

The ground-state statistical mechanics for the two sites Hubbard model André M. C. Souza

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In this work we develop the details of the calculation for the ground-state statistical mechanics properties of the Hubbard model for two electrons in two sites. The ground-state Helmholtz free energy, mean energy, specific heat and entropy have been obtained.

Keywords: ground-state, statistical mechanics, Hubbard model

1. INTRODUCTION

In a recent work, we have introduced a statistical mechanics description to analyze the ground state of quantum systems [1]. The scheme of this formalism is applied to Hamiltonians defined as

$$\hat{H} = \hat{H}_0 + T\hat{V}, \quad (1)$$

where \hat{H}_0 and \hat{V} are, respectively, the one-particle and interaction operator, and T is the dimensionless interaction parameter. We consider that $T > 0$ and \hat{V} is positively defined. One good example of this class of Hamiltonians is the one of the Hubbard model [2]. The Hamiltonian of the Hubbard model is defined by

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where $c_{i\sigma}^+$, $c_{i\sigma}$ and $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ are respectively the creation, annihilation and number operators for an electron with spin σ in an orbital localized at site i on a lattice of N sites; the $\langle ij \rangle$ denotes pairs i, j of nearest-neighbor sites on lattice; U is the Coulombian repulsion that operates when the two electrons occupy the same site; and t is the electron transfer integral connecting states localized on nearest-neighbor sites.

Here, we discuss detail of the simplest example to the formalism introduced in Ref. 1 applied to the Hubbard model, namely, the problem of two electrons in two sites. In section 2 we solve the Hubbard model for the case of two electrons in two sites to find its spectrum of energy, in section 3 we apply the formalism of the ground-state statistical mechanics for this system, and, finally in section IV we present our conclusion and final remarks.

2. THE SPECTRUM

For the case of two sites (**a** and **b**) the Hubbard Hamiltonian can be written as [3]

$$\hat{H} = \sum_{\sigma} (a_{\sigma}^+ b_{\sigma} + b_{\sigma}^+ a_{\sigma}) + U (a_{\uparrow}^+ a_{\uparrow} b_{\downarrow}^+ b_{\downarrow} + a_{\downarrow}^+ a_{\downarrow} b_{\uparrow}^+ b_{\uparrow}), \quad (3)$$

where a_{σ}^+ (b_{σ}^+) and a_{σ} (b_{σ}) are the creation and annihilation operators in the **a**(**b**) site.

Considering two electrons in the system, the six spin configurations are given by

$$\text{Configuration 1: } |\uparrow, \uparrow\rangle = a_{\uparrow}^+ b_{\uparrow}^+ |vacuum\rangle$$

$$\text{Configuration 2: } |\downarrow, \downarrow\rangle = a_{\downarrow}^+ b_{\downarrow}^+ |vacuum\rangle$$

$$\text{Configuration 3: } |\uparrow, \downarrow\rangle = a_{\uparrow}^+ b_{\downarrow}^+ |vacuum\rangle$$

Configuration 4: $|\downarrow, \uparrow\rangle = a_{\downarrow}^{\dagger} b_{\uparrow}^{\dagger} |vacuum\rangle$

Configuration 5: $|\downarrow, \downarrow\rangle = a_{\downarrow}^{\dagger} a_{\downarrow}^{\dagger} |vacuum\rangle$

Configuration 6: $|\uparrow, \downarrow\rangle = b_{\downarrow}^{\dagger} b_{\uparrow}^{\dagger} |vacuum\rangle$

We define $|A\rangle = \frac{1}{\sqrt{2}}(|\downarrow, \downarrow\rangle - |\uparrow, \downarrow\rangle)$, $|B\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)$, $|C\rangle = \frac{1}{\sqrt{2}}(|\downarrow, \uparrow\rangle + |\uparrow, \downarrow\rangle)$ and $|D\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle)$. The application of the Hamiltonian (Eq. (3)) in this configuration yields

$$\hat{H}|\uparrow, \uparrow\rangle = 0|\uparrow, \uparrow\rangle \tag{4a}$$

$$\hat{H}|\downarrow, \downarrow\rangle = 0|\downarrow, \downarrow\rangle \tag{4b}$$

$$\hat{H}|A\rangle = U|A\rangle \tag{4c}$$

$$\hat{H}|B\rangle = 0|B\rangle \tag{4d}$$

$$\hat{H}|C\rangle = U|C\rangle - 2t|D\rangle \tag{4e}$$

$$\hat{H}|D\rangle = -2t|C\rangle. \tag{4f}$$

The four first states are eigenvectors of \hat{H} which eigenvalues given by $E_1=0$, $E_2=0$, $E_3=U$ and $E_4=0$. The two last eigenvalues are determined by the equation

