



Describing the ground state of quantum systems through statistical mechanics

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ABSTRACT

We present a statistical mechanics description to study the ground state of quantum systems. In this approach, averages for the complete system are calculated over the non-interacting energy levels. Taking a different interaction parameter, the particles of the system fall into non-interacting microstates, corresponding to different occupation probabilities for these energy levels. Using this novel thermodynamic interpretation we study the Hubbard model for the case of two electrons in two sites and for the half-filled band on a one-dimensional lattice. We show that the form of the entropy depends on the specific system considered.

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1. Introduction

Statistical Mechanics (SM) provides useful concepts to study systems with a large number of particles. For example, based on standard SM, Edwards [1] proposed a thermodynamic description of granular matter in which thermodynamic quantities are computed as flat averages over configurations where the grains are static or jammed, leading to a definition of configurational temperature. A numerical diffusion-mobility experiment of a granular system has supported the Edwards' statistical ensemble idea [2]. Another example is the relation between entropy and the horizon area of a black hole [3], which provides a new approach for studying black holes and quantum gravity theory. Furthermore, four laws of black hole mechanics can be demonstrated using this thermodynamic description. The microscopic origin of the black hole entropy, originally calculated thermodynamically, has been explained from string theory [4].

Recently, Cejnar et al. [5] analyzed quantum phase transitions in finite systems [6] by defining an analog of the absolute temperature scale connected to the interaction parameter of the Hamiltonian. And thus, they were capable of establishing a thermodynamic analogy for the quantum phase transition. However, they did not identify the correspondence with statistical mechanics and consequently the new scenario opened by this microscopic analysis. This correspondence and these consequences are the goal of this paper.

Here, we use tools developed in SM to study the ground-state of quantum systems. We observe that, for certain classes of quantum systems, taking different intensities of the interaction between particles of the system corresponds to taking different occupation probabilities for non-interacting microstates energy levels. With this observation we can define an analog of the absolute temperature scale in such a manner that it is possible to make a thermodynamic interpretation for the interaction in the ground-state of quantum systems. The Hubbard Hamiltonian [7] is a typical model in which this approach can be applied. Here, we analyze two exact solvable limits of the Hubbard model.

This paper is organized as follow. The formalism is described in Section 2. The study of the two exact solvable problems based on the Hubbard model are presented in Section 3. Finally, we present the conclusions in Section 4.

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2. Formalism

The scheme of our formalism can be applied to a broad class of Hamiltonians defined as

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

where we assume that \hat{H}_0 is a one-particle Hamiltonian operator and the interaction term is given by the \hat{V} operator and T is the dimensionless interaction parameter. Here, we must consider that $T \geq 0$ and the operator \hat{V} is positively defined. In this way we have established that the energy is a concave function of T .

A good example of this class of Hamiltonians is the one of the Hubbard model [7]. In this model, which is amongst the most important magnetic ones, the eigenstates of the Hamiltonian in the absence of interaction ($T = 0$) are just the non-interacting states $|\phi_i\rangle$, whose respective energy eigenvalues, $E_i(0)$ are defined through the relation $\hat{H}_0|\phi_i\rangle = E_i(0)|\phi_i\rangle$. The eigenvalues $E_i(T)$ of \hat{H} for nonvanishing T are obtained from the equation $\hat{H}|\psi_i\rangle = E_i(T)|\psi_i\rangle$. Moreover, the expectation value of an operator \hat{X} on the ground-state $|\psi_0\rangle$ is given by $\langle\psi_0|\hat{X}|\psi_0\rangle$.

Now, we can provide an approach for obtaining expectation values of physical quantities on the ground-state in the base of non-interacting states. This simply means to find the expectation values of \hat{X} on the ground-state in the $|\phi_i\rangle$ representation.

The ground-state $|\psi_0\rangle$ can be expanded in terms of the non-interacting states $|\phi_i\rangle$ as

$$|\psi_0\rangle = \sum_i a_i(T)|\phi_i\rangle, \quad (2)$$

where the coefficients $a_i(T) = \langle\phi_i|\psi_0\rangle$. We recall that the quantity $|a_i(T)|^2$ has a *probabilistic* interpretation. In other words, we can write $p_i(T) \equiv |a_i(T)|^2 \in [0, 1]$ and $\sum_i p_i(T) = \sum_i |a_i(T)|^2 = 1$. This establishes the connection to SM: the expectation value of \hat{H}_0 ,

$$\langle\hat{H}_0(T)\rangle = \langle\psi_0|\hat{H}_0|\psi_0\rangle = \sum_i p_i(T)E_i(0), \quad (3)$$

can be interpreted as a usual average, which is computed over the set of non-interacting energy levels $E_i(0)$, each one with probability $p_i(T)$. It is an analog of the mean energy $\langle E \rangle = \sum_i p_i E_i$.

We can easily verify that $\partial E_0(T)/\partial T = \partial\langle\psi_0|\hat{H}|\psi_0\rangle/\partial T = \langle\psi_0|\hat{V}|\psi_0\rangle$. It is straightforward to find that $\langle\psi_0|\hat{V}|\psi_0\rangle > V_0$, where V_0 is the lower bound to the eigenvalues of \hat{V} . We have considered that \hat{V} is positively defined. An immediate consequence is that $V_0 \geq 0$ and it finally follows that $\partial E_0(T)/\partial T \geq 0$, leading to the monotonically increasing behavior of $E_0(T)$ as a function of T , i.e., $E_0(T_1) \leq E_0(T_2)$ for $T_1 \leq T_2$. Before we continue on the presentation of the method, let us observe that we also can consider $T \leq 0$ with \hat{V} being negatively defined. In this situation, observing now that \hat{V} has an upper bound eigenvalue, we can also easily prove that $\partial E_0(T)/\partial T \geq 0$. In the above cases, in analogy to SM, for the non-interacting case $T = 0$ the system has the lowest energy $E_0(0)$ and $p_i(0) = \delta_{i0}$. If $T > 0$, like thermal energy, the interaction favors other energy levels of the non-interacting case. In this description, only the non-interacting microscopic states are used to compute the *thermodynamic* properties. This enables us to define an analog of the absolute temperature scale, called ground-state temperature, as $T_g = T/k$, where k is a constant measured in K^{-1} .

This description is illustrated in Fig. 1. Similar to the usual canonical ensemble of the SM, we can consider that taking different ground-state temperatures T_g , i.e., different values of the interaction parameter, the particles of the system fall into non-interacting microstates, corresponding to different occupation probabilities for these energy levels.

In addition, an analogy to the standard thermodynamics is also reproduced by this description. We can introduce a so-called ground-state thermodynamics, defining the ground-state internal energy, ground-state free energy and ground-state entropy, respectively, as

$$U(T_g) = \langle\hat{H}_0(T_g)\rangle = \sum_i p_i(T_g)E_i(0), \quad (4)$$

$$F(T_g) = \langle\hat{H}(T_g)\rangle - kT_g\langle\hat{V}(0)\rangle, \quad (5)$$

$$S(T_g) = k(\langle\hat{V}(0)\rangle - \langle\hat{V}(T_g)\rangle). \quad (6)$$

It can be easily seen that $S(T_g)$ is a non-negative monotonically increasing function of T_g . We can trivially verify that, using Eqs. (4)–(6), the ground-state thermodynamics precisely satisfies the standard thermodynamics relation for the Helmholtz free energy

$$F(T_g) = U(T_g) - T_g S(T_g). \quad (7)$$

Furthermore, we can derive the thermal response function, in correspondence to the heat capacity

$$C(T_g) = T_g \frac{dS(T_g)}{dT_g} = -T_g \frac{d^2 F(T_g)}{dT_g^2}. \quad (8)$$

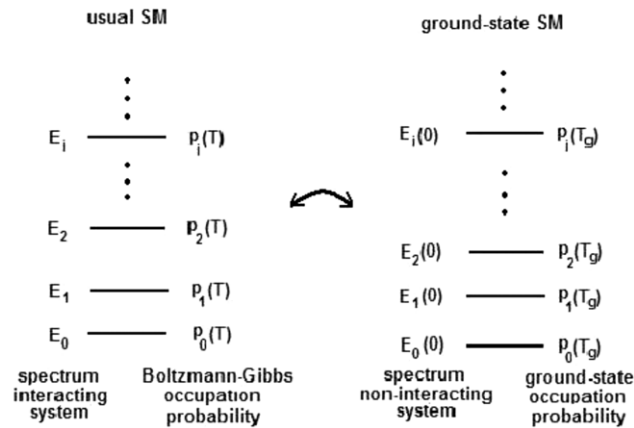


Fig. 1. Similar to the usual canonical ensemble of the SM, taking a different ground-state temperature T_g (interaction parameter), the particles of the system fall into non-interacting microstates, corresponding to different occupation probabilities for these energy levels.

It is interesting to observe that the expression above can be calculated using the Hellmann-Feynman theorem which allows one to find the ground-state expectation values of a general operator \hat{X} by differentiating the ground state energy of a perturbed Hamiltonian $\hat{H}_0 + \lambda\hat{X}$ with respect to λ [8].

Unfortunately, the identification of the entropy as an expectation value of an observable used in Eq. (6) suggests that we do not have a closed theory since in Statistical Mechanics the entropy is not dependent on the eigenvalues of an observable. However, as we will see in the next section, in a particular application, we can express the entropy as a quantity exclusively depending on the probabilities that describe the system and that it is a symmetrical function of these probabilities, as one expects in Statistical Mechanics. The general fundamental question remains open.

Furthermore, it is important to mention that the canonical ensemble is characterized by an entropic variational principle under the constraint imposed by the mean energy [9]. In more general cases, as studied for example in Ref. [10], we can use a more general entropic variational principle using constraints imposed by the mean values of more than one relevant observable. However, it has not yet been established what is the role played by the maximum entropy principle within our scheme. Understanding this point is an open problem.

3. Applications

For illustrating the approach introduced in this letter, let us study two exact solvable problems based on the Hubbard model [7]. The Hamiltonian of the Hubbard model is defined as

$$\hat{H} = -t \sum_{\langle ij \rangle \alpha} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{9}$$

where $\hat{c}_{i\alpha}^\dagger$, $\hat{c}_{i\alpha}$ and $\hat{n}_{i\alpha} \equiv \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha}$ are respectively the creation, annihilation and number operators for an electron with spin α 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 the lattice; U is the Coulomb 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. First and second terms of Eq. (9) correspond to, respectively, one-particle \hat{H}_0 and interaction terms of Eq. (1).

The problem of two electrons in two sites is the simplest example to our approach. By using direct calculus, it is easy to obtain the ground-state eigenvalue and eigenfunction, respectively, as

$$E_0(U) = -\frac{1}{2}(U - \sqrt{U^2 + (4t)^2}), \tag{10}$$

and

$$|\psi_0\rangle = a_- |\phi_-\rangle + a_+ |\phi_+\rangle \tag{11}$$

where $|\phi_\pm\rangle$ are eigenfunctions for the case $U = 0$, with $a_- = \sqrt{1 - a_+^2}$ and

$$a_+ = 2t / \sqrt{(2\sqrt{U^2 + (4t)^2} - U)\sqrt{U^2 + (4t)^2}}. \tag{12}$$

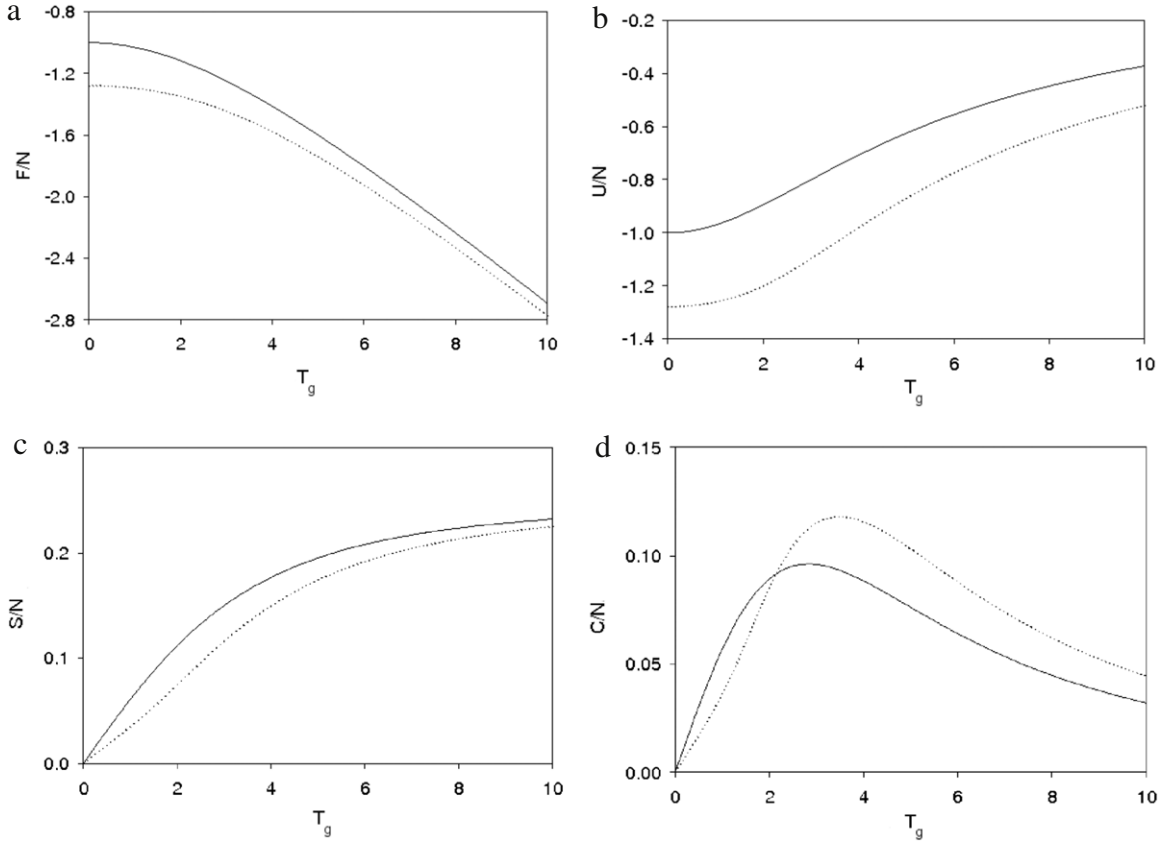


Fig. 2. Ground-state (a) free energy $F(T_g)$, (b) internal energy $U(T_g)$, (c) entropy $S(T_g)$ and (d) heat capacity $C(T_g)$ versus temperature T_g for the Hubbard model ($k = 1$ and $t = 1$). The full line represents the case $N = 2$ and two electrons, while the dotted line represents the half-filled band for the one-dimensional case in the thermodynamic limit ($N \rightarrow \infty$).

Thus, we define $T_g = U/kt$, and using Eqs. (4)–(6) into Eqs. (10) and (11), we find (from now $k = 1$ and $t = 1$ for simplicity)

$$F(T_g) = -\frac{1}{2}\sqrt{T_g^2 + 16}, \quad (13)$$

$$S(T_g) = \frac{T_g}{2\sqrt{T_g^2 + 16}}, \quad (14)$$

$$U(T_g) = -\frac{8}{\sqrt{T_g^2 + 16}}, \quad (15)$$

and

$$C(T_g) = \frac{8T_g}{2(T_g^2 + 16)^{3/2}}. \quad (16)$$

Fig. 2 shows curves (full lines) of $F(T_g)$, $U(T_g)$, $S(T_g)$ and $C(T_g)$ versus the temperature T_g for the expression above representing the case of two electrons on two sites for the Hubbard model. As is clearly seen in these figures, the behavior of these new variables is exactly as expected from the usual thermodynamics.

Now, let us consider the functional dependence for the entropy given by Eq. (14) in terms of the occupation probability of the non-interacting quantum states. Using the energetic constraint (Eq. (4)), this dependence generates the concept of thermostat temperature, if we focus on the canonical ensemble of the SM formalism. It is easy to show from Eqs. (11)–(12) that the occupation probabilities for the eigenfunctions $|\phi_{\pm}\rangle$ of the non-interacting case are

$$p_{\pm}(T_g) = \frac{1}{2} \mp \frac{2}{\sqrt{T_g^2 + 16}}. \quad (17)$$

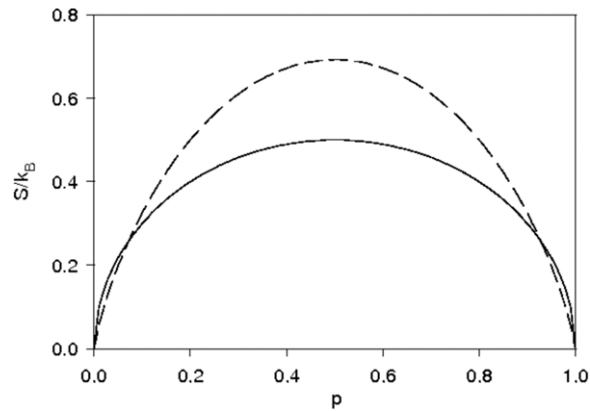


Fig. 3. Functional forms of the entropies $S(p)$ associated with the Boltzmann–Gibbs (dashed line) and with Eq. (18) for 2 states (full line).

We straightforwardly obtain the entropic form

$$S(p) = \sqrt{p_+ p_-}, \quad (18)$$

which 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 SM and the ground-state SM. For the standard SM we always use the Boltzmann–Gibbs entropy $S(p) = -\sum_i p_i \ln p_i$, while for the ground-state SM, this universality is broken, and the form of the entropy depends on the particular quantum system. On the other hand, this issue does not rule out the possibility that many different systems fall into some basic classes exhibiting qualitatively similar behavior. In Fig. 3, we show the functional forms of the entropies associated with the Boltzmann–Gibbs and with Eq. (18) assuming 2 states.

In what follows, we shall illustrate the above procedure by addressing the exact solution for the half-filled band of the Hubbard model for the one-dimensional case in the thermodynamic limit. This famous solution was obtained by Lieb and Wu in the sixties [11] using the Bethe ansatz. Since then, this result is considered one of the most important ones, owing to the lack of exact solution for the Hubbard Model. The ground-state as a function of the electron–electron interactions U , for N sites in the limit $N \rightarrow \infty$, is given by

$$E_0(U) = -4N \int_0^\infty \frac{J_0(w)J_1(w)dw}{w[1 + \exp(wU/2)]}, \quad (19)$$

where $J_0(w)$ and $J_1(w)$ are Bessel functions. It is, then, simple to obtain the quantities associated to the ground-state thermostatics:

$$F(T_g)/N = -\frac{T_g}{4} - 4 \int_0^\infty \frac{J_0(w)J_1(w)dw}{w[1 + \exp(wT_g/2)]}, \quad (20)$$

$$S(T_g)/N = \frac{1}{4} - \frac{1}{2} \int_0^\infty \frac{J_0(w)J_1(w)dw}{\cosh^2(wT_g/4)}, \quad (21)$$

$$U(T_g)/N = - \int_0^\infty \frac{J_0(w)J_1(w)f(w, T_g)dw}{w[1 + \exp(wT_g/2)]^2}, \quad (22)$$

where $f(w, T_g) = [4 + (4 + wT_g/2) \exp(wT_g/2)]$ and

$$C(T_g)/N = \frac{T_g}{4} \int_0^\infty \frac{wJ_0(w)J_1(w) \sinh(wT_g/4)dw}{\cosh^3(wT_g/4)}. \quad (23)$$

We show the behavior of $F(T_g)$, $U(T_g)$, $S(T_g)$ and $C(T_g)$ versus the temperature T_g for the solution of the one-dimensional Hubbard model in Fig. 2. These curves correspond to the dotted lines and, as well noticed from the case of two electrons, they are also expected from the usual thermodynamics.

4. Conclusions

In summary, we introduce an approach to solve problems of quantum mechanics using concepts of statistical mechanics. We can consider that taking different ground-state temperatures T_g , i.e., different values of the interaction parameter, the particles of the system fall into non-interacting microstates, corresponding to different occupation probabilities for these energy levels.

We found that the functional form of the ground-state entropy depends on the particular quantum system. The breakdown of universality of the entropy is consistent with the concept of generalized entropies [12] associated with a specific quantum Hamiltonian. However, there have to be further investigations for identifying the entropic variational principle in our scheme.

Finally, the ideas presented here can eventually provide a mechanism for new approximation methods, such as the usage of the geometric average of the quantum states probability in the high dimensional limit for the Hubbard model. We can envisage in further works the study of the possibility that many different systems may fall into some basic classes of the ground-state entropy.

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