Analytical results of the one-dimensional Hubbard model in the high-temperature limit

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We investigate the grand potential of the one-dimensional Hubbard model in the high-temperature limit, calculating the coefficients of the high-temperature expansion (β-expansion) of this function up to order β^4 by an alternative method. The results derived are analytical and do not involve any perturbation expansion in the hopping constant, being valid for arbitrary density of electrons in the one-dimensional model. In the half-filled case, we compare our analytical results for the specific heat and the magnetic susceptibility, in the high-temperature limit, with the ones obtained by Beni *et al.* [Phys. Rev. B **8**, 3329 (1973)] and Takahashi's integral equations, showing that the latter result does not take into account the complete energy spectrum of the one-dimensional Hubbard model. The exact integral solution by Jüttner *et al.* [Nucl. Phys. B **522**, 471 (1998)] is applied to the determination of the range of validity of our expansion in β in the half-filled case, for several different values of U.

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I. INTRODUCTION

The Hubbard model has been an important candidate to explain distinct physical phenomena such as itinerant magnetism in $4d$ metals,[1] quasi-one-dimensional[2] organic salts, and superconductivity in high T_c for two-dimensional materials.[3]

Since the earliest papers on what today is known as the Hubbard model,[1] perturbation theory has been used due to the absence of exact solutions in dimensions higher than one. For the special case of the one-dimensional Hubbard model, Lieb and Wu[4] applied the Bethe ansatz in order to get the analytical expression of the ground-state wave function of the model with periodic space conditions in the half-filled case. The wave functions of the excited states of the Bethe ansatz and their corresponding energies were derived by Ovchinnikov[5] from Lieb and Wu ground-state wave function. That was the situation of the one-dimensional Hubbard model at $T=0$ in the early 1970s.

At that time, Takahashi[6,7] derived an integral equation for the grand potential of the one-dimensional Hubbard model, based on the known energy spectrum of the Bethe ansatz solutions besides the string hypothesis. The functions that appear in such integral equation satisfy an infinite set of coupled equations. At the same time, Shiba and Pincus[8] numerically studied the exact thermodynamics of the Hubbard model of a one-dimensional model with a finite number of space sites. The longest chain included six sites with a periodic space boundary condition. Based on these results, they extended their conclusions on the behavior of the specific heat and the magnetic susceptibility to the thermodynamic limit. Later, Beni *et al.*[9] applied the standard high-temperature expansion (a perturbation theory in the hopping constant t) to derive the grand potential of the one-dimensional Hubbard model up to order t^2. The literature offers many examples of high temperature expansions of the grand canonical partition function for the Hubbard model in d-dimensions for $d \geqslant 2$, some of them up to order β^9 ($\beta = 1/kT$).[10–12] However, all these works refer to some perturbative scheme where one of the characteristic constants of the model (i.e., its parameters) must be much larger than the other ones.

More recently, the interest on theoretical aspects of the one-dimensional Hubbard model returned when Shastry[13–15] proved its integrability. A very interesting approach was developed where a d-dimensional quantum system at finite temperature is mapped onto a $(d+1)$-dimensional classical model. In this method, the calculation of the grand potential of the quantum system reduces to obtaining the largest eigenvalue of the quantum transfer matrix of the $(d+1)$-dimensional classical model. This was successfully applied to many quantum systems and, in particular, to the one-dimensional Hubbard model by Klümper and Bariev in 1996 for the half-filled case.[16] In 1998, Martins and Ramos[17] and Jüttner *et al.*[18] fully performed the study of this model at finite temperature. In both references, the largest eigenvalue of the appropriate quantum matrix transfer was obtained through the Bethe ansatz approach. In Ref. 18, Jüttner *et al.* extended the results obtained by Klümper and Bariev to any particle density. Differently from Takahashi's integral solution, the solution obtained by the quantum-transfer matrix approach includes the solutions with SO(4) symmetry for the one-dimensional Hubbard model.[19]

Charret *et al.*[20] developed a method to calculate the analytical expression of the exact coefficient of the high-temperature expansion of the grand canonical partition func-

tion at each order in β, applying this method to the calculation of the first three terms of the grand canonical partition function for the one-dimensional generalized Hubbard model.[21] The method is *not* based on the knowledge of the energy spectrum of the one-dimensional Hubbard model.

In the present paper, we will apply the approach developed in Ref. 20 to get the coefficients associated to orders β^3 and β^4 of the high-temperature expansion of the grand potential per site of the one-dimensional Hubbard model subject to a periodic space boundary condition. Our results are *analytical* and do not rest upon any additional hypothesis on the constants that characterize the model. We should point out that we do *not* perform a perturbative expansion besides the high-temperature expansion, that is we do a β expansion of the grand canonical partition function for any density of electrons. In Sec. II we present the Grassmannian functions associated to the model, necessary to the application of the results of Ref. 20. In Sec. III we present the coefficients at orders β^4 and β^5 of the β expansion of the grand canonical partition function of the one-dimensional Hubbard model. Section IV is devoted to comparing our results to the ones known in the literature.[6,9,18] In Sec. IV A we compare our results to the perturbation expansion carried out by Beni *et al.*[9] of the grand potential per site in the hopping term t. In Sec. IV B we present a numerical comparison between Takahashi's results and ours, in the half-filled case. Finally, in Sec. IV C we study, for different values of U, the range of validity of our expressions in β, by comparing them to the numerical solutions provided by Jüttner *et al.* integral equations for the specific heat and magnetic susceptibility. Section V contains our conclusions.

II. ONE-DIMENSIONAL HUBBARD MODEL

The Hamiltonian that describes the one-dimensional Hubbard model in the presence of an external constant magnetic field in the $\hat{z}$ direction is:[1]

$$\mathbf{H}=t\sum_{i=1}^{N}\sum_{\sigma=-1,1}(\mathbf{a}_{i\sigma}^{\dagger}\mathbf{a}_{i-1,\sigma}+\mathbf{a}_{i\sigma}^{\dagger}\mathbf{a}_{i+1,\sigma})+U\sum_{i=1}^{N}\mathbf{a}_{i\uparrow}^{\dagger}\mathbf{a}_{i\uparrow}\mathbf{a}_{i\downarrow}^{\dagger}\mathbf{a}_{i\downarrow}+\lambda_B\sum_{i=1}^{N}\sum_{\sigma=-1,1}\sigma\mathbf{a}_{i\sigma}^{\dagger}\mathbf{a}_{i\sigma}, \tag{1}$$

where $\mathbf{a}_{i\sigma}^{\dagger}$ is the creation operator of an electron with spin σ in the ith site, and $\mathbf{a}_{i\sigma}$ is the destruction operator of an electron with spin σ in the ith site. The first term on the right-hand side (rhs) of Eq. (1) is the hopping term of the kinetic energy operator with constant t. U is the strength of the interaction between electrons in the same site but with different spins. We have defined $\lambda_B=\frac{1}{2}g\mu_B B$, where g is the Landé's factor, μ_B is the Bohr's magneton, and B is the constant external magnetic field in the $\hat{z}$ direction. N is the number of space sites in the one-dimensional lattice. We use the convention: $\sigma=\uparrow\equiv 1$ and $\sigma=\downarrow\equiv -1$. The periodic boundary condition in space is implemented by imposing that $\mathbf{a}_{0\sigma}\equiv\mathbf{a}_{N\sigma}$ and $\mathbf{a}_{N+1,\sigma}\equiv\mathbf{a}_{1\sigma}$. Therefore, the hopping terms $\mathbf{a}_{1\sigma}^{\dagger}\mathbf{a}_{0\sigma}$ and $\mathbf{a}_{N\sigma}^{\dagger}\mathbf{a}_{N+1,\sigma}$ become $\mathbf{a}_{1\sigma}^{\dagger}\mathbf{a}_{N\sigma}$ and $\mathbf{a}_{N\sigma}^{\dagger}\mathbf{a}_{1\sigma}$, respectively. We point out that the Hamiltonian (1) is already in normal order, and the method by Charret *et al.*[20] can be applied directly.

First of all, the high-temperature expansion $\beta\ll 1$ for the grand canonical partition function $\mathcal{Z}(\beta;\mu)$ is

$$\mathcal{Z}(\beta;\mu)=\mathrm{Tr}[e^{-\beta\mathbf{K}}]=\mathrm{Tr}[\mathbb{1}]+\sum_{n=1}^{\infty}\frac{(-\beta)^n}{n!}\mathrm{Tr}[\mathbf{K}^n], \tag{2}$$

where $\mathbf{K}=\mathbf{H}-\mu\mathbf{N}$, $\mathbf{H}$ is the Hamiltonian of the system, $\mathbf{N}$ is the total number of electrons operator, and μ is the chemical potential with $\beta=1/kT$; k is the Boltzmann constant and T is the absolute temperature.

We showed in Ref. 20 that for any self-interacting fermionic quantum system, the coefficients of the β expansion (2) can be written as multivariable Grassmann integrals. For the one dimensional ($d=1$), these coefficients are

$$\mathrm{Tr}[\mathbf{K}^n]=\int\prod_{I=1}^{2nN}d\eta_I d\overline{\eta}_I\exp\left[\sum_{I,J=1}^{2nN}\overline{\eta}_I A_{IJ}\eta_J\right]\times\mathcal{K}^{(n)}(\overline{\eta},\eta;\nu=0)\mathcal{K}^{(n)}(\overline{\eta},\eta;\nu=1)\cdots\times\mathcal{K}^{(n)}(\overline{\eta},\eta;\nu=n-1), \tag{3}$$

where $\overline{\eta},\eta$ are Grassmann generators, $\mathcal{K}^{(n)}$ is the kernel of the $\mathbf{K}$ operator and the matrix $\mathbf{A}$ is given by

$$\mathbf{A}=\begin{pmatrix}\mathbf{A}^{\uparrow\uparrow} & \mathbb{0}\\ \mathbb{0} & \mathbf{A}^{\downarrow\downarrow}\end{pmatrix} \tag{4}$$

so that

$$\mathbf{A}^{\uparrow\uparrow}=\mathbf{A}^{\downarrow\downarrow}=\begin{pmatrix}\mathbb{1}_{N\times N} & -\mathbb{1}_{N\times N} & \mathbb{0}_{N\times N} & \cdots & \mathbb{0}_{N\times N}\\ \mathbb{0}_{N\times N} & -\mathbb{1}_{N\times N} & -\mathbb{1}_{N\times N} & \cdots & \mathbb{0}_{N\times N}\\ \vdots & & & & \vdots\\ \mathbb{1}_{N\times N} & \mathbb{0}_{N\times N} & \mathbb{0}_{N\times N} & \cdots & \mathbb{1}_{N\times N}\end{pmatrix}. \tag{5}$$

Each matrix $\mathbf{A}^{\sigma\sigma}$ has dimension $nN\times nN$, $\mathbb{1}_{N\times N}$, and $\mathbb{0}_{N\times N}$ being the identity and null matrices in dimension $N\times N$, respectively. Here, N is the number of space sites and n is the power of the β term. The matrix $\mathbf{A}$ is independent of the particular model under consideration.[20]

The kernel of the operator $\mathbf{K}$ for the one-dimensional Hubbard model on the lattice, written in terms of the Grassmann generators $\overline{\eta}_I$ and η_J, is equal to

$$\mathcal{K}^{\textcircled{n}}(\overline{\eta},\eta;\nu)=\sum_{l=1}^{N}\sum_{\sigma=\pm 1}(\sigma\lambda_B-\mu)\,\overline{\eta}_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}\,\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}$$
$$+\sum_{l=1}^{N}\sum_{\sigma=\pm 1}t\left[\overline{\eta}_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}\,\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l+1}\right.$$
$$\left.+\overline{\eta}_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}\,\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l-1}\right]+\sum_{l=1}^{N}U\,\overline{\eta}_{(n+\nu)N+l}\,\eta_{(n+\nu)N+l}\,\overline{\eta}_{\nu N+l}\,\eta_{\nu N+l}, \tag{6}$$

where the mapping[20]

$$\eta_\sigma(x_l,\tau_\nu)\equiv\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l} \tag{7}$$

has been used. The generators $\overline{\eta}_\sigma(x_l,\tau_\nu)$ have an equivalent mapping. These generators satisfy the boundary conditions:

a. Periodic boundary conditions in space.

$$\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+N+1}\equiv\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+1}$$

and

$$\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N}\equiv\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+N}.$$

b. Anti-periodic boundary condition in the temperature (ν).

$$\eta_{\left[\frac{(1-\sigma)}{2}n+n\right]N+l}=-\eta_{\left[\frac{(1-\sigma)}{2}n\right]N+l},$$
$$\text{for } l=1,2,\cdots,N, \text{ and } \sigma=\mp 1.$$

In order to write down the terms that contribute to $\mathcal{K}^{\textcircled{n}}(\overline{\eta},\eta;\nu)$ in a simplified way, we define

$$\mathcal{E}(\overline{\eta},\eta;\nu;\sigma)\equiv\sum_{l=1}^{N}\overline{\eta}_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}\,\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}; \tag{8}$$

$$\mathcal{T}^{\mp}(\overline{\eta},\eta;\nu;\sigma)\equiv\sum_{l=1}^{N}\overline{\eta}_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l}\,\eta_{\left[\frac{(1-\sigma)}{2}n+\nu\right]N+l\pm 1}. \tag{9}$$

We also define

$$\mathcal{E}(\overline{\eta},\eta;\nu)\equiv\sum_{\sigma=\pm 1}E(\sigma)\mathcal{E}(\overline{\eta},\eta;\nu;\sigma), \tag{10}$$

$$\mathcal{T}^{\mp}(\overline{\eta},\eta;\nu)\equiv\sum_{\sigma=\pm 1}t\mathcal{T}^{\mp}(\overline{\eta},\eta;\nu;\sigma), \tag{11}$$

and

$$\mathcal{U}(\overline{\eta},\eta;\nu)\equiv U\sum_{l=1}^{N}\overline{\eta}_{(n+\nu)N+l}\,\eta_{(n+\nu)N+l}\,\overline{\eta}_{\nu N+l}\,\eta_{\nu N+l}, \tag{12}$$

where $E(\sigma)\equiv\sigma\lambda_B-\mu$. Now, for the one-dimensional Hubbard model, the Grassmannian function $\mathcal{K}^{\textcircled{n}}(\overline{\eta},\eta;\nu)$ can be written as [see Eq. (6)]

$$\mathcal{K}^{\textcircled{n}}(\overline{\eta},\eta;\nu)=\mathcal{E}(\overline{\eta},\eta;\nu)+\mathcal{T}^{-}(\overline{\eta},\eta;\nu)+\mathcal{T}^{+}(\overline{\eta},\eta;\nu)$$
$$+\mathcal{U}(\overline{\eta},\eta;\nu). \tag{13}$$

III. THE COEFFICIENTS OF THE β EXPANSION OF THE GRAND POTENTIAL FOR THE ONE-DIMENSIONAL HUBBARD MODEL

In Ref. 21, we calculated the coefficients of the terms of order β^2 and β^3 in Eq. (2) for the one-dimensional Hubbard model, for arbitrary values of the constants t, U, μ, and B (the external magnetic field). In this section, the coefficients of orders β^4 and β^5 are calculated.

The evaluation of integrals has been performed by a number of procedures (computer programs) developed by the authors in the symbolic system MAPLE 5.1. This collection of procedures is the computational implementation of the method described in Ref. 20. We have called this package[22] of procedures `gint`.

The procedure `perm`, contained in the package, is a useful tool to calculate the independent non-null terms that contribute to $\mathrm{Tr}[\mathbf{K}^4]$ and $\mathrm{Tr}[\mathbf{K}^5]$, and implements the symmetries discussed in Ref. 21. The procedure `gint`, in its turn, calculates the multivariable Grassmann integrals, taking into account the property of factorization into subgraphs (for details, see Ref. 21).

We introduce a simplified notation,

$$\langle\mathcal{O}_1(\nu_1)\cdots\mathcal{O}_m(\nu_m)\rangle$$
$$\equiv\int\prod_{I=1}^{2nN}d\,\eta_I d\,\overline{\eta}_I\exp\left(\sum_{I,J=1}^{2nN}\overline{\eta}_I A_{IJ}\eta_J\right)$$
$$\times\mathcal{O}_1(\overline{\eta},\eta;\nu_1)\cdots\mathcal{O}_m(\overline{\eta},\eta;\nu_m), \tag{14}$$

which let us write the independent terms that contribute to $\mathrm{Tr}[\mathbf{K}^4]$ in Eq. (2) with $n=4$ as

$$\begin{aligned}\mathrm{Tr}[\mathbf{K}^4] = {} & \langle \mathcal{E}\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 4\langle \mathcal{U}\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 2\langle \mathcal{U}\mathcal{E}\mathcal{U}\mathcal{E}\rangle + 8\langle \mathcal{U}\mathcal{T}^-\mathcal{T}^+\mathcal{E}\rangle \\ & + 4\langle \mathcal{U}\mathcal{U}\mathcal{E}\mathcal{E}\rangle + 4\langle \mathcal{U}\mathcal{U}\mathcal{U}\mathcal{E}\rangle + \langle \mathcal{U}\mathcal{U}\mathcal{U}\mathcal{U}\rangle + 4\langle \mathcal{T}^-\mathcal{E}\mathcal{T}^+\mathcal{E}\rangle \\ & + 8\langle \mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{E}\rangle + 4\langle \mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{U}\rangle + 8\langle \mathcal{T}^-\mathcal{T}^+\mathcal{E}\mathcal{E}\rangle \\ & + 8\langle \mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{E}\rangle + 8\langle \mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{U}\rangle + 2\langle \mathcal{T}^-\mathcal{T}^+\mathcal{T}^-\mathcal{T}^+\rangle \\ & + 4\langle \mathcal{T}^-\mathcal{T}^-\mathcal{T}^+\mathcal{T}^+\rangle. \end{aligned} \tag{15}$$

In order to calculate the terms on the rhs of Eq. (15), we need the result of a set of Grassmann multivariable integrals. The procedure `gint` is used for obtaining such results. In Ref. 21 we give a lengthy explanation on how to handle those integrals applying the results of Ref. 23, where multivariable Grassmann integrals are written as co-factors of **A**.

Letting $n=5$, the expression of $\mathrm{Tr}[\mathbf{K}^5]$ output by `perm` is

$$\begin{aligned}\mathrm{Tr}[\mathbf{K}^5] = {} & 5\langle \mathcal{U}\mathcal{E}\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 5\langle \mathcal{U}\mathcal{E}\mathcal{U}\mathcal{E}\mathcal{E}\rangle + 5\langle \mathcal{U}\mathcal{U}\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 5\langle \mathcal{U}\mathcal{U}\mathcal{E}\mathcal{U}\mathcal{E}\rangle + 10\langle \mathcal{U}\mathcal{U}\mathcal{T}^-\mathcal{T}^+\mathcal{E}\rangle + 5\langle \mathcal{U}\mathcal{U}\mathcal{U}\mathcal{E}\mathcal{E}\rangle + 5\langle \mathcal{U}\mathcal{U}\mathcal{U}\mathcal{U}\mathcal{E}\rangle \\ & + \langle \mathcal{U}\mathcal{U}\mathcal{U}\mathcal{U}\mathcal{U}\rangle + \langle \mathcal{E}\mathcal{E}\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{T}^-\mathcal{T}^+\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{T}^-\mathcal{T}^+\mathcal{U}\rangle + 10\langle \mathcal{T}^-\mathcal{U}\mathcal{U}\mathcal{T}^+\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{E}\mathcal{U}\mathcal{E}\rangle \\ & + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{E}\mathcal{E}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{E}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{U}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{U}\mathcal{U}\rangle + 10\langle \mathcal{T}^-\mathcal{E}\mathcal{T}^+\mathcal{U}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{E}\mathcal{T}^+\mathcal{E}\mathcal{E}\rangle \\ & + 10\langle \mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{E}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{U}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{U}\mathcal{U}\rangle + 10\langle \mathcal{T}^+\mathcal{T}^-\mathcal{T}^-\mathcal{T}^+\mathcal{E}\rangle + 10\langle \mathcal{T}^+\mathcal{T}^-\mathcal{T}^-\mathcal{T}^+\mathcal{U}\rangle + 10\langle \mathcal{U}\mathcal{T}^-\mathcal{U}\mathcal{T}^+\mathcal{E}\rangle \\ & + 10\langle \mathcal{U}\mathcal{T}^-\mathcal{E}\mathcal{T}^+\mathcal{E}\rangle + 10\langle \mathcal{U}\mathcal{T}^-\mathcal{T}^+\mathcal{E}\mathcal{E}\rangle + 10\langle \mathcal{U}\mathcal{T}^-\mathcal{T}^+\mathcal{U}\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^-\mathcal{T}^+\mathcal{T}^+\mathcal{E}\rangle + 10\langle \mathcal{T}^-\mathcal{T}^-\mathcal{T}^+\mathcal{T}^+\mathcal{U}\rangle. \end{aligned} \tag{16}$$

The relation between the grand potential per site $\mathcal{W}(\beta;\mu)$ and the grand canonical partition function $\mathcal{Z}(\beta;\mu)$ is

$$\mathcal{W}(\beta;\mu) = -\lim_{N\to\infty}\frac{1}{N\beta}\ln \mathcal{Z}(\beta;\mu). \tag{17}$$

From Eqs. (15), (16), (17) and the results (up to order β^3) derived in Ref. 21, we get the grand potential per site up to order β^4 for the one-dimensional Hubbard model,

$$\begin{aligned}\mathcal{W}(\beta;\mu) = -\Bigg\{ & \frac{2}{\beta}\ln 2 + \left(-\frac{1}{16}Ut^2\lambda_B^2 - \frac{1}{16}U^2t^2\mu + \frac{1}{1024}U^5 + \frac{1}{16}Ut^2\mu^2 + \frac{13}{768}U^3\mu^2 - \frac{1}{768}U^3\lambda_B^2 - \frac{1}{96}U\lambda_B^4 + \frac{1}{96}U\mu^4 \right. \\ & \left. - \frac{5}{768}U^4\mu - \frac{1}{48}U^2\mu^3 + \frac{1}{64}U^3t^2 \right)\beta^4 - \left(-\frac{1}{8}t^2U\mu - \frac{1}{16}U\mu\lambda_B^2 + \frac{1}{96}\mu^4 + \frac{1}{16}t^4 + \frac{1}{96}\lambda_B^4 + \frac{1}{1024}U^4 - \frac{1}{48}U\mu^3 \right. \\ & \left. + \frac{1}{8}t^2\mu^2 - \frac{1}{192}U^3\mu + \frac{5}{96}t^2U^2 + \frac{1}{64}U^2\lambda_B^2 + \frac{1}{64}U^2\mu^2 + \frac{1}{16}\mu^2\lambda_B^2 + \frac{1}{8}t^2\lambda_B^2 \right)\beta^3 \\ & + \left(-\frac{U^3}{64} + \frac{1}{16}U\lambda_B^2 - \frac{1}{16}\mu^2U + \frac{1}{16}\mu U^2 \right)\beta^2 + \left(\frac{1}{4}\mu^2 + \frac{1}{4}\lambda_B^2 - \frac{1}{4}\mu U + \frac{t^2}{2} + \frac{3}{32}U^2 \right)\beta - \left(-\mu + \frac{U}{4} \right) + \mathcal{O}(\beta^5) \Bigg\}. \end{aligned} \tag{18}$$

It is important to stress that the coefficients of the β expansion of $\mathcal{W}(\beta;\mu)$ are exact for any set of constants (t, U, μ, and B) of this model. From Eq. (18) we can obtain the strong limit approximation having $U \gg t$, as well as the atomic limit approximation having $U \ll t$. No matter how large the values of the constants, the high-temperature expansion still makes sense, provided that those values are finite. In this case, the β region where expression (18) is *bona fide* is diminished.

From expression (18), we can derive any physical quantity for the model at thermal equilibrium at high temperature. In the following we consider the two quantities:

(i) the specific heat at constant length and fixed chemical potential $C_L(\beta)$,

$$C_L(\beta) = -k\beta\frac{\partial}{\partial\beta}\left[\beta^2\frac{\partial\mathcal{W}(\beta;\mu)}{\partial\beta}\right]; \tag{19}$$

(ii) the magnetic susceptibility $\chi(\beta)$,

$$\chi(\beta) = -\left(\frac{1}{2}g\mu_B\right)^2\frac{\partial^2\mathcal{W}(\beta;\mu)}{\partial\lambda_B^2}. \tag{20}$$

In general, the available information is in terms of the density of electrons in the chain, instead of the chemical potential. The density of electrons is given by

$$\frac{N_A}{N} = -\frac{\partial \mathcal{W}(\beta;\mu)}{\partial \mu}, \tag{21}$$

where N_A is the number of electrons in the chain and β, λ_B and all the other constants of the model, are kept constants in the partial derivative. From Eq. (18) we get

$$\begin{aligned}\rho \equiv \frac{N_A}{N} = &\left(-\frac{1}{16}t^2U^2 + \frac{1}{8}U\mu t^2 + \frac{13}{384}\mu U^3 \right. \\ &\left. + \frac{1}{24}U\mu^3 - \frac{5}{768}U^4 - \frac{1}{16}U^2\mu^2 \right)\beta^4 \\ &- \left(-\frac{1}{8}Ut^2 - \frac{1}{16}U\lambda^2 + \frac{1}{24}\mu^3 - \frac{1}{16}\mu^2 U \right. \\ &\left. + \frac{1}{4}t^2\mu - \frac{1}{192}U^3 + \frac{1}{32}\mu U^2 + \frac{1}{8}\mu\lambda^2 \right)\beta^3 \\ &+ \left(-\frac{1}{8}\mu U + \frac{1}{16}U^2 \right)\beta^2 + \left(\frac{1}{2}\mu - \frac{1}{4}U \right)\beta + 1.\end{aligned} \tag{22}$$

IV. COMPARISON TO PREVIOUS RESULTS

In this section, we compare our results derived in Sec. III to the ones presented by Beni *et al.*,[9] as well as to Takahashi's integral solution[6] and to the exact integral solution derived by Jüttner *et al.*[18] We explore the results of these references in the high-temperature region, where our expressions are valid, comparing two derived thermodynamical quantities, namely, the specific heat and the magnetic susceptibility, obtained by each particular approach.

Throughout this section we have chosen $t=1$; all the remaining constants in the model are expressed in units of t.

A. Comparison to Beni *et al.*

The high-temperature expansion (HTSE) has been applied to the calculation of the coefficients of the β expansion in Eq. (2). Henderson *et al.*[12] calculated the terms up to $(\beta t)^9$ of this series for the single-band Hubbard model in two- and three-dimensional lattices. Bartkowiak *et al.*[24] calculated the high-temperature expansion of the extended Hubbard model on the simple cubic lattice up to order $(\beta t)^6$. On the other hand, the high-temperature expansion of the one-dimensional Hubbard model was carried out by Beni *et al.*[9] up to order t^2 only, but to all orders in β. We believe that it is always interesting to compare analytical results, mainly because in Ref. 9 the perturbation expansion is done under the condition $t/U \ll 1$ and in the temperature region where $\beta t \ll 1$ whereas our results are valid for *any* ratio t/U.

We compare our main result [Eq. (18)] for the grand potential per site of the one-dimensional Hubbard model to the expansion of Eq. (8) of Ref. 9 up to order β^4. Even though both calculations allow us to handle the problem with arbitrary density of electrons in the chain, we consider here the half-filled case ($\rho=1$) only, when we have $\mu=U/2$. The difference between the expressions derived for the grand potential per site in both calculations is

$$\mathcal{W}(\beta) - \mathcal{W}_{BPH}(\beta) = \frac{1}{16}\beta^3 t^4, \tag{23}$$

where $\mathcal{W}_{BPH}(\beta)$ is the grand potential per site derived from the expressions of Beni *et al.* Such difference has diverse consequences for distinct physical quantities. In the case of the specific heats $C_L(\beta)$ and $C_{BPH}(\beta)$, the difference between our result and the one derived by Beni *et al.* is

$$C_L(\beta) - C_{BPH}(\beta) = \frac{3}{4}\beta^4 t^4, \tag{24}$$

where $C_{BPH}(\beta)$ is the specific heat derived from Ref. 9. The difference between these two expressions is independent of U, but the relative error decreases as U increases.

The magnetic susceptibility is obtained from the grand potential per site $\mathcal{W}(\beta)$ through Eq. (20). We see from Eq. (23) that the difference between $\mathcal{W}(\beta)$ and $\mathcal{W}_{BPH}(\beta)$ is independent of the external magnetic field. Both approaches give the same expression for the magnetic susceptibility up to order β^4. It is worth noticing that the result for this thermodynamic function derived in Ref. 9 was obtained for $t/U \ll 1$, whereas the approach presented here allows one to affirm that, up to this order in β, it is valid for *arbitrary* values of t/U.

In Ref. 24 Bartkowiak *et al.* asserted: "*The HTSE method is exact at each order in the inverse temperature* β." We have a simple argument to understand this assertion. In the β expansion of the grand canonical partition function [see Eq. (2)], the β^n term is multiplied by $\mathrm{Tr}[\mathbf{K}^n]$, that is proportional to $t^{2n_1}E^{n_2}U^{n_3}$, with $2n_1+n_2+n_3=n$. For *even* values of n, the term of highest order in the hopping constant t that contributes to order β^n is t^n. Actually, this is the only term to be calculated in order to get the exact coefficient of the β expansion of $\mathcal{Z}(\beta;\mu)$, since all the other terms proportional to t^{2n_1} $(n_1=0,\ldots,n/2)$ would have been calculated in lower orders in the t expansion after the standard high temperature expansion.[25] When we include the term $(t\beta)^n$ in the standard high-temperature expansion, we lift the restriction $t/U \ll 1$, under which perturbation theory is usually done. When n takes odd values, we do not have the term t^n since we calculate traces in expansion (2). Therefore all the coefficients of the term β^n would have been calculated already in the terms proportional to t^{2n_1}, $[n_1=0,1,\ldots,(n-1)/2]$. We only need to collect all the terms of the form $t^{2n_1}E^{n_2}U^{n_3}$, under the condition $2n_1+n_2+n_3=n$ and drop the restriction $t/U \ll 1$.

This analysis is coherent with result (23), where only the term of order β^4 in $\mathcal{W}(\beta;\mu)$ yielded a correction to the expansion obtained by Beni *et al.*[9]

B. Comparison to Takahashi's integral solution

In Ref. 6, Takahashi presents a set of coupled integral equations of infinite order for the grand potential [see Eqs. (3.5b) and (3.6) in Ref. 6]. Equation (3.6a) in Ref. 6 has a typographical error, which has been corrected in Ref. 7.

We have obtained a numerical solution of Takahashi's equations by recursively iterating those equations up to third

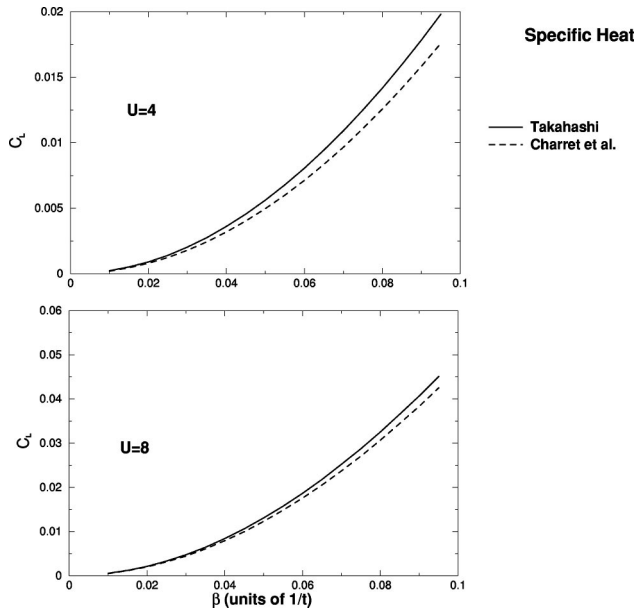

FIG. 1. Specific heat from Takahashi's equations (solid line) and Charret *et al.* (dashed line) for $U=4$ and $U=8$.

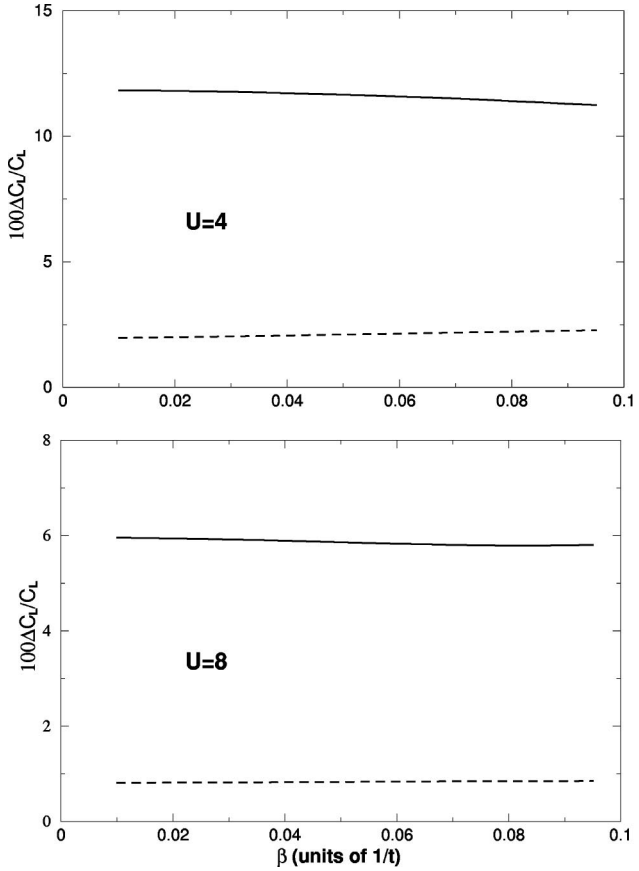

FIG. 2. Relative error in the specific heat obtained from two successive approximations to Takahashi's equations (dashed lines) and the difference between Takahashi's and Charret *et al.* results (solid lines) for $U=4$ and $U=8$.

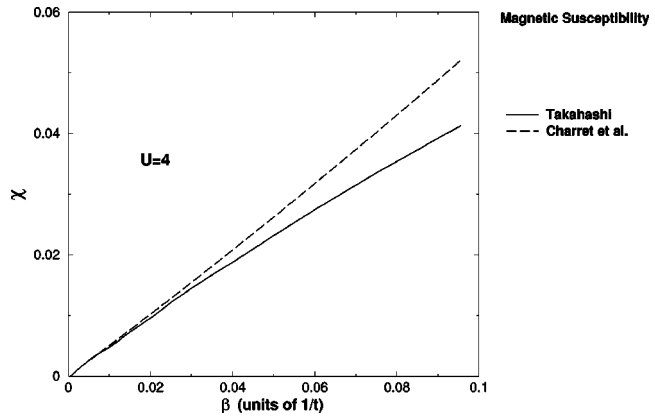

FIG. 3. Magnetic susceptibility from Takahashi's equations (solid line) and Charret *et al.* (dashed line) for $U=4$.

order. Doing so, we have obtained the specific heat and magnetic susceptibility in the half-filled case.

More explicitly, we did our numerical analysis of Eqs. (3.6) for $n=1,2,3$. For $n=1$, we took into account Eqs. (3.6a), (3.6b), and (3.6c), we considered several initial conditions where $\eta_1=\eta_1'=\eta_2=\eta_2'\equiv\theta$, by choosing some distinct values of θ. The numerical results obtained are independent of the particular choice of θ. For $n=2$, the new variables (η_3,η_3') where included, as well as Eqs. (3.6d) and (3.6e) with $n=2$. We chose initial conditions such that $\eta_1=\eta_1'=\cdots=\eta_3=\eta_3'\equiv\theta$ for several different values of θ, and again the results were independent of θ. For $n=3$, two more variables $(\eta_3=\eta_3')$ and two more equations [namely, (3.6d) and (3.6e) with $n=3$] were included in the computations, and the same type of initial condition was used. Again, the particular value of θ did not interfere with the results.

Such iterated solutions showed a good convergence: the difference between the calculated grand potentials with $n=2$ and $n=3$ is smaller than 1%. The difference between Takahashi's and Charret *et al.* results are much greater.

We compare our results and those coming from Takahashi's equations for two different values of U; namely, $U=4$ and $U=8$ (in units of t). We have β ranging over the interval [0,0.1]. Within this range (and for the values of U under consideration) our results are almost exact (see Sec. IV C). We compare two physical quantities: the specific heat and the magnetic susceptibility. The specific heat curves are shown in Fig. 1, for $U=4$ and $U=8$. The difference between our results and Takahashi's solutions is not due to numerical approximations. To make this point clear, we show in Fig. 2 that the relative error between the approaches is larger than the estimated numerical error. In Fig. 3 we compare the results for the magnetic susceptibility. They agree for small values of β, but as β increases their difference again cannot be explained by numerical errors.

We conclude that, since our results can be considered exact in the given range of β, something must be missing in Takahashi's result. For such small values of β, both results should agree perfectly, but that is not the case.

C. Comparison to the exact integral solution by Jüttner *et al.*

In Refs. 17 and 18, the thermodynamic properties of the one-dimensional Hubbard model are fully determined by two

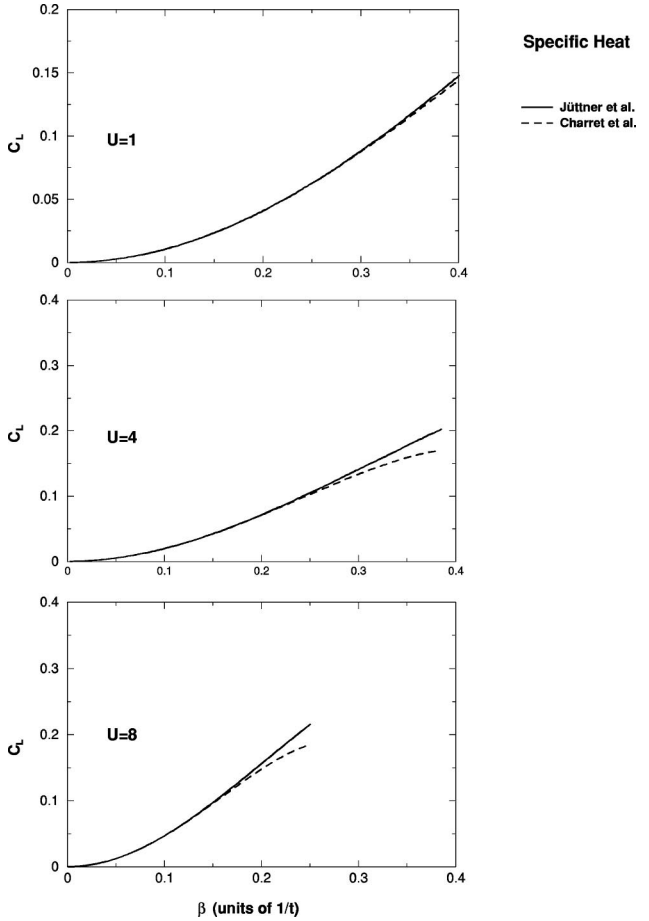

FIG. 4. Specific heat from Jüttner *et al.* equations (solid line) and Charret *et al.* (dashed line) for $U=1$, $U=4$, and $U=8$.

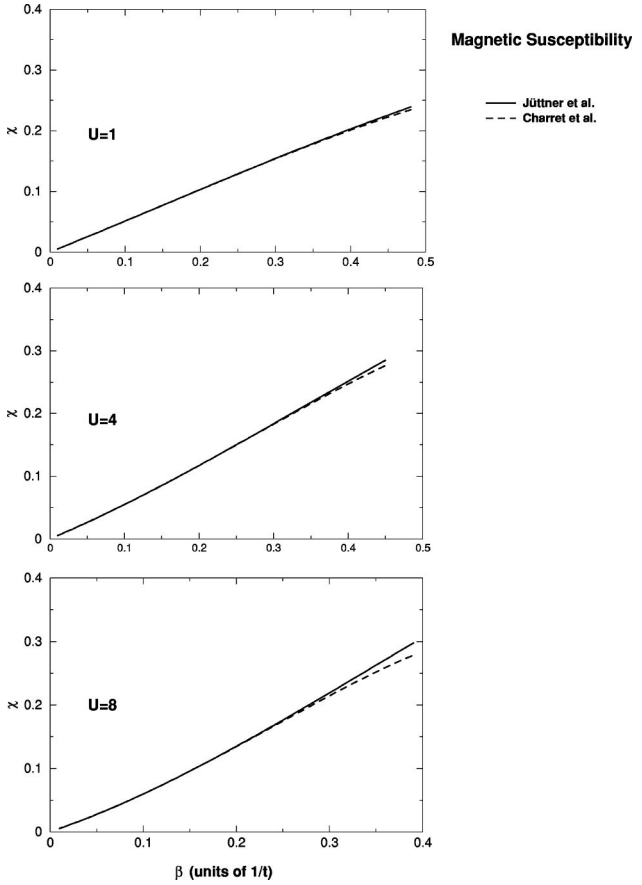

FIG. 5. Magnetic susceptibility from Jüttner *et al.* equations (solid line) and Charret *et al.* (dashed line) for $U=1$, $U=4$, and $U=8$.

independent approaches; one important point is that solutions with built-in SO(4) symmetry appear in both, making their results exact. The same applies to Ref. 16.

We take the results by Jüttner *et al.*[18] to discuss the validity of our expressions, since they have managed to write the largest eigenvalue of the suitable quantum transfer matrix as the solution of a few coupled integral equations.

In Ref. 18 Jüttner *et al.* extended the results of Ref. 16 for arbitrary particle densities, obtaining a new set of coupled integral equations. In the half-filled case, even though this set is equivalent to the one presented in Ref. 16, it offers much better numerical convergence.

We restrict the comparison of our results with the ones derived in Ref. 18 to the half-filled case. Our physical results are obtained by differentiating properly the grand potential per site in Eq. (18). This comparison can show the range for β which are suitable in describing the thermodynamics of the one-dimensional Hubbard model, for different values of U (in units of t). As in the previous sections, we focus on the specific heat and the magnetic susceptibility.

For the specific heat (see Fig. 4) for $U=1$ at $\beta=0.3$ the relative error between results is 0.63%; at $\beta=0.4$ it amounts to 2.26%. For $U=4$ and $\beta=0.2$, the error is 0.71%; at $\beta=0.24$ it becomes 2%. For $U=8$ our result at $\beta=0.1$ shows an error of 0.15% and at $\beta=0.16$ it is 2%.

For the magnetic susceptibility we get even better results, as shown in Fig. 5. For $U=1$ and $\beta=0.3$ the error is 0.27%; at $\beta=0.4$ it is 0.88% (still less than 1% !). For $U=4$ and $\beta=0.3$ the error is 0.39%; for $\beta=0.4$ it is 1.98%. Finally, for $U=8$ and $\beta=0.2$ the error is 0.3% and for $\beta=0.29$ it becomes 2%.

These comparisons stress that in all studied cases, the precision of our analytical solution turned out to be far better than our initial expectations.

V. CONCLUSIONS

The method developed in Ref. 20 can be easily applied to the one-dimensional Hubbard model, allowing us to derive exact analytical coefficients at each order of the β expansion of the grand potential. With the help of the procedure `gint`, written in the symbolic language MAPLE 5.1, the multivariable Grassmann integrals can be easily calculated. Besides, the property of factorization of graphs into subgraphs, described in Ref. 21, allows us to reduce the number of integrals to be actually calculated. Besides, the method does not involve any further approximation scheme. Even though the physics for $U>0$ and $U<0$ are different, the results of Sec. III apply equally well for both cases.

Beni *et al.*[9] derived a perturbative expansion in the hopping constant t, valid in the temperature range $\beta t \ll 1$. It is

simple to compare our results to theirs, since both methods yielded analytical results. For the sake of comparison, we consider the one-dimensional Hubbard model in the half-filled case. Equation (23) shows that the difference between our result for the grand potential per site and Beni *et al.* is proportional to $t^4\beta^3$; it gives a correction to the specific heat but keeps the magnetic susceptibility unchanged. Our result is compatible with the assertion of Bartkowiak *et al.*[24] that the coefficients derived by the standard high-temperature expansion are exact at each order of β^n. With our correction to the grand potential per site derived by Beni *et al.*, we can drop the condition $t/U \ll 1$ under which it was derived.

Takahashi's integral solution[6] is derived from the energy spectrum of the Bethe ansatz solution of the one-dimensional Hubbard model plus the so-called string hypothesis. In the case of the specific heat, our correction to Takahashi's result is not associated with any numerical approximation or error. We present Fig. 2 to show this fact. For the magnetic susceptibility there is a larger correction to the Takahashi's solution in the high-temperature region. Certainly, these differences come from the fact that Takahashi's calculation does not take into account solutions to the one-dimensional Hubbard model with SO(4) symmetry.[19]

In order to determine the range of validity in β of our analytical solution for the grand potential per site for different values of U (in units of t), we considered the curves of the specific heat and magnetic susceptibility for $U=1$, $U=4$, and $U=8$. In all cases studied the validity of our expressions are far beyond our initial expectations. For example, for $U=1$ the error of our result for the magnetic susceptibility at $\beta=0.4$ is less than 1%. The result of the standard high-temperature expansion is not reliable for $U=1$ and the numerical solution of the coupled integral equations in the approach of Jüttner *et al.*[18] are very much involved, while our analytical result is a very good approximation for $U=1$ up to $\beta=0.4$.

Finally, we should mention that the present approach opens the possibility of calculating the first terms of the β expansion of the grand canonical partition function of the Hubbard model in two space dimensions, as well as of one-dimensional models with inhomogeneities. We believe that improvements on the present approach will render a valuable tool for tackling such problems.

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