$$\begin{vmatrix} -E+U & -2t \\ -2t & -E \end{vmatrix} = 0. \tag{5}$$

By using direct calculus, it is easy to obtain the two eigenvalues as [3]

$$E_{\pm} = \frac{1}{2} \left(U \pm \sqrt{U^2 + 16t^2} \right). \tag{6}$$

The eigenvector are $|\psi_{\pm}\rangle = a_{\pm}|C\rangle + b_{\pm}|D\rangle$, where

$$a_{\pm} = \mp \sqrt{1 - b_{\pm}^2} \quad \text{and} \quad b_{\pm} = \frac{4t}{\sqrt{2(\pm U + \sqrt{U^2 + 16t^2})\sqrt{U^2 + 16t^2}}}. \tag{7}$$

Thus, the energy of the ground-state is

$$E_0 = \frac{1}{2} \left(U - \sqrt{U^2 + 16t^2} \right), \tag{8}$$

and its eigenvector is given by

$$|\psi_0\rangle = a_-|C\rangle + b_-|D\rangle. \tag{9}$$

Table 1 shows the energy eigenvalues and its respective eigenvectors $|\phi_i\rangle$ in the absence of interaction ($U=0$), obtained from Eqs. (4)-(7). Using Tab. 1 and Eq. (9), we can observe that the ground-state $|\psi_0\rangle$ for the case with interaction can be expanded in terms only of the two non-interacting states, namely, $|\phi_0\rangle$ and $|\phi_1\rangle$. We can immediately obtain

$$|\psi_0\rangle = \left(\frac{a_- + b_-}{\sqrt{2}} \right) |\phi_0\rangle + \left(\frac{b_- - a_-}{\sqrt{2}} \right) |\phi_1\rangle, \tag{10}$$

Table 1: Spectrum of energy of the Hubbard model in the absence of interaction ($U=0$) for two electrons in two sites.

| energy | eigenvector |
|--------|---|
| $-2t$ | $ \phi_0\rangle = \frac{1}{2}(\downarrow, \uparrow\rangle + \downarrow, \uparrow\rangle + \downarrow \uparrow, \rangle + \downarrow \uparrow\rangle)$ |
| $2t$ | $ \phi_1\rangle = \frac{1}{2}(\downarrow, \uparrow\rangle + \downarrow, \uparrow\rangle - \downarrow \uparrow, \rangle - \downarrow \uparrow\rangle)$ |
| 0 | $ \phi_2\rangle = \frac{1}{\sqrt{2}}(\downarrow \uparrow, \rangle - \downarrow \uparrow\rangle)$ |
| 0 | $ \phi_3\rangle = \frac{1}{\sqrt{2}}(\uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle)$ |
| 0 | $ \phi_4\rangle = \uparrow, \uparrow\rangle$ |
| 0 | $ \phi_5\rangle = \downarrow, \downarrow\rangle$ |

3. GROUND-STATE STATISTICAL MECHANICS

The key of our description is to obtain the expectation values of the physical quantities on the ground-state in the base of non-interacting states of the system, considering an absolute temperature scale, called ground-state temperature, as [1]

$$T_g = U/k, \tag{11}$$

where k is a constant measured in Kelvins⁻¹. Similar to the usual statistical mechanics, we consider that taking different T_g the particles of the system fall into non-interacting microstates.

The ground-state $|\psi_0\rangle$ is expanded in terms of the non-interacting states $|\phi_i\rangle$ as $|\psi_0\rangle = \sum_i \alpha_i(T_g) |\phi_i\rangle$ where the occupation probability for the $|\phi_i\rangle$ is $p_i(T_g) = |\alpha_i(T_g)|^2$. From Eq. (10) we get

$$p_0(T_g) = \frac{|a_- + b_-|^2}{2} = \frac{1}{2} + |a_- b_-|, \tag{12a}$$

$$p_1(T_g) = \frac{|b_- - a_-|^2}{2} = \frac{1}{2} - |a_- b_-|. \tag{12b}$$

Of course, $p_0(T_g) + p_1(T_g) = 1$, $p_0(T_g) \geq p_1(T_g)$ and $p_0(0) = 1$. Substituting Eq. (7) into Eq. (12), we found that

$$p_0(T_g) = \frac{|a_- + b_-|^2}{2} = \frac{1}{2} + \frac{2t}{\sqrt{16t^2 + U^2}} = \frac{1}{2} + \frac{2}{\sqrt{16 + (kT_g/t)^2}}, \tag{13a}$$

$$p_1(T_g) = \frac{|b_- - a_-|^2}{2} = \frac{1}{2} - \frac{2t}{\sqrt{16t^2 + U^2}} = \frac{1}{2} - \frac{2}{\sqrt{16 + (kT_g/t)^2}}. \tag{13b}$$

Figure 1 presents the occupation probabilities as a function of temperature T_g . $p_0(T_g)$ ($p_1(T_g)$) decreases (increases) slowly with T_g . That is to say, if the ground-state temperature T_g increases then the probability of an electron is in the non-interacting ground-state decreases. If the electronic interaction is sufficiently large, i.e. $T_g \gg 1$, all the quantum states have the same occupation probability values.

