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Statistical mechanics of the strongly-correlated Hubbard chain: I. Formulation

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Abstract. We show with the aid of a canonical transformation that separates charge and spin degrees of freedom that the strongly correlated one-dimensional Hubbard model with infinite ($U = \infty$) on-site repulsion is related to a corresponding spinless free-fermion lattice model. Thermodynamic properties of the two models are shown to be closely related whereas the single-particle two-site function for the $U = \infty$ model is shown to be related to a modified many site function for the spinless model which involves many-point correlations The latter is shown to be expressible in terms of the inverse of a certain matrix which should be amenable to numerical and analytical analysis.

1. Introduction

The Hubbard model [1] has received considerable attention over the years as a possible model for itinerant ferromagnetism [2–4], and more recently as a prototype model for strongly correlated electron systems, of which the high-temperature superconductors are thought to be an example [5, 6].

In spite of much effort there are very few rigorous results for the Hubbard model. Certain ground-state properties are known exactly for the one-dimensional model [7, 8], and in higher dimensions it is known that with one hole in an otherwise half-filled band, the ground state is ferromagnetic [9]. The only claimed exact results at finite temperature, of which the authors are aware, are the expressions derived by Sokoloff [10] and Beni *et al* [11] for certain properties of the one-dimensional model in the strong correlation limit of infinite ($U = \infty$) on-site repulsion. Unfortunately, both sets of results contain errors which are due in the main to an incorrect mixing of canonical and grand-canonical descriptions of the model. Nevertheless, the basic observation by Sokoloff and Beni *et al* , which is correct and has been noted subsequently by other authors [12], is that for the $U = \infty$ model in one dimension, the charge and spin degrees of freedom separate and hence the model is in essence equivalent to a corresponding spinless free-fermion model.

Our aim in this paper is to demonstrate this equivalence explicitly through a canonical transformation to operators corresponding to new particles which have only 'charge' or 'spin'. The special feature of the one-dimensional $U = \infty$ model, that spin configurations of the fermions must be preserved, allows us to easily eliminate one of the new species of particles.

As we will show, the thermodynamic properties of the $U = \infty$ model are in fact equivalent to those of a spinless free-fermion model but care needs to be exercised in relating the chemical potentials of the two models. We will also show that the single-particle two-site function for the $U = \infty$ model is expressible in terms of a modified many-site function for the spinless model which is unfortunately quite complex from a computational point of view.

In outline this paper is organized as follows. In section two we define the problem and summarize our main results. The canonical transformation to 'charge' and 'spin' particles is introduced in section 3 and a simple relation connecting the canonical partition functions for the $U = \infty$ and the spinless free-Fermion model is derived. Similar, but more complicated relations, for the single-particle two-site functions in the canonical and grand-canonical ensembles are derived in sections 4 and 5 respectively and in section 6 we derive some thermodynamic properties of the model. We conclude in section 7 with a discussion of our results.

2. The model and statement of the main results

In the strong correlation limit with infinite on-site repulsion, the Hamiltonian for the one-dimensional Hubbard model with V-sites and nearest-neighbour hopping energy t can be written as [13]

$$\mathcal{H}_\infty = -t \sum_{\substack{i=1 \\ \sigma}}^{V} \left(\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+1\sigma} + \tilde{c}_{i+1\sigma}^\dagger \tilde{c}_{i\sigma} \right) \tag{2.1}$$

where

$$\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i-\sigma}). \tag{2.2}$$

In (2.2) $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the usual destruction (creation) operator for a fermion with spin $\sigma = \uparrow, \downarrow$ on site i and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator for a fermion with spin σ on site i.

The canonical partition function for the model (2.1) with N particles of either spin is given by

$$Z_N^\infty(V,T) = \mathrm{Tr}_{\{N\}} \left[\mathcal{P} \exp\left(-\beta \mathcal{H}_\infty\right) \mathcal{P} \right] \tag{2.3}$$

where

$$\mathcal{P} = \prod_{i=1}^{V} \left(1 - n_{i\uparrow} n_{i\downarrow}\right) \tag{2.4}$$

projects out doubly occupied sites in the trace ($\mathrm{Tr}_{\{N\}}$) which is taken over all N-particle states.

In the following section we show that

$$Z_{V-K}^\infty(V,T) = 2^{V-K} Z_K^0(V,T) \tag{2.5}$$

where

$$Z_K^0(V, K) = \mathrm{Tr}_{\{K\}}\left[\exp(-\beta\mathcal{H}_0)\right] \tag{2.6}$$

is the canonical partition function for K spinless Fermions with Hamiltonian

$$\mathcal{H}_0 = -t\sum_{i=1}^{V}\left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right) \tag{2.7}$$

and a_i ($a_i^\dagger$) is the destruction (creation) operator for a spinless fermion at site i.

The relation (2.5) is a direct consequence of the fact that for the $U = \infty$ model in one dimension the only way particles can move on the lattice is by exchanging their position with a hole. Spin degeneracy gives rise to the factor 2^{V-K} in (2.5) and the K spinless particles in (2.5) and (2.7) are essentially the holes in the $U = \infty$ model. A detailed derivation of (2.5) is given in the following section using a canonical transformation that separates the charge and spin degrees of freedom.

In a similar fashion we show in section 4 that ($m \geqslant l + 2$)

$$\begin{aligned}\mathrm{Tr}_{\{V-K\}}&\left[\mathcal{P}\exp\left(-\beta\mathcal{H}_\infty\right)\mathcal{P}\frac{1}{2}\left(c_{l\uparrow}^\dagger c_{m\uparrow} + c_{l\downarrow}^\dagger c_{m\downarrow}\right)\right] \\ &= 2^{V-K}(-1)^{m-l}\,\mathrm{Tr}_{\{K\}}\left[\exp\left(-\beta\mathcal{H}_0\right)a_l a_m^\dagger \prod_{j=l+1}^{m-1}\frac{1}{2}\left(1 + a_j^\dagger a_j\right)\right]\end{aligned} \tag{2.8}$$

where we have used the notation developed above.

In essence, the complicating product term in (2.8) allows for the fact that configurations with spin $-\sigma$ particles between sites l and m do not contribute to the left-hand side of (2.8), and hence spin degrees of freedom are reduced by a factor of two to the power of $m - l - 1$ minus the number of holes between sites l and m.

3. The canonical transformation

To begin, we first consider the vacuum state $|0)$ for the spinless Fermi particles in (2.7) which we define to be the state where all sites are occupied by either up or down spin electrons with no doubly occupied sites. Such a state may be expressed as

$$|0) = \prod_{i=1}^{V} 2^{-1/2}\left(c_{i\uparrow}^\dagger + c_{i\downarrow}^\dagger\right)|0\rangle \tag{3.1}$$

where $|0\rangle$ denotes the true vacuum. The expression (3.1) is not the only possible definition of the vacuum but it will prove most convenient for our purposes. In particular, given (3.1), it is natural to define new operators h_i and s_i by

$$h_i = 2^{-1/2}\left(c_{i\uparrow} + c_{i\downarrow}\right) \tag{3.2}$$

and

$$s_i = 2^{-1/2}\left(c_{i\uparrow} - c_{i\downarrow}\right) \tag{3.3}$$

We observe that (3.2) and (3.3) constitute a canonical transformation on the operators $c_{i\uparrow}$, $c_{i\downarrow}$ and hence both sets of operators $\{h_i\}$, $\{s_i\}$ and their Hermitian conjugates $\{h_i^\dagger\}, \{s_i^\dagger\}$ satisfy the usual Fermi anticommutation relations. We also note that $h_i^\dagger$ creates a particle at site i which has 'charge' but no 'spin' while $s_i^\dagger$ creates a particle at site i which has 'spin' but no 'charge'.

We will subsequently refer to these new Fermi particles as h- and s-particles.

Again, it should be noted that (3.2), (3.3) is not the only possible canonical transformation on $c_{i\uparrow}$, $c_{i\downarrow}$. A rotation through any 'angle', including $\pi/4$ in (3.2), (3.3), in fact produces identical results but without the interpretation mentioned above.

In order to re-express $\mathcal{H}_\infty$ (2.1) in terms of h_i and s_i operators, it is convenient to define the dressed operators $\tilde{h}_i$ and $\tilde{s}_i$ by

$$\tilde{h}_i = h_i(1 - s_i^\dagger s_i) \qquad \tilde{s}_i = s_i(1 - h_i^\dagger h_i). \tag{3.4}$$

It then follows easily from the definitions (2.2), (3.2) and (3.3) that

$$\tilde{c}_{i\uparrow} = 2^{-1/2}(\tilde{h}_i + \tilde{s}_i) \qquad \tilde{c}_{i\downarrow} = 2^{-1/2}(\tilde{h}_i - \tilde{s}_i) \quad . \tag{3.5}$$

and on substitution into (2.1) that

$$\mathcal{H}_\infty = -t\sum_{i=1}^{V}[\tilde{h}_i^\dagger \tilde{h}_{i+1} + \tilde{h}_{i+1}^\dagger \tilde{h}_i + \tilde{s}_i^\dagger \tilde{s}_{i+1} + \tilde{s}_{i+1}^\dagger \tilde{s}_i]. \tag{3.6}$$

In order to evaluate the trace in (2.3) we note that the projection operator $\mathcal{P}$ in (2.4) can be expressed in terms of the h_i and s_i operators as

$$\mathcal{P} = \prod_{i=1}^{V}(1 - h_i^\dagger h_i s_i^\dagger s_i) \tag{3.7}$$

After projection by $\mathcal{P}$ each site can be occupied by either a hole, an h-particle or an s-particle, giving rise to a total of 3^V allowed states for a lattice of V sites.

The special feature now of one dimension in the strong correlation limit, is that h- and s-particles cannot hop over one another and hence movement of these particles is only made possible by movement of holes. This means that once a configurational arrangement of h- and s-particles is specified on a one-dimensional lattice, it must be left invariant during motion of holes. This restriction causes a great deal of degeneracy in the diagonal elements of $\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}$. To be more specific, if we consider a chain of V sites, of which K are occupied by holes, the remaining $N = V - K$ sites may be occupied by either h- or s-particles. However, so far as the diagonal elements in the trace (2.3) are concerned, both h- and s-particles play the same role and hence all configurations with the same value of N give the same contribution to the trace. It thus follows that for given N, $2^N = 2^{V-K}$ different configurations give rise to the same contribution to the trace (2.3) and we can write

$$\mathrm{Tr}_{\{N\}}[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}] = 2^{V-K}\,\mathrm{Tr}_{[K]}^{(h)}[\exp(-\beta\mathcal{H}_\infty)] \tag{3.8}$$

where $\mathrm{Tr}_{[K]}^{(h)}$ denotes a trace over the subspace in which K holes and $V - K$ h-particles only are included. In this particular subspace where there are no s-particles, the s_i-operators in $\mathcal{H}_\infty$ have a null effect and thus $\mathcal{H}_\infty$ on the right-hand side of (3.8) can be replaced by

$$\mathcal{H}_\infty^{(h)} = -t\sum_{i=1}^{V}(h_i^\dagger h_{i+1} + h_{i+1}^\dagger h_i). \tag{3.9}$$

Finally, if we define the destruction operator for a hole on site i by

$$a_i = (-1)^{i-1}h_i^\dagger \tag{3.10}$$

where the factor $(-1)^{i-1}$ in (3.10) is chosen so that

$$a_i^\dagger|0) = h_1^\dagger h_2^\dagger\cdots h_{i-1}^\dagger h_{i+1}^\dagger\cdots h_V^\dagger|0\rangle \tag{3.11}$$

then $\mathcal{H}_\infty^{(h)}$ is transformed into $\mathcal{H}_0$ defined by (2.7) and

$$\mathrm{Tr}_{[K]}^{(h)}[\exp(-\beta\mathcal{H}_\infty)] = \mathrm{Tr}_{\{K\}}[\exp(-\beta\mathcal{H}_0)] \tag{3.12}$$

where $\mathrm{Tr}_{\{K\}}$ is now the trace in the space spanned by the states

$$|i_1 i_2\cdots i_K\rangle = a_{i_1}^\dagger a_{i_2}^\dagger\cdots a_{i_K}^\dagger|0) \tag{3.13}$$

with K holes and $|0)$ is the vacuum state defined by (3.1).

Combining (3.8) and (3.12) gives the stated result (2.5).

4. Canonical form of the single-particle two-site function

For our present purposes we define the canonical single-particle two-site function by

$$\left\langle\frac{1}{2}(c_{l\uparrow}^\dagger c_{m\uparrow} + c_{l\downarrow}^\dagger c_{m\downarrow})\right\rangle$$
$$= Z_N^\infty(V,T)^{-1}\,\mathrm{Tr}_{\{N\}}\left[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}\frac{1}{2}(c_{l\uparrow}^\dagger c_{m\uparrow} + c_{l\downarrow}^\dagger c_{m\downarrow})\right] \tag{4.1}$$

where we have used the notation developed in the previous two sections. For want of a better name we call (4.1) the single-particle two-site function in the canonical ensemble.

As we will see in a moment, even though charge and spin degrees of freedom separate in the one-dimensional $U = \infty$ model and the thermodynamic properties are essentially equivalent to those of a spinless free-fermion model, correlations between particles are maintained and it is by no means an easy task to evaluate (4.1) for arbitrary lattice sites l and m.

In terms of the h_i- and s_i-operators (3.2), (3.3) the trace in (4.1) can be written as

$$\mathrm{Tr}_{\{N\}}[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}h_l^\dagger h_m]$$
$$\equiv {\sum_{\{x\}}}'\langle x_1x_2\cdots x_V|\exp(-\beta\mathcal{H}_\infty)h_l^\dagger h_m|x_1x_2\cdots x_V\rangle \tag{4.2}$$

where use has been made of the fact that the transformed Hamiltonian (3.6) is symmetric with respect to h- and s-particles. In order to clarify our subsequent argument, we have expressed the trace in (4.2) as a sum over all 3^V allowed states $\{x\} = (x_1, x_2, \ldots, x_V)$, with $x_i = 0, h, s$ denoting occupation of the ith site by a hole, an h-particle or an s-particle respectively, and the prime on the sum denoting a sum over such states with a fixed total number N of h- and s-particles.

Since, by definition,

$$h_l^\dagger h_m |x_1 x_2 \cdots x_V\rangle = \begin{cases} |x_1 \cdots x_{l-1} h\, x_{l+1} \cdots x_{m-1} 0\, x_{m+1} \cdots x_V\rangle & x_l = 0 \text{ and } x_m = h \\ 0 & \text{otherwise} \end{cases} \tag{4.3}$$

it follows that

$$\mathrm{Tr}_{\{N\}}\{\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}h_l^\dagger h_m\} = \sum_{\{x\}_{l,m}}{}' \langle x_1 \cdots x_{l-1} 0\, x_{l+1} \cdots x_{m-1} h\, x_{m+1} \cdots x_V | \exp(-\beta\mathcal{H}_\infty) \times |x_1 \cdots x_{l-1} h\, x_{l+1} \cdots x_{m-1} 0\, x_{m+1} \cdots x_V\rangle \tag{4.4}$$

where $\{x\}_{l,m} = (x_1, \ldots, x_{l-1}, x_{l+1}, \ldots, x_{m-1}, x_{m+1}, \ldots, x_V)$ and the primed sum is over these restricted configurations with a total number of $N-1$ h- and s-particles.

Again, since $\mathcal{H}_\infty$ prevents the exchange of an h- and an s-particle, the matrix elements in (4.4) between states which have an s-particle between sites l and m must vanish. For an open chain, this means that x_i for $l+1 \leqslant i \leqslant m-1$ must be either 0 or h. For the periodic chain $x_i = 0$ or h for $m+1 \leqslant i \leqslant V$ or $1 \leqslant i \leqslant l-1$ is an additional possibility but since this involves a macroscopic number of particle movements in (4.4) its contribution is negligible in the thermodynamic limit.

In order to reduce the evaluation of (4.4) to a spinless free-fermion problem, we follow the argument leading to (3.8) to write

$$\mathrm{Tr}_{\{N\}}[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}h_l^\dagger h_m] = 2^{V-K}\,\mathrm{Tr}_{[K]}^{(h)}[\exp(-\beta\mathcal{H}_\infty)h_l^\dagger h_m \mathcal{Q}] \tag{4.5}$$

where $N = V - K$, the notation is as before, and the operator $\mathcal{Q}$ is introduced to correct for the fact that there is no double degeneracy factor for sites between l and m. Thus if we consider a state $|H\rangle$ which has H h-particles between site l and m, the degeneracy factor should be 2^{N-H} rather than 2^N in (3.8). We therefore require

$$\mathcal{Q}|H\rangle = 2^{-H}|H\rangle \tag{4.6}$$

that is,

$$\mathcal{Q} = \prod_{i=l+1}^{m-1}(1 - \tfrac{1}{2}h_i^\dagger h_i) \tag{4.7}$$

Finally, when we combine the above results and transform to the hole operators a_i defined by (3.10) we obtain

