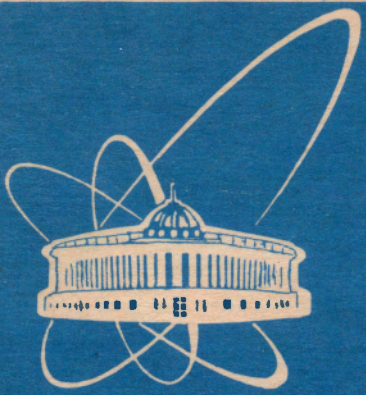

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GROUND-STATE ENERGY OF THE ONE-DIMENSIONAL HUBBARD MODEL IN A SIMPLE SELF-CONSISTENT VERSION OF THE LADDER APPROXIMATION

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1 Introduction

By taking into account only the on-site interactions between the electrons, the Hubbard model (HM) [1, 2, 3] is the simplest improvement of the tight binding approximation; however, it incorporates essential features of strongly correlated electrons leading to a large variety of phenomena such as itinerant magnetism, metal-insulator transition or superconductivity.The one-dimensional (1D) version of the HM is of particular interest because an exact (Bethe-ansatz) solution is available [4]; even in this case, the knowledge of its properties is far from a complete one. Besides their intrinsic importance, the exact results can be also used to test the validity of some approximate theories, many times closer to our intuition than more rigorous methods. The aim of this paper is to compare the Bethe-ansatz (BA) results for the ground-state energy (GSE) of the 1D HM , in both repulsive and attractive case, with those obtained in a simple perturbative approach described below.

The GSE at half filling and zero magnetization (equal number of spins up and down) was obtained analytically by Lieb and Wu [4] ; its dependence on the magnetization was determined by Takahashi [5] . Approximating the Lieb and Wu equations by a set of coupled linear algebraic equations, Shiba [6] calculated the GSE for a positive Hubbard constant U (repulsive case) and arbitrary concentration n ; for $U < 0$ (attractive case), Krivnov and Ovchinnikov [7] found in a similar manner a universal behavior of the GSE in terms of the model parameters. Real space renormalization studies for $U > 0$ and several band fillings [8] show a good agreement with the exact results. For $U < 0$ a simple approximation scheme [9] for the Lieb and Wu equations, arising from weak coupling and low density limit, gives practicaly the same universal behavior of the GSE as that found in the reference [7].

In computing the GSE for the 1D HM we start with the ladder approximation (LA) [10]. This approximation was used by Nagano and Singwi [11] to calculate the GSE for a 1D Fermi gas with a repulsive $\delta-$function interaction whose exact (BA) solution was given by Yang [12] (see also [13]) ; they found that the LA results are the closest to the exact ones in comparison with other approximate many-boby schemes , the maximum deviation in the extreme case of an infinte coupling constant being no more than 20% . For the repulsive HM, it is shown in the next section that the LA gives good results at low densities ($n < 1/2$) or weak coupling regime ($U < 4t$) . In principle, the LA can be improved by imposing a self-consistent condition [14] which amounts to treat the problem in the manner of Brueckner and Gammel [15] ; however, we will consider here that only the bandwidth parameter t is affected by a simplified self-consistent requirement, leading to an effective value t_{ef} determined below. The results for the GSE obtained in this simplified self-consistent ladder

approximation (SCLA) are rather good for every $U > 0$ and all densities. The case of the attractive HM reduces to that of the repulsive HM at half filling and a given magnetization; the results obtained in our SCLA and a comparison with the exact ones are presented in the last section.

2 The repulsive case

The Hamiltonian corresponding to the 1D HM in the Wannier representation is

$$\mathcal{H} = -t\sum_{j,\sigma}\left(c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + H.c.\right) + U\sum_{j} n_{j,\uparrow}n_{j,\downarrow} \quad ; \quad t > 0, \tag{1}$$

where $n_{j,\sigma} = c^{\dagger}_{j,\sigma}c_{j,\sigma}$ $(\sigma = \uparrow, \downarrow)$; in the Bloch representation it is given by

$$\mathcal{H} = \sum_{k.\sigma}\varepsilon(k)\, c^{\dagger}_{k,\sigma}c_{k,\sigma} + \frac{U}{2N}\sum_{k_1,k_2,k_3;\sigma} c^{\dagger}_{k_1,\sigma}c^{\dagger}_{k_2,-\sigma}c_{k_1\oplus k_2\ominus k_3,-\sigma}c_{k_3,\sigma} \tag{2}$$

with

$$\varepsilon(k) = -2tcos(ak) \quad , \quad k \in BZ = \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]. \tag{3}$$

Every k in Eq.(2) belongs to the first Brillouin zone (BZ), a is the lattice constant; and N, the number of sites ; the $\oplus$ ($\ominus$) symbol stands for the usual addition (subtraction) operation and reduction to the BZ.

