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EXACT SPECTRUM FOR n ELECTRONS IN THE SINGLE BAND HUBBARD MODEL

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The energy spectrum and the correlation functions for n electrons in the one-dimensional single band Hubbard model with periodic boundary conditions are calculated exactly. For that purpose the Hamiltonian is transformed into a set of Hamiltonians, corresponding to systems of spinless fermions.

Our results include the results of Mei and Chen, presented in a recent paper.

1. Introduction

The Hubbard Hamiltonian is widely believed to describe the new high-T_C superconductors. For dimension $d = 1$ it reads [1]

$$H = -T \sum_{j=1}^{N} \sum_{\sigma=\uparrow,\downarrow} (\mathbf{c}_{j,\sigma}^{\dagger} \mathbf{c}_{j+1,\sigma} + \mathbf{c}_{j+1,\sigma}^{\dagger} \mathbf{c}_{j,\sigma}) + U \sum_{j=1}^{N} \mathbf{n}_{j,\uparrow} \mathbf{n}_{j,\downarrow} \qquad (T > 0)\,, \tag{1}$$

where $\mathbf{c}_{j,\sigma}^{\dagger}$ ($\mathbf{c}_{j,\sigma}$) is the creation (annihilation) operator for an electron on site j with z-component σ of the spin. Because the $\mathbf{c}$'s are fermion operators the number operators $\mathbf{n}_{j,\sigma} = \mathbf{c}_{j,\sigma}^{\dagger} \mathbf{c}_{j,\sigma}$ have the eigenvalues 0 and 1. In (1) we suppose periodic boundary conditions, so: $\mathbf{c}_{N+1,\sigma}^{(\dagger)} = \mathbf{c}_{1,\sigma}^{(\dagger)}$.

Quite recently Mei and Chen [2] studied this model in the limit $U \to \infty$, the so-called single band Hubbard model, in which double occupation of a lattice site is prohibited, due to the second term in (1). The Hamiltonian in this infinite repulsion limit may be written as

$$H_{\text{eff}} = -T \sum_{j=1}^{N} \sum_{\sigma=\uparrow,\downarrow} [(1 - \mathbf{n}_{j,-\sigma}) \mathbf{c}_{j,\sigma}^{\dagger} \mathbf{c}_{j+1,\sigma} (1 - \mathbf{n}_{j+1,-\sigma}) + \text{h.c.}]\,. \tag{2}$$

Mei and Chen calculated the ground-state energy and the correlation functions in the case of two electrons in the band. In this work we will give an extension of their results, this extension being obtained, however, by a different, more general, method in which we transform H_{eff} into a set of Hamiltonians, corresponding to systems of spinless fermions. We are able to calculate the complete energy spectrum and the correlation functions for an arbitrary number of spins n on a lattice with N sites.

In section 2 we will describe these transformations, while in section 3 some examples will be presented.

2. The transformation

We consider a ring with N sites. There are n ($n \leq N$) electrons. As a basis for the states space for this system we can take

$$\{\mathbf{c}^{\dagger}_{j_1\sigma_1}\mathbf{c}^{\dagger}_{j_2\sigma_2}\cdots\mathbf{c}^{\dagger}_{j_n\sigma_n}|0\rangle\}, \qquad 1 \leq j_1 < j_2 < \cdots < j_n \leq N\,, \tag{3}$$

which represent for fixed j_i, σ_i states of n electrons on the singly occupied sites j_i with spins $\sigma_i (i = 1, 2, \ldots, n)$.

Now we consider the cyclic permutation P acting on the n spin variables:

$$P\colon \{\sigma_1, \sigma_2, \ldots, \sigma_n\} \rightarrow \{\sigma_2, \sigma_3, \ldots, \sigma_1\}\,. \tag{4}$$

It is clear that by applying P^n each configuration of the spins reproduces itself. However, there are configurations (with some kind of symmetry) which reproduce themselves already after applying the cyclic permutation n' ($<n$) times (where n' is necessarily a divisor of n). We give two simple examples: $n' = 1$ for the configuration $\{\uparrow\uparrow\uparrow\uparrow\ldots\}$, while $n' = 2$ for $\{\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots\}$.

It is important to notice that the Hamiltonian H_{eff} can transport electrons with fixed spin over the lattice sites; however it cannot change the sequence of $\uparrow$ and $\downarrow$. Of course the number of electrons n is also a preserved quantity. So there exist subspaces that are invariant under the action of H_{eff}. The states within one subspace all have the same spin configuration or one that is obtained by applying a number of times the cyclic permutation operator P. We will now describe a method to give a diagonalization of H_{eff} in each of these subspaces. We will see that for each subspace the obtained Hamiltonian corresponds with a Hamiltonian for a system of spinless fermions.

We introduce the state which is the fourier sum over the cyclic permutations of the spin variables. This state has a wavenumber k:

$$|\Phi_{j_1 j_2 \cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle = \left[\frac{1}{\sqrt{n'}}\sum_{m=0}^{n'-1} e^{imk}\mathbf{c}^{\dagger}_{j_1 p^m(\sigma_1)}\cdots\mathbf{c}^{\dagger}_{j_n p^m(\sigma_n)}\right]|0\rangle$$

$$= \frac{1}{\sqrt{n'}}\left[\mathbf{c}^{\dagger}_{j_1\sigma_1}\mathbf{c}^{\dagger}_{j_2\sigma_2}\cdots\mathbf{c}^{\dagger}_{j_n\sigma_n} + e^{ik}\mathbf{c}^{\dagger}_{j_1\sigma_2}\mathbf{c}^{\dagger}_{j_2\sigma_3}\cdots\mathbf{c}^{\dagger}_{j_n\sigma_1}\right.$$
$$\left. + e^{2ik}\mathbf{c}^{\dagger}_{j_1\sigma_3}\cdots\mathbf{c}^{\dagger}_{j_n\sigma_2} + \cdots + e^{ik(n'-1)}\mathbf{c}^{\dagger}_{j_1\sigma_{n'}}\mathbf{c}^{\dagger}_{j_2\sigma_{n'+1}}\cdots\mathbf{c}^{\dagger}_{j_n\sigma_{n'-1}}\right]|0\rangle\,, \tag{5}$$

and k can take the values

$$k = (2\pi/n')\mu \qquad (\mu = 0, 1, 2, \ldots, n'-1)\,. \tag{6}$$

For the effect of the Hamiltonian on the state $|\Phi_{j_1 j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle$ we first consider the cases I for which:

$$\text{I:}\quad 1 < j_1 < j_2 < \cdots < j_n < N\,. \tag{7}$$

Then:

$$H_{\text{eff}}|\Phi_{j_1 j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle = -T[|\Phi_{j_1-1\ j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle$$
$$+ |\Phi_{\substack{j_1+1\ j_2\cdots j_n \\ (j_1+1\neq j_2)}}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle + \cdots + |\Phi_{j_1 j_2\cdots j_n+1}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle]\,. \tag{8}$$

In (8) there are no state vectors for which two of the site indices are equal.

Now we define the set of "stripped" states $|\Psi_{j_1 j_2\cdots j_n}\rangle$ in which we don't see the quantum numbers k and σ_j anymore, and a corresponding Hamiltonian H_0, such that the effect of H_0 on the "stripped" state $|\Psi_{j_1 j_2\cdots j_n}\rangle$ is the same as the effect of H_{eff} on the state $|\Phi_{j_1 j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle$. The correspondence is obtained by

$$|\Phi_{j_1 j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle \to |\Psi_{j_1 j_2\cdots j_n}\rangle = \mathbf{d}^{\dagger}_{j_1}\mathbf{d}^{\dagger}_{j_2}\cdots\mathbf{d}^{\dagger}_{j_n}|0\rangle\,,$$
$$H_{\text{eff}} \to H_0 = -T\sum_{j=1}^{N-1}(\mathbf{d}^{\dagger}_j\mathbf{d}_{j+1} + \mathbf{d}^{\dagger}_{j+1}\mathbf{d}_j)\,, \tag{9}$$

in which $\mathbf{d}^{(\dagger)}_j$ are fermion operators. It is easy to see that

$$H_0|\Psi_{j_1 j_2\cdots j_n}\rangle = -T[|\Psi_{j_1-1 j_2\cdots j_n}\rangle + \cdots + |\Psi_{j_1 j_2\cdots j_n+1}\rangle]\,. \tag{10}$$

Now we consider the cases for which

$$\text{IIa:}\quad 1 = j_1 < j_2 < \cdots < j_n < N\,,$$

or (11)

$$\text{IIb:}\quad 1 < j_1 < j_2 < \cdots < j_n = N\,.$$

Notice that if $j_1 = 1$ and $j_n = N$, H_{eff} cannot result in a shift of an electron from position 1 to N or vice versa. So I, IIa and IIb cover all interesting possibilities.

We concentrate on the cases IIa (the case IIb follows in a similar way) and because of the periodic boundary conditions we may write

$$H_{\text{eff}}|\Phi_{1j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle = -T[|\Phi_{Nj_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle + |\Phi_{\substack{2j_2\cdots j_n\\(j_2\neq 2)}}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle + \cdots + |\Phi_{1j_2\cdots j_n+1}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle]\,. \tag{12}$$

Because in the definition (5) of the Φ's, the $\mathbf{c}$'s are fermion operators with the well-known anti-commutation rules, we may rewrite the first state in the right-hand side of (12),

$$\begin{aligned}|\Phi_{Nj_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle &= (-1)^{n-1}|\Phi_{j_2\cdots j_nN}(k;\sigma_2\sigma_3\cdots\sigma_n\sigma_1)\rangle\\ &= (-1)^{n-1}\,\mathrm{e}^{-\mathrm{i}k}|\Phi_{j_2\cdots j_nN}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle\,.\end{aligned} \tag{13}$$

The first of the equalities (13) follows from the anti-commutation relations (we perform $n-1$ pair interchanges of the $\mathbf{c}$-operators, each of which leaves us with a minus sign), while the second identity is also a direct consequence of the definition (5).

For a set of indices obeying one of the conditions (11) we can define a "stripped" state in the same way we did in (9) for the cases I. However, for these states we need to add an extra term H_1 to the Hamiltonian H_0 (cf. (9)). This term, corresponding to $j = N$ in the sum in (9), cannot have the simple form $(\mathbf{d}_N^\dagger\mathbf{d}_1 + \mathbf{d}_1^\dagger\mathbf{d}_N)$, because of the additional factor $(-1)^{n-1}\mathrm{e}^{\mathrm{i}k}$ that occurs in (13). Therefore we write H_1 as

$$H_1 = -(t_{N1}\mathbf{d}_N^\dagger\mathbf{d}_1 + t_{1N}\mathbf{d}_1^\dagger\mathbf{d}_N), \qquad t_{N1} = t_{1N}^*\,. \tag{14}$$

This particular choice for H_1 covers both the cases IIa as well as IIb: In the first (second) one only the first (second) term of (14) is active. We consider the effect of H_1 on states belonging to the category IIa.

$$H_1|\Psi_{1j_1\cdots j_n}\rangle = H_1\mathbf{d}_1^\dagger\mathbf{d}_{j_2}^\dagger\cdots\mathbf{d}_{j_n}^\dagger|0\rangle = -t_{N1}\mathbf{d}_N^\dagger\mathbf{d}_{j_2}^\dagger\cdots\mathbf{d}_{j_n}^\dagger|0\rangle$$
$$= -(-1)^{n-1}t_{N1}\mathbf{d}_{j_2}^\dagger\cdots\mathbf{d}_{j_n}^\dagger\mathbf{d}_N^\dagger|0\rangle$$
$$= -T\,\mathrm{e}^{-\mathrm{i}k}(-1)^{n-1}\mathbf{d}_{j_2}^\dagger\cdots\mathbf{d}_{j_n}^\dagger\mathbf{d}_N^\dagger|0\rangle\,. \tag{15}$$

The last identity follows from the periodic boundary conditions (the sites N and 1 are neighbours). From (15) it now follows directly that

$$t_{N1} = T\,\mathrm{e}^{-\mathrm{i}k} \Leftrightarrow t_{1N} = T\,\mathrm{e}^{\mathrm{i}k}\,. \tag{16}$$

For an arbitrary state $|\Phi_{j_1j_2\cdots j_n}(k;\sigma_1\sigma_2\cdots\sigma_n)\rangle$ the effect of H_{eff} is the analogue of the effect of $H^* = H_0 + H_1$ on an arbitrary state $|\Psi_{j_1j_2\cdots j_n}\rangle$, with

$$H^* = -T\Big[\sum_{j=1}^{N-1}(\mathbf{d}_j^\dagger\mathbf{d}_{j+1} + \mathbf{d}_{j+1}^\dagger\mathbf{d}_j) + \mathrm{e}^{-\mathrm{i}k}\mathbf{d}_N^\dagger\mathbf{d}_1 + \mathrm{e}^{\mathrm{i}k}\mathbf{d}_1^\dagger\mathbf{d}_N\Big]\,. \tag{17}$$

By writing down this Hamiltonian we have established the fact that the spectrum of H_{eff} is the superposition of the spectra for a set of free fermion Hamiltonians. Each invariant subspace of H_{eff} can be characterized by a configuration $\{\sigma_j\}$ $(j = 1, \ldots, n)$: it contains the n-electron states (3) with spin configuration $\{\sigma_j\}$ or one of its cyclic permutations.

The energy spectrum in each subspace, however, is completely determined by $n'\{\sigma_j\}$, which gives us the possible values for k. So H_{eff} can have identical spectra in different subspaces (i.e. with different $\{\sigma_j\}$). The conclusion is that the total space of states can be written as the sum of a set of invariant subspaces $\{V(n, n')\}$ $(n \leq N, n/n' \in \mathbb{N})$. The state vectors in $V(n, n')$ are interpreted (cf. (9)) as states for a system of n spinless fermions.

Our next goal is to make the Hamiltonian H^* translational invariant. For that purpose we make the following transformation to new fermion operators:

$$\begin{cases}\mathbf{d}_j = \mathrm{e}^{\mathrm{i}\phi_j}\mathbf{a}_j\,,\\ \mathbf{d}_j^\dagger = \mathrm{e}^{-\mathrm{i}\phi_j}\mathbf{a}_j^\dagger\,.\end{cases} \tag{18}$$

Expressed in terms of the operators $\mathbf{a}_j^{(\dagger)}$ the Hamiltonian (17) becomes one in which the phase shift due to the boundary effect is spread out over the total lattice,

$$H^* = -T\Big[\sum_{j=1}^{N-1}(\mathrm{e}^{\mathrm{i}(\phi_{j+1}-\phi_j)}\mathbf{a}_j^\dagger\mathbf{a}_{j+1} + \mathrm{e}^{-\mathrm{i}(\phi_{j+1}-\phi_j)}\mathbf{a}_{j+1}^\dagger\mathbf{a}_j) + \mathrm{e}^{\mathrm{i}(\phi_1-\phi_N-k)}\mathbf{a}_N^\dagger\mathbf{a}_1$$
$$+ \mathrm{e}^{-\mathrm{i}(\phi_1-\phi_N-k)}\mathbf{a}_1^\dagger\mathbf{a}_N\Big]\,. \tag{19}$$

In order to make H^* translational invariant we choose

$$\phi_j = j\,\Delta\phi \Rightarrow \phi_{j+1} - \phi_j = \Delta\phi\,. \tag{20}$$

Because of the periodic boundary conditions ($N+1 \equiv 1$) we get (cf. (19))

$$\begin{aligned}\Delta\phi &= \phi_1 - \phi_N - k + \lambda 2\pi = -(N-1)\,\Delta\phi - k + \lambda 2\pi \\ &\Rightarrow \Delta\phi = -k/N + \lambda 2\pi/N\,,\end{aligned} \tag{21}$$

where the possible values for k are given by (6). If we make the choice $\lambda = 0$ we finally obtain

$$H^* = -T\sum_{j=1}^{N}(\mathrm{e}^{\mathrm{i}\Delta\phi}\mathbf{a}_j^\dagger\mathbf{a}_{j+1} + \text{h.c.})\,. \tag{22}$$

The expression (22) is symmetric in all neighbour pairs.

All possible spectra (corresponding to the possible values for $\Delta\phi$) for the Hamiltonian (22) together constitute the spectrum of H_{eff}.

3. The energy spectrum and correlation functions

In order to obtain the energy spectrum of H^* we make one more transformation,

$$\mathbf{a}_j^\dagger = \frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{-\mathrm{i}qj}\mathbf{b}_q^\dagger\,, \tag{23}$$

with

$$q = \nu 2\pi/N \qquad (\nu = 0, 1, \ldots, N-1)\,. \tag{24}$$

Our final expression for the Hamiltonian reads

$$H^* = -2T\sum_q \cos(\Delta\phi + q)\mathbf{b}_q^\dagger\mathbf{b}_q\,. \tag{25}$$

The number operator $\mathbf{n}_q = \mathbf{b}_q^\dagger\mathbf{b}_q$ has eigenvalues $n_q = 0, 1$ so the eigenvalues of the Hamiltonian are

$$E_{\{n_q\}} = -2T\sum_q \cos(\Delta\phi + q)n_q\,, \tag{26}$$

where the set $\{n_q\}$ has to satisfy the constraint

$$\sum_q n_q = n \,. \tag{27}$$

Now we are able to derive the spectrum for H^* (and thus for H_{eff}): the possible values for q are given in (24), those for $\Delta\phi$ in (21), with $\lambda = 0$. Combination of the possibilities, together with the constraint (27) gives us all possible eigenvalues. The ground-state energy $E_0(N, n, n')$ is obtained by taking the combination with minimal energy.

As an example we will calculate the ground-state energy for two electrons ($n = 2$) on a lattice of arbitrary length N.

For $n = 2$ there are two possible values for n':

A: $n = 2$ and $n' = 1$ ($|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$). It follows that $k = \Delta\phi = 0$. The optimal choice is obtained by taking $q_1 = 0$, $q_2 = 2\pi/N$. We get:

$$E_0(N, 2, 1) = -2T(1 + \cos 2\pi/N) = -4T\cos^2(\pi/N) \,. \tag{28}$$

B: $n = 2$ and $n' = 2$ ($|\uparrow\downarrow\rangle$ or $|\uparrow\downarrow\rangle$). There are two possibilities for k and $\Delta\phi$:

(1) $k = \Delta\phi = 0$. The optimal combination here too is $q_1 = 0$, $q_2 = 2\pi/N$ and the resulting energy $E_0(N, 2, 2)_1$ equals $E_0(N, 2, 1)$.

(2) $k = \pi \Rightarrow \Delta\phi = -\pi/N$. Again for $q_1 = 0$, $q_2 = 2\pi/N$ we find the lowest energy

$$E_0(N, 2, 2)_2 = -4T\cos\pi/N \,. \tag{29}$$

For an infinitely large lattice ($N \to \infty$) the energies (28) and (29) become equal, i.e. $-4T$, but for a finite system the energy $E_0(N, 2, 2)_2$ is the ground-state energy. E.g. for $N = 4$ we find

$$E_0(N = 4, n = 2) = -2T\sqrt{2} \,, \tag{30}$$

and we see that the result of Mei and Chen [2] is included in our scheme.

