Thermal equilibrium emerging in a subsystem of a pure ground state by quantum entanglement

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(Dated: May 13, 2020)

By numerically exact calculations of spin-1/2 antiferromagnetic Heisenberg models on small clusters, we demonstrate that quantum entanglement between subsystems $A$ and $B$ in a pure ground state of a whole system $A + B$ can induce thermal equilibrium in subsystem $A$. Temperature $T_A$ of subsystem $A$ is not a parameter but can be determined from the entanglement von Neumann entropy $S_A$ and the total energy $E_A$ of subsystem $A$ calculated for the ground state of the whole system. Temperature $T_A$ is essentially identical to the thermodynamic temperature, for which the entropy and the internal energy evaluated using the canonical ensemble in statistical mechanics for the isolated subsystem $A$ are almost indistinguishable numerically from the entanglement entropy $S_A$ and the total energy $E_A$ of subsystem $A$. Fidelity calculations ascertain that the reduced density matrix operator of subsystem $A$ for the pure but entangled ground state of the whole system $A + B$ is almost identical to the Gibbs state (i.e., thermodynamic density matrix operator) of subsystem $A$ at temperature $T_A$. We argue that quantum fluctuation in an entangled pure state can mimic thermal fluctuation in a subsystem. We also provide two simple but nontrivial examples of free bosons and free fermions for which these statements can be exactly proved analytically. We furthermore discuss implications and possible applications of our finding.

I. INTRODUCTION

How thermal equilibrium arises in a pure quantum state has been an attractive subject of study in statistical mechanics [1]. This is often addressed by examining how the time average of an expectation value of observable for a pure quantum state after relaxation dynamics approaches an ensemble average of the corresponding observable [2–8]. Recently, the eigenstate-thermalization hypothesis (ETH) [9–13] is widely exploited as a useful concept for investigating the thermalization in isolated quantum systems. The ETH hypothesizes that expectation values of few-body observables with respect to energy eigenstates in a given energy shell behave as microcanonical expectation values of the corresponding energy shell (see Ref. [14] for details). However, not all quantum states satisfy the ETH [15] and systems that do not follow the ETH can be systematically constructed [16, 17].

The typicality [18–21], which characterizes thermal equilibrium rather than thermalization, is also considered as an important concept for foundation of statistical mechanics. The typicality states that for almost every pure state randomly sampled from the Hilbert space, a single measurement of observable converges to the corresponding statistical expectation value with probability close to 1 (see Ref. [22] for detail). Based on the typicality, it has been shown that statistical mechanics can be formulated in terms of the thermal pure quantum (TPQ) states [23–25], rather than conventional mixed states. Note that construction of a TPQ state involves multiplications of Hamiltonian in non-unitary forms.

Another key ingredient for foundation of statistical mechanics from a quantum-mechanical point of view is the entanglement [18]. Consider a normalized pure state $|\Psi\rangle$ in a Hilbert space $\mathcal{H}$, and divide the Hilbert space into two, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The reduced density matrix operator $\hat{\rho}_A$ on $\mathcal{H}_A$ is defined as $\hat{\rho}_A = \text{Tr}_B[|\Psi\rangle\langle\Psi|]$, where $\text{Tr}_B[\cdot]$ denotes the trace over $\mathcal{H}_B$. Since $\hat{\rho}_A$ is hermitian ($\hat{\rho}_A^\dagger = \hat{\rho}_A$), positive semidefinite ($\hat{\rho}_A \geq 0$), and normalized ($\text{Tr}_A[\hat{\rho}_A] = 1$), it has the form of $\hat{\rho}_A = \exp(-\hat{\mathcal{I}}_A)$ with $\hat{\mathcal{I}}_A$ being a hermitian operator on $\mathcal{H}_A$. $\hat{\mathcal{I}}_A$ is referred to as entanglement Hamiltonian and its spectrum [26] is the entanglement spectrum. Following Li and Haldane [27], one can consider $\hat{\rho}_A$ as the Gibbs state of “Hamiltonian” $\hat{\mathcal{I}}_A$ at “temperature” $T = 1$.

The entanglement Hamiltonian or the entanglement spectrum has been studied for various quantum states, such as the quantum Hall state [26, 28], Tomonaga-Luttinger liquids [29, 30], the ground state of the Heisenberg model [31, 32], the ground state of the Hubbard model [33], the ground states in different phases of magnetic impurity models [34, 35], and the valence-bond solid states [36], either by numerical or analytical techniques. Remarkably, it has been shown for the quantum Hall state that the entanglement Hamiltonian is proportional to the Hamiltonian at the boundary [28]. Also, near the limit of maximal entanglement under certain conditions, a proportionality between the entanglement Hamiltonian and the Hamiltonian of a subsystem has been found [37]. These results imply a possibility to find a physical interpretation for the entanglement Hamiltonian, at least, in some cases. Moreover, a recent cold-atom experiment [38] has shown that through a unitary evolution of a pure state, thermalization occurs on a local scale, and has pointed out the importance of the entanglement entropy for thermalization.

Such formal similarities between a reduced density matrix operator and a Gibbs state may naturally raise a question as to whether a thermal equilibrium state in statistical mechanics can emerge from a pure quantum state described by quantum mechanics. To this end, disentangling the “temperature” from the entanglement Hamiltonian in a reduced density matrix operator is a crucial step. In this paper, we address this issue by numerically analyzing the ground states of spin-1/2 antiferromagnetic Heisenberg models in two coupled one-dimensional
(1D) chains (i.e., two-leg ladder) and in two coupled two-dimensional (2D) square and triangular lattices (i.e., bilayer lattice) (see Fig. 1 and Fig. 2). We demonstrate that thermal equilibrium emerges in a partitioned subsystem of a pure ground state with the temperature that is not a parameter but is determined by the entanglement von Neumann entropy and the total energy of the subsystem. This is further ascertained numerically by the fidelity calculation of the reduced density matrix operator and the Gibbs state. We also provide two simple but nontrivial examples, relevant to the Unruh effect or a two-mode squeezed state in quantum optics and a BCS-type superconducting state, to support this statement analytically.

The rest of the paper is organized as follows. In Sec. II, we introduce the Heisenberg Hamiltonian and describe the setup of bipartitioning the system. We also briefly review the reduced density matrix operator for a subsystem of a pure ground state and the Gibbs state. We also provide two simple examples, relevant to the Unruh effect or a two-mode squeezed state in quantum optics and a BCS-type superconducting state, to support this statement analytically.

IV. MODEL AND FORMALISM

A. Model and bipartitioning

We consider the spin-1/2 antiferromagnetic Heisenberg model described by the following Hamiltonian:

\[ \hat{H} = \sum_{\langle i, j \rangle} J_{ij} \hat{S}_i \cdot \hat{S}_j \] (1)

where \( \langle i, j \rangle \) runs over all pairs of nearest-neighbor sites \( i \) and \( j \) in two coupled 1D chains (i.e., two-leg ladder) or in two coupled 2D square or triangular lattices (i.e., bilayer lattice). \( \hat{S}_i \) is the spin-1/2 operator located at the \( i \)th site and the nearest-neighbor spins are connected with the exchange interaction \( J_{ij} = J_A, J_B, \) or \( J \) (see Fig. 1). We denote by \( N \) the number of spins and thus the dimension of the total Hilbert space \( \mathcal{H} \) is \( D = \dim \mathcal{H} = 2^N \). We consider the case where the exchange interactions are antiferromagnetic (\( J_{ij} > 0 \)).

To study the entanglement in the ground state of \( \hat{H} \), we bipartition the Hilbert space \( \mathcal{H} \) of the whole system into those of subsystems \( A \) and \( B \) as \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). Accordingly, the Hamiltonian \( \hat{H} \) can be written as

\[ \hat{H}(\lambda) = \hat{H}_A \otimes I_B + I_A \otimes \hat{H}_B + \hat{V}_{AB}(\lambda), \] (2)

where

\[ \hat{H}_A = J_A \sum_{\langle i, j \rangle \in A} \hat{S}_i \cdot \hat{S}_j, \] (3)

\[ \hat{H}_B = J_B \sum_{\langle i, j \rangle \in B} \hat{S}_i \cdot \hat{S}_j, \] (4)

\[ \hat{V}_{AB}(\lambda) = A \sum_{\langle i, j \rangle \in A, \lambda B} \hat{S}_i \cdot \hat{S}_j, \] (5)

and \( I_A(B) \) is the identity operator on \( \mathcal{H}_A(B) \) (see Fig. 1). \( \hat{H}_A(B) \) is the Hamiltonian of subsystem \( A \) (\( B \)) and \( \hat{V}_{AB}(\lambda) \) describes the exchange interaction between subsystems \( A \) and \( B \). The subsystem \( B \) considered here is essentially a copy of the subsystem \( A \) except that its interaction strength \( J_B \) may differ from \( J_A \). We denote by \( N_A(B) \) the number of spins in subsystem \( A \) (\( B \)) and thus the dimension of the Hilbert space for subsystem \( A \) (\( B \)) is \( D_A(B) = \dim \mathcal{H}_A(B) = 2^{N_A(B)} \). Note that \( N = N_A + N_B \) and \( D = D_A D_B \). The exchange interaction \( \lambda \) controls the entanglement between subsystems \( A \) and \( B \).

Let \( |\Psi_0(\lambda)\rangle \) be the normalized ground state of \( \hat{H}(\lambda) \). Note that the \( \lambda \) dependency of \( \hat{H} \) and \( |\Psi_0\rangle \) is explicitly denoted since we consider the entanglement between subsystems \( A \) and \( B \) in the ground state \( |\Psi_0(\lambda)\rangle \) with varying \( \lambda \). Although the ground state should depend on the exchange interactions as \( |\Psi_0\rangle = |\Psi_0(J_B/J_A, \lambda/J_A)\rangle \), here we simply assume the \( J_A \) and \( J_B \) dependency of these quantities.

Four remarks are in order. In our setup, (i) we assume any finite temperature in neither subsystem \( A \) nor subsystem \( B \); (ii) the volume \( N_B \) of subsystem \( B \) is not necessarily sufficiently larger than the volume \( N_A \) of subsystem \( A \) (and vice versa); (iii) we do not assume that the coupling term \( \hat{V}_{AB}(\lambda) \) between subsystems \( A \) and \( B \) is negligible as compared to \( \hat{H}_A \) and \( \hat{H}_B \),
and (iv) a pure state of the whole system $A+B$ is always chosen as its ground state $|\Psi_0(\lambda)i\rangle$, and thus any stochastic sampling of pure states from $\mathcal{H}$ does not apply. Remarks (i)-(iii) imply that the role of subsystem $B$ is not the heat bath for subsystem $A$, unlike in the conventional statistical mechanics. Remark (iv) implies that our approach do not make use of the typicality argument.

B. Entanglement entropy and energy of subsystem $A$

The ground state can be expanded as

$$|\Psi_0(\lambda)i\rangle = \sum_{j=1}^{D_A} c_i(\lambda)|j\rangle_B,$$

where $\{|j\rangle\}^{D_B}_{j=1}$ is the orthonormal basis set in $\mathcal{H}$, and $\{|i\rangle\}^{D_A}_{i=1}$ is the orthonormal basis set in $\mathcal{H}_{A(B)}$. The coefficients $c_i(\lambda)$ are rewritten as $c_{i,j}(\lambda)$ simply by using the labels $i$ and $j$ for subsystems $A$ and $B$. The reduced density matrix $\hat{\rho}_{A}^{\text{red}}(\lambda)$ of subsystem $A$ is now given as

$$\hat{\rho}_{A}^{\text{red}}(\lambda) = \text{Tr}_B \hat{\rho}_{A}^{\text{red}}(\lambda) = \sum_{i=1}^{D_A} \sum_{j=1}^{D_A} c_{i,j}^{*}(\lambda) c_{i,j}(\lambda) |j\rangle_A \langle i|_A,$$

where the reduced density matrix

$$\hat{\rho}_{A}^{\text{red}}(\lambda) \equiv \sum_{k=1}^{D_A} \hat{\rho}_{A,k}^{\text{red}}(\lambda) = [c(\lambda)c^{\dagger}(\lambda)]_{ij}$$

is introduced with $[c(\lambda)]_{ij} = c_{i,j}(\lambda)$. The reduced density matrix $\hat{\rho}_{A}^{\text{red}}(\lambda)$ is hermitian, positive semidefinite, and satisfies $\text{Tr}[\hat{\rho}_{A}^{\text{red}}(\lambda)] = \langle \Psi_0(\lambda)|\Psi_0(\lambda)\rangle = 1$ [39]. The positive semidefiniteness of $\hat{\rho}_{A}^{\text{red}}(\lambda)$ follows from the fact that $\hat{\rho}_{A}^{\text{red}}(\lambda)$ is a Gram matrix as apparently noticed in Eq. (8).

The entanglement entropy $S_A(\lambda)$ of subsystem $A$ is here defined as the von Neumann entropy of the reduced density matrix operator,

$$S_A(\lambda) \equiv \text{Tr}_A \left[ \hat{\rho}_{A}^{\text{red}}(\lambda) \ln \hat{\rho}_{A}^{\text{red}}(\lambda) \right] = -\text{Tr}_A \left[ \hat{\rho}_{A}^{\text{red}}(\lambda) \ln \hat{\rho}_{A}^{\text{red}}(\lambda) \right]$$

with $\hat{\rho}_{A}^{\text{red}}(\lambda) = -\ln \hat{\rho}_{A}^{\text{red}}(\lambda)$ being the entanglement Hamiltonian. The entanglement entropy satisfies $0 \leq S_A \leq \ln D_A$, where the lower bound is achieved when $\hat{\rho}_{A}^{\text{red}}(\lambda)$ is a pure state and the upper bound is obtained when $\hat{\rho}_{A}^{\text{red}}(\lambda)$ is the maximally mixed state. The energy $\mathcal{E}_A(\lambda)$ of subsystem $A$ is calculated as

$$\mathcal{E}_A(\lambda) \equiv \text{Tr}_A \left[ \hat{\rho}_{A}^{\text{red}}(\lambda) \hat{H}_A \right] = \langle \Psi_0(\lambda)|\hat{H}_A \otimes \hat{I}_B|\Psi(\lambda)\rangle.$$

Note that these quantities are defined using the ground-state wavefunction $|\Psi_0(\lambda)i\rangle$ of the whole system $\hat{H}(\lambda)$.

C. Canonical ensemble of subsystem $A$

Let us consider the canonical ensemble in statistical mechanics for the isolated subsystem $A$ without subsystem $B$. In the canonical ensemble, the heat bath with temperature $T$ is assumed and the average of an observable $\hat{O}$ in subsystem $A$ is given as

$$\langle \hat{O} \rangle_{\beta}^{\text{can}} = \text{Tr}_A \left[ \hat{\rho}_{A}^{\text{can}}(\beta) \hat{O} \right],$$

where

$$\hat{\rho}_{A}^{\text{can}}(\beta) = \frac{e^{-\beta \hat{H}_A}}{Z_A(\beta)},$$

is the Gibbs state, i.e., thermodynamic density matrix operator, $\beta = 1/T$ is the inverse temperature, and $Z_A(\beta) = \text{Tr}_A \left[ e^{-\beta \hat{H}_A} \right]$ is the partition function. The entropy $S_A(\beta)$ and the internal energy $E_A(\beta)$ are given, respectively, as

$$S_A(\beta) = \langle \hat{H}_A \rangle_{\beta}^{\text{can}} = -\text{Tr}_A \left[ \hat{\rho}_{A}^{\text{can}}(\beta) \ln \hat{\rho}_{A}^{\text{can}}(\beta) \right],$$

$$E_A(\beta) = \langle \hat{H}_A \rangle_{\beta}^{\text{can}} = \text{Tr}_A \left[ \hat{\rho}_{A}^{\text{can}}(\beta) \hat{H}_A \right].$$

III. NUMERICAL RESULTS

By numerically analyzing the Heisenberg models described above, we now demonstrate the emergence of thermal equilibrium in the partitioned subsystem $A$ by quantum entanglement, provided that the temperature is appropriately introduced. First, we briefly review two limiting cases when $\lambda = 0$ (i.e., zero entanglement limit) and $\lambda = \infty$ (i.e., maximal entanglement limit). Next, we show numerical results for general values of $\lambda$.

A. Zero entanglement and zero-temperature limit

When $\lambda = 0$, there exists no entanglement between subsystems $A$ and $B$ and any eigenstate of $\hat{H}(\lambda = 0)$ is separable. In particular, the ground state $|\Psi_0(\lambda = 0)i\rangle$ is the product state of the ground states $|\psi_A^0\rangle$ and $|\psi_B^0\rangle$ of subsystems $A$ and $B$, i.e., $|\Psi_0(\lambda = 0)i\rangle = |\psi_A^0\rangle |\psi_B^0\rangle$. Thus, the subsystem $A$ is a pure state and the reduced density matrix operator of subsystem $A$ is

$$\hat{\rho}_{A}^{\text{red}}(\lambda = 0) = |\psi_A^0\rangle \langle \psi_A^0|$$

with the entanglement von Neumann entropy of subsystem $A$

$$S_A(\lambda = 0) = 0,$$

which is the lower bound of $S_A$. The thermodynamic density matrix operator in the zero-temperature limit is apparently identical with the reduced density matrix operator at $\lambda = 0$, i.e.,

$$\hat{\rho}_{A}^{\text{can}}(\beta = \infty) = \hat{\rho}_{A}^{\text{red}}(\lambda = 0),$$

and the thermodynamic entropy is $S_A(\beta = \infty) = 0$. 
B. Maximal entanglement and infinite-temperature limit

When $\lambda = \infty$, the total Hamiltonian $\hat{H}(\lambda)$ is dominated by $\hat{V}_{AB}(\lambda)$ and the corresponding ground state $|\Psi_0(\lambda = \infty)\rangle$ is a singlet-pair product state, i.e., the direct product of the spin singlet states formed by two neighboring spins, each locating in subsystems A and B. Thus, $|\Psi_0(\infty)\rangle$ has the maximal entanglement between subsystems A and B. After tracing out subsystem B, the subsystem A is described by the maximally mixed state (see a similar argument in Ref. [40]) and the reduced density matrix operator of subsystem A is

$$\hat{\rho}_A^{\text{red}}(\lambda = \infty) = \frac{1}{D_A} \hat{I}_A$$

(18)

with the entanglement von Neumann entropy of subsystem A

$$S_A(\lambda = \infty) = \ln D_A = N_A \ln 2,$$

(19)

which is the upper bound of $S_A$. The thermodynamic density matrix operator in the infinite-temperature limit is identical with the reduced density matrix operator at $\lambda = \infty$, i.e.,

$$\hat{\rho}_A^{\text{can}}(\beta = 0) = \hat{\rho}_A^{\text{red}}(\lambda = \infty),$$

(20)

and the thermodynamic entropy is $S_A(\beta = 0) = N_A \ln 2$.

C. General values of $\lambda$ and $\beta$

We calculate the ground state $|\Psi_0(\lambda)\rangle$ of $\hat{H}(\lambda)$ by the Lanczos method, and evaluate $S_A(\lambda)$ and $E_A(\lambda)$ of subsystem A, accordingly to the formalism described in Sec. II B. We also calculate $S_A(\beta)$ and $E_A(\beta)$ of the isolated subsystem A at the inverse temperature $\beta = 1/T$ by numerically diagonalizing the Hamiltonian $\hat{H}_A$ (see Sec. II C). The finite-size systems used for these calculations are shown in Fig. 2. We should emphasize that the ground state $|\Psi_0(\lambda)\rangle$ of $\hat{H}(\lambda)$ is spin singlet (i.e., total spin and thus the $z$ component of the total spin being both zero) and the total momentum of $|\Psi_0(\lambda)\rangle$ is zero, while the canonical ensemble described in Sec. II C averages over all eigenstates of $\hat{H}_A$ in all spin and momentum symmetry sectors.

Figure 3 shows the $\lambda$ dependence of $S_A(\lambda)$ and $E_A(\lambda)$ with different values of $J_B/J_A$. For comparison, the $T$ dependence of $S_A(\beta)$ and $E_A(\beta)$ is also shown. It is clearly observed that $S_A(\lambda)$ and $E_A(\lambda)$ increase monotonically with $\lambda$. Moreover, as discussed in Sec. III A and Sec. III B, the ranges of the entanglement von Neumann entropy $S_A(\lambda)$ and the thermodynamic entropy $S_A(\beta)$ with varying $\lambda$ and $T$, respectively, as well as those of $E_A(\lambda)$ and $E_A(\beta)$, agree with each other.

Figure 4 shows the same quantities $S_A(\lambda)$ and $E_A(\lambda)$ but as a function of an effective temperature defined as $T_A(\lambda) = 1/\mathcal{B}_A(\lambda)$ with

$$\mathcal{B}_A(\lambda) = \lim_{\Delta \lambda \to 0} \frac{S_A(\lambda + \Delta \lambda) - S_A(\lambda)}{E_A(\lambda + \Delta \lambda) - E_A(\lambda)} = \frac{\partial S_A(\lambda)}{\partial E_A(\lambda)}.$$  

(21)

In the numerical calculations, we evaluate $\mathcal{B}_A(\lambda)$ for $\lambda \geq \Delta \lambda$ by a central finite difference $\mathcal{B}_A(\lambda) \approx (S_A(\lambda + \Delta \lambda) - S_A(\lambda) - \Delta \lambda)/(E_A(\lambda + \Delta \lambda) - E_A(\lambda))$ with $\Delta \lambda/J_A = 0.02$ fixed. For comparison, $T$ dependencies of $S_A(\beta)$ and $E_A(\beta)$ of the canonical ensemble are also shown in Fig. 4. Remarkably, for each lattice structure, $S_A(\lambda)$ for all $J_B/J_A$ values are on a universal curve [Figs. 4(a), 4(c), and 4(e)]. Moreover, such a universal curve essentially coincides with the temperature dependence of the thermodynamic entropy $S_A(\beta)$ for the corresponding lattice. The same is also found in the energy $E_A(\beta)$, as shown in Figs. 4(b), 4(d), and 4(f).

Note that a lack of data points around the limit of $T_A(\lambda) = 0$ in Fig. 4 is due to the finite-difference scheme employed for evaluating $\mathcal{B}_A(\lambda) = T_A(\lambda)^{-1}$ in Eq. (21). If smaller $\Delta \lambda$ is chosen, one may find more data points around this limit. We also note that the form of Eq. (21) for the effective temperature is apparently analogous to the definition of the inverse temperature in thermodynamics [41], except that there is the microscopic parameter $\lambda$, through which $S_A(\lambda)$ and $E_A(\lambda)$ are
mediated. The motivation for introducing $B_A(\lambda)$ in the form of Eq. (21) is further discussed in Sec. V A.

Excellent collapse of different quantities, $S_A(\lambda) \approx S_A(B_A(\lambda))$ and $E_A(\lambda) \approx E_A(B_A(\lambda))$, implies that the relation

$$\tilde{\rho}_A^{\text{red}}(\lambda) \approx \rho_A^{\text{can}}(B_A(\lambda))$$

holds between the reduced density matrix operator $\tilde{\rho}_A^{\text{red}}(\lambda)$ and the thermodynamic density matrix operator $\rho_A^{\text{can}}(\beta)$, independently of the detail of the subsystem $B$ whose degrees of freedom are traced out, as schematically shown in Fig. 5. To quantify the similarity between these two density matrix operators, we calculate the fidelity $F$ of density matrix operators $\hat{\rho}$ and $\hat{\sigma}$ on $\mathcal{H}_A$ defined as

$$F(\hat{\rho}, \hat{\sigma}) = \left( \text{Tr}_A \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2$$

for $\hat{\rho} = \tilde{\rho}_A^{\text{can}}(B_A(\lambda))$ and $\hat{\sigma} = \rho_A^{\text{red}}(\lambda)$. Note that the fidelity $F(\hat{\rho}, \hat{\sigma}) = 1$ if and only if $\hat{\rho} = \hat{\sigma}$, and generally $0 < F(\hat{\rho}, \hat{\sigma}) < 1$. Figure 6 shows the fidelity calculated for the three different lattice structures with $J_B/J_A = 1$. As expected from the discussion in Sec. III A and Sec. III B, the fidelity tends to 1 in the limits of $T_A(\lambda) \to 0$ and $T_A(\lambda) \to \infty$. More interestingly, the fidelity is kept large even at intermediate $T_A(\lambda)$, verifying Eq. (22) quantitatively. However, except for the triangular lattice, the fidelity tends to become smaller with increasing the system size. Obviously, calculations with larger clusters are desirable to further examine the finite-size effects, but currently are not feasible due to the exponentially large computational cost. We note that the fidelity with $J_B/J_A = 0.5$ and $J_B/J_A = 1.5$ does not significantly differ from that with $J_B/J_A = 1$.  

FIG. 3. (a,c,e) The entanglement von Neumann entropy $S_A(\lambda)$ of subsystem $A$ as a function of $\lambda/J_A$ for several values of $J_B$ (symbols) and the thermodynamic entropy $S_A(\beta)$ of the isolated subsystem $A$ as a function of temperature $T$ (solid line). (b,d,f) The energy $E_A(\lambda)$ of subsystem $A$ as a function of $\lambda/J_A$ for several values of $J_B$ (symbols) and the internal energy $E_A(\beta)$ of the isolated subsystem $A$ as a function of temperature $T$ (solid line). In (a) and (b), $S_A(\lambda)$ and $E_A(\lambda)$ are calculated for the two coupled 1D chains (i.e., two-leg ladder) with $N_A = N_B = 12$, and $S_A(\beta)$ and $E_A(\beta)$ are calculated for the 1D chain with $N_A = 12$. In (c) and (d), $S_A(\lambda)$ and $E_A(\lambda)$ are calculated for the two coupled 2D square lattices (i.e., bilayer square lattice) with $N_A = N_B = 12$, and $S_A(\beta)$ and $E_A(\beta)$ are calculated for the 2D square lattice with $N_A = 12$. In (e) and (f), $S_A(\lambda)$ and $E_A(\lambda)$ are calculated for the two coupled 2D triangular lattices (i.e., bilayer triangular lattice) with $N_A = N_B = 12$, and $S_A(\beta)$ and $E_A(\beta)$ are calculated for the 2D triangular lattice with $N_A = 12$.  

\[ F(\hat{\rho}, \hat{\sigma}) = \left( \text{Tr}_A \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2 \]
IV. TWO ANALYTICAL EXAMPLES

To support the numerical finding in Sec. III, here we consider two examples, free bosons and free fermions under pairing field, which can be solved analytically, and show that the reduced density matrix operator of a partitioned subsystem of a ground state is identical to the thermodynamic density matrix operator of a partitioned subsystem of a ground state, which can be solved analytically, and show that the effective temperature is properly introduced as in Eq. (21).

A. Bosons under pairing field

First we analyze the entanglement between free bosons under pairing field by considering the Hamiltonian of the form in Eq. (2) with

\[ \hat{H}_A = \omega_A \left( \hat{a}_A^\dagger \hat{a}_A + \frac{1}{2} \right), \]

\[ \hat{H}_B = \omega_B \left( \hat{b}_B^\dagger \hat{b}_B + \frac{1}{2} \right), \]

\[ \mathcal{V}_{AB}(\lambda) = \lambda \left( \hat{a}_A \hat{b}_B + \hat{b}_B \hat{a}_A \right), \]

where \( \hat{a} \) and \( \hat{b} \) are boson annihilation operators on \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively. The operators satisfy the commutation relations \([\hat{a}, \hat{a}^\dagger] = 1, [\hat{b}, \hat{b}^\dagger] = 1, [\hat{a}, \hat{b}^\dagger] = 0, \) and \([\hat{a}, \hat{b}] = 0 \). We assume that \( \omega_A > 0, \omega_B > 0, \) and \( |\lambda| < (\omega_A + \omega_B)/2 \). More precise restrictions on the parameters are discussed after Eq. (34). By introducing new bosonic operators \( \hat{\alpha} \) and \( \hat{\beta} \) via a Bogoliubov transformation as

\[ \begin{bmatrix} \hat{\alpha} \\ \hat{\beta}^\dagger \end{bmatrix} = \begin{bmatrix} \cosh \theta & \sinh \theta \\ \sinh \theta & \cosh \theta \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b}^\dagger \end{bmatrix} \]

(27)

with \( \theta \) satisfying

\[ \lambda = \omega \tanh(2\theta), \]

(28)

\[ \omega = \frac{\omega_A + \omega_B}{2}, \]

(29)

the Hamiltonian \( \hat{H}(\lambda) \) can be diagonalized as

\[ \hat{H}(\lambda) = \Omega_\alpha \hat{\alpha}^\dagger \hat{\alpha} + \Omega_\beta \hat{\beta}^\dagger \hat{\beta} + E_0, \]

(30)
FIG. 5. Schematic figure featuring that thermal equilibrium at temperature $T = 1/\beta$ (right) emerges in a bipartitioned subsystem of a pure ground state by quantum entanglement controlled with $A$ (left). This implies that the quantum fluctuation mimics the thermal fluctuation.

FIG. 6. The fidelity $F(\hat{\rho}, \hat{\sigma})$ for $\hat{\rho} = \hat{\rho}_{A}^{\text{red}}(\lambda)$ and $\hat{\sigma} = \hat{\rho}_{A}^{\text{can}}(B_{A}^{\langle \lambda \rangle})$ as a function of the effective temperature $T_{A}(\lambda)$ for clusters of $N_{A} = N_{B} = 8$, 10, and 12 on (a) the 1D chain, (b) the 2D square lattice, and (c) the 2D triangular lattice.

where

$$
\Omega_{\alpha} = \frac{\omega_{A} \cosh^{2} \theta - \omega_{B} \sinh^{2} \theta}{\cosh^{2} \theta + \sinh^{2} \theta},
$$

$$
\Omega_{\beta} = \frac{\omega_{B} \cosh^{2} \theta - \omega_{A} \sinh^{2} \theta}{\cosh^{2} \theta + \sinh^{2} \theta},
$$

$$
E_{0} = \frac{\omega}{\cosh^{2} \theta + \sinh^{2} \theta} = \frac{\Omega_{\alpha} + \Omega_{\beta}}{2}.
$$

Let us assume

$$
\Omega_{\alpha} > 0 \quad \text{and} \quad \Omega_{\beta} > 0.
$$

These inequalities are satisfied for any $\theta$ if $\omega_{A} = \omega_{B}$. However, if $\omega_{A} \neq \omega_{B}$, these inequalities are satisfied only in a limited range of $\theta$. For example, if $\omega_{B}/\omega_{A} < 1$, $\Omega_{\beta} > 0$ is satisfied for any $\theta$ but $\Omega_{\beta} > 0$ is satisfied only if $\tanh^{2} \theta > \omega_{B}/\omega_{A} < 1$. A similar condition can be found for $\omega_{A}/\omega_{B} < 1$. Below we only consider the parameter region that satisfies the inequalities in Eq. (34).

Since $\Omega_{\alpha} > 0$ and $\Omega_{\beta} > 0$, the ground state $|\Psi_{0}(\lambda)\rangle$ of $\hat{H}(\lambda)$ should be a vacuum state of bosons $\hat{a}$ and $\hat{b}$ satisfying $\hat{a}|\Psi_{0}(\lambda)\rangle = 0$ and $\hat{b}|\Psi_{0}(\lambda)\rangle = 0$. Using the vacuum states $|0\rangle_{A}$ and $|0\rangle_{B}$ in $\mathcal{H}_{A}$ and $\mathcal{H}_{B}$, respectively satisfying $\hat{a}|0\rangle_{A} = 0$ and $\hat{b}|0\rangle_{B} = 0$, the ground state can be given explicitly as

$$
|\Psi_{0}(\lambda)\rangle = \frac{1}{\cosh \theta} e^{-(\tanh \theta)\lambda} |0\rangle_{A} |0\rangle_{B} = \frac{1}{\cosh \theta} \sum_{n=0}^{\infty} (-\tanh \theta)^{n} |n\rangle_{A} |n\rangle_{B},
$$

with $|n\rangle_{A} = (n!)^{-1/2} (\hat{a}^{\dagger})^{n} |0\rangle_{A}$ and $|n\rangle_{B} = (n!)^{-1/2} (\hat{b}^{\dagger})^{n} |0\rangle_{B}$. The entangled state of the form in Eq. (35) has several applications including the Unruh effect [42, 43] and a two-mode squeezed state in quantum optics [44].

By tracing out the degrees of freedom in $\mathcal{H}_{B}$ from the ground-state density matrix operator $|\Psi_{0}\rangle\langle\Psi_{0}|$, we obtain the reduced density matrix operator of subsystem $A$:

$$
\rho_{A}^{\text{red}}(\lambda) = \frac{1}{\cosh^{2} \theta} \sum_{n=0}^{\infty} (\tanh^{2} \theta)^{n} |n\rangle_{AA} \langle n|.
$$

On the other hand, by noticing $\hat{H}_{A}|n\rangle_{A} = \omega_{A}(n + \tfrac{1}{2})|n\rangle_{A}$, the thermodynamic density matrix operator of the isolated subsystem $A$ is given by

$$
\hat{\rho}_{A}^{\text{can}}(\beta) = (1 - e^{-\beta_{A}}) \sum_{n=0}^{\infty} e^{-\beta_{A}n} |n\rangle_{AA} \langle n|
$$

$$
= (e^{\beta_{A}/2} - e^{-\beta_{A}/2}) \sum_{n=0}^{\infty} e^{-\beta_{A}(n + \tfrac{1}{2})} |n\rangle_{AA} \langle n|,
$$

By comparing Eq. (36) with Eq. (37), it is found that $\hat{\rho}_{A}^{\text{red}}(\lambda)$ is exactly the same as $\hat{\rho}_{A}^{\text{can}}(\beta)$ when $\beta = \beta_{A}^{*}$ with

$$
\beta_{A}^{*} = -\frac{1}{\omega_{A}} \ln \tanh^{2} \theta,
$$

$$
= -\frac{1}{\omega_{A}} \ln \left[ \frac{\omega_{A} \pm \sqrt{(\omega_{A}^{2} - 1)^{2}}}{2} \right].
$$
where \( (+ (-) \) sign is taken for \( \theta > 0 \) \( \theta < 0 \). Figures 7(a) and 7(b) show \( \theta \) and \( \lambda \) dependence of \( \beta^* \) and \( T^*_1 \) \( 1/\beta^* \), respectively. We can furthermore find that the entanglement Hamiltonian \( \hat{H}_A = -\ln \hat{\rho}_A^{\text{red}} \) is proportional to \( \hat{H}_A \) with coefficient \( \beta^* \):

\[
\hat{H}_A = \beta^* \hat{H}_A + \frac{1}{2} \ln Z_A^2, \quad (41)
\]

where \( Z_A^2 = \cosh^2 \theta \sinh^2 \theta = (e^{2\beta^* \omega_A} - e^{-2\beta^* \omega_A})^{-2} \) and the spectral representation of the number operator \( \hat{n} = \sum_{n=0}^{\infty} n n_{A}^{n} \) is used. Next, we shall show that the inverse temperature \( \beta^* \) given in Eq. (39) is the same as the effective inverse temperature \( B_A(\lambda) = \partial_\lambda S_A / \partial_\lambda E_A \) introduced in Eq. (21).

The effective inverse temperature \( B_A(\lambda) \) is evaluated from the entanglement von Neumann entropy \( S_A(\lambda) \) and the energy \( E_A(\lambda) \) of subsystem \( A \) for the ground state \( |\Psi_0(\lambda)\rangle \). Equation (36) implies that \( \hat{\rho}_A^{\text{red}}(\lambda) \) contains the eigenstate \( n_{A}^{\lambda} \) of \( \hat{H}_A \) with the probability

\[
p_n = \frac{(\tanh^2 \theta)^n}{\cosh^2 \theta}. \quad (42)
\]

Therefore, the entanglement von Neumann entropy \( S_A(\lambda) \) is calculated as

\[
S_A(\lambda) = -\text{Tr} \left[ \hat{\rho}_A^{\text{red}}(\lambda) \ln \hat{\rho}_A^{\text{red}}(\lambda) \right] = -\sum_{n=0}^{\infty} p_n \ln p_n = (\cosh^2 \theta) \ln \cosh^2 \theta - (\sinh^2 \theta) \ln \sinh^2 \theta, \quad (43)
\]

where \( \sum_{n=0}^{\infty} p_n = 1 \) is used. We thus find that \( \partial_\lambda S_A = -2 \cosh \theta \sinh \theta \) \( \ln \cosh^2 \theta \) and \( \partial_\lambda E_A = 2 \omega_A \cosh \theta \sinh \theta \). Therefore, the effective inverse temperature \( B_A(\lambda) \) is calculated as

\[
B_A(\lambda) = \frac{\partial_\lambda \theta \partial_\lambda \hat{S}_A}{\partial_\lambda \theta \partial_\lambda \hat{E}_A} = -\frac{1}{\omega_A} \ln \cosh^2 \theta = \beta^* \lambda. \quad (45)
\]

From Eqs. (36)–(39) and (45), we can conclude that the relation

\[
\hat{\rho}_A^{\text{red}} \left( B_A(\lambda) \right) = \hat{\rho}_A^{\text{red}}(\lambda) \quad (46)
\]

holds exactly and thus is no longer a conjecture in this case.

We note that the relation in Eq. (45) can also be derived by directly calculating \( \partial S_A / \partial E_A \). Namely, it follows from Eq. (44) that \( \sinh^2 \theta = \frac{\omega_A}{e^{\beta^* \omega_A}} - \frac{1}{\omega_A} \) and \( \cosh^2 \theta = \frac{\omega_A}{e^{\beta^* \omega_A}} + \frac{1}{\omega_A} \). Therefore, \( S_A \) can be expressed in terms of \( E_A \) as

\[
S_A = \left( \frac{E_A}{\omega_A} + \frac{1}{2} \right) \ln \left( \frac{E_A}{\omega_A} + \frac{1}{2} \right) - \left( \frac{E_A}{\omega_A} - \frac{1}{2} \right) \ln \left( \frac{E_A}{\omega_A} - \frac{1}{2} \right). \quad (47)
\]

and thus one can readily show that

\[
\frac{\partial S_A}{\partial E_A} = \beta^*. \quad (48)
\]

To confirm more specifically the correspondence between the two density matrix operators in Eq. (46), let us rewrite the entanglement von Neumann entropy \( S_A \) and the energy \( E_A \) in terms of \( \beta^* \), instead of \( \theta \). It follows from Eq. (39) that

\[
\tanh^2 \theta = e^{-2\beta^* \omega_A}, \quad (49)
\]

\[
\cosh^2 \theta = 1 + n_{\beta^*}(\omega_A), \quad (50)
\]

\[
\sinh^2 \theta = n_{\beta^*}(\omega_A), \quad (51)
\]

where

\[
n_{\beta^*}(\omega_A) = \frac{1}{e^{\beta^* \omega_A} - 1}. \quad (52)
\]

is the Bose-Einstein distribution function at inverse temperature \( \beta^* \). Substituting Eqs. (50) and (51) into Eqs. (43) and (44) yields

\[
S_A = (1 + n_{\beta^*})(1 + n_{\beta^*}) - n_{\beta^*} \ln n_{\beta^*}, \quad (53)
\]

\[
E_A = \omega_A \left( n_{\beta^*} + \frac{1}{2} \right), \quad (54)
\]

which are familiar forms of the thermodynamic entropy and the internal energy of free bosons, respectively. One can also readily find that the positive square root \( Z_A = \left( e^{\beta^* \omega_A / 2} - e^{-\beta^* \omega_A / 2} \right)^{-1} > 0 \) of \( Z_A \) gives the corresponding partition function, i.e., \( Z_A = \text{Tr} [e^{-\beta^*_A \hat{H}_A}] \).

By doing the same analysis for subsystem \( B \), one can find the relation between the effective temperatures \( T_A(\lambda) = B_A^{-1}(\lambda) \) and \( T_B(\lambda) = B_B^{-1}(\lambda) \) as

\[
T_A(\lambda) / \omega_A = T_B(\lambda) / \omega_B. \quad (55)
\]

Finally, we note that all these analyses given above are based on the ground state in Eq. (35) under the conditions in Eq. (34). One can readily show that if \( \omega_A \neq \omega_B \), the maximum of the effective temperature is bounded. For example, when \( \omega_A / \omega_B < 1 \), \( \tanh^2 \theta < \omega_B / \omega_A \) should be satisfied in order to satisfy the conditions in Eq. (34). This implies that \( \ln (\omega_A / \omega_B) = \beta A \omega_A < \infty \), or equivalently \( 0 < T_A / \omega_A < 1 / \ln (\omega_A / \omega_B) \).

### B. Fermions under pairing field

Next we analyze the entanglement between free fermions under pairing field by considering the Hamiltonian of the form
in Eq. (2) with
\[
\hat{H}_A = \epsilon_A \left( \hat{a}^\dagger \hat{a} - \frac{1}{2} \right),
\]
(56)
\[
\hat{H}_B = \epsilon_B \left( \hat{b}^\dagger \hat{b} - \frac{1}{2} \right),
\]
(57)
\[
\hat{V}_{AB}(\lambda) = \lambda \left( \hat{a}\hat{b} + \hat{b}^\dagger \hat{a}^\dagger \right),
\]
(58)
where \(\hat{a}\) and \(\hat{b}\) are fermion annihilation operators on \(\mathcal{H}_A\) and \(\mathcal{H}_B\), respectively. The subtraction of 1/2 in Eqs. (56) and (57) is made simply to find a formal similarity with the bosonic case. The operators satisfy the anticommutation relations \([\hat{a}, \hat{a}^\dagger] = 1, [\hat{b}, \hat{b}^\dagger] = 1, [\hat{a}, \hat{b}^\dagger] = 0,\) and \([\hat{a}, \hat{b}] = 0\). Here we assume that \(\epsilon_A > 0\) and \(\epsilon_B > 0\). An interpretation of this assumption is, for example, that we consider the coupling between two fermion particles (holes) added above (below) the Fermi sea, with the energies \(\epsilon_A\) and \(\epsilon_B\) measured from the Fermi level. More precise restrictions on the parameters are discussed after Eq. (66).

By introducing new fermionic operators \(\hat{\alpha}\) and \(\hat{\beta}\) via a Bogoliubov transformation as
\[
\begin{bmatrix}
\hat{\alpha} \\
\hat{\beta}^\dagger
\end{bmatrix}
= \begin{bmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{bmatrix}
\begin{bmatrix}
\hat{a} \\
\hat{b}^\dagger
\end{bmatrix},
\]
(59)
with \(\theta\) satisfying
\[
\lambda = \epsilon \tan(2\theta),
\]
(60)
\[
\epsilon = \frac{\epsilon_A + \epsilon_B}{2},
\]
(61)
the Hamiltonian \(\hat{H}(\lambda)\) can be diagonalized as
\[
\hat{H}(\lambda) = \xi_\alpha \hat{\alpha}^\dagger \hat{\alpha} + \xi_\beta \hat{\beta}^\dagger \hat{\beta} + E_0,
\]
(62)
where
\[
\xi_\alpha = \epsilon_A \cos^2 \theta - \epsilon_B \sin^2 \theta,
\]
(63)
\[
\xi_\beta = \epsilon_B \cos^2 \theta - \epsilon_A \sin^2 \theta,
\]
(64)
\[
E_0 = -\epsilon(\cos^2 \theta - \sin^2 \theta) = -\frac{\xi_\alpha + \xi_\beta}{2}.
\]
(65)
Similarly to the bosonic case, we assume
\[
\xi_\alpha > 0 \quad \text{and} \quad \xi_\beta > 0.
\]
(66)
If \(\epsilon_A = \epsilon_B\), these inequalities are satisfied for \(-\frac{\pi}{4} < \theta < \frac{\pi}{4}\), implying that \(-\infty < \lambda < \infty\). However, if \(\epsilon_A \neq \epsilon_B\), the range of \(\theta\) and hence \(\lambda\) allowed is more restricted. For example, if \(\epsilon_B/\epsilon_A < 1, \xi_\alpha > 0\) is satisfied for any \(\theta\) but \(\xi_\beta > 0\) is satisfied only if \(\tan^2 \theta < \epsilon_B/\epsilon_A < 1\). A similar condition can be found for \(\epsilon_A/\epsilon_B < 1\). Below we only consider the parameter region that satisfies the inequalities in Eq. (66).

Since \(\xi_\alpha > 0\) and \(\xi_\beta > 0\), the ground state \(|\Psi_0(\lambda)\rangle\) of \(\hat{H}(\lambda)\) should be a vacuum state of fermions \(\hat{\alpha}\) and \(\hat{\beta}\) satisfying \(\hat{\alpha}|\Psi_0(\lambda)\rangle = 0\) and \(\hat{\beta}|\Psi_0(\lambda)\rangle = 0\). Using the vacuum states \(|0\rangle_A\) and \(|0\rangle_B\) in \(\mathcal{H}_A\) and \(\mathcal{H}_B\), respectively satisfying \(\hat{\alpha}|0\rangle_A = 0\) and \(\hat{\beta}|0\rangle_B = 0\), the ground state can be given explicitly as
\[
|\Psi_0(\lambda)\rangle = \cos \theta \sum_{n=0}^{\infty} (\tan \theta)^n |n\rangle_A |n\rangle_B,
\]
(67)
with $|n\rangle_A = (\hat{a}^{\dagger})^n |0\rangle_A$ and $|n\rangle_B = (\hat{b}^{\dagger})^n |0\rangle_B$. The multi-mode-
generalization of the entangled state of the form in Eq. (67) is the Bardeen-Cooper-Schrieffer (BCS) wave function [45].

By tracing out the degrees of freedom in $\mathcal{H}_B$ from the ground-state density matrix operator $|\Psi_0\rangle\langle\Psi_0|$, we obtain the reduced density matrix operator of subsystem $A$:

$$\hat{\rho}^{\text{red}}_A(\lambda) = \cos^2 \theta \sum_{n=0}^{\infty} (\tan^2 \theta)^n |n\rangle_A \langle n|.$$  \hspace{1cm} (68)

On the other hand, by noticing $\hat{H}_A |n\rangle_A = \epsilon_A (n + \frac{1}{2}) |n\rangle_A$, the thermodynamic density matrix operator of subsystem $A$ is given by

$$\hat{\rho}^{\text{can}}_A(\beta) = \frac{1}{1 + e^{-\beta \epsilon_A}} \sum_{n=0}^{\infty} e^{-\beta \epsilon_A |n\rangle_A \langle n|}$$

$$= \frac{1}{1 + e^{-\beta \epsilon_A}} \sum_{n=0}^{\infty} e^{-\beta \epsilon_A (n + \frac{1}{2})} |n\rangle_A \langle n|.$$ \hspace{1cm} (69)

By comparing Eq. (68) with Eq. (69), it is found that $\hat{\rho}^{\text{red}}_A(\lambda)$ is exactly the same as $\hat{\rho}^{\text{can}}_A(\beta)$ when $\beta = \beta^*_A$ with

$$\beta^*_A = \frac{1}{\epsilon_A} \ln \tan^2 \theta$$ \hspace{1cm} (71)

$$= - \frac{1}{\epsilon_A} \ln \left[ \frac{\epsilon_A}{\lambda} \pm \sqrt{\frac{\epsilon_A^2}{\lambda^2} + 1} \right],$$ \hspace{1cm} (72)

where $+$ ($-$) sign is taken for $\theta > 0$ ($\theta < 0$). Figures 7(c) and 7(d) show $\theta$ and $\lambda$ dependence of $\beta^*_A$ and $T^*_A = 1/\beta^*_A$, respectively. We can furthermore find that the entanglement Hamiltonian $\hat{I}^{\text{red}}_A = -\ln \hat{\rho}^{\text{red}}_A$ is proportional to $\hat{H}_A$ with coefficient $\beta^*_A$:

$$\hat{I}^{\text{red}}_A = \beta^*_A \hat{H}_A + \frac{1}{2} \ln Z^2_A,$$ \hspace{1cm} (73)

where $Z^2_A = 1/\cos^2 \theta \sin^2 \theta = (e^{\beta \epsilon_A/2} + e^{-\beta \epsilon_A/2})^2$ and the spectral representation of the number operator $\hat{n}_A = \sum_{n=0}^{\infty} n |n\rangle_A \langle n|$ is used. Next, we shall show that the inverse temperature $\beta^*_A$ given in Eq. (71) is the same as the effective inverse temperature $\beta_A(\lambda) = \partial_\lambda S_A/\partial_\lambda E_A$ introduced in Eq. (21).

The effective inverse temperature $\beta_A(\lambda)$ is evaluated from the entanglement von Neumann entropy $S_A(\lambda)$ and the energy $E_A(\lambda)$ of subsystem $A$ for the ground state $|\Psi_0(\lambda)\rangle$. Equation (68) implies that $\hat{\rho}^{\text{red}}_A(\lambda)$ contains the eigenstate $|n\rangle_A$ of $\hat{H}_A$ with the probability

$$p_n = \cos^2 \theta (\tan^2 \theta)^n,$$ \hspace{1cm} (74)

or more explicitly $p_0 = \cos^2 \theta$ and $p_1 = \sin^2 \theta$. Therefore, the entanglement von Neumann entropy $S_A(\lambda)$ is calculated as

$$S_A(\lambda) = -\text{Tr}_A \left[ \hat{\rho}^{\text{red}}_A(\lambda) \ln \hat{\rho}^{\text{red}}_A(\lambda) \right]$$

$$= - \sum_{n=0}^{\infty} p_n \ln p_n$$

$$= -(\cos^2 \theta) \ln \cos^2 \theta - (\sin^2 \theta) \ln \sin^2 \theta,$$ \hspace{1cm} (75)

Similarly, the energy $E_A(\lambda)$ is calculated as

$$E_A(\lambda) = \text{Tr}_A \left[ \hat{\rho}^{\text{red}}_A(\lambda) \hat{H}_A \right]$$

$$= \epsilon_A \sum_{n=0}^{\infty} p_n \left( n - \frac{1}{2} \right)$$

$$= \epsilon_A \left( \sin^2 \theta - \frac{1}{2} \right).$$ \hspace{1cm} (76)

We thus find that $\partial_\lambda S_A = (2 \cos \theta \sin \theta) \ln \tan^2 \theta$ and $\partial_\lambda E_A = -2 \epsilon_A \cos \theta \sin \theta$. Therefore, the effective inverse temperature $\beta_A(\lambda)$ is calculated as

$$\beta_A(\lambda) = \frac{\partial_\lambda S_A}{\partial_\lambda E_A} = -\frac{1}{\epsilon_A} \ln \tan^2 \theta = \beta^*_A.$$ \hspace{1cm} (77)

From Eqs (68)–(71) and (77), we can conclude that the relation

$$\hat{\rho}^{\text{can}}_A(\beta_A(\lambda)) = \hat{\rho}^{\text{red}}_A(\lambda)$$ \hspace{1cm} (78)

holds exactly and thus is no longer a conjecture in this case.

We note that the relation in Eq. (77) can be derived also by directly calculating $\partial_\lambda S_A/\partial_\lambda E_A$. Namely, it follows from Eq. (76) that $\sin^2 \theta = \frac{1}{2} + \frac{\epsilon_A}{\epsilon_1}$ and $\cos^2 \theta = \frac{1}{2} - \frac{\epsilon_A}{\epsilon_1}$. Therefore, $S_A$ can be expressed in terms of $E_A$ as

$$S_A = - \frac{1}{2} \left( 1 - \frac{\epsilon_A}{\epsilon_1} \right) \ln \left( \frac{1}{2} + \frac{\epsilon_A}{\epsilon_1} \right) - \frac{1}{\epsilon_1} \ln \left( \frac{1}{2} + \frac{\epsilon_A}{\epsilon_1} \right).$$ \hspace{1cm} (79)

and thus one can readily show that

$$\frac{\partial S_A}{\partial E_A} = \beta^*_A.$$ \hspace{1cm} (80)

To confirm more specifically the correspondence between the two density matrix operators in Eq. (78), let us rewrite the entanglement von Neumann entropy $S_A$ and the energy $E_A$ in terms of $\beta^*_A$, instead of $\theta$. It follows from Eq. (71) that

$$\tan^2 \theta = e^{-\beta^*_A \epsilon_1},$$ \hspace{1cm} (81)

$$\cos^2 \theta = 1 - f_{\beta^*_A}(\epsilon_A),$$ \hspace{1cm} (82)

$$\sin^2 \theta = f_{\beta^*_A}(\epsilon_A),$$ \hspace{1cm} (83)

where

$$f_{\beta^*_A}(\epsilon_A) = \frac{1}{e^{\beta^*_A \epsilon_1} + 1}$$ \hspace{1cm} (84)

is the Fermi-Dirac distribution function at inverse temperature $\beta^*_A$. Substituting Eqs. (82) and (83) into Eqs. (75) and (76) yields

$$S_A = - (1 - f_{\beta^*_A}) \ln (1 - f_{\beta^*_A}) - f_{\beta^*_A} \ln f_{\beta^*_A},$$ \hspace{1cm} (85)

$$E_A = \epsilon_A \left( f_{\beta^*_A} - \frac{1}{2} \right),$$ \hspace{1cm} (86)

which are familiar forms of the thermodynamic entropy and the internal energy of free fermions, respectively. One can
also readily find that the positive square root $Z_A = e^{\beta_A \epsilon_A/2} + e^{-\beta_A \epsilon_A/2} > 0$ of $Z_A^2$ gives the corresponding partition function, i.e., $Z_A = \text{Tr}_A \left[ e^{-\beta_A \hat{H}_A} \right]$.

By doing the same analysis for subsystem $B$, one can find the relation between the effective temperatures $T_A(\lambda) = B^{-1}_{\lambda}(\lambda)$ and $T_B(\lambda) = B^{-1}_{\lambda}(\lambda)$ as

$$T_A(\lambda)/\epsilon_A = T_B(\lambda)/\epsilon_B.$$  

(87)

We also note that all these analyses given above are based on the ground state in Eq. (67) under the conditions in Eq. (66). As in the bosonic case, one can readily show that if $\epsilon_A \neq \epsilon_B$, the maximum of the effective temperature is bounded. For example, when $\epsilon_B/\epsilon_A < 1$, $\tan^2 \theta < \epsilon_B/\epsilon_A$ should be satisfied in order to satisfy the conditions in Eq. (66). This implies that $\ln (\epsilon_A/\epsilon_B) < B_1^\lambda \epsilon_A < \infty$, or equivalently $0 < T_A(\lambda)/\epsilon_A < 1/\ln (\epsilon_A/\epsilon_B)$.

Finally, we briefly describe the correspondence between the BCS Hamiltonian and the present Hamiltonian discussed in this section. The BCS Hamiltonian $\hat{H}_{\text{BCS}}$ is generally described by the following Hamiltonian in the momentum space:

$$\hat{H}_{\text{BCS}} = \sum_{k,\sigma} \xi_k \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} + \Delta \sum_k \left( \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow} + \hat{c}_{-k\downarrow}^\dagger \hat{c}_{k\uparrow} \right).$$  

(88)

where $\hat{c}_{k\sigma}$ ($\hat{c}_{k\sigma}$) is the creation (annihilation) operator of electron with momentum $k$ and spin $\sigma (=\uparrow, \downarrow)$. $\xi_k = \epsilon_k - \mu$, $\epsilon_k$ is the single-particle dispersion of electrons, and $\mu$ is the chemical potential. Note that the spatial dimensionality is not assumed. We now introduce the following canonical transformation:

$$\hat{c}_{k\uparrow}^\dagger \rightarrow \hat{a}_{k\uparrow}^\dagger, \quad \hat{c}_{-k\downarrow}^\dagger \rightarrow \hat{b}_k^\dagger \quad \text{(for } \xi_k > 0),$$  

$$\hat{c}_{k\downarrow} \rightarrow \hat{a}_{k\downarrow}, \quad \hat{c}_{-k\uparrow} \rightarrow \hat{b}_k \quad \text{(for } \xi_k < 0),$$  

(89)

(90)

where $\hat{a}_{k\sigma}$ and $\hat{a}_{k\sigma}^\dagger$ ($\hat{b}_k^\dagger$ and $\hat{b}_k$) satisfy the anticommutation relations, e.g., $\{\hat{a}_{k\sigma}, \hat{a}_{k'\sigma}^\dagger\} = \delta_{k,k'} \delta_{\sigma,\sigma'}$ and $\{\hat{b}_k, \hat{b}_k^\dagger\} = 0$. With this canonical transformation, the BCS Hamiltonian $\hat{H}_{\text{BCS}}$ is rewritten as

$$\hat{H}_{\text{BCS}} = \sum_{k, (\xi_k > 0)} \left[ \xi_k \left( \hat{a}_{k\uparrow}^\dagger \hat{a}_{k\uparrow} + \hat{b}_k^\dagger \hat{b}_k \right) + \Delta \left( \hat{a}_{k\uparrow}^\dagger \hat{b}_k + \hat{b}_k^\dagger \hat{a}_{k\uparrow} \right) \right]$$

$$+ \sum_{k, (\xi_k < 0)} \left[ -\xi_k \left( \hat{a}_{k\downarrow}^\dagger \hat{a}_{k\downarrow} + \hat{b}_k \hat{b}_k^\dagger \right) + \Delta \left( \hat{a}_{k\downarrow}^\dagger \hat{b}_k + \hat{b}_k \hat{a}_{k\downarrow}^\dagger \right) \right]$$

$$+ 2 \sum_{k, (\xi_k = 0)} \xi_k$$  

$$= \sum_k \left[ |\xi_k| \left( \hat{a}_{k\uparrow}^\dagger \hat{a}_{k\uparrow} - \frac{1}{2} \right) + |\xi_k| \left( \hat{b}_k^\dagger \hat{b}_k - \frac{1}{2} \right) \right]$$

$$+ \Delta \left( \hat{a}_{k\uparrow}^\dagger \hat{b}_k + \hat{b}_k^\dagger \hat{a}_{k\uparrow}^\dagger \right) + \sum_k \xi_k.$$  

(91)

(92)

Here $\sum_{k, (\xi_k > 0)} (\sum_{k, (\xi_k = 0)} \sum_{k, (\xi_k < 0)})$ indicates the sum over $k$ with $\xi_k > 0$ ($\xi_k < 0$) and we assume that $\xi_k = \xi_{-k}$. Therefore, apart from the irrelevant constant term, each component with a given momentum $k$ in the BCS Hamiltonian $\hat{H}_{\text{BCS}}$ is exactly the same as the Hamiltonian $\hat{H}(\lambda) = \hat{H}_A + \hat{H}_B + \hat{V}_{\text{AB}}(\lambda)$ in Eqs. (56)–(58) with the correspondence of $\epsilon_A = \epsilon_B \leftrightarrow |\xi_k|$ and $\lambda \leftrightarrow \Delta$.

For example, the ground state of $\hat{H}_{\text{BCS}}$ is thus given simply as a product state of $|\Psi_0(\lambda = \Delta)\rangle$ in Eq. (67) over all momenta. Following the same argument given above in this section, we can conclude that the reduced density matrix operator of subsystem $A$ for the ground state of the BCS Hamiltonian is exactly the same as the thermodynamic density matrix operator of the isolated subsystem $A$ with the effective temperature introduced in Eq. (21). However, we should note that bipartitioning of the whole Hilbert space is not trivial because the subsystem $A$ consists of Hilbert space for up electrons with $\xi_k > 0$ and down electrons with $\xi_k < 0$, i.e., the subsystem $A$ being described by

$$\hat{H}_A = \sum_k |\xi_k| \left( \hat{a}_{k\uparrow}^\dagger \hat{a}_{k\uparrow} - \frac{1}{2} \right)$$

$$+ \sum_{k, (\xi_k > 0)} \xi_k \left( \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} - \frac{1}{2} \right) + \sum_{k, (\xi_k < 0)} \xi_k \left( \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} - \frac{1}{2} \right).$$  

(93)

V. DISCUSSIONS

A. Insights of the effective inverse temperature $B_A(\lambda)$

The observation from the numerical calculations in Sec. III as well as two analytical examples in Sec. IV leads us to conjecture that a canonical ensemble with the inverse temperature

$$\beta = B_A(\lambda)$$  

(94)

could emerge by quantum entanglement in a partitioned subsystem of a pure ground state. This assertion is highly non-trivial as $\beta$ in the left-hand side is a given inverse temperature in the canonical ensemble, while $B_A(\lambda)$ in the right-hand side is evaluated in the entangled pure ground state $|\Psi_0(\lambda)\rangle$ of $\hat{H}(\lambda)$. Here, we further discuss the observation summarized in Eqs. (22) and (94) to gain more insights. Note however that we intend to prove neither Eq. (22) nor Eq. (94).

1. Product state and additivity

Let us first briefly review the additivity of the entanglement von Neumann entropy by considering a product state [46]. Consider a system $W$ that is composed of subsystems $X$ and $Y$. Note that these are nothing to do with system $A + B$ consisting of subsystems $A$ and $B$ considered in the previous sections. Let $\hat{\rho}_{X(Y)}$ be the density matrix operator of subsystem $X (Y)$, and suppose that the density matrix operator $\hat{\rho}_W$ of the total system is given as a product state of $\hat{\rho}_X$ and $\hat{\rho}_Y$, i.e.,

$$\hat{\rho}_W = \hat{\rho}_X \otimes \hat{\rho}_Y,$$  

(95)

implying no entanglement between subsystems $X$ and $Y$. Then the entanglement von Neumann entropy $S_s (s = W, X, or Y)$ defined as

$$S_s = -\text{Tr}_s \left[ \hat{\rho}_s \ln \hat{\rho}_s \right]$$  

(96)
possesses the additivity
\[ S_W = S_X + S_Y. \] (97)

Next, let us consider the additivity of the energy. For this purpose, we introduce Hamiltonian. Let \( \hat{H}_X(Y) \) be the Hamiltonian of subsystem \( X \) (\( Y \)), and suppose that the total Hamiltonian \( \hat{H}_W \) of the system \( W \) is given as
\[ \hat{H}_W = \hat{H}_X \otimes \hat{1}_Y + \hat{1}_X \otimes \hat{H}_Y, \] (98)
implying no interaction between subsystems \( X \) and \( Y \). Notice that any eigenstate of \( \hat{H}_W \) is given as a product of eigenstates of \( \hat{H}_X \) and \( \hat{H}_Y \), satisfying the form in Eq. (95). Then the energy \( E_\varepsilon \) defined as
\[ E_\varepsilon = \text{Tr} \left[ \hat{\rho}_s \hat{H}_s \right] \] (99)
possesses the additivity
\[ E_\varepsilon = E_X + E_Y. \] (100)

2. Functional form of density matrix operator

Now we show that the Gibbs state, i.e., the thermodynamic density matrix operator, arises if a particular functional form of the Hamiltonian \( \hat{H} \) is provided that the spectrum of \( \hat{H} \) is bounded. Obviously from the assumption in Eq. (101), \( \hat{H} \) is common in subsystems \( X \) and \( Y \) as well as the system \( W \), otherwise Eq. (103) does not satisfy Eq. (102) in general. Such a “common temperature” property of \( \beta^* \) required for the additivity of the entanglement entropy of subsystem \( \hat{H}_s \) and the energy is analogous to the property of the thermodynamic temperature characterizing equilibrium between subsystems \( X \) and \( Y \). Thus the Gibbs state as well as the inverse-temperature-like real number \( \beta^* \) have arisen from the assumption in Eq. (101).

3. \( \beta^* \) as a derivative of entanglement entropy and energy

Now we derive Eq. (94) by assuming the functional form of Eq. (101) even when there exists an interaction between subsystems, as in the case studied in Sec. III. Under this assumption, the reduced density matrix operator \( \hat{\rho}_A^\text{red}(\lambda) \) of subsystem \( A \) has the form as in Eq. (103), i.e.,
\[ \hat{\rho}_A^\text{red}(\lambda) = \hat{\rho}_A^\text{can}(\beta^*) = \frac{e^{-\beta^* \hat{H}_A}}{Z_A(\beta^*)} \] (104)
with \( \beta^* \) real. In our setting, the parameter \( \lambda \) does not enter in \( \hat{H}_A \) but \( \hat{\rho}_A^\text{red}(\lambda) \) should depend on \( \lambda \) through \( \beta^* \), i.e.,
\[ \beta^* = \beta^*(\lambda). \] (105)

As described in details in Appendix A, considering the relative entropy \( D(\hat{\rho}_1|\hat{\rho}_0) = \text{Tr}[\hat{\rho}_1 \ln \hat{\rho}_1] - \text{Tr}[\hat{\rho}_1 \ln \hat{\rho}_0] \) with \( \hat{\rho}_0 = \hat{\rho}_A^\text{red}(\lambda) \) and \( \hat{\rho}_1 = \hat{\rho}_A^\text{red}(\lambda + \Delta \lambda) \), we obtain that
\[ D(\hat{\rho}_1|\hat{\rho}_0) = \beta^*(\lambda) [E_A(\lambda + \Delta \lambda) - E_A(\lambda)] - [S_A(\lambda + \Delta \lambda) - S_A(\lambda)]. \] (106)

Since \( D(\hat{\rho}_1|\hat{\rho}_0) = O((\Delta \lambda)^2) \) [see Ref. [47] and also Eq. (A6) in Appendix A], we finally obtain, by solving the above equation with respect to \( \beta^*(\lambda) \), that
\[ \beta^*(\lambda) = \frac{S_A(\lambda + \Delta \lambda) - S_A(\lambda)}{E_A(\lambda + \Delta \lambda) - E_A(\lambda) + O((\Delta \lambda)^2)} \] (107)
leading to the form of Eq. (21) and consistent with the observation in Eqs. (22) and (94).

Remarkably, the functional form of the reduced density matrix operator as in Eq. (101) has been proven to be valid for a certain class of topological quantum states [28] and we have also already shown that it is the case for the two examples described in Sec. IV. Although such a dependence of the reduced density matrix operator on the Hamiltonian is in general not necessarily valid, our numerical results suggest that the reduced density matrix operator of a partitioned subsystem for the ground state of the Heisenberg models in the two-leg ladder and the bilayer lattices can be well approximated in the form of Eq. (101), which describes the Gibbs state with the effective inverse temperature \( B_A(\lambda) \). Finally, we note that the effective inverse temperature \( B_A(\lambda) \) of subsystem \( A \) differs in general from the effective inverse temperature \( B_0(\lambda) \) of subsystem \( B \) (see Sec. IV and Appendix B).

B. Thermal and quantum fluctuations

Let us now discuss an association between thermal and quantum fluctuations. The quantities \( W_A \equiv e^{S_A} \) and \( W_A^{\text{red}} \equiv e^{S_A^{\text{red}}} \), each satisfying \( 1 \leq W_A \leq D_A \) and \( 1 \leq W_A^{\text{red}} \leq D_A \), can be regarded as effective numbers of microscopic pure states that contribute to the thermodynamic and reduced density matrix operators, respectively. Considering that fluctuations are induced by a statistical mixture of microscopic states in a density matrix operator, \( S_A \) and \( S_A^{\text{red}} \) may serve as a measure of the
thermal fluctuation due to the temperature and as a measure of 
the quantum fluctuation due to the quantum entanglement, re-
respectively. The almost indistinguishable agreement between 
$S_A$ vs. $T$ and $S_A$ vs. $T_A(\lambda)$ found numerically in Sec. III 
(and also the exact agreement in the case of two analytical ex-
amples in Sec. IV) suggests that the quantum fluctuation in 
the partitioned subsystem $A$ coupled to the other subsystem 
via the coupling parameter $\lambda$ can mimic the thermal fluctua-
tion in the isolated subsystem $A$ at the temperature $T = T_A(\lambda)$ 
and vice versa (see Fig. 5). In other words, the mixture of 
microscopic states caused by either temperature or quantum 
entanglement is essentially indistinguishable, at least, for the 
quantities studied here. A related discussion on thermal and 
quantum fluctuations has also been reported in Ref. [48].

VI. CONCLUSION AND REMARKS

In conclusion, by numerically analyzing the spin-1/2 an-
tiferromagnetic Heisenberg model in the two-leg ladder and 
the bilayer lattices, we have demonstrated that thermal equi-
rium can emerge in a partitioned subsystem $A$ of a pure 
ground state by quantum entanglement. The emergent ther-
mