Thermal entanglement witness for interacting itinerant fermion systems

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The Hubbard model describes interacting itinerant fermion systems and is the simplest model capable of describing the essential physics of strongly correlated electron systems. In this model, both spin correlations and charge correlations are important for the entanglement, thus the magnetic susceptibility is not an appropriate thermal entanglement witness. The specific heat reflects spin correlations and charge correlations. We obtain a relation that permits the specific heat to be used directly as a thermal entanglement witness. We calculate, away from half filling, the entanglement critical temperature T_E, below which entanglement is detected, for small linear clusters and the hypercubic lattice in the limit of infinite dimensions by using the exact numerical diagonalization method and the dynamical mean-field theory, respectively. We find, in both cases, that T_E increases with increasing strength of the on-site Coulomb repulsion U.

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I. INTRODUCTION

The state of a system is said to be entangled whenever it cannot be written as a product of states of subsystems (separable or product states) [1–5]. The study of quantum entanglement in macroscopic systems is important for three basic reasons: to investigate the quantum-to-classical transition, to determine whether entanglement indicates a phase transition, and because the development of quantum computing depends on the handling of entangled macroscopic systems [2]. It is difficult to determine whether a state of many subsystems is entangled and also to quantify this entanglement, particularly if the state is mixed, such as states of systems at finite temperatures. Thus it is extremely important to have a tool for detecting the entanglement: the entanglement witness has this function. The entanglement witness is an observable whose expectation value exceeds a certain bound only if the state under consideration is entangled [1,3].

Ghosh *et al.* showed that quantum entanglement is crucial for describing the behavior of the experimental magnetic susceptibility of the insulator magnetic salt $LiHo_{0.045}Y_{0.955}F_4$ [6]. Calculations revealed that at low temperature the values of the magnetic susceptibility, magnetization, internal energy, and specific heat in some magnetic systems could only be explained by assuming that the states of these systems are entangled [6–12]. Consequently, these properties can be used as thermal entanglement witnesses. In particular, Wiesniak *et al.* showed that for an Ising ring in a transverse magnetic field and a Heisenberg antiferromagnetic ring, under the assumption that only separable states exist, the specific heat diverges when the temperature approaches absolute zero [12]. Thus, for systems described by these Hamiltonians, the validity of the third law of thermodynamics relies on quantum entanglement.

Although several studies in the literature describe thermodynamic properties as thermal entanglement witnesses for localized spin models, this scenario changes when the Hamiltonian describes interacting itinerant particles in a solid. Souza and Almeida presented an entanglement witness that depends on both the magnetic susceptibility and the local spin-spin correlation function [8]. This witness is adequate for studying systems with variable local spin lengths and permits the analysis of quantum entanglement in both conducting and insulating materials. Nevertheless, the magnetic susceptibility and the spin-spin correlation functions take into account only the spin correlations of the system, but in interacting itinerant electron systems, the charge correlations also play an important role in the entanglement, as demonstrated by Zhu *et al.* [13]. Thus, when studying the entanglement in these systems, it is more appropriate to use a witness that takes into account both charge and spin correlations.

The simplest model capable of describing the essential physics of strongly correlated electron systems is the Hubbard model [14,15]. Here the word correlated refers to those consequences of the particle-particle interaction that arise beyond the mean-field approximation, while in the context of quantum information theory, the expression quantum correlation is used in a more general sense, indicating the presence of correlations between different subsystems that exceed any correlation allowed by classical physics [16]. Quantum entanglement is one type of quantum correlation, but quantum correlations can be present even in separable quantum states [17,18]. The quantum discord is a good indicator of the quantum nature of correlations in a bipartite system [19,20]; zero quantum discord is a necessary condition for classical-only correlations.

In Sec. II we demonstrate a criterion that determines, by measuring the specific heat, if the thermal state of a system described by the Hubbard Hamiltonian is entangled, for the case away from half filling and with a constant number of particles. That is, we obtain a relation that uses the specific heat directly as a thermal entanglement witness. This result is important because the specific heat reflects both spin and charge correlations, which makes it adequate for the study of quantum entanglement in interacting itinerant electron systems. In addition, measuring the specific heat of a solid is a well-established experimental routine [12]. Note that the relation between entanglement and specific heat is not new, even for itinerant fermion systems. There are studies relating fidelity and specific heat in the context of phase transition [21,22]. In particular, You *et al.* introduced the concept of fidelity susceptibility, which defines the response of the fidelity to the driving parameter of the Hamiltonian, and studied the fidelity and fidelity susceptibility of the one-dimensional Hubbard model at temperature zero [21]. They also showed that the fidelity susceptibility driven by temperature is related to the specific heat. Because fidelity is a measure of the similarity between two states, it can be used to signal the change of state of a system from an entangled thermal state (state of the system at temperatures lower than the critical temperature) to a separable thermal state (state of the system at temperatures higher than the critical temperature) and thus to determine the critical temperature. This indicates that the specific heat (by means of the fidelity) could be regarded as an entanglement witness for itinerant and localized systems.

Using the specific heat as witness, we analyze the thermal entanglement for linear clusters and the hypercubic lattice in the limit of infinite dimensions. The results and discussion are presented in Sec. III. We summarize in Sec. IV.

II. THE HUBBARD MODEL AND THE SPECIFIC HEAT AS AN ENTANGLEMENT WITNESS

The Hubbard Hamiltonian is given by [14]

$$H = \sum_{\substack{i,j \\ i\neq j}} \sum_{\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}, \qquad (1)$$

where t_{ij} is the hopping amplitude between sites i and j, U is the on-site Coulomb interaction, $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) is the fermionic creation (annihilation) operator, which creates (destroys) a particle on site i with spin projection $\sigma = \uparrow (+1), \downarrow (-1)$, and $\hat{n}_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ is the number operator. In this work the first and second terms on the right-hand side of Eq. (1) will be called H_t and H_U, respectively.

For a system with N_s sites, considering each site as an elementary subsystem, the fully separable states (N_s-partite states) have the form [1]

$$|\psi\rangle = \otimes_{i=1}^{N_s} |\psi\rangle_i = |\psi\rangle_1 \otimes |\psi\rangle_2 \otimes \cdots \otimes |\psi\rangle_{N_s}, \qquad (2)$$

with, in general,

$$|\psi\rangle_i = a_0^i|0\rangle_i + a_{+1}^i|\uparrow\rangle_i + a_{-1}^i|\downarrow\rangle_i + a_2^i|\uparrow\downarrow\rangle_i \big(|a_0^i|^2 + |a_{+1}^i|^2 + |a_{-1}^i|^2 + |a_2^i|^2 = 1\big), \qquad (3)$$

where the label $i = 1, 2, \ldots, N_s$ refers to the lattice site. If there is entanglement among elementary subsystems, then the state of the system cannot have the form (2). If the state is bipartite $|\psi\rangle = |\psi\rangle_A \otimes |\psi\rangle_B$ [where A (B) denote a subsystem with N_{S_A} (N_{S_B}) sites and $N_{S_A} + N_{S_B} = N_S$], then the subsystem A (B) is entangled because if it is not entangled, then the state is not only bipartite but multipartite. Thus, if the state is bipartite, then $|\psi\rangle_A \neq \otimes_{i=1}^{N_{S_A}} |\psi\rangle_{A_i}$ ($A_i = 1, 2, \ldots,$ or N_s) and similarly $|\psi\rangle_B \neq \otimes_{i=1}^{N_{S_B}} |\psi\rangle_{B_i}$ ($B_i = 1, 2, \ldots,$ or N_s and the B_i's are different from the A_i's). Consequently, $|\psi\rangle \neq |\psi\rangle_{A_1} \otimes \cdots \otimes |\psi\rangle_{A_{N_{S_A}}} \otimes |\psi\rangle_{B_1} \otimes \cdots \otimes |\psi\rangle_{B_{N_{S_B}}}$; therefore it does not have the form of Eq. (2).

Theorem of the separability of eigenstates (SE theorem). The only fully separable eigenstates of the Hamiltonian H are $|\psi\rangle = \otimes_{i=1}^{N_S}|0\rangle_i$, $|\psi\rangle = \otimes_{i=1}^{N_S}|\uparrow\rangle_i$, $|\psi\rangle = \otimes_{i=1}^{N_S}|\downarrow\rangle_i$, and $|\psi\rangle = \otimes_{i=1}^{N_S}|\uparrow\downarrow\rangle_i$.

Proof. Suppose that $|\psi\rangle = \otimes_{i=1}^{N_S}|\psi\rangle_i$ is an eigenstate of H; then it also must be an eigenstate of H_t, that is, $H_t|\psi\rangle = \Sigma_{i\neq j}\Sigma_\sigma t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma}|\psi\rangle = E_0|\psi\rangle$. The state $|\psi\rangle$ must be an eigenstate of $c^{\dagger}_{i,\sigma} c_{j,\sigma}$ for any i, j, and σ because these operators act in different subspaces. Consider a specific set but arbitrary $\{i, j, \sigma\}$; then $|\psi\rangle$, to be an eigenstate of $c^{\dagger}_{i,\sigma} c_{j,\sigma}$, requires that both $|\psi\rangle_i$ be an eigenstate of $c^{\dagger}_{i,\sigma}$ and $|\psi\rangle_j$ be an eigenstate of $c_{j,\sigma}$. Thus $|\psi\rangle_i = |\psi(\sigma)\rangle_i \equiv a^i_\sigma|\sigma\rangle_i + a^i_2|\uparrow\downarrow\rangle_i$ and $|\psi\rangle_j = |\tilde{\psi}(\sigma)\rangle_j \equiv a^j_0|0\rangle_j + a^j_{-\sigma}|-\sigma\rangle_j$, and so $c^{\dagger}_{i,\sigma}|\psi(\sigma)\rangle_i = 0$ and $c_{j,\sigma}|\tilde{\psi}(\sigma)\rangle_j = 0$, and consequently, $c^{\dagger}_{i,\sigma} c_{j,\sigma}|\psi\rangle = 0$. Nevertheless, for this last equation to hold, it is sufficient that only one of the two equations is valid: $c^{\dagger}_{i,\sigma}|\psi\rangle_i = 0$ or $c_{j,\sigma}|\psi\rangle_j = 0$. The first possibility is $|\psi\rangle_i = |\psi(\sigma)\rangle_i$ and $|\psi\rangle_j$ given by Eq. (3). As $|\psi\rangle$ must be an eigenstate of $c^{\dagger}_{j,\sigma} c_{i,\sigma}$ and $c_{i,\sigma}|\psi(\sigma)\rangle_i \neq 0$, one has that $c^{\dagger}_{j,\sigma}|\psi\rangle_j = 0 \Rightarrow |\psi\rangle_j = |\psi(\sigma)\rangle_j$, and as $|\psi\rangle$ also must be an eigenstate of $c^{\dagger}_{i,-\sigma} c_{j,-\sigma}$, one has that $c^{\dagger}_{i,-\sigma}|\psi(\sigma)\rangle_i = -\sigma a^i_\sigma|\uparrow\downarrow\rangle_i = 0$ or $c_{j,-\sigma}|\psi(\sigma)\rangle_j = -\sigma a^j_2|\sigma\rangle_j = 0$. Hence $|\psi\rangle = \otimes_{i=1}^{N_S}|\sigma\rangle_i$ and $|\psi\rangle = \otimes_{i=1}^{N_S}|\uparrow\downarrow\rangle_i$ are the eigenstates of H_t. As these separable states are clearly also eigenstates of H_U, they are eigenstates of H. The second possibility is $|\psi\rangle_i$ given by Eq. (3) and $|\psi\rangle_j = |\tilde{\psi}(\sigma)\rangle_j$. Utilizing a procedure analogous to the one adopted for the first possibility, one finds that $|\psi\rangle = \otimes_{i=1}^{N_S}|0\rangle_i$ and $|\psi\rangle = \otimes_{i=1}^{N_S}|-\sigma\rangle_i$ are also eigenstates of H. Q.E.D.

When the system described by H is in thermal equilibrium at a temperature T, its state is mixed and given, with the canonical ensemble, by $\rho_T = \exp(-H/k_B T)/Z$, where Z is the partition function. The specific heat is given by $C = \langle \Delta^2 H\rangle_{\rho_T}/N_S k_B T^2$, where $\langle(\cdots)\rangle_{\rho_T} \equiv \mathrm{Tr}\{\rho_T(\cdots)\}$ and $\langle \Delta^2 H\rangle_{\rho_T} = \langle H^2\rangle_{\rho_T} - \langle H\rangle^2_{\rho_T}$ is the variance of H. The thermal state ρ_T of an N_s-site system is fully separable if $\rho_T = \Sigma_\nu p_\nu |\psi\rangle^{(\nu)(\nu)}\langle\psi| = \Sigma_\nu p_\nu |\psi\rangle_1^{(\nu)(\nu)}{}_1\langle\psi| \otimes |\psi\rangle_2^{(\nu)(\nu)}{}_2\langle\psi| \otimes \cdots \otimes |\psi\rangle_{N_S}^{(\nu)(\nu)}{}_{N_S}\langle\psi|$, where $p_\nu \geqslant 0$ is the weight of the fully separable pure state $|\psi\rangle^{(\nu)}$ [Eq. (2)] in the mixture, with $\Sigma_\nu p_\nu = 1$. Hofmann and Takeuchi have shown that if the thermal state ρ_T is a mixture of separable states, then $\langle \Delta^2 H\rangle_{\rho_T} \geqslant \langle \Delta^2 H\rangle_{\min}$, where $\langle \Delta^2 H\rangle_{\min}$ is the lowest value of the variance obtained over the pure states, that is, $\langle \Delta^2 H\rangle_{\min} = \min\{^{(\nu)}\langle\psi|\Delta^2 H|\psi\rangle^{(\nu)}\}$ [23]. Therefore, if $C < \langle \Delta^2 H\rangle_{\min}/N_S k_B T^2$, then the state of the system described by H must contain entanglement. In this manner, the entanglement critical temperature T_E, where for $T < T_E$ it is possible to guarantee that the system state is entangled, is given by the equation $T_E^2 C(T_E) = \langle \Delta^2 H\rangle_{\min}/N_S k_B$, that is, T_E is the temperature where C intersects with $\langle \Delta^2 H\rangle_{\min}/N_S k_B T^2$. Thus, to determine T_E, it is necessary to calculate $\langle \Delta^2 H\rangle_{\min}$.

Let us consider a system described by H with a fixed particle number N. Then, for the separable state (2), $N = \sum_i \langle \hat{n}_i\rangle_i$, where $\hat{n}_i \equiv \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}$ and $\langle(\cdots)\rangle_i \equiv {}_i\langle\psi|(\cdots)|\psi\rangle_i$. From Eq. (3) one finds that $\langle \hat{n}_i\rangle_i = 0|a^i_0|^2 + 1|a^i_{+1}|^2 + 1|a^i_{-1}|^2 + 2|a^i_2|^2$, which can assume values between 0 and 2. Let us analyze the separable state $|\psi'\rangle$ for a two-site system:

$$|\psi'\rangle = \left(a_0^1|0\rangle_1 + a_{+1}^1|\uparrow\rangle_1 + a_{-1}^1|\downarrow\rangle_1 + a_2^1|\uparrow\downarrow\rangle_1\right) \otimes \left(a_0^2|0\rangle_2 + a_{+1}^2|\uparrow\rangle_2 + a_{-1}^2|\downarrow\rangle_2 + a_2^2|\uparrow\downarrow\rangle_2\right)$$
$$= \begin{cases} a_0^1 a_0^2|0\rangle_1 \otimes |0\rangle_2 \quad \text{if} \quad N=0 \\ a_0^1|0\rangle_1 \otimes \left(a_{+1}^2|\uparrow\rangle_2 + a_{-1}^2|\downarrow\rangle_2\right) + \left(a_{+1}^1|\uparrow\rangle_1 + a_{-1}^1|\downarrow\rangle_1\right) \otimes a_0^2|0\rangle_2 \quad \text{if} \quad N=1 \\ \left(a_{+1}^1|\uparrow\rangle_1 + a_{-1}^1|\downarrow\rangle_1\right) \otimes \left(a_{+1}^2|\uparrow\rangle_2 + a_{-1}^2|\downarrow\rangle_2\right) + a_0^1 a_2^2|0\rangle_1 \otimes |\uparrow\downarrow\rangle_2 + a_2^1 a_0^2|\uparrow\downarrow\rangle_1 \otimes |0\rangle_2, \quad \text{if} \quad N=2 \\ a_2^1|\uparrow\downarrow\rangle_1 \otimes \left(a_{+1}^2|\uparrow\rangle_2 + a_{-1}^2|\downarrow\rangle_2\right) + \left(a_{+1}^1|\uparrow\rangle_1 + a_{-1}^1|\downarrow\rangle_1\right) \otimes a_2^2|\uparrow\downarrow\rangle_2 \quad \text{if} \quad N=3 \\ a_2^1 a_2^2|\uparrow\downarrow\rangle_1 \otimes |\uparrow\downarrow\rangle_2 \quad \text{if} \quad N=4, \end{cases} \tag{4}$$

where the constant a's are nonzero. Defining $|1\rangle_i \equiv a_{+1}^i|\uparrow\rangle_i + a_{-1}^i|\downarrow\rangle_i$ and $|2\rangle_i \equiv |\uparrow\downarrow\rangle_i$, which satisfies $\hat{n}_i|1\rangle_i = 1|1\rangle_i$ and $\hat{n}_i|2\rangle_i = 2|2\rangle_i$, one has

$$|\psi'\rangle = \begin{cases} a_0^1 a_0^2|0\rangle_1 \otimes |0\rangle_2 \quad \text{if} \quad N=0 \\ a_0^1|0\rangle_1 \otimes |1\rangle_2 + a_0^2|1\rangle_1 \otimes |0\rangle_2 \quad \text{if} \quad N=1 \\ |1\rangle_1 \otimes |1\rangle_2 + a_0^1 a_2^2|0\rangle_1 \otimes |2\rangle_2 + a_2^1 a_0^2|2\rangle_1 \otimes |0\rangle_2 \quad \text{if} \quad N=2 \\ a_2^1|2\rangle_1 \otimes |1\rangle_2 + a_2^2|1\rangle_1 \otimes |2\rangle_2 \quad \text{if} \quad N=3 \\ a_2^1 a_2^2|2\rangle_1 \otimes |2\rangle_2 \quad \text{if} \quad N=4. \end{cases} \tag{5}$$

This equation reveals that for $N = 1$, 2, and 3, $|\psi'\rangle$ is not a separable state. If we perform a local measure on a site for determining its occupation, the result indicates the particle number on the other site. In the case of $N = 1$ it may seem counterintuitive that a single particle could have nonlocal properties because the detection of the particle at one location nullifies any possibility of simultaneous recording of the particle at another location. However, the nonlocal properties of a single particle are comprehended by means of its wavelike properties [24]. This analysis shows that when N is constant, $|\psi\rangle_i$ is an eigenstate of $\hat{n}_i$, that is, $\langle\hat{n}_i\rangle_i = n_i = 0, 1,$ or 2 (where n_i is the particle number on site i); otherwise Eq. (2) would produce entangled states. In the general case with N_s sites, this result remains valid. If $|\psi\rangle_i$ is not an eigenstate of $\hat{n}_i$, then from Eq. (2) $|\psi\rangle = |\psi\rangle_A \otimes |\psi\rangle_i = a_0^i|\psi\rangle_A \otimes |0\rangle_i + |\psi\rangle_A \otimes |1\rangle_i + a_2^i|\psi\rangle_A \otimes |2\rangle_i$ and $N = N_A + n_i$ (where $|\psi\rangle_A$ is the state of the system with the site i out and N_A is the particle number in the subsystem A), but as N is fixed, a local measure on the site i for determining if n_i is 0, 1, or 2 determines N_A and thus $|\psi\rangle$ given by Eq. (2) contains entanglement. Hence, for fixed N, any fully separable state of an N_s-site system has the form given by Eq. (2), but with

$$|\psi\rangle_i = \begin{cases} |0\rangle_i \\ a_{+1}^i|\uparrow\rangle_i + a_{-1}^i|\downarrow\rangle_i \quad \text{for} \quad \left|a_{+1}^i\right|^2 + \left|a_{-1}^i\right|^2 = 1 \\ |\uparrow\downarrow\rangle_i. \end{cases} \tag{6}$$

The separable states given by Eqs. (2) and (6) are eigenstates of H_U: $H_U|\psi\rangle = UD_\psi|\psi\rangle$, where $D_\psi = \Sigma_i n_{i,\uparrow}n_{i,\downarrow}$ is the number of doubly occupied sites in state $|\psi\rangle$, with $n_{i,\sigma} = 0$ or 1 the particle number on site i with spin projection σ. To obtain the mean value of H_t, we use the following result, which is valid for Eq. (6):

$$\langle c_{i,\sigma}^\dagger\rangle_i = \langle c_{i,\sigma}\rangle_i = 0. \tag{7}$$

With these equations, one finds that $\langle\psi|c_{i,\sigma}^\dagger c_{j,\sigma}|\psi\rangle = 0$ for $i \neq j$. Thus

$$\langle\psi|\,H_t|\psi\rangle = \sum_{\substack{i,j\\ i\neq j}}\sum_\sigma t_{ij}\,\langle\psi|\,c_{i,\sigma}^\dagger c_{j,\sigma}|\psi\rangle = 0. \tag{8}$$

This result implies that $\langle\psi|H|\psi\rangle = UD_\psi$. Therefore, the lowest possible value E_B of the energy (for $U > 0$) over fully separable states of an N_s-sites system with a fixed particle number is $E_B = 0$ for $0 \leqslant N \leqslant N_S$ and $E_B = (N - N_S)U$ for $N_S < N \leqslant 2N_S$.

The variance $\langle\Delta^2 H\rangle$ with respect to an arbitrary fixed-N fully separable state is given by

$$\begin{aligned}\langle\Delta^2 H\rangle &= \langle\psi|H_t^2|\psi\rangle + \langle\psi|H_t H_U|\psi\rangle + \langle\psi|H_U H_t|\psi\rangle \\ &\quad + \langle\psi|H_U^2|\psi\rangle - (\langle\psi|H_t|\psi\rangle + \langle\psi|H_U|\psi\rangle)^2 \\ &= \langle\psi|H_t^2|\psi\rangle,\end{aligned} \tag{9}$$

where Eq. (8), the equality $\langle\psi|H_U^2|\psi\rangle = \langle\psi|H_U|\psi\rangle^2$, and the equation $\langle\psi|H_t H_U|\psi\rangle = (\langle\psi|H_U H_t|\psi\rangle)^\dagger = 0$ were used. On account of Eq. (7), Eq. (9) becomes

$$\begin{aligned}\langle\Delta^2 H\rangle &= \sum_{\substack{i,j\\ i\neq j}}\sum_{\substack{p,q\\ p\neq q}}\sum_{\sigma,\xi} t_{ij}t_{pq}\langle\psi|c_{i,\sigma}^\dagger c_{j,\sigma}c_{p,\xi}^\dagger c_{q,\xi}|\psi\rangle \\ &= \sum_{\substack{i,j\\ i\neq j}}\sum_{\substack{p,q\\ p\neq q}}\sum_{\sigma,\xi} t_{ij}t_{pq}[\delta_{i,j}\delta_{p,q} + (1-\delta_{i,j})\delta_{i,q}\delta_{j,p}\delta_{\sigma,\xi}] \\ &\quad \times \langle\psi|c_{i,\sigma}^\dagger c_{j,\sigma}c_{p,\xi}^\dagger c_{q,\xi}|\psi\rangle \\ &= \sum_{\substack{i,j\\ i\neq j}}\sum_\sigma t_{ij}t_{ji}\langle\psi|\hat{n}_{i,\sigma}(1-\hat{n}_{j,\sigma})|\psi\rangle,\end{aligned} \tag{10}$$

where $\delta_{i,j}$ is the Kronecker delta. Writing $\Sigma_\sigma\hat{n}_{i,\sigma}\hat{n}_{j,\sigma} = 1/2(\hat{n}_i\hat{n}_j + 4\hat{S}_i^Z\hat{S}_j^Z)$, where $\hat{S}_i^Z = 1/2(\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})$ is the Z component of the spin operator on site i, and assuming that the lattice is isotropic, that is, $t_{ij} = t_{ji}$, one has

$$\langle \Delta^2 H \rangle = \sum_{\substack{i,j \\ i \neq j}} (t_{ij})^2 \left[\langle \hat{n}_i \rangle_i - \frac{1}{2} \left(\langle \hat{n}_i \rangle_i \langle \hat{n}_j \rangle_j + 4 \langle \hat{S}_i^Z \rangle_i \langle \hat{S}_j^Z \rangle_j \right) \right]. \tag{11}$$

This equation shows that the variance of H with respect to any fully separable state [Eq. (2)] depends on $\langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$ and $\langle \hat{S}_i^Z \rangle \langle \hat{S}_j^Z \rangle$, which is generally different from $\langle \hat{n}_i \hat{n}_j \rangle$ and $\langle \hat{S}_i^Z \hat{S}_j^Z \rangle$. Therefore, we conclude that both charge and spin correlations are important for the entanglement in the Hubbard model (this result has already been obtained by Zhu *et al.* using another approach [13]). Thus the specific heat is more suitable for studying the entanglement in this model than the magnetic susceptibility, which is given by the variance of the spin.

Considering that the lattice is homogenous and the hopping occurs only between nearest-neighbor sites, that is, $t_{ij} = -t$ if i and j refer to nearest-neighbor sites and $t_{ij} = 0$ otherwise, Eq. (11) becomes

$$\langle \Delta^2 H \rangle = t^2 N z - \frac{1}{2} t^2 \sum_{\langle i,j \rangle} \left(n_i n_j + 4 \langle \hat{S}_i^Z \rangle_i \langle \hat{S}_j^Z \rangle_j \right), \tag{12}$$

where $\Sigma_{\langle i,j \rangle}$ refers to a sum over nearest-neighbor sites and z is the coordination number of the lattice. Thus $\langle \Delta^2 H \rangle_{\min}$ is obtained when $\Sigma_{\langle i,j \rangle} (n_i n_j + 4 \langle \hat{S}_i^Z \rangle \langle \hat{S}_j^Z \rangle_j)$ is maximum. This maximization occurs for the states $|\psi\rangle_{\min} = \otimes_{i=1}^{N_S} |n_{i\uparrow}, n_{i\downarrow}\rangle_i$ with both saturated magnetization and particles occupying each other's nearest-neighbor sites, that is, states where the hopping is minimum (the SE theorem asserts that the only fully separable eigenstates are those where hopping does not occur). For these states, $\langle \Delta^2 H \rangle = 0$ at $N = 0$, N_s, or $2N_s$, which is consistent with the SE theorem, thus it is not possible to obtain information about the entanglement of the system when $n \equiv N/N_s = 1$ by using the specific heat as an entanglement witness. Therefore, we must study systems away from half filling, that is, $n \neq 1$. From Eq. (10) one finds that an N_s-site system with a fixed particle number is entangled if

$$C/k_B < \frac{\min\left\{ \frac{t^2}{N_S} \sum_{\langle i,j \rangle} \sum_\sigma n_{i,\sigma}(1 - n_{j,\sigma}) \right\}}{(k_B T)^2}, \tag{13}$$

where the specific heat must be calculated over the canonical ensemble and $\Sigma_{\langle i,j \rangle} \Sigma_\sigma n_{i,\sigma}(1 - n_{j,\sigma})$ is calculated over the separable states $|\psi\rangle = \otimes_{i=1}^{N_S} |n_{i\uparrow}, n_{i\downarrow}\rangle_i$.

III. THERMAL ENTANGLEMENT IN LINEAR CLUSTERS AND IN THE HYPERCUBIC LATTICE

For $n < 1$ the state of saturated magnetization is given, for example, by $n_i = n_{i,\uparrow}$. Thus $\min\{\Sigma_{\langle i,j \rangle} n_{i,\uparrow}(1 - n_{j,\uparrow})\}$ is obtained for states where the allowed hopping number is at its minimum. Hence, assuming periodic boundary conditions, $|\psi\rangle_{\min} = \otimes_{i=1}^{N_S} |n_{i\uparrow}\rangle_i$ with the unoccupied (occupied) sites being nearest-neighbor sites of each other for $0.5 \leqslant n < 1$ $(0 < n < 0.5)$ (see Fig. 1). Analyzing Fig. 1, one finds that for a d-dimensional hypercubic lattice with $0.5 \leqslant n < 1$ $(0 < n < 0.5)$, the minimal value of $\Sigma_{\langle i,j \rangle} n_{i,\uparrow}(1 - n_{j,\uparrow})$ is greater than or equal to $(\sqrt[d]{N_X})^{d-1} 2d$, where $N_X = N_h$ $(N_X = N)$ denotes the number of unoccupied (occupied) sites and $N_h = N_S - N$ is the number of holes. Thus, for a density of particles $n < 1$, the state of the system described by the Hubbard Hamiltonian on a d-dimensional hypercubic lattice with nearest-neighbor hopping is entangled if

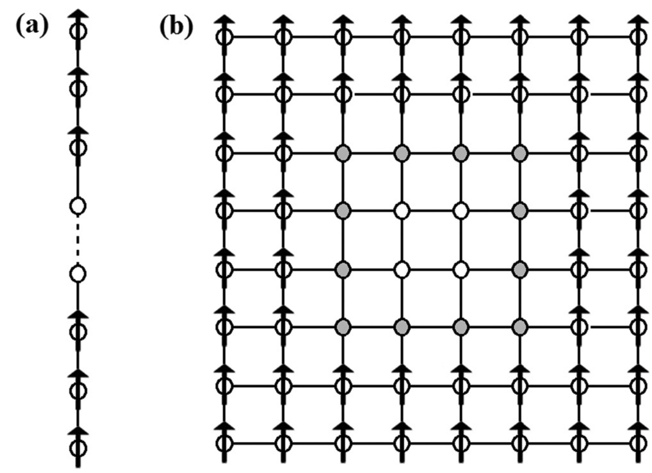

FIG. 1. State that minimizes the variance $\langle \Delta^2 H \rangle$ for (a) a linear lattice and (b) a square lattice, using periodic boundary conditions, at $0.5 < n < 1$. For these states $\langle \Delta^2 H \rangle_{\min} = \min\{t^2 \Sigma_{\langle i,j \rangle} n_{i,\uparrow}(1 - n_{j,\uparrow})\}$. The quantity $\Sigma_{\langle i,j \rangle} n_{i,\uparrow}(1 - n_{j,\uparrow})$ is equal to the allowed hopping number and is minimal for the states shown in (a) and (b). In (a) only two hops are allowed and in (b) nearest-neighbor hopping is allowed only to the gray sites. For a d-dimensional hypercubic lattice with $0.5 < n < 1$ the minimal hopping number between nearest-neighbor sites, and consequently $\langle \Delta^2 H \rangle_{\min}$, is greater than or equal to $(\sqrt[d]{N_X})^{d-1} 2d$, where N_X is the number of unoccupied sites.

$$C/k_B < \frac{(n_X)^{1-1/d}}{(k_B T)^2} \frac{t^2 2d}{(N_S)^{1/d}}, \tag{14}$$

where $n_X \equiv N_X/N_S$. Note that in the thermodynamic limit ($N_S \to \infty$ with fixed n_X) Eq. (14) becomes $C < 0$, which apparently makes its use of limited value. Nevertheless, the value of N_S is actually of the order of Avogadro's number N_A and Eq. (14) can be used to analyze the entanglement in real systems. For example, setting $t \approx 1$ eV and $n_X \approx 1$, for a three-dimensional system with $N_S \approx N_A$, Eq. (14) becomes C (J/mol K) $< 79.5/T^2$ [in Eq. (14) the value of C is given per site]. Besides, for the Hubbard Hamiltonian on a hypercubic lattice in the limit of infinite dimensions, the right-hand side of Eq. (14) is finite even in the thermodynamic limit because the nearest-neighbor hopping t must be scaled as $t = t^*/\sqrt{2d}$ (t^* is a constant) to keep the kinetic energy per site finite [25].

We studied rings with six and four sites by using the exact numerical diagonalization method (see Fig. 2) and the hypercubic lattice in the limit of infinite dimensions by using the dynamical mean-field theory (DMFT) in the paramagnetic phase (see Fig. 3). In this limit the noninteracting ($U = 0$) density of states of the hypercubic lattice acquires a Gaussian form [25]. The DMFT reduces the problem of the dynamics of interacting electrons on a lattice to a single-site problem (described by the Anderson impurity model, for example) with effective parameters being self-consistently determined and becomes exact in the limit of infinite dimensions [26]. We solved the equations of the DMFT by using an algorithm based on the exact numerical diagonalization of the Anderson

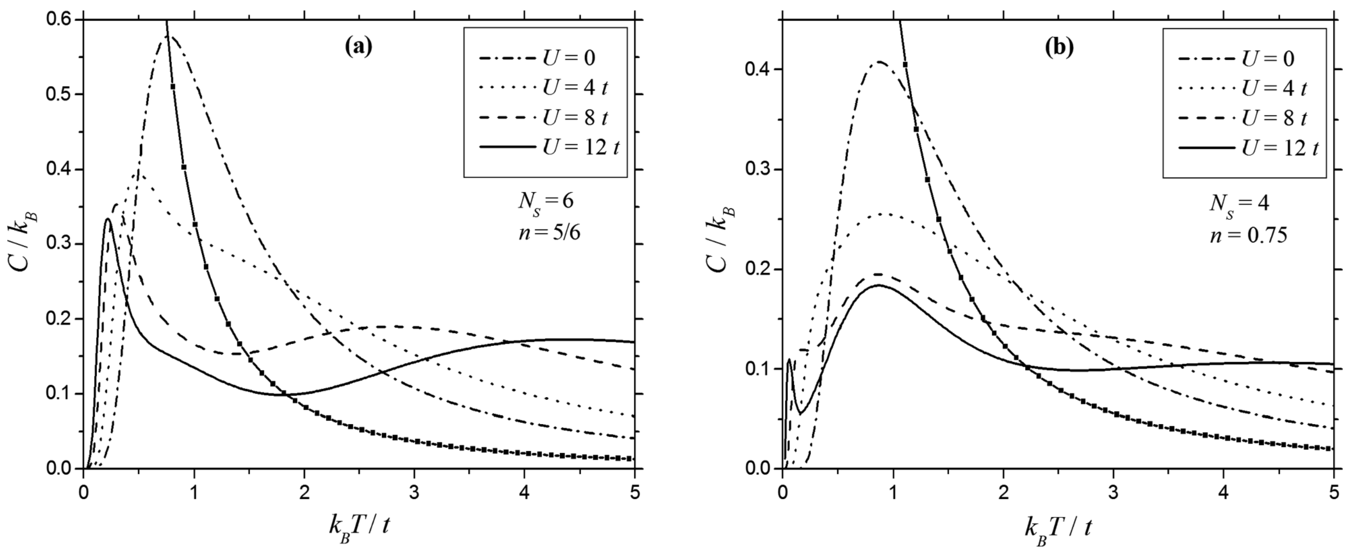

FIG. 2. Specific heat C of the Hubbard model on rings with (a) $N_S = 6$ and (b) $N_S = 4$ as a function of the temperature T for $N = N_S - 1$ and several values of U. The line with small squares is our entanglement witness; from Eq. (14) it is given by $(2/N_S)/(k_B T/t)^2$. The entanglement critical temperature T_E is the temperature at which the specific-heat curve intersects the line with small squares. For temperatures lower than T_E, the state of the system is entangled.

impurity model with a finite number of sites (in this work we use six sites) presented by Caffarel and Krauth [27]. The numerical program that we used is based on the one indicated in Ref. [26].

It is interesting to observe that as the strength of the Coulomb interaction increases, the entanglement critical temperature increases as well (see Figs. 2–4). This behavior of T_E as a function of U is analogous to the behavior of T_E as a function of the magnetic field for a transverse antiferromagnetic Ising chain reported by Wiesniak *et al.* also by using the specific heat as an entanglement witness [12]. Nevertheless, our results, calculated away from half filling, are qualitatively different from those obtained by Souza and Almeida and Zhu *et al.* at half filling. Using a thermal entanglement witness that takes into account only spin correlations, Souza and Almeida found that for the Hubbard model on rings with four and six sites, $T_E \propto U^{-1}$ in the regime $U \gg t$ [8]; Zhu *et al.* studied the entanglement in the Hubbard model on a ring of four sites using the negativity and found that the various pairwise entanglements are generally suppressed by the on-site repulsion U [13]. This difference can be understood as follows. At half filling, when U increases, the spin correlations increase, the charge correlations decrease ($\langle \hat{n}_i \hat{n}_j \rangle \to 1 = \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$ and $\langle \hat{S}_i^Z \hat{S}_j^Z \rangle \to \pm 1/4 \neq \langle \hat{S}_i^Z \rangle \langle \hat{S}_j^Z \rangle =$

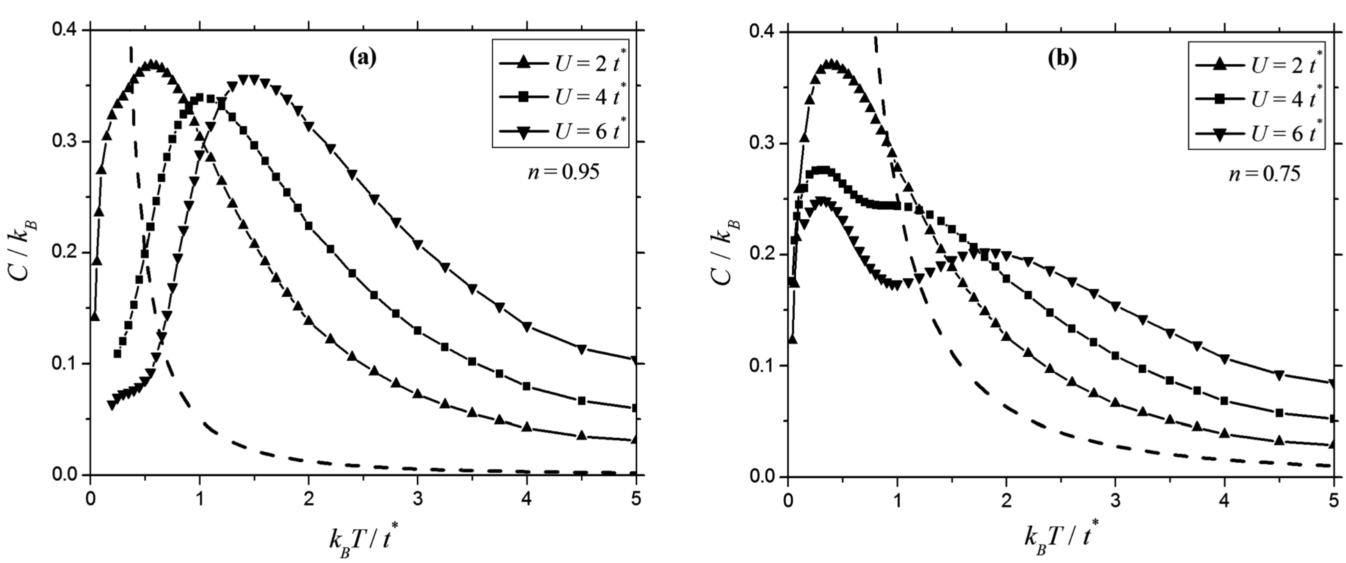

FIG. 3. Specific heat C of the Hubbard model on a hypercubic lattice in the limit of infinite dimensions as a function of the temperature T, in the thermodynamic limit, with (a) $n = 0.95$ and (b) $n = 0.75$, for several values of U. The dashed line is our entanglement witness; from Eq. (14) it is given by $(1 - n)/(k_B T/t^*)^2$. The entanglement critical temperature T_E is the temperature at which the specific-heat curve intersects the dashed line. For temperatures lower than T_E, the state of the system is entangled.

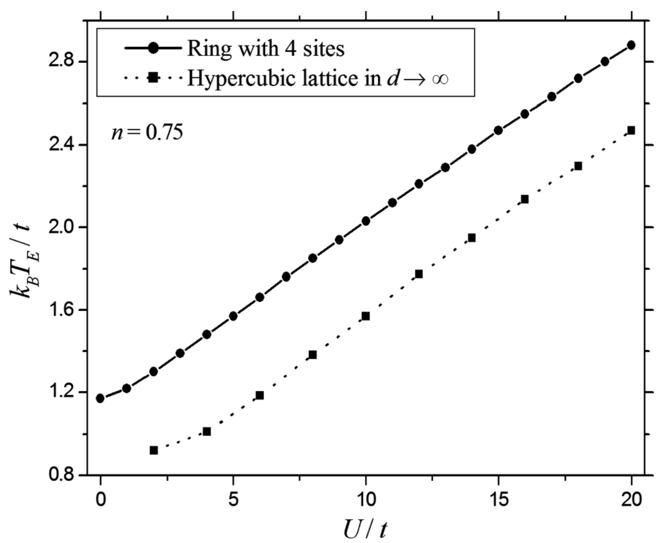

FIG. 4. Entanglement critical temperature T_E versus on-site Coulomb interaction U for a ring with four sites and a hypercubic lattice in the limit of infinite dimensions, with $n = 0.75$. In the region below the line, the state of the corresponding system is entangled. The points $U/t \geqslant 6$ are well fitted by a linear curve with angular coefficient $\cong 0.09$ in both cases. For the hypercubic lattice in $d \to \infty$, the parameter t in the scale must be changed to t^*.

0), and, in general, the charge correlations are weakened more quickly than the spin correlations are enhanced, so the entanglement is suppressed by U and is mainly determined by spin correlations at large U [13]. However, away from half filling, the hopping exists even with $U \to \infty$. Therefore, $\langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$ decreases to a nonzero value as U increases toward infinity and the charge correlations are weakened more slowly than the spin correlations are enhanced. Consequently, the entanglement is enlarged by the on-site Coulomb repulsion and is determined by both spin correlations and charge correlations.

IV. CONCLUSION

We presented a thermal entanglement witness that analyzes interacting itinerant electron systems described by the Hubbard model. Our witness is based on the specific heat, a thermodynamic property whose measurement is a well-established experimental technique in solid-state physics and that reflects both spin and charge correlations; consequently, our witness can be used to investigate the entanglement in magnetic or nonmagnetic materials as well as conducting or insulating materials.

For a fixed particle number, we found that the lowest possible value of the specific heat over fully separable states of the nearest-neighbor Hubbard model is given by α/T^2, where the constant α depends on the geometry and dimension of the lattice and on the site and electron number of the system. At half filling the constant α is zero. This occurs because at $n = 1$ there are fully separable states that are eigenstates of the Hubbard Hamiltonian, while for $0 < n < 1$ and $1 < n < 2$, all the eigenstates of this Hamiltonian are not N_s partite. The constant α also is zero in the thermodynamic limit for lattices with finite dimensions. We calculated, away from half filling, the entanglement critical temperature T_E below which entanglement is detected for small linear clusters and for the hypercubic lattice in the limit of infinite dimensions. We found that T_E increases with increasing strength of the on-site Coulomb repulsion U.

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