimensional Hubbard model described by the Hamiltonian

$$H=-\sum_{i=1}^{N}\sum_{\sigma}(c_{i+1\sigma}^{+}c_{i\sigma}+\mathrm{HC})+U\sum_{i=1}^{N}c_{i\uparrow}^{+}c_{i\uparrow}c_{i\downarrow}^{+}c_{i\downarrow}\qquad N+1\equiv 1 \tag{2}$$

(where $c_{i\sigma}$ are electron creation and destruction operators) can be diagonalised by solving the set of equations (Lieb and Wu 1968)

$$Nk_j=2\pi I_j-\sum_{\beta=1}^{M}2\tan^{-1}\frac{\sin k_j-\lambda_\beta}{U/4} \tag{3}$$

$$\sum_{j=1}^{N_e}2\tan^{-1}\frac{\lambda_\alpha-\sin k_j}{U/4}=2\pi J_\alpha+\sum_{\beta=1}^{M}2\tan^{-1}\frac{\lambda_\alpha-\lambda_\beta}{U/2}. \tag{4}$$

Here k_j are the momenta of the electrons and λ_α are connected with the spin distribution. I_j and J_α are the actual quantum numbers. The magnetisation and the energy per site of the N_e electrons described by a solution of (3) and (4) are given by

$$S=\tfrac{1}{2}N_e-M \tag{5}$$

$$\varepsilon=-\frac{1}{N}\sum_{j=1}^{N_e}2\cos k_j. \tag{6}$$

In order to obtain the lowest energy state of the half-filled band ($N_e=N(=\text{even})$) with a given magnetisation one has to choose the I_j and J_α sets as

$$I_{j+1}=I_j+1\qquad I_1=-N/2+\begin{cases}0 & (N/2-S=\text{even})\\ \frac{1}{2} & (N/2-S=\text{odd})\end{cases}\qquad j=1,2,\ldots,N \tag{7}$$

$$J_{\alpha+1}=J_\alpha+1\qquad J_1=-[N/2-(S+1)]/2\qquad \alpha=1,2,\ldots,N/2-S. \tag{8}$$

The ground and first excited states are characterised by (7) and (8) with $S=0$ and $S=1$, respectively.

In calculating the finite-size effects we closely follow the method given by de Vega and Woynarovich (1985) and further developed by Woynarovich and Eckle (1987). We introduce the functions

$$w(k)=\frac{1}{2\pi}\left(k+\frac{1}{N}\sum_{\beta}2\tan^{-1}\frac{\sin k-\lambda_\beta}{U/4}\right)\qquad \frac{\mathrm{d}w(k)}{\mathrm{d}k}=\rho_N(k) \tag{9}$$

$$z(\lambda)=\frac{1}{2\pi}\left(\frac{1}{N}\sum_{j}2\tan^{-1}\frac{\lambda-\sin k_j}{U/4}-\frac{1}{N}\sum_{\beta}2\tan^{-1}\frac{\lambda-\lambda_\beta}{U/2}\right)\qquad \frac{\mathrm{d}z(\lambda)}{\mathrm{d}\lambda}=\sigma_N(\lambda). \tag{10}$$

With these definitions (3) and (4) take the form

$$w(k_j)=I_j/N \tag{11}$$

$$z(\lambda_\alpha)=J_\alpha/N \tag{12}$$

and a straightforward manipulation leads to the energy per site

$$\varepsilon = \varepsilon_\infty^{(0)} - \int_{-\pi}^{\pi} \varepsilon_c(k) R(k) - \int_{-\infty}^{\infty} \varepsilon_s(\lambda) S(\lambda). \tag{13}$$

Here $\varepsilon_\infty^{(0)}$ is the ground-state energy per site for an infinite system

$$\varepsilon_\infty^{(0)} = -4 \int_0^\infty J_0(\omega) J_1(\omega) \frac{\exp(-\omega U/2)}{1+\exp(-\omega U/2)} \frac{d\omega}{\omega} \tag{14}$$

and $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$ are the same as the excitation energies connected with the charge and spin excitations (holes in the k and λ distributions, respectively) (Woynarovich 1983):

$$\varepsilon_c(k) = 2\cos k + 4 \int_0^\infty J_1(\omega) \frac{\exp(-\omega U/2)}{1+\exp(-\omega U/2)} \cos(\omega \sin k) \frac{d\omega}{\omega} \tag{15}$$

$$\varepsilon_s(\lambda) = 2 \int_0^\infty \frac{J_1(\omega) \cos \omega\lambda}{\cosh(\omega U/4)} \frac{d\omega}{\omega}. \tag{16}$$

The $R(k)$ and $S(\lambda)$ are shorthand notations for

$$R(k) = \frac{1}{N} \sum_j \delta(k - k_j) - \rho_N(k) \qquad S(\lambda) = \frac{1}{N} \sum_\beta \delta(\lambda - \lambda_\beta) - \sigma_N(\lambda) \tag{17}$$

while $J_0(\omega)$ and $J_1(\omega)$ are Bessel functions.

We note that, similarly to the excitation energies, the finite-size corrections to the ground state also split up into two contributions, one coming from the charge, the other from the spin degrees of freedom. Now we show that for a state characterised by an I_j set given by (7) the charge contribution is negligible in the sense that as $N \to \infty$ it disappears faster than any power of $1/N$. For this we use the formula

$$\frac{1}{N} \sum_{I=I_4}^{I_N} f\left(\frac{I}{N}\right) - \int_{(I_1-1/2)/N}^{(I_N+1/2)/N} f(w)\, dw = \sum_{m=1}^{\mu} \frac{A_m}{N^{2m}} \left(f^{(2m-1)}\left(\frac{I_N+1/2}{N}\right) - f^{(2m+1)}\left(\frac{I_1-1/2}{N}\right)\right) + \frac{A_\mu(f, N)}{N^{2\mu+1}}. \tag{18}$$

Here A_m are f and N independent constants and $A_\mu(f, N)$ depends on both f and N, but if the $(2\mu+1)$th derivative of f is finite then it has an N-independent upper bound. If f is a smooth periodic function with a period 1, all the terms on the RHS are zero except the last one. Since μ can be any large value, the LHS disappears faster than any power of $1/N$ as $N \to \infty$.

Changing the variables in the contribution of the charge part from k to w (k_j to I_j/N) transforms this contribution into the form of the LHS of (18), with $f = \varepsilon_c(k(w))$, which is, for any $u > 0$, a smooth periodic function with a period of 1. Thus according to the above paragraph this contribution is negligible. This is not a surprising result: the charge excitation spectrum possesses a gap, so its contribution is expected to be exponentially small (de Vega and Woynarovich 1985).

According to the previous paragraph, the contribution of $R(k)$ can be neglected. Moreover, also in (10), we may replace $(1/N)\sum_j$ by $\int dk\, \rho_N(k)$ without introducing a significant error. The remaining equation

$$\sigma_N(\lambda) = \frac{1}{2\pi}\left(\frac{1}{2\pi} \int_{-\pi}^{\pi} 2\frac{U/4}{(U/4)^2 + (\lambda - \sin k)^2}\, dk - \int_{-\infty}^{\infty} 2\frac{U/2}{(U/2)^2 + (\lambda - \lambda')^2} (\sigma_N(\lambda) + S(\lambda))\, d\lambda \right) \tag{19}$$

is extremely similar to the analogous equation of the isotropic Heisenberg model. Actually it can be treated in the same way (Woynarovich and Eckle 1987). Using the formula

$$\frac{1}{2N}\left(g\left(\frac{J_1}{N}\right)+2\sum_{\alpha=2}^{N/2-S-1} g\left(\frac{J_\alpha}{N}\right)+g\left(\frac{J_{N/2-S}}{N}\right)\right)$$
$$=\frac{1}{12N^2}\left(g'\left(\frac{J_{N/2-S}}{N}\right)-g'\left(\frac{J_1}{N}\right)\right)+\mathrm{O}\left(\frac{\max g'''}{N^3}\right) \qquad (20)$$

to calculate the contributions of $S(\lambda)$, denoting the largest $\lambda_\alpha(\lambda_{N/2-S})$ by Λ, introducing the functions

$$\sigma_N^+(\lambda)=\begin{cases}\sigma_N(\lambda+\Lambda) & \text{if } \lambda>0\\ 0 & \text{if } \lambda<0\end{cases}$$
$$\sigma_N^-(\lambda)=\begin{cases}0 & \text{if } \lambda>0\\ \sigma_N(\lambda+\Lambda) & \text{if } \lambda<0\end{cases} \qquad (21)$$

and using Fourier transforms, (19), (12) and (13) can be transformed into the set of equations

$$\tilde\sigma_N^-(\omega)+\frac{\tilde\sigma_N^+(\omega)}{1+\exp(-|\omega|U/2)}$$
$$=\frac{1}{2\pi}\frac{1}{2\cosh(\omega U/4)}\exp(\mathrm{i}\omega\Lambda)J_0(\omega)-\frac{1}{2\pi}\left[\left(\frac{1}{2N}-\frac{\mathrm{i}\omega}{12N^2\sigma(\Lambda)}\right)\right.$$
$$\left.+\left(\frac{1}{2N}+\frac{\mathrm{i}\omega}{12N^2\sigma(\Lambda)}-2\pi\tilde\sigma_N^+(-\omega)\right)\exp(\mathrm{i}\omega 2\Lambda)\right]\frac{\exp(-|\omega|U/2)}{1+\exp(-|\omega|U/2)} \qquad (22)$$

$$2\pi\tilde\sigma_N^+(0)=(S+\tfrac{1}{2})/N \qquad (23)$$

$$\sigma_N(\Lambda)=\int_{-\infty}^{\infty}(\tilde\sigma_N^+(\omega)+\tilde\sigma_N^-(\omega))\,\mathrm{d}\omega \qquad (24)$$

$$\varepsilon_N^{(S)}-\varepsilon_\infty^{(0)}=16\pi\exp(-2\pi\Lambda/U)I_1\left(\frac{2\pi}{U}\right)\left[\tilde\sigma+\left(-\frac{\mathrm{i}2\pi}{U}\right)-\frac{1}{2\pi}\frac{1}{2N}+\frac{1}{12N^2\sigma_N(\Lambda)U}\right]$$
$$+\mathrm{O}\left[I_1\left(\frac{6\pi}{U}\right)\exp(-6\pi\Lambda/U)\tilde\sigma_N^+\left(-\frac{\mathrm{i}6\pi}{U}\right)\right] \qquad (25)$$

with $J_0(\omega)$ and $I_1(x)$ being Bessel functions. Solving (22) by the method given by Yang and Yang (1966) (23)-(25) can be calculated giving

$$\varepsilon_N^{(0)}-\varepsilon_\infty^{(0)}=-\frac{\pi}{3}\frac{I_1(2\pi/U)}{I_0(2\pi/U)}\frac{1}{N^2}\left[1+0.3433\frac{1}{\ln[NI_0(2\pi/U)]^3}+\mathrm{O}\left(\frac{\ln(\ln N)}{(\ln N)^2}\right)\right] \qquad (26)$$

$$\varepsilon_N^{(S)}-\varepsilon_\infty^{(0)}=2\pi\frac{I_1(2\pi/U)}{I_0(2\pi/U)}\frac{S^2}{N^2}\left[1-\frac{1}{2}\frac{1}{\ln[NI_0(2\pi/U)]}+\mathrm{O}\left(\frac{\ln(\ln N)}{(\ln N)^2}\right)\right]. \qquad (27)$$

Since the dispersion of the spin excitations is given by (Woynarovich 1983)

$$p_s(\lambda)=\frac{\pi}{2}-\int_0^\infty\frac{J_0(\omega)\sin(\omega\lambda)}{\omega\cosh(\omega U/4)}\mathrm{d}\omega \qquad (\sim\exp(-2\pi\lambda/U)I_0(2\pi/U) \text{ for } \lambda\gg 1)$$
$$\varepsilon_s(\lambda)=2\int_0^\infty\frac{J_1(\omega)\cos(\omega\lambda)}{\omega\cosh(\omega U/4)}\frac{\mathrm{d}\omega}{\omega} \qquad (\sim 4\exp(-2\pi\lambda/U)I_1(2\pi/U) \text{ for } \lambda\gg 1) \qquad (28)$$

after properly normalising the Hamiltonian (von Gehlen *et al* 1986) (i.e. to have instead of (28) the simple relation $\varepsilon_s(\lambda) = p_s(\lambda)$ for small momenta) and returning from the energy per site to the energy, (26) and (27) yield (1) with the same c and x_S as the isotropic Heisenberg model, i.e. with $c = 1$ and $x_S = S^2/2$. Moreover, the powers and the coefficients of the first logarithmic corrections are also the same in the two models:

$$E_N^{(0)} = N\varepsilon_\infty^{(0)} - \frac{\pi}{6N}\left(1 + 0.3433\frac{1}{\{\ln[NI_0(2\pi/U)]\}^3} + \dots\right) \tag{29}$$

$$E_N^{(S)} - E_N^{(0)} = 2\pi\frac{S^2}{2}\left(1 - \frac{1}{2}\frac{1}{\ln[NI_0(2\pi/U)]} + \dots\right). \tag{30}$$

Based on the above results one may expect the half-filled Hubbard model to exhibit the same critical behaviour as the isotropic Heisenberg model. We have to stress, however, that this analogy holds only for $U > 0$ for two reasons. One is that in the $U \to 0$ limit the corrections due to the charge degrees of freedom grow up: for small U the derivatives of $\varepsilon_c(k(w))$ grow up, and in the $U = 0$ limit $\varepsilon_c(k(w))$ is not a smooth (although it is still a periodic) function, and the argument presented just after (18) does not hold. Actually, in this limit the contribution of the charge degrees of freedom is just as large as that of the spins. The other reason is that the spin part of the corrections itself cannot be continued down to $U = 0$ due to the essential singularity of the model at this point. In our calculation $\Lambda \gg 1$ has been supposed, but for $U = 0$ for all λ_α, and so for Λ too, $|\lambda| < 1$. Actually, at the point $U = 0$ one can solve the equations which describe the spin contribution only (equations (31) and (32)) exactly, and one finds that the result for the correction to the ground state does not coincide with (26).

We also carried out numerical calculations for the finite-size corrections. We have solved numerically by iteration for $N = 8, 16, 32, \dots, 512$ and several U values that form of (4) in which the Σ_i is replaced by the $N\int\rho_N(k)$, i.e.

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} 2\tan^{-1}\frac{\lambda_\alpha - \sin k}{U/4}\,\mathrm{d}k = 2\pi J_\alpha + \sum_{\beta=1}^{M} 2\tan^{-1}\frac{\lambda_\alpha - \lambda_\beta}{U/2}. \tag{31}$$

For the energy per site we used the expression

$$\begin{aligned}\varepsilon &= -\int_{-\pi}^{\pi} 2\cos k\rho_N(k)\,\mathrm{d}k = -\frac{4}{N}\sum_\alpha \{[(U/4)^2 + \cos^2(x_\alpha/2)]^{1/2} - U/4\}\\ x_\alpha &= 2\sin^{-1}\left(\frac{[(U/4)^2 + (\lambda_\alpha + 1)^2]^{1/2} - [(U/4)^2 + (\lambda - 1)^2]^{1/2}}{2}\right)\end{aligned} \tag{32}$$

and for $\varepsilon_\infty^{(0)}$ we used (14).

Note that (31) and (32) do not contain the finite-size corrections due to the charge degrees of freedom. Our findings are plotted in figures 1 and 2. Both the correction to the ground state and the mass gap are normalised to their values for $N \to \infty$. The individual curves are labelled by the value of U and ∞ indicates the Heisenberg limit. On the both sets of curves one can observe the tendency that, for fixed but large enough N with decreasing U, the points approach the $N \to \infty$ values. This is due to the fact that in the argument of the logarithm N enters together with $I_0(2\pi/U)$ which increases with decreasing U. It is striking, however, that for small U and not large enough N the corrections to the ground-state energy are very far away from their $N \to \infty$ values. This is due to the power law type corrections (indicated in (25) but not in (26)). The

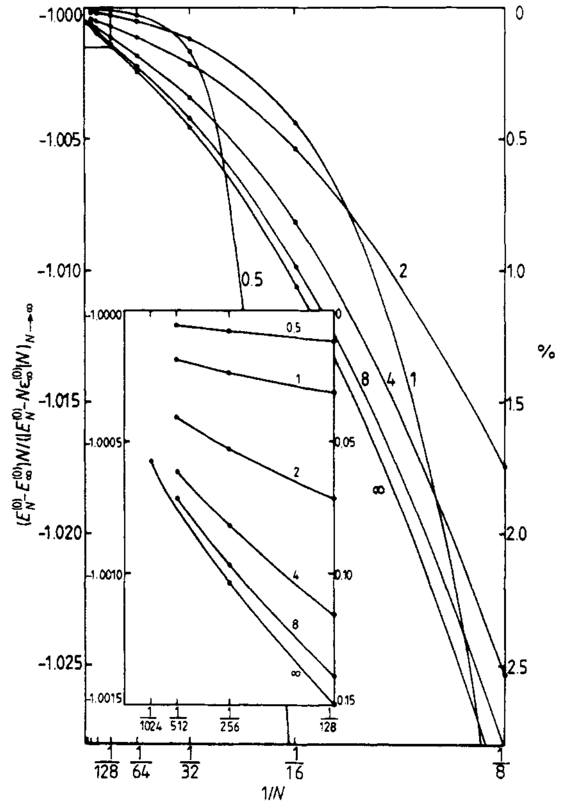

Figure 1. Corrections to the ground-state energy normalised to -1 in the $N\to\infty$ limit plotted against $1/N$. The individual curves are labelled by the value of U.

terms yielding power type corrections are in general of the form

$$\left[I_1\left(\frac{(2n+1)2\pi}{U}\right)\exp\{-[(2n+1)2\pi\Lambda]/U\}\right]$$
$$\times\left[I_0\left(\frac{(2m+1)2\pi}{U}\right)\exp\{-[(2m+1)2\pi\Lambda]/U\}\right]. \tag{33}$$

Since

$$\exp(-2\pi\Lambda/U)/I_0(2\pi/U)\sim N \tag{34}$$

for small U the terms of (33) take the form

$$\left[I_1\left(\frac{(2n+1)2\pi}{U}\right)I_0\left(\frac{(2m+1)2\pi}{U}\right)\{[I_0(2\pi/U)]^{2(m+n)+2}\}^{-1}\right]$$
$$\times\frac{1}{N^{2(m+n)+2}}\sim\frac{1}{N^2}\frac{1}{(\sqrt{U}N)^{2(m+n)}} \tag{35}$$

i.e. their significance is enhanced when U is small. Nevertheless they decay faster than the logarithmic terms. The form (35) is an indication that our calculation breaks down in the $U\to 0$ limit, as discussed earlier.

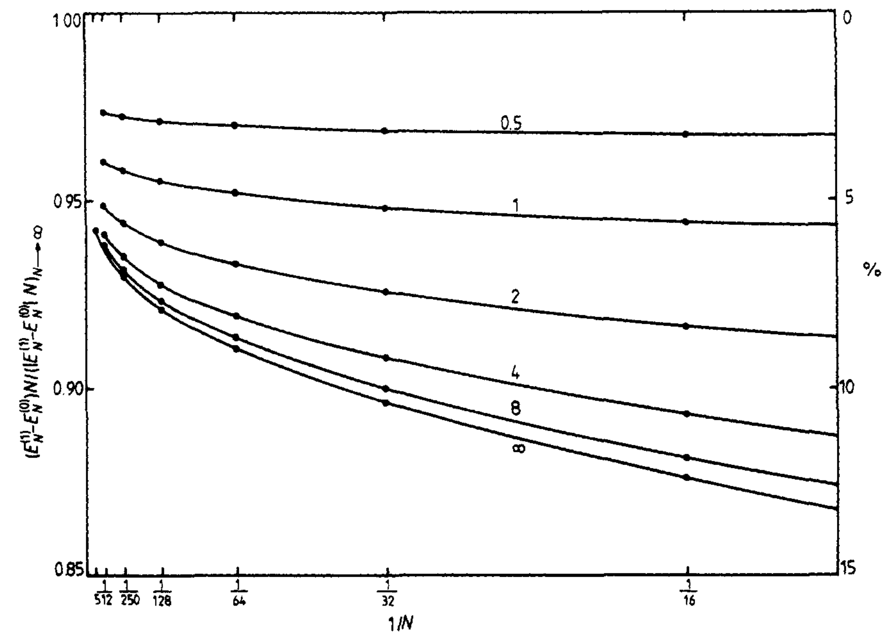

Figure 2. The gap between the first excited and ground states normalised to 1 in the $N \to \infty$ limit plotted against $1/N$. The individual curves are labelled by the value of U.

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