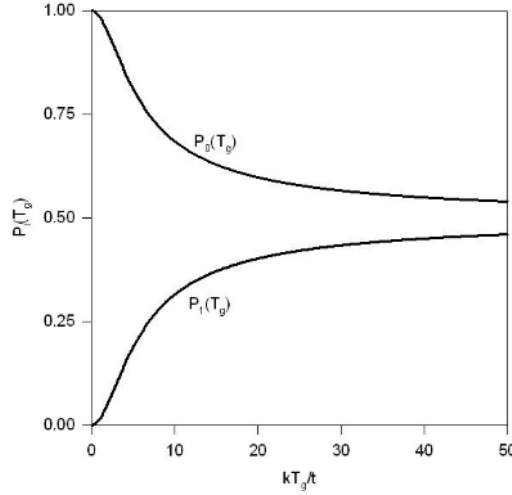


Figure 1. Occupation probabilities versus ground-state temperature T_g .

We can introduce a called ground-state thermodynamics [1], defining the ground-state internal energy, ground-state free energy and ground-state entropy, respectively, as

$$U(T_g) = \langle E(T_g) \rangle = \sum_i p_i(T_g) E_i(0) \tag{14}$$

$$F(T_g) = E_0(T_g) - kT_g d(0) \tag{15}$$

$$S(T_g) = k \{ d(0) - d(T_g) \}, \tag{16}$$

as well as, we can derive the heat capacity

$$C(T_g) = T_g \frac{dS(T_g)}{dT_g} = -T_g \frac{d^2 F(T_g)}{dT_g^2}, \tag{17}$$

where $d(T_g) = \langle \psi_0 | \hat{d} | \psi_0 \rangle$ and $\hat{d} = \sum_i n_{i\uparrow} n_{i\downarrow}$ is the double occupancy operator. In the non-interacting limit each site is equivalent and it has the same possibility of to be occupied by zero, one up, one down or two electrons. Therefore, $d(0) = N/4$. Hence:

A. mean energy

Using Eq. (14),

$$U(T_g) = -2tp_0(T_g) + 2tp_1(T_g) = -4tp_0(T_g) + 2t. \tag{18}$$

Substituting Eq. (13) into Eq. (18), we obtain

$$U(T_g) = -\frac{8t}{\sqrt{(kT_g/t)^2 + 16}}. \tag{19}$$

B. Ground-state free energy

Substituting Eq. (11) into Eq. (8),

$$F(T_g) = \frac{1}{2} \left(kT_g - \sqrt{(kT_g)^2 + 16t^2} \right) - kT_g \frac{2}{4} \tag{20}$$

and we get

$$F(T_g) = -\frac{t}{2} \sqrt{\left(\frac{kT_g}{t} \right)^2 + 16}. \tag{21}$$

C. Ground-state heat capacity

From Eqs. (17) and (21)

$$C(T_g) = -T_g \frac{d^2 F(T_g)}{dT_g^2} = \frac{8k(kT_g/t)}{\sqrt{[(kT_g/t)^2 + 16]^3}}. \quad (22)$$

D. Entropy

From Eq. (9)

$$d(T_g) = \langle \psi_0 | \hat{d} | \psi_0 \rangle = \langle \langle C | a^* - + \langle D | b^* - \rangle (a_- | C \rangle) = |a_-|^2, \quad (23)$$

using Eqs. (7) and (11)

$$d(T_g) = \frac{1}{2} - \frac{(kT_g/t)}{2\sqrt{(kT_g/t)^2 + 16}}, \quad (24)$$

and from Eq. (16), we straightforwardly obtain the entropy

$$S(T_g) = \frac{k}{2} \frac{(kT_g/t)}{\sqrt{(kT_g/t)^2 + 16}}. \quad (25)$$

Figure 2(a)-(d) shows curves of $F(T_g)$, $U(T_g)$, $C(T_g)$ and $S(T_g)$ versus the temperature T_g for the expression above representing the case of two electrons on two sites for the Hubbard model. The picture presented is analogous to those ones of the usual thermodynamics.

