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Thermodynamic signatures of an underlying quantum phase transition: A grand canonical approach

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ABSTRACT

The grand canonical formalism is employed to study the thermodynamic structure of a model displaying a quantum phase transition when studied with respect to the canonical formalism. A numerical survey shows that the grand partition function diverges following a power law when the interaction parameter approaches a limiting constant. The power-law exponent takes a distinctive value when such limiting constant coincides with the critical point of the subjacent quantum phase transition. An approximated expression for the grand partition function is derived analytically implementing a mean field scheme and a number of thermodynamic observables are obtained. The system observables show signatures that can be used to track the critical point of the underlying transition. This result provides a simple fact that can be exploited to verify the existence of a quantum phase transition avoiding the zero temperature regime.

1. Introduction

The observation of quantum-interference effects in many-body systems is often deterred by the very short coherence times displayed by quantum pure states in nature. This affects in particular cooperative states resulting from interaction-dominated phases in many-body systems. These states have important applications in quantum computation and nanoelectronics because interaction is key to develop control mechanisms. In contrast to pure states, mixed states are less prone to be demolished by decoherence [1], especially when they correspond to equilibrium states because their entropies are maximal and the system cannot loss any more information to the environment. As a result, it is reasonable to assume that the observation of specific effects in many-body systems through thermodynamic states is feasible, even practical, as long as it be possible to easily keep the system in equilibrium.

Quantum Phase Transitions (QPTs) are physical processes arising from a change in the ground state structure of a system as a parameter crosses a transition- or critical-point [2]. These transitions occur at zero temperature and they are strongly influenced by quantum correlations. In fact, it is known that the amount of entanglement present in a system is maximal at, or close to, the critical point of a second order QPT [3]. The universality class of a QPT is determined by the power law exponents that define the scaling behavior of characteristic variables in the vicinity of the critical point. Recently, there has been interest in knowing how correlations, either classical or quantum, behave at finite temperature in models showing well understood QPTs [4,5]. These investigations have been made using canonical ensemble theory: the system is in thermodynamic equilibrium with a bath at fixed temperature and the number of particles is fixed. In contrast, applications of the grand-canonical ensemble theory to the same kind of systems are, to the best of the authors' knowledge, not available so far. The element that is added in the grand canonical formulation is the notion of fluctuations of the number of particles. In this case an open quantum system interacts with a bath in such a way that not only energy but also particles can be exchanged. This additional consideration might better describe the conditions encountered in some low-temperature- and solid-state-experiments. Let us consider a system governed by the following Hamiltonian

$$\hat{H}_M = \hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 - \frac{\lambda}{M}\left(\hat{a}_1^\dagger \hat{a}_1 \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_2\right). \qquad (1)$$

The operators that describe the Hamiltonian follow bosonic commuting relations $[\hat{a}_1, \hat{a}_1^\dagger] = [\hat{a}_2, \hat{a}_2^\dagger] = 1$ and $[\hat{a}_1, \hat{a}_2] = 0$. Symbols M and λ represent the number of particles and the intensity of the interaction among bosons respectively. By definition $\hat{H}_0 = 0$. The Hamiltonian has been normalized so that λ is dimensionless and the energy unit is half the energy difference between the eigenenergies of $\hat{H}_1$. In this letter only the case $\lambda > 0$ is considered. It is possible to change the sign of the single particle term so that it better resembles a kinetic energy contribution applying a unitary transformation producing $\hat{a}_1 \to i\hat{a}_1$ and $\hat{a}_2 \to -i\hat{a}_2$. This scheme

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can be seen as a simple model describing a system of cold atoms tunneling between symmetric adjacent wells and undergoing attractive interactions [6,7]. It is known that in actual experiments both the double-well profile and the interaction intensity can be controlled to a great degree [8]. Usually, the confining profile is realized using counter-propagating laser beams that form a periodic super-lattice while the interaction can be tuned applying a magnetic field near a Feshbach resonance [9]. In numerical studies it is useful to exploit the fact that $\hat{H}_M$ commutes with the following operators,

$$\hat{M} = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2, \qquad \hat{\Pi} = e^{i\frac{\pi}{2}\left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1\right)}. \tag{2}$$

These commutation properties imply that the eigenstates of (1) display fixed number of particles and, for non-degenerate spectra, parity. This latter symmetry emerges as a consequence of the invariance of the Hamiltonian under the swap of labels (wells) $1 \leftrightarrow 2$. The system behavior is determined by the trade-off between hopping and attractive interaction. Hamiltonian (1) can be written in terms of angular momenta through the following Schwinger transformation,

$$\hat{J}_z = \frac{\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1}{2}, \quad \hat{J}_x = \frac{\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2}{2}. \tag{3}$$

Inserting these identities in Eq. (1) and after a few arrangements we arrive to,

$$2\hat{J}_z - \frac{2\lambda}{M}\hat{J}_x^2 - \frac{M\lambda}{2}, \tag{4}$$

which corresponds to a particular case of the Lipkin–Meshkov–Glick (LMG) model [10]. This model undergoes a QPT at $\lambda_c = 1$ and a phase transition at finite temperature $\beta_c = \tanh^{-1}\frac{1}{\lambda^2}$. The Hamiltonian form shown in Eq. (4) has been extensively studied with reference to, among many others, its scaling behavior [11–13], energy spectrum [14], correlations at finite temperature [4] and applications to quantum metrology [15]. If the angular momenta are written as sums of spins, $\hat{J}_{x,z} = \frac{1}{2}\sum_{j=1}^{M}\hat{\sigma}_j^{x,z}$, where $\hat{\sigma}^{x,z}$ are Pauli matrices, the model becomes

$$\sum_{j=1}^{M}\hat{\sigma}_j^z - \frac{\lambda}{M}\sum_{j=1}^{M}\sum_{k=1}^{j-1}\hat{\sigma}_k^x\hat{\sigma}_j^x - M\lambda. \tag{5}$$

In this notation, and up to a constant factor, the model is known as the infinite range Ising model because the interaction among spins is completely homogeneous with respect to the spin index. It is worth mentioning that Hamiltonian (1) is not completely equivalent to either Hamiltonian (5) or Hamiltonian (4), as can be seen by comparing their respective Hilbert space dimensions. Indeed, the sums of spins give rise to various irreducible representations of Hamiltonian (4) corresponding to different values of total angular momentum. The representation with the biggest total angular momentum corresponds to Hamiltonian (1). It can be shown that, up to an additive constant proportional to M, Hamiltonian (1) is the bosonic second quantization of Hamiltonian (5) and as such it is spanned by the symmetric states of the spin basis. This affects the density of states and eventually derives in the fact that Hamiltonians (4) and (5) exhibit a QPT as well as a phase transition at finite temperature, while Hamiltonian (1) displays only a QPT. Such a QPT can be studied by assuming that the ground state is given as follows [6]

$$|G(\theta)\rangle = \frac{\hat{b}^{\dagger M}|0\rangle}{\sqrt{M!}}, \ \hat{b}^\dagger = \hat{a}_1^\dagger\cos\theta - \hat{a}_2^\dagger\sin\theta, \tag{6}$$

where θ is bounded to the interval $[0, \pi]$ in order to avoid redundancies. The angle θ takes the value that minimizes the energy

$$E_G = Min_\theta\langle G(\theta)|\hat{H}_M|G(\theta)\rangle. \tag{7}$$

After some direct calculations we obtain to leading order in M

$$\text{if } \lambda < 1, \ \theta^* = \frac{\pi}{4} \text{ and } E_G = -M\left(1 + \frac{\lambda}{2}\right). \tag{8}$$

Otherwise

$$\text{if } \lambda \geq 1, \ \theta_1^* = \frac{1}{2}\arcsin\left(\frac{1}{\lambda}\right) \text{ or } \theta_2^* = \frac{\pi}{2} - \theta_1^*, \tag{9}$$

and $E_G = -M\left(\lambda + \frac{1}{2\lambda}\right)$. Canonical ensemble theory dictates that the statistical state becomes $|G(\theta^*)\rangle$ for $\lambda < 1$ and

$$\frac{1}{2}\left(|G(\theta_1^*)\rangle\langle G(\theta_1^*)| + |G(\theta_2^*)\rangle\langle G(\theta_2^*)|\right), \tag{10}$$

for $\lambda \geq 1$. The QPT is characterized by a structural change in the spectrum of the Hamiltonian, which goes from a gaped phase with non-degenerate energy levels for $\lambda < 1$, to a gapless phase with a double degeneration of every level for $\lambda \geq 1$.[1] Such a change in the density of states takes place only in the limit $M \to \infty$ (the thermodynamic limit) and is marked by a discontinuity at $\lambda = 1$ in the second derivative of the rescaled free energy.[2] As the free energy is continuous at the critical point, the transition is classified as a second order QPT. Neither $|G(\theta_1^*)\rangle$ nor $|G(\theta_2^*)\rangle$ are invariant under parity transformations, because they display different occupation numbers at each side of the double well. Contrariwise, both state (10) and $|G(\theta^*)\rangle$ are invariant, and as such it can be said that symmetry is preserved across the critical point as long as the system remains in thermodynamic equilibrium so that the transition be reversible. The general purpose of this work is to analyze the thermodynamic properties of a system governed by Hamiltonian (1) using the grand canonical formalism, i.e., assuming that the number of particles is not fixed but subject to statistical fluctuations determined by the characteristic conditions of a surrounding bath. In particular, it is of interest to examine whether signatures of the aforementioned QPT can be in any way seen in the resulting framework. The underlying intention is to establish a connection of physical significance between the properties of the system in the thermodynamic limit and its finite size structure as a whole.

2. Grand canonical approach

The thermodynamics of the model is determined by the grand canonical partition function,

$$\Xi = \sum_{M=0}^{\infty} Tr\left(e^{-\beta(\hat{H}_M - \mu\hat{M})}\right), \tag{11}$$

where β and μ indicate the inverse temperature and chemical potential respectively. For a set of parameters λ, μ and β, a corresponding state in thermodynamic equilibrium is well defined as long as Ξ converges to a positive real number. One way of ensuring convergence is by requiring that the terms having large M in (11) go to zero fast enough as M goes to infinity. A convergence analysis can be done using the fact that the system's ground state energy in the thermodynamic limit E_G is known. It is in this way found that in order to guarantee the convergence of Ξ the interaction parameter must fulfill $\lambda < \lambda_D$, where

$$\lambda_D = -2(1 + \mu) \to \mu = -\left(1 + \frac{\lambda_D}{2}\right), \tag{12}$$

[1] Here only the ground state degeneration is shown. Numerical simulations show that this also happens to the rest of the spectrum.

[2] At zero temperature the free energy is just $f = E_G$.