The ground-state correlation function for two electrons is given by

$$\langle \mathbf{n}_{j_1}\mathbf{n}_{j_2}\rangle_N = \langle \mathbf{a}^\dagger_{j_1}\mathbf{a}_{j_1}\mathbf{a}^\dagger_{j_2}\mathbf{a}_{j_2}\rangle_N = N^{-2}\Big[4 + \sum_{q\neq 0,2\pi/N} \cos(j_1 - j_2)q\Big] \,. \tag{31}$$

For $j_1 = j_2 = j$ (31) gives ($n_j = n_j^2 = 0, 1$)

$$\langle \mathbf{n}_{j_1}\rangle_N = \langle \mathbf{n}_{j_1}\mathbf{n}_{j_1}\rangle_N = N^{-2}[4 + 2(N-2)] = 2/N \,, \tag{32}$$

which is not a surprise while there are two electrons spread out over N sites, so the density is $2/N$.

We now calculate $\langle \mathbf{n}_{j_1} \mathbf{n}_{j_2} \rangle_4$, so we study the ring consisting of four sites. The trivial result (1/2) is obtained for $j_1 = j_2 = j$, but for $j_1 \neq j_2$ the result is

$$\begin{aligned} |j_1 - j_2| = 1 &\rightarrow \langle \mathbf{n}_{j_1} \mathbf{n}_{j_2} \rangle_4 = 1/8 , \\ |j_1 - j_2| = 2 &\rightarrow \langle \mathbf{n}_{j_1} \mathbf{n}_{j_2} \rangle_4 = 1/4 , \end{aligned} \tag{33}$$

which is also the result in ref. [2]. Notice that for the sum of all correlations

$$\sum_{j_1 < j_2} \langle \mathbf{n}_{j_1} \mathbf{n}_{j_2} \rangle = 1 . \tag{34}$$

In (33) we already see a manifestation of the repulsion between the electrons. If the electrons are close to each other they are restricted in their mobility, because of the wall ($U \rightarrow \infty$) between them. Electrons separated by a large distance can move undisturbed. Therefore Gutzwiller's approximation [3], which is a uniform superposition of states in which the two electrons are joined in a singlet, so $\langle \mathbf{n}_{j_1} \mathbf{n}_{j_2} \rangle_N$ is independent of $|j_1 - j_2|$, cannot be exact, as already may be concluded from the energies that follow from this method.

4. Conclusions, remarks

In this work we have studied the one-dimensional Hubbard model in the limit $U \rightarrow \infty$. This so-called single-band Hubbard model turned out to be equivalent to a set of systems, consisting of spinless fermions. For an arbitrary number of electrons in the band we are able to calculate the energy spectrum and the correlation functions. The results of Mei and Chen [2] are included in ours.

However, for the ground-state energy we find the expression (29). Using the expansion: $\cos(x) \approx 1 - x^2/2 (1 \gg x)$ we obtain for large N:

$$\lim_{N \rightarrow \infty} E_0(N, 2, 2)_2 = -4T(1 - \beta \cdot N^{-2}) , \qquad \beta = \pi^2/2 , \tag{35}$$

whereas in ref. [2], eq. (13) the finite-size correction is of the order N^{-1}.

In the infinite repulsion limit it is possible to give the total spectrum of the Hamiltonian (1), and we can give the eigenvalues in the subspaces corresponding to n and S, where n is the number of electrons and S is the total spin. The total spin S is in this case a good quantum number while in this limit the Hamiltonian becomes rotational invariant.

It would be interesting to study the single-band two-dimensional Hubbard model, while for the high-T_c superconductors two-dimensional lattices are important. In these systems U is believed to be much larger than $T(U/T \approx 5\text{–}20)$. The case $U = 0$ can be treated exactly. When we are able to describe the differences between the two limits ($U = 0, U \to \infty$) we perhaps will gain more insight in the critical behaviour for large U.

However the generalization of our method to two dimensions is not a trivial one, because of the lack of an ordering principle in two dimensions. We have used the ordering in one dimension to make the classification of the invariant subspaces for the one-dimensional Hamiltonian.

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