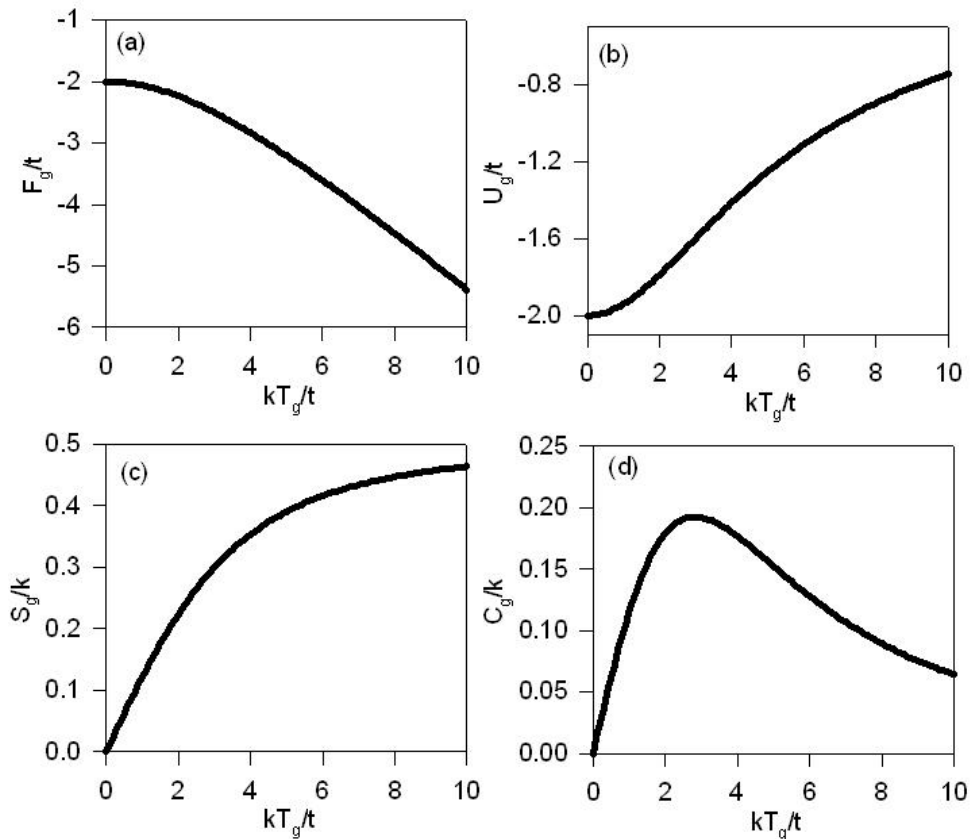


Figure 2. Ground-state (a) free energy $F(T_g)$, (b) internal energy $U(T_g)$, (c) entropy $S(T_g)$ and (d) heat capacity $C(T_g)$ versus temperature T_g for the Hubbard model for two electrons in two sites.

Now, let us consider the functional dependence for the entropy of the Eq. (16) in terms of the occupation probability of the non-interacting quantum states. It is easy to show of the Eqs. (13) and (21) that

$$p_0(T_g) = \frac{1}{2} - \frac{1}{F(T_g)} \quad \text{and} \quad p_1(T_g) = \frac{1}{2} + \frac{1}{F(T_g)}. \quad (26)$$

Then

$$p_0(T_g)p_1(T_g) = \frac{1}{4} - \frac{1}{F(T_g)^2} = \frac{1}{4} - \frac{4}{[(kT_g)^2 + 16t^2]} = \frac{(kT_g/t)^2}{4[(kT_g/t)^2 + 16]}, \quad (27)$$

and, using Eq. (25), we obtain

$$S(p) = k\sqrt{p_0p_1} = k\sqrt{p_i(1-p_i)}, \quad (28)$$

that is a concave function representing the geometric average of the quantum states probability, where certainty corresponds to $S = 0$. Here, we can see the difference between the standard statistical mechanics and the ground-state statistical mechanics. For the standard we always use the Boltzmann-Gibbs entropy $S(p) = k \sum_i p_i \ln p_i$, while for the ground-state statistical mechanics, this universality is broken, and the entropic form depends on the particular quantum system.

4. CONCLUSIONS

We have discussed the connection between interaction and statistical mechanics of the ground-state for the Hubbard model with interacting particles in the Hilbert space of lowest dimensionality. Specifically, we have investigated the case of two particles into two sites. Considering the ground-state thermodynamics [1], we obtain the ground-state internal energy, ground-state free energy, ground-state entropy and ground-state heat capacity as a function of the ground-state temperature, as well as, we find the functional dependence for the entropy in terms of the occupation probability of the non-interacting quantum states.

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