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Ground-state structural transitions in small clusters within the effective temperature framework

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ABSTRACT

Ground-state structural transitions in finite-sized systems are studied in the Hubbard model. We use the concept of an effective temperature γ that is directly related to the interactions among electrons. We have studied all the possible clusters, with nearest-neighbour hopping, for two, three and four sites. Furthermore, we have also analysed the octahedron and the seven-site Apollonian networks. We show that the clusters in which there is a ground-state phase transition are antiferromagnetically frustrated. The low temperature dependence for the specific heat and entropy allow us to infer that there is a V-shaped universal phase in finite clusters.

1. Introduction

The study of thermodynamic properties of finite systems has proved a fascinating and challenging research field, particularly when it involves phase transitions. It has been greatly focused upon in view of its application in, for example, Bose–Einstein condensation in magnetically or optically trapped alkali atoms [1], the nuclear liquid–gas transition in heavy ion reactions [2], and the solid–liquid phase transition of sodium clusters [3].

Finite clusters are far away from the thermodynamic limit and the standard description of a phase transition is not applicable. For example, the specific heat of finite small systems cannot exhibit the sharp peak or discontinuity observed in phase transition regions. Typically, the specific heat curves of finite small systems present smooth peaks in temperature associated with some destruction of the short-range ordering [4–8].

Recently, several theoretical descriptions, identifications and classifications of phase transitions in finite clusters have been put forward [9–13]. For example, Borrmann et al. [9] have shown that the distribution of zeros of the canonical partition function in the complex temperature plane provides a powerful tool for detecting phase changes and creating classification schemes concerning the order of the transition. For a parabolically trapped ideal Bose gas in d dimensions, Mulken et al. [14] obtained a second-order transition for $d = 2$, and a third-order transition for all other higher dimensions.

These features are expected for thermal phase transitions in finite systems. However, further studies are relevant for our understanding of the class of the quantum phase transition (QPT) in finite quantum systems. The QPT takes place at absolute zero and is driven by quantum fluctuations associated with competing ground states [15–19]. One of the most important aspects that has been analysed for the QPT is its universal nature. The concept of universality in the scaling form of the thermodynamic properties close to the quantum critical point (QCP) is used as for the thermal phase transition. Many generic features of conventional phase transitions cannot, however, be applied for the QPT. For example, a QPT can occur between two disordered phases without any symmetry breaking and we cannot consider any conventional Landau-type order parameters [20]. A comprehensive characterization of different kinds of QPT must be carefully considered in the theoretical approaches, since there are several remaining open questions about it.

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In this paper, we investigate the ground-state transition in some finite systems. This transition is associated with changes in the ground-state spatial symmetry. The purpose is to examine finite clusters as a function of the Coulombian interaction on the Hubbard model [21–23] by using cluster diagonalization [4–6] in order to obtain the exact ground-state and thermodynamic properties. This approach offers an opportunity to study a set of universal properties associated with the QPT in finite clusters. We consider a statistical mechanics description for the ground state in order to study the QCP [24,25].

In the next section, we describe the methodology used in this work. The results are discussed in Sections 3 and 4. Conclusions are presented in Section 5.

2. Methodology

The main characteristics of the QPT are theoretically well-known [15]. Its behaviour has been interpreted with remarkable success using the simplest interacting lattice systems, exemplified by the Ising model in a transverse field, and Kondo, and bosonic and fermionic Hubbard models. The QPT can be accessed by analysis of the ground state of the model that describes the system as a function of a parameter g of the Hamiltonian. In experiments, g is a parameter, such as the magnetic field or pressure. In the transition, $g = g_c$, the ground state changes, and its energy, in infinite lattice systems, is a non-analytic function of g. Close to temperature $T = 0$, the dynamics of excited states and the thermodynamics are intimately tied to each other.

Our study will be based on the Hubbard model [21–23]. Its Hamiltonian is defined by

$$\hat{H} = \hat{H}_0 + I\hat{V} = -t \sum_{\langle ij\rangle\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + I \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\alpha}$, $c_{i\alpha}$ and $n_{i\alpha} \equiv c^{\dagger}_{i\alpha} c_{i\alpha}$ are respectively the creation, annihilation and number operators for an electron with spin α in an orbital localized at site i, and $\langle ij\rangle$ denotes pairs i, j of nearest-neighbour sites on lattice; I is the Coulombian repulsion that operates when the two electrons occupy the same site; and t is the electron transfer integral connecting localized states in nearest-neighbour sites.

Here, we use the formalism recently introduced by Cejnar et al. [24] and Souza [25]. Cejnar et al. [24] established a thermodynamics connection for the QPT as an analogy to the Borrmann et al. [9] procedure for the thermodynamic phase transition in finite systems. Souza [25] identified the correspondence between statistical mechanics and this. It has been observed that assuming different intensities of the interaction I is equivalent to taking different occupation probabilities for the energy levels of the non-interacting microstates, in such a way that it is possible to construct a thermodynamic interpretation of the interaction within the ground state for quantum systems. Along these lines, we can define an analogue of the absolute temperature scale, called the effective temperature, as $\gamma = I/k$, where k is a constant measured in joules/kelvins. We verified that γ presents a behaviour very similar to those found in standard thermodynamics as one changes the absolute temperature T. Moreover, important relations, analogous to those of standard thermodynamics, are found for the effective temperature γ.

We can introduce an effective thermodynamics, defining the ground-state internal energy, ground-state free energy, ground-state entropy and ground-state heat capacity, respectively, as

$$U_{GS}(\gamma) = \langle \hat{H}_0(\gamma)\rangle, \tag{2}$$

$$F_{GS}(\gamma) = \langle \hat{H}(\gamma)\rangle - I\langle \hat{V}(0)\rangle, \tag{3}$$

$$\gamma S_{GS}(\gamma) = I(\langle \hat{V}(0)\rangle - \langle \hat{V}(\gamma)\rangle), \tag{4}$$

$$C_{GS}(\gamma) = \gamma \frac{dS_{GS}(\gamma)}{d\gamma} = -\gamma \frac{d^2 F_{GS}(\gamma)}{d\gamma^2}, \tag{5}$$

where the expectation value of an operator $\hat{X}$ on the ground state $|\psi_0(\gamma)\rangle$ of $\hat{H}$ (i.e., $\hat{H}|\psi_n(\gamma)\rangle = E_n|\psi_n(\gamma)\rangle$) is given by $\langle \hat{X}(\gamma)\rangle = \langle \psi_0(\gamma)|\hat{X}|\psi_0(\gamma)\rangle$. Consistently, $F_{GS}(\gamma) = U_{GS}(\gamma) - \gamma S_{GS}(\gamma)$, and $\left(\frac{\partial S_{GS}}{\partial U_{GS}}\right)_t = \frac{1}{\gamma}$.

The standard statistical mechanics is described by Boltzmann–Gibbs (BG) statistical mechanics. In this framework, the functional form of the entropy in terms of the probability density p_i is $S(p) = -k_B \sum_i p_i \ln p_i$. However, for the effective statistical mechanics presented here, this is different. For example, for the Hubbard model with two electrons in two sites the entropy is written as $S(p)_{GS} = k\sqrt{p(1-p)}$ [25]. In general, the entropic form depends on the quantum system considered [25].

It is interesting to note that the lack of universality of the entropy, imposing that we cannot apply the Boltzmann–Gibbs entropy, yields major implications for the QPT in finite systems. The ground-state statistical mechanics transcends the validity of the Yang–Lee theorem [26]. Thus there is no reason to believe that it is not possible to obtain a QPT in finite systems.