The GSE in LA is determined from

$$E = E_0 + E_{int} \tag{4}$$

with

$$E_0 = -\frac{4}{\pi}tN\sin(ak_f) \tag{5}$$

and

$$E_{int} = \frac{1}{N}\sum_{|k_1|,|k_2|\le k_F}\gamma(k_1,k_2) \tag{6}$$

γ from Eq.(6) obeys in general an integral equation [16] ; in the particular case of the HM this equation reduces to an algebraic one with the solution

$$\gamma(k_1,k_2) = \frac{U}{1 + Ud_0(k_1,k_2)} \tag{7}$$

In other words, the sum of the ladder diagrams for γ is in fact a geometrical series with the ratio Ud_0 , where

$$d_0(k_1,k_2) \equiv -\frac{1}{N}\sum_{k\in\mathcal{D}}\frac{1}{\varepsilon(k_1) + \varepsilon(k_2) - \varepsilon\left(\frac{K}{2}\oplus k\right) - \varepsilon\left(\frac{K}{2}\ominus k\right)} \quad ; \quad K = k_1 \oplus k_2 \tag{8}$$

and

$$\mathcal{D} \equiv \left\{k \in BZ \,\Big/ \left|\frac{K}{2}\oplus k\right| > k_F, \left|\frac{K}{2}\ominus k\right| > k_F\right\}. \tag{9}$$

For $k_1, k_2 \le k_F \le \frac{\pi}{2a}$, the range $\mathcal{D}$ takes the form

$$\mathcal{D} = \left(-\frac{\pi}{a}, -k_F - \frac{|K|}{2}\right) \cup \left(k_F + \frac{|K|}{2}, \frac{\pi}{a}\right] \tag{10}$$

and passing in Eq.(8) from sum to integral we get

$$d_0(p,q) = \frac{1}{4\pi t\cos(ap)}\begin{cases} \dfrac{1}{\sin(aq)}\ln\left|\dfrac{\sin\left[\frac{a}{2}(k_F + p + q)\right]}{\sin\left[\frac{a}{2}(k_F + p - q)\right]}\right| & , \quad q \neq 0 \\ \tan^{-1}\left[\frac{a}{2}(k_F + p)\right] & , \quad q = 0, \end{cases} \tag{11}$$

where

$$p \equiv \frac{|k_1 + k_2|}{2}, q \equiv \frac{|k_1 - k_2|}{2}. \tag{12}$$

The results for the GSE are represented in Fig.1 by dashed lines ; by comparing them with the BA results from Fig.2 [6], we can see that the deviation grows with the increasing of U or of the density n , defined through

$$ak_F = \frac{\pi}{2}n \tag{13}$$

The previous treatment can be in principle improved by imposing a self-consistency condition : as in the Brueckner theory , we can ask $\varepsilon(k)$ used in finding γ not to have the 'free' expression (3) but an effective form $\varepsilon_{ef}(k)$ which can be determined self-consistently from :

$$\varepsilon_{ef}(k) = \varepsilon(k) + \frac{1}{N}\sum_{|k'|<k_F}\gamma[\varepsilon_{ef}(k), \varepsilon_{ef}(k')] \tag{14}$$

Obviously, Eq.(14) can be solved only numerically, as will be disscused in a forthcoming paper ; here we assume that only the bandwidth parameter modifies, i.e.

$$\varepsilon_{ef}(k) = -2t_{ef}\cos(ak). \tag{15}$$

Because Eq.(14) entails a k-dependence of t_{ef}, we will replace it by a weaker condition: we ask that the interaction energy in LA , calculated with t_{ef}, to

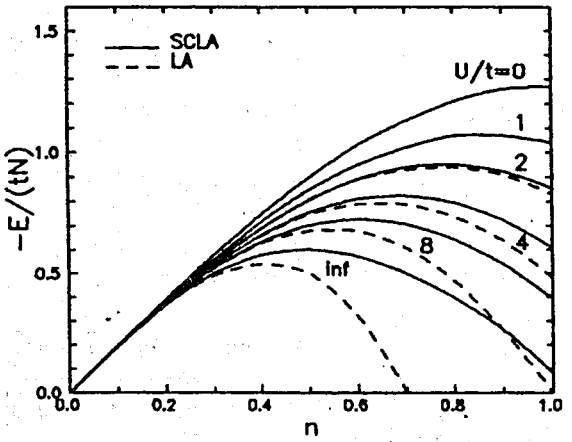

Figure 1. Ground-state energy of the one-dimensional Hubbard model in the ladder approximation (LA) and self-consistent ladder approximation (SCLA).

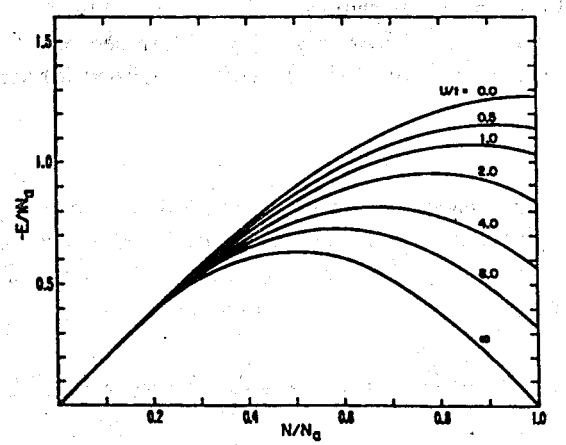

Figure 2 [6]. Bethe-ansatz results for the ground-state energy of the one-dimensional Hubbard model.

coincide with the difference between the ground state energies of a 'free' system with the bandwidth parameter t_{ef} and respectively t, i.e.

$$E_0(t_{ef}) = E_0(t) + E_{int}(t_{ef}) \tag{16}$$

Eq.(16) looks like an average of Eq.(14) over k. Moreover, in order to simplify the expression of t_{ef}, we will consider that $\gamma(k_1, k_2)$ from Eq.(6) can be approximated by $\gamma(0,0)$, assumption which in the 3D case introduces quite small errors ($\sim 5\%$) [3] . From Eq.(16) we get then

$$t_{ef}(n, U/t) = \frac{t}{2}\left\{1 - C(n)\frac{U}{t} + \sqrt{\left[1 - C(n)\frac{U}{t}\right]^2 + \frac{\tan^{-1}(\pi n/4)}{\pi}\frac{U}{t}}\right\}, \tag{17}$$

where

$$C(n) = \frac{1}{4\pi}\left[\frac{\pi^2}{4}\frac{n^2}{\sin(\pi n/2)} + \tan^{-1}(\pi n/4)\right]. \tag{18}$$

The dependence of t_{ef}/t on n for various coupling constant U/t is presented in Fig.3 ; the effective bandwidth always decreases with increasing of n or U/t. The results for the GSE computed from $E_0(t) + E_{int}(t_{ef})$ are drawn in Fig. 1 by solid lines; a clear improvement in comparison with the LA results can be observed. We expect even a better agreement with the exact results by solving Eq.(14) numerically.

3 The attractive case

From the conservation of the number of electrons with a given spin (up or down) and from the electron-hole symmetry of the Hamiltonian (1) it follows that the GSE of the 1D HM with $U < 0$, concentration n and zero magnetization is related to that of $U > 0$ case , half filling and magnetization $s = (1-n)/2$ [4] ; the correspondence can be written as

$$\frac{E}{tN}\left(\frac{n}{2}, \frac{n}{2}; -\frac{|U|}{t}\right) = -\frac{n}{2}\frac{|U|}{t} + \frac{E}{tN}\left(1 - \frac{n}{2}, \frac{n}{2}; \frac{|U|}{t}\right). \tag{19}$$

The formalism presented in the previous section can be adapted to the case of a nonzero magnetization; this can be done by introducing two k_F, one for each spin

$$k_{F1} = \frac{\pi}{a}n_1 \quad , \quad k_{F2} = \frac{\pi}{a}n_2 \,. \tag{20}$$

The summation over $|k_1|, |k_2| \leq k_F$ will be replaced by the summation over $|k_1| \leq k_{F1}$, $|k_2| \leq k_{F2}$ and the domain $\mathcal{D}$ given by Eq.(9) will pass now in the

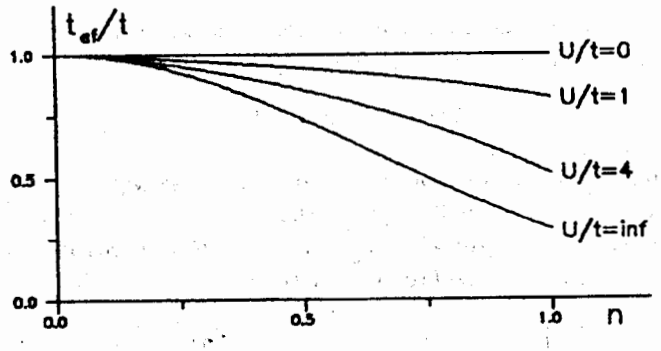

Figure 3. The effective bandwidth parameter as a function of concentration and for different U/t values.

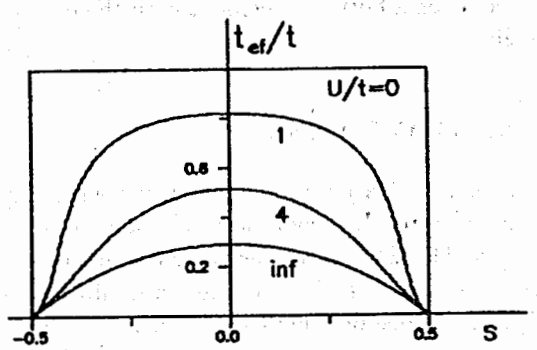

Figure 4. The effective bandwidth parameter at half filling as a function of the magnetization and for some U/t values.

range $\mathcal{R}$

$$\mathcal{R} \equiv \left\{ k \in ZB \Big/ \left|\frac{K}{2} \oplus k\right| > k_{F1},\ \left|\frac{K}{2} \ominus k\right| > k_{F2} \right\}. \tag{21}$$

In our case

$$k_{F1} + k_{F2} = \frac{\pi}{a} \quad (n_1 + n_2 = 1) \tag{22}$$

and we can consider, without loss of generality, that $k_{F2} > k_{F1}$; it can be shown then that the range $\mathcal{R}$ takes the following form.

$$\mathcal{R} = \begin{cases} \left(-\frac{\pi}{a}, \frac{K}{2} \ominus k_{F2}\right) \cup \left(\frac{K}{2} \oplus k_{F2}, \frac{\pi}{a}\right] \ , & |\frac{K}{2}| < min\left\{k_{F1}, \frac{k_{F2}-k_{F1}}{2}\right\} \\ \left[\zeta k_{F2} \oplus |\frac{K}{2}| \oplus \theta_{-}\frac{\pi}{a}, \zeta k_{F2} \ominus |\frac{K}{2}| \ominus \theta_{+}\frac{\pi}{a}\right) \ , & |\frac{K}{2}| > max\left\{k_{F1}, \frac{k_{F2}-k_{F1}}{2}\right\} \\ \left(-\frac{\pi}{a}, \zeta k_{F2} \ominus \theta_{+}\frac{\pi}{a}\right] \cup \left(\zeta k_{F2} \oplus |\frac{K}{2}| \oplus \theta_{-}\frac{\pi}{a}, \frac{\pi}{a}\right] \ , & \frac{k_{F2}-k_{F1}}{2} \le |\frac{K}{2}| < k_{F1} \\ \quad or \\ \left[\frac{K}{2} \oplus k_{F2}, \frac{K}{2} \ominus k_{F2}\right) \ , & k_{F1} \le |\frac{K}{2}| < \frac{k_{F2}-k_{F1}}{2} \ , \end{cases} \tag{23}$$

where

$$\theta_{\pm} \equiv \theta(\pm K) \quad , \quad \zeta \equiv sgn(K). \tag{24}$$

Instead of the coefficient d_0 given by (12), will appear now another coefficient, denoted by f_0 , with the following expression

$$f_0 = \begin{cases} f_{01} \ , & |K| < (k_{F2} - k_{F1}) \\ f_{02} \ , & |K| \ge (k_{F2} - k_{F1}) \ , \end{cases} \tag{25}$$

where

$$f_{01}(p, q; k_{F2}) = \frac{1}{2}[d_0(p, q; k_{F2}) + d_0(-p, q; k_{F2})] \tag{26}$$

$$f_{02}(p, q; k_{F2}) = \frac{1}{2}[d_0(p, q; k_{F2}) + d_0(p, q; \pi/a - k_{F2})] \tag{27}$$

with the same notations as in Eq.(12).

At half filling, even in the case of zero magnetization, the LA gives rather good results only for small U/t. As the magnetization grows the errors become greater and greater; for $s = \pm\frac{1}{2}$ (total magnetization) γ vanishes only for

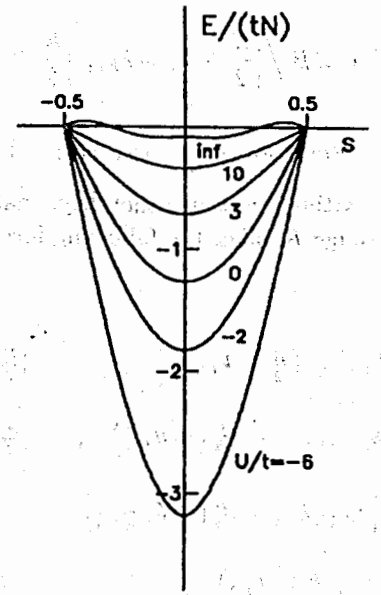

Figure 5. Ground-state energy of the one-dimensional Hubbard model at half filling as a function of the magnetization and for different U/t values in the self-consistent ladder approximation.

certain values of k_1 and k_2. Let us aplly now the same self-consistent condition (16) but at half filling and with the only exception that

$$\begin{aligned} E_0(t) &= -\frac{2}{\pi} tN \left[\sin(ak_{F1}) + \sin(ak_{F2})\right] \\ &= -\frac{4}{\pi} tN \cos(\pi s). \end{aligned} \tag{28}$$

We get in this way an effective bandwidth parameter with the same form (17) but at $n = 1$ and depending on the magnetization

$$t_{ef}(1, s; U/t) = \frac{t}{2}\left\{1 - C(1,s)\frac{U}{t} + \sqrt{\left[1 - C(1,s)\frac{U}{t}\right]^2 + \frac{1}{\pi}\frac{U}{t}}\right\} \tag{29}$$

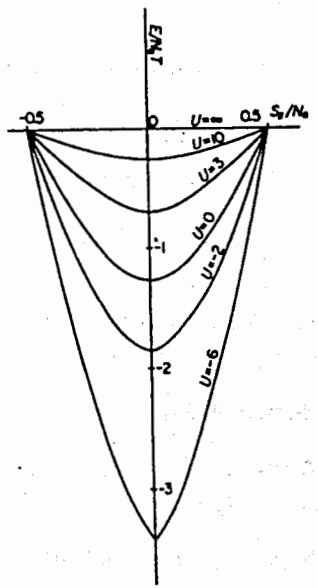

Figure 6 [5]. Bethe-ansatz results for the ground-state energy of the one-dimensional Hubbard model at half filling as a function of the magnetization.

where

$$C(1;s) = \frac{1}{4\pi}\left[\frac{\pi^2}{4}\frac{1}{\cos(\pi s)} + 1\right] \tag{30}$$

The dependence of t_{ef} on the magnetization for various coupling constants is presented in Fig.4 where it can be seen that in the case of a total magnetization the bandwidth parameter becomes zero and consequently the effective interaction vanishes for every value of U/t .

The results for the GSE of the repulsive HM at half filling and a given magetization s are presented in Fig.5 . Let us note that for $U < 0$ (at $n = 1$) the results can be obtained directly from the case $U > 0$ and concentration $n = 1 - 2s$. The comparison with the Bethe-ansatz results from Fig.6 [5] indicates a good agreement up to rather large values of U/t.

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Энергия основного состояния одномерной
модели Хаббарда в простом самосогласованном подходе
в лестничном приближении

Энергия основного состояния одномерной модели Хаббарда вычислена в лестничном приближении; из сравнения с точными результатами в случае отталкивания следует, что приближение хорошо выполняется в пределе низкой плотности и слабого взаимодействия. Лестничное приближение может быть улучшено наложением условия самосогласования; с использованием простых предположений результаты становятся близкими к точным при всех плотностях и значениях констант взаимодействия как в случае отталкивания, так и притяжения.

Работа выполнена в Лаборатории теоретической физики им. Н.Н.Боголюбова ОИЯИ.

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Buzatu F.D. E17-95-64

Ground-State Energy of the One-Dimensional
Hubbard Model in a Simple Self-Consistent Version
of the Ladder Approximation

The ground-state energy of the one-dimensional Hubbard model is calculated within the ladder approximation; from the comparison with the exact results in the repulsive case, it follows that the approximation is good at low densities or small couplings. The ladder approximation can be improved by imposing a self-consistency condition; using a simple assumption, the results become close to the exact ones at all densities and coupling constants in both the repulsive and attractive case.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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