Thermal entanglement witness for materials with variable local spin lengths

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We show that the thermal entanglement in a spin system using only magnetic-susceptibility measurements is restricted to the insulator materials. We develop a generalization of the thermal entanglement witness that allows us to get information about the system entanglement with variable local spin lengths that can be used experimentally in conductor or insulator materials. As an application, we study thermal entanglement for the half-filled Hubbard model for linear, square, and cubic clusters. We note that it is the itinerancy of electrons that favors the entanglement. Our results suggest a weak dependence between entanglement and external spin freedom degrees.

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I. INTRODUCTION

The manipulation of quantum systems in an entangled state that can be used as a quantum information channel is one of the main challenges of science today. Information theory, teleportation, and cryptography are just some of the areas that may advance enormously through the amount of technological applications, which can potentially make use of entanglement [1–4]. It is also of great interest to explore the role played by entanglement systems in order to understand the basis of quantum mechanics [3,4]. However, even the quantification of entanglement remains an open question. Current research is focusing on measures for precisely quantifying entanglement [5–7]. As an example, entanglement of indistinguishable particles calculated using different measures has shown that a same quantum state can have several different characterizations because of the lack of individual identity of the entangled particles [8–11].

The use of uncertainty relations has provided an efficient approach for obtaining one of the most precise experimental measures of entanglement [12]. A quantitative evaluation of the entangled states can be defined in terms of expectation values of a convenient witness operator. This operator, called the entanglement witness, is defined as taking positive values for separable states and negative ones for entangled states. Thus, an appropriate uncertainty relation allows us to choose macroscopic properties which define an entanglement witness.

A good level of interest has been focused on the special case of entanglement in macroscopic properties which has been particularly motivated by experiments that have shown the presence of entanglement in solid-state systems [13–16]. Wieśniak *et al.* [17] recently explored some aspects of the connection between entanglement and magnetic susceptibility for an arbitrary Hamiltonian with spin length s.

Experimental observations of thermal entanglement in spin systems using susceptibility measurements have been reported. Souza *et al.* [13] studied the compound $Na_2Cu_5Si_4O_14$. They found entanglement confined to the small clusters, with tripartite entanglement being stronger than bipartite entanglement. A similar result was obtained by Vértesi and Bene [14] in the $Na_2V_3O_7$ system that formed a nanotubular structure of weakly coupled nine-site rings. Brukner *et al.* [15] and Bose and Tribedi [16] showed entanglement in antiferromagnetic spin systems.

Since these experimental susceptibility measurements are applicable to systems with spins localized in sites of the lattice, they are in accordance with the entanglement witness as defined by Wieśniak *et al.* [17]. However, this powerful tool is not adequate for systems with variable local spin lengths, which is an important feature for conductor materials. The present work addresses this issue. We will show that new aspects of the entanglement can appear when we consider systems with variable local spin lengths. The extension of the entanglement witness across variable local spins can be related to the itinerant electron models such as Hubbard and Falikov-Kimball.

In this paper, we investigate the Hubbard model [18]. The purpose was to choose appropriated macroscopic variables in order to define an entanglement witness adequate for the Hubbard model, or any other model that can be applied to systems with variable local spin lengths.

There are some works about entanglement associated to the Hubbard model [8,19–25]. For example, the entanglement for the Hubbard dimer was investigated by Dowling *et al.* [8] and Zanardi [19]. Gun *et al.* studied the entanglement entropy on the extended Hubbard model and proposed that the entanglement can be used to identify quantum phase transitions [20]. Larsson and Johannesson found exact expressions for the local entanglement entropy on the one-dimensional (1D) Hubbard model at a quantum phase transition driven by a change in the magnetic field or chemical potential, related to the zero-temperature spin and charge susceptibilities [21]. Hudak modeled $CeAl_2$ nanoparticles by the Hubbard model with negative chemical potential and by using entanglement entropy he studied the quantum phase transitions present in this system [22].

Some experimental results have indicated that the entanglement is restricted to small clusters within the materials [13,14]. Exploring this fact, we studied the critical temperature, below which there is thermal entanglement for finite chains and rings, using the standard direct diagonalization method [26,27]. This approach is very well suited for small-sized clusters since it produces exact results for thermodynamic quantities. Furthermore, it is also interesting to study

the limit of large clusters. In this case, using the quantum Monte Carlo approach [28–30] we obtained the temperature dependence of the entanglement witness for linear, square, and simple-cubic lattices as described by the Hubbard model. Summarizing, we will show how the cluster length, itinerancy of the electrons, and system dimensions influence the thermal entanglement on the Hubbard model using direct diagonalization and quantum Monte Carlo methods.

The organization of this paper is as follows. Entanglement witness for constant and variable local spin is presented in Sec. II, the results in Sec. III, and the conclusions in Sec. IV.

II. ENTANGLEMENT WITNESS

The total magnetic susceptibility at null magnetic field

$$\chi = \chi_x + \chi_y + \chi_z = \frac{\langle \vec{M}^2 \rangle - \langle \vec{M} \rangle^2}{(\mu_B)^2 N k_B T} \tag{1}$$

has been a useful variable to study the witness of thermal entanglement. Here, $\vec{M}$ is the total magnetization of N spins and $\langle \ldots \rangle$ is the thermodynamic average. Considering s_i to be the length of the ith spin in the system, the entanglement condition for a thermal state of N spins of same length s ($s_i=s$ for $i=1,\ldots,N$) is given by [17]

$$\chi < \frac{s}{k_B T}. \tag{2}$$

The above condition is deduced based on the method of entanglement detection using the uncertainty relations [12]. In summary, an arbitrary thermal state of spin s has the following conditions:

$$\begin{aligned} \langle \vec{S}_i^2 \rangle &= s(s+1) \\ \langle \vec{S}_i \rangle^2 &\leq s^2, \end{aligned} \tag{3}$$

where $\vec{S}_i$ is the spin vector of the individual site i. Therefore, if the thermal state is actually a product of N states of individual spins, the variance of magnetization would be the sum of variances of individual sites $Nk_BT\chi = \Sigma_{i=1}^N \langle \vec{S}_i^2 \rangle - \langle \vec{S}_i \rangle^2 \geq [s(s+1)-s^2] = s$, which is also valid for the general case of separable states due to the convexity of the mixture.

However, we notice that entanglement condition (2) fails if the N individual spins have different lengths $s_i \neq s$. Itinerant systems are an example of this phenomenon because the N individual sites can have different spin lengths due to the variety of ways in which they can be filled with particles. It can also occur in localized systems since the sites can be filled in different ways. Thus, Eq. (3) must be generalized as follows:

$$\begin{aligned} \textstyle\sum_{i=1}^N \langle \vec{S}_i^2 \rangle &= N \langle L_0 \rangle \\ \langle \vec{S}_i \rangle^2 &\leq s_{\max}^2, \end{aligned} \tag{4}$$

where $s_{\max}$ is the largest spin length which the individual sites can take and $L_j \equiv \frac{1}{N}\Sigma_{i=1}^N \vec{S}_i \cdot \vec{S}_{i+j}$ is the spin spin-correlation function. Therefore, we can rewrite the condition for entanglement (2) as

$$\chi < \frac{\langle L_0 \rangle - s_{\max}^2}{k_B T}. \tag{5}$$

Note that this is also valid for sites with same spin $s_i=s$ because $\langle L_0 \rangle = s(s+1)$, $s_{\max}=s$, and consequently the condition above is reduced to Eq. (2).

Particularly, assume an N-sites system in which the basis states are given by $|n_{1\uparrow}, n_{1\downarrow}\rangle \otimes \ldots \otimes |n_{N\uparrow}, n_{N\downarrow}\rangle$, where $n_{i\alpha}=0$ or 1 (due to the Pauli exclusion principle) is the number of electrons with α orientation of S^z at the individual state i. Thus, $s_i=0$ for $|0,0\rangle$ (vacuum state) or $|1,1\rangle$ (singlet state of two electrons) and $s_i=1/2$ for $|1,0\rangle$ or $|0,1\rangle$ (single-electron states). Therefore, $s_{\max}=1/2$ and taking into account isotropy $L_j^x = L_j^y = L_j^z$ (and consequently $\chi^x = \chi^y = \chi^z$), the generalized condition of thermal entanglement can be expressed as

$$\mathcal{E} \equiv \chi^z - \frac{\langle L_0^z \rangle - 1/12}{k_B T} < 0. \tag{6}$$

Note that if the individual state can only assume single electron states ($|1,0\rangle$ or $|0,1\rangle$), $s_i=s=1/2$ is fixed, $\langle L_0^z \rangle = 1/4$ and the condition of entanglement above reduces to Eq. (2) as hoped.

The generalization of the entanglement witness for variable local spins introduces, besides the magnetic susceptibility, L_0 as an experimental measurement. Called local moment, the quantity L_0 shows the degree of localization of electrons. This measurement is much less common and more difficult that the magnetic susceptibility. However, it can be obtained by neutron-diffraction methods [31–33].

III. RESULTS

Using witness (6), we investigated the thermal entanglement for the half-filled itinerant electron systems described by the Hubbard model. The Hamiltonian is

$$\mathcal{H} = -t \sum_{\langle ij \rangle \alpha} (c_{i\alpha}^\dagger c_{j\alpha} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{7}$$

where $c_{i\alpha}^\dagger (c_{i\alpha})$ are the creation (annihilation) operators for electrons at site i, $n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$, U is the on-site Coulomb (electron-electron) interaction, and t is the nearest-neighbor hopping integral representing the overlap of electron wave functions.

We have obtained exact results for linear chains and rings with two, four, and six sites using the numerical method of direct diagonalization of small clusters over the canonical and the grand canonical ensembles [26,27]. We have observed that witness (6) for small odd numbers of sites provides no information about entanglement due to $\mathcal{E} \gg 0$ for all T since χ^z diverges at null temperature [26].

It is illustrated in Fig. 1 that there is a critical temperature T_c where $\mathcal{E}(T_c)=0$ and the system is entangled for $T<T_c$ because $\mathcal{E}(T<T_c)<0$. Therefore, we can understand T_c as the highest temperature below which the system is certainly entangled since there is no certainty about the entanglement when $\mathcal{E}(T \geq T_c) \geq 0$ [12].

Figure 2 exhibits T_c versus U for 1D systems. A comparison between results for different ensembles shows a good

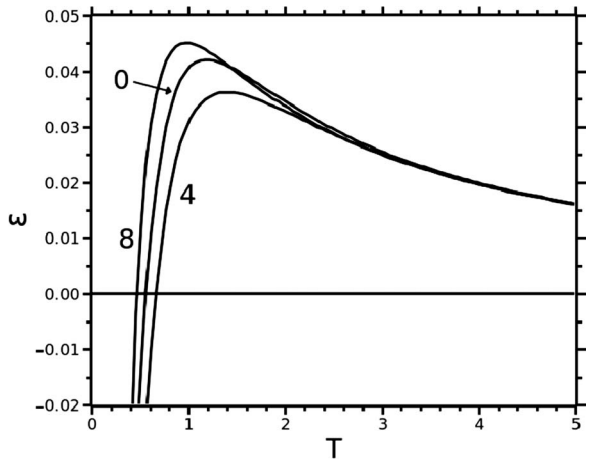

FIG. 1. Temperature dependence of the witness given by expression (6) for the four site linear chain of the half-filled Hubbard model using the grand canonical ensemble with $U=0$, 4, and 8. We adopt units $k_B=1$ and $t=1$.

agreement at large Coulomb interaction, but not at small ones. We have found a rich dependence on U and N. With fixed N for small U/t, we see that the value of T_c increases as the value of U/t is increased and tends to a maximum value. All curves have presented a value of interaction U which produces the maximum T_c (global maximum of T_c vs U). For the strong Coulombian interaction $U \gg t$, we notice that all curves present a hyperbolic behavior $T_c \propto U^{-1}$. We will define the parameter $\eta(N,U) \equiv A_N k_B T_c/(4t^2/U)$, where A_N is a

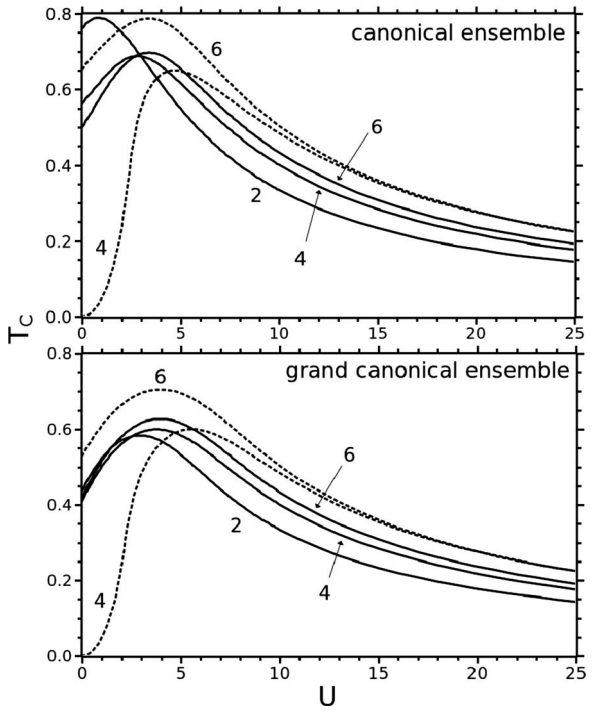

FIG. 2. Coulombian interaction dependence of the critical temperature for the finite one-dimensional half-filled Hubbard model. We adopt units $k_B=1$ and $t=1$. The solid and dashed lines are related to chains and rings, respectively. Each curve is labeled by its number of sites.

function of N. $\eta(N,U)$ is convenient to compare our results with the Heisenberg model ones, considering that in the asymptotic regime $U \gg t$ there is an equivalence between the half-filled Hubbard and the Heisenberg models with exchange interaction $J=4t^2/U$ [34].

For the grand canonical ensemble, as the size of an even sites system increases, the values of the maximum global $U^{\max}$ and $T_c^{\max}$ also increase. Although the canonical ensemble has a similar increasing relation between $U^{\max}$ and N, there is no monotonic behavior of $T_c^{\max}$ versus N. We performed a numerical extrapolation using the grand canonical ensemble for linear chains with two, four, and six sites. Our extrapolation analysis predicts $k_B T_c^{\max}=0.712t$ at $U^{\max}=4.1t$ in the thermodynamic limit. We also obtained $\eta(\infty,\infty) \cong 1.568 \pm 0.003$, which is very close to the exact value $\eta(\infty,\infty)=k_B T_c/J=1.6$ for $\frac{1}{2}-s$ Heisenberg model [17].

The direct diagonalization approach is very suitable for small-sized clusters, but becomes inefficient when the system has its size increased. On the other hand, the quantum Monte Carlo (QMC) method [28,29] is an efficient approach to study large systems. Using it we have studied the entanglement witness for linear, square, and cubic lattices.

The QMC method treats the exponentials of the grand partition function with the Suzuki-Trotter decomposition scheme. Using a discrete Hubbard-Stratonovich transformation it converts the electron-electron interaction into one of free electrons interacting with a time-dependent Ising field. With it we compute the relative weights of the Ising field configurations. The algorithm follows the lines of those for classical systems, except for the Boltzmann weight that is expressed as a sum over Ising spins of a product of determinants. For the Hubbard model at half filling, the product of determinants is always positive. We have used the imaginary time discretization of the QMC $\Delta\tau=0.125$ [30].

Figure 3 shows the QMC results for a 64-site ring, and for 100-site square and cubic lattices. Our T_c cannot be estimated accurately for large U/t because the QMC becomes unstable at low temperatures and with strong Coulombian interaction [30].

Furthermore, we include in Fig. 3 the thermodynamic limit extrapolation obtained through the linear-chain results from the direct diagonalization for small clusters. Note that the extrapolation is consistent with the simulation. Notice that for different lattices, the results for T_c are similar revealing no new behavior.

IV. CONCLUSION

Wesniak *et al.* [17] suggested that magnetic susceptibility can be a macroscopic (thermodynamical) spin entanglement witness without complete knowledge of the specific model (Hamiltonian) of the solid. However, we observed here that its applicability is restricted to the insulator materials because local features of the spin length affect the deviation of the witness. We have developed a generalization that allows us to get information about system entanglement with variable local spin lengths such as found in itinerant electron systems. Moreover, our witness is also valid for fixed local spin lengths and consequently, it can be used experimentally in conductor or insulator materials.

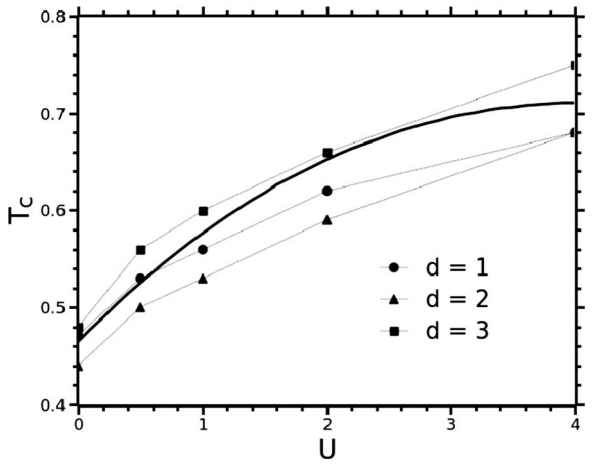

FIG. 3. Coulombian interaction dependence of the critical temperature for the one, two, and three dimensional half-filled Hubbard model. We adopt units $k_B=1$ and $t=1$. The scatter is related to the quantum Monte Carlo method and the solid line is an extrapolation of the thermodynamic limit for a linear chain.

As an application, we studied thermal entanglement for the one, two and three dimensional half-filled Hubbard model. We obtained the critical temperature T_c below which the system is certainly entangled. We have shown that there is a Coulombian repulsion that presents a global T_c maximum. This feature is relevant for quantum information science since it reveals the optimal Coulombian repulsion referent to the highest temperature where the system is definitely entangled. In addition, the decrease in T_c for $t \ll U$ indicates that the itinerancy of electrons favors the entanglement. Furthermore, at the asymptotic regime $U \gg t$ we show, through a numerical extrapolation to the thermodynamic limit, that T_c is in accordance with the exact result for the $\frac{1}{2}-s$ Heisenberg model. A recent study has shown that higher spin length increases the T_c. [17] Since higher spin length means higher internal degrees of freedom, the above result shows a strong favoring of entanglement according to the increases in the internal degrees of freedom. In this work, from the results of T_c for linear, square, and cubic lattices, we notice that an increase in the external spin degrees of freedom produces similar results. These results suggest that the dependence between entanglement and internal spin degrees of freedom is far stronger than between entanglement and external spin degrees of freedom.

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