$$\mathrm{Tr}_{\{V-K\}}[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}h_l^\dagger h_m]$$
$$= 2^{V-K}(-1)^{m-l}\,\mathrm{Tr}_{\{K\}}\left[\exp(-\beta\mathcal{H}_0)a_l a_m^\dagger \prod_{i=l+1}^{m-1}\frac{1}{2}(1+a_i^\dagger a_i)\right] \tag{4.8}$$

which, together with the steps leading to (4.2), gives the stated result (2.8)

5. Grand-canonical form of the single-particle two-site function

In the grand-canonical ensemble we define the single-particle two-site function by

$$G_{lm} = [Z_G^\infty(z,V,T)]^{-1}\sum_{N=0}^{V} z^N\,\mathrm{Tr}_{\{N\}}\left[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}\frac{1}{2}(c_{l\uparrow}^\dagger c_{m\uparrow}+c_{l\downarrow}^\dagger c_{m\downarrow})\right] \tag{5.1}$$

where

$$Z_G^\infty(z,V,T) = \sum_{N=0}^{V} z^N\,\mathrm{Tr}_{\{N\}}[\mathcal{P}\exp(-\beta\mathcal{H}_\infty)\mathcal{P}] \tag{5.2}$$

is the grand-canonical partition function.

Using (2.5) and (2.8) and the fact that since $(a_j^\dagger a_j)^2 = (a_j^\dagger a_j)$,

$$\prod_{j=l+1}^{m-1}(1+a_j^\dagger a_j) = \exp\left(\sum_{j=l+1}^{m-1}(\log 2)a_j^\dagger a_j\right) \tag{5.3}$$

we can write

$$G_{lm} = (-2)^{l-m+2}\sum_{K=0}^{V}(2z)^{-K}\,\mathrm{Tr}_{\{K\}}\left[\exp(-\beta\mathcal{H}_0)a_l a_m^\dagger\prod_{j=l+1}^{m-1}(1+a_j^\dagger a_j)\right]$$
$$\times\left\{\sum_{K=0}^{V}(2z)^{-K}\,\mathrm{Tr}_{\{K\}}[\exp(-\beta\mathcal{H}_0)]\right\}^{-1}$$
$$= (-2)^{l-m+2}\,\mathrm{Tr}\left[\exp\left(\frac{1}{2}\sum_{i,j=1}^{V}A_{ij}a_i^\dagger a_j\right)\exp\left(\sum_{i,j=1}^{V}B_{ij}a_i^\dagger a_j\right)\right.$$
$$\left.\times\exp\left(\frac{1}{2}\sum_{i,j=1}^{V}A_{ij}a_i^\dagger a_j\right)a_l a_m^\dagger\right]\left\{\mathrm{Tr}\left[\exp\left(\sum_{i,j=1}^{V}B_{ij}a_i^\dagger a_j\right)\right]\right\}^{-1} \tag{5.4}$$

where

$$A_{ij} = \begin{cases}\log 2 & \text{when } i=j=l+1,\ldots,m-1\\ 0 & \text{otherwise}\end{cases} \tag{5.5}$$

$$B_{ij} = \begin{cases}\beta t & j=i\pm 1\\ -\log 2z & j=i\\ 0 & \text{otherwise}\end{cases} \tag{5.6}$$

and in choosing the symmetrical exponential form in (5.4), we have made use of the fact that the operator on the left-hand side of (5.3) commutes with $a_l a_m^\dagger$.

In order to simplify (5.4), we use the following elementary result.

Theorem. If a_i ($a_i^\dagger$) are Fermi destruction (creation) operators, then for arbitrary matrices $A = (A_{ij})$ and $B = (B_{ij})$,

$$\exp\left(\frac{1}{2}\sum_{i,j} A_{ij} a_i^\dagger a_j\right) \exp\left(\sum_{i,j} B_{ij} a_i^\dagger a_j\right) \exp\left(\frac{1}{2}\sum_{i,j} A_{ij} a_i^\dagger a_j\right) = \exp\left(\sum_{i,j} C_{ij} a_i^\dagger a_j\right) \tag{5.7}$$

where the matrix $C = (C_{ij})$ is defined by

$$e^C = e^{A/2} e^B e^{A/2}. \tag{5.8}$$

Proof. From the Baker–Hausdorf theorem [14]

$$e^Z = e^{X/2} e^Y e^{X/2} \tag{5.9}$$

where Z is a sum of Lie elements generated from X and Y under commutation

$$[X, Y] = XY - YX \tag{5.10}$$

The required results (5.8) follows immediately from this observation by noting that for Fermi operators a_i, $a_i^\dagger$,

$$\left[\sum_{i,j} A_{ij} a_i^\dagger a_j, \sum_{i,j} B_{ij} a_i^\dagger a_j\right] = \sum_{i,j} [A, B]_{ij} a_i^\dagger a_j. \tag{5.11}$$

The following useful corollaries, which hold for Fermi operators a_i, $a_i^\dagger$, self-adjoint matrices A and B and self-adjoint matrix C defined by (5.8), are a direct consequence of the above theorem.

Corollary I.

$$\mathrm{Tr}\left[\exp\left(\sum_{i,j} C_{ij} a_i^\dagger a_j\right)\right] = \det(\mathbb{I} + e^A e^B). \tag{5.12}$$

Corollary II.

$$\mathrm{Tr}\left[\exp\left(\sum_{i,j} C_{ij} a_i^\dagger a_j\right) a_l a_m^\dagger\right] = (\mathbb{I} + e^{A/2} e^B e^{A/2})^{-1}_{lm} \det(\mathbb{I} + e^A e^B). \tag{5.13}$$

In order to prove the corollaries, we make a canonical (unitary) transformation

$$a_i = \sum_{i'} u_{ii'} c_{i'} \qquad a_i^\dagger = \sum_{i'} u_{ii'}^* c_{i'}^\dagger \tag{5.14}$$

to Fermi operators $c_{i'}$, $c_{i'}^\dagger$ in which the exponent on the right-hand side of (5.7) is diagonal. In this representation, the left-hand side of (5.12) can be written as

$$\mathrm{Tr}\left[\exp\left(\sum_j \lambda_j c_j^\dagger c_j\right)\right] = \prod_j (1 + e^{\lambda_j}) = \det(\mathbb{I} + e^C) \tag{5.15}$$

where $\{\lambda_j\}$ are the eigenvalues of the matrix C. The required result (5.12) follows from (5.8) and (5.15) using elementary properties of determinants.

Similarly, the left-hand side of (5.13) can be written as

$$\begin{aligned}\sum_{l',m'} u_{ll'}u^*_{mm'}\,\mathrm{Tr}\left[c_{l'}c^\dagger_{m'}\exp\left(\sum_j \lambda_j c^\dagger_j c_j\right)\right] \\ &= \sum_{l'} u_{ll'}u^*_{ml'}\,\mathrm{Tr}\left[c_{l'}c^\dagger_{l'}\exp\left(\sum_j \lambda_j c^\dagger_j c_j\right)\right] \\ &= \sum_{l'} u_{ll'}(1+\mathrm{e}^{\lambda_{l'}})^{-1}u^*_{ml'}\prod_j(1+\mathrm{e}^{\lambda_j}) \\ &= (\mathbb{I}+\mathrm{e}^C)^{-1}_{lm}\det(\mathbb{I}+\mathrm{e}^C)\end{aligned} \tag{5.16}$$

from which the stated result (5.13) easily follows.

Combining the above results, we then see that the grand-canonical single-particle two-site function (5.4) can be written in the form

$$G_{lm} = (-2)^{l-m+2}(\mathbb{I}+\mathrm{e}^{A/2}\mathrm{e}^B\mathrm{e}^{A/2})^{-1}_{lm}\det(\mathbb{I}+\mathrm{e}^A\mathrm{e}^B)\left[\det(\mathbb{I}+\mathrm{e}^B)\right]^{-1} \tag{5.17}$$

where the matrices A and B are defined by (5.5) and (5.6).

The expression (5.17) can be further simplified by noting from (5.5) that $\exp(A)$ is a diagonal matrix which can be written in the form

$$\mathrm{e}^A = \mathbb{I} + \mathcal{P}(l,j) \tag{5.18}$$

where $\mathcal{P}(l,m)$ is a (diagonal) projection matrix with unit elements in positions $i = j = l+1,\ldots,m-1$ and zeros elsewhere. Since $[\exp(A/2)]_{ll} = [\exp(A/2)]_{mm} = 1$, it is then an elementary exercise to check that

$$G_{lm} = (-2)^{l-m+2}(\mathbb{I}+\mathrm{e}^A\mathrm{e}^B)^{-1}_{lm}\det(\mathbb{I}+\mathcal{P}(l,m)M) \tag{5.19}$$

where

$$M = \mathrm{e}^B(\mathbb{I}+\mathrm{e}^B)^{-1}. \tag{5.20}$$

6. Thermodynamic properties

In order to derive thermodynamic properties of the $U=\infty$ model, we use the relation (2.5) connecting the canonical partition functions for the $U=\infty$ model and the spinless Fermion model (2.7). Thus from (2.5) the grand-canonical partition function for the $U=\infty$ model is given by

$$\begin{aligned}Z^\infty_{\mathrm{G}}(z,V,T) &= \sum_{N=0}^{V} z^N Z^\infty_N(V,T) = \sum_{K=0}^{V}(2z)^{V-K}Z^0_K(V,T) \\ &= (2z)^V Z^0_{\mathrm{G}}[(2z)^{-1},V,T] = \prod_{k=1}^{V}[2z+\exp(\beta\epsilon_k)]\end{aligned} \tag{6.1}$$

where Z_G^0 denotes the grand-canonical partition function for the spinless fermion model,

$$\epsilon_k = 2t\ \cos(2\pi k/V) \tag{6.2}$$

and in the last step of (6.1), we have used the well known result

$$\begin{aligned} Z_G^0(z', V, T) &= \mathrm{Tr}\left[\exp\left(\beta\sum_{i=1}^{V}\{t(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \mu' a_i^\dagger a_i\}\right)\right] \\ &= \prod_{k=1}^{V}(1 + z' \mathrm{e}^{\beta\epsilon_k}) \end{aligned} \tag{6.3}$$

where $z' = \exp(\beta\mu')$.

The density of fermions in the $U = \infty$ model is thus given from (6.1) by

$$\rho = V^{-1} z \frac{\partial}{\partial z} \log Z_G^\infty(z, V, T) = V^{-1}\sum_{k=1}^{V} 2z(2z + \mathrm{e}^{\beta\epsilon_k})^{-1} \tag{6.4}$$

and the average energy per site is given by

$$E = -V^{-1}\frac{\partial}{\partial\beta}\log Z_G^\infty(z, V, T) = -V^{-1}\sum_{k=1}^{V}\epsilon_k \mathrm{e}^{\beta\epsilon_k}(2z + \mathrm{e}^{\beta\epsilon_k})^{-1}. \tag{6.5}$$

In the thermodynamic limit $V \to \infty$, these two expressions become

$$\begin{aligned} \rho &= \pi^{-1}\int_0^\pi \left[1 + (2z)^{-1}\exp(2\beta t\cos\theta)\right]^{-1}\mathrm{d}\theta \\ &= \pi^{-1}\int_{-1}^{1}\left[1 + \tfrac{1}{2}\exp[\beta(2t\epsilon - \mu)]\right]^{-1}\left[1 - \epsilon^2\right]^{-1/2}\mathrm{d}\epsilon \end{aligned} \tag{6.6}$$

and

$$\begin{aligned} E &= -\pi^{-1}\int_0^\pi 2t\cos\theta\left[1 + 2z\exp(-2\beta t\cos\theta)\right]^{-1}\mathrm{d}\theta \\ &= -\pi^{-1}\int_{-1}^{1} 2t\epsilon\{1 + 2\exp[\beta(\mu - 2t\epsilon)]\}^{-1}\left[1 - \epsilon^2\right]^{-1/2}\mathrm{d}\epsilon \end{aligned} \tag{6.7}$$

where $z = \exp(\beta\mu)$ and we have made the change of variable $\epsilon = \cos\theta$.

The energy E is then expressed as a function of temperature and density by 'solving' (6.6) for the chemical potential μ and substituting the result into (6.7). For example, at zero temperature ($\beta \to \infty$), (6.6) gives

$$\rho = \pi^{-1}\int_{-1}^{\mu/2t}(1 - \epsilon^2)^{-1/2}\mathrm{d}\epsilon = 1 - \pi^{-1}\cos^{-1}(\mu/2t) \tag{6.8}$$

or in other words, the Fermi energy

$$\epsilon_{\mathrm{F}} = \mu = 2t\cos\pi(1-\rho). \tag{6.9}$$

Similarly, in the limit of zero temperature, the ground-state energy from (6.7) is given by

$$\begin{aligned} E_0 &= -\pi^{-1}\int_{\mu/2t}^{1} 2t\epsilon\left(1-\epsilon^2\right)^{-1/2}\mathrm{d}\epsilon \\ &= -2t\pi^{-1}\left[1-(\mu/2t)^2\right]^{1/2} = -2t\pi^{-1}\sin\pi\rho \end{aligned} \tag{6.10}$$

in agreement with the results of Lieb and Wu [7] where in the last step, we have made use of (6.9).

Magnetic properties of the $U=\infty$ model are also easy to obtain by the methods developed in previous sections. Thus in the presence of a magnetic field H, the Hamiltonian (2.1) is replaced by

$$\mathcal{H}_\infty = -t\sum_{\substack{i=1\\ \sigma}}^{V}\left(\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{i+1\sigma} + \tilde{c}_{i+1\sigma}^{\dagger}\tilde{c}_{i\sigma}\right) - H\sum_{i=1}^{V}\left(\tilde{n}_{i\uparrow} - \tilde{n}_{i\downarrow}\right). \tag{6.11}$$

Separating the charge and spin degrees of freedom as in section 3, we obtain in place of (2.5) the result

$$Z_{V-K}^{\infty}(V,T) = \left(2\cosh B\right)^{V-K} Z_K^0(V,T) \tag{6.12}$$

where Z_K^0 is defined as before by (2.6) and $B = \beta H$.

It easily follows that the grand-canonical partition function is now given by

$$Z_{\mathrm{G}}^{\infty}(z,V,T,B) = \prod_{k=1}^{V}\left(2z\cosh B + \mathrm{e}^{\beta\epsilon_k}\right) \tag{6.13}$$

and hence the isothermal susceptibility is given by

$$\begin{aligned} \chi &= \beta\frac{\partial^2}{\partial B^2}V^{-1}\log Z_{\mathrm{G}}^{\infty}(z,V,T,B) \\ &= \beta V^{-1}\sum_{k=1}^{V}\left\{2z\cosh B\left(2z\cosh B + \mathrm{e}^{\beta\epsilon_k}\right)^{-1}\right. \\ &\qquad \left. - \left(2z\sinh B\right)^2\left(2z\cosh B + \mathrm{e}^{\beta\epsilon_k}\right)^{-2}\right\}. \end{aligned} \tag{6.14}$$

In particular in zero field, we obtain

$$\chi_0 = \beta V^{-1}\sum_{k=1}^{V} 2z\left(2z + \mathrm{e}^{\beta\epsilon_k}\right)^{-1} = \beta\rho \tag{6.15}$$

in agreement with Sokolof [10] and Beni *et al* [11].

7. Discussion

In this paper we have shown with the aid of a canonical transformation, that separates charge and spin degree of freedom, that the strongly correlated one-dimensional Hubbard model with infinite ($U = \infty$) on-site repulsion is related to a corresponding spinless free-Fermion lattice model.

The thermodynamic properties of the two models were shown to be very closely related whereas the single-particle two-site function for the $U = \infty$ model was shown to be related to a modified many-site function for the spinless model which involves many-point correlation functions. The latter was shown to be expressible in terms of the inverse of a certain matrix which should be amenable to numerical analysis.

In a subsequent paper, we will study the expressions derived in this paper numerically for finite and infinite lattices. The single-particle two-site function G_{lm} (5.1) and (5.19) in particular, which is related to the momentum distribution through

$$n(k) = V^{-1} \sum_{l=1}^{V} \sum_{m=1}^{V} \exp[2\pi \mathrm{i} k(l-m)/V] G_{lm} \tag{7.1}$$

is of significant interest in the study of strongly correlated systems such as the Hubbard model. In this regard our results should provide an alternative test of Ogata and Shiba's suggestion [12] that at zero temperature the momentum distribution for the $U = \infty$ one-dimensional model has a weak algebraic singularity at the Fermi momentum k_{F}, given from (6.9) by

$$k_{\mathrm{F}} = \pi(1 - \rho). \tag{7.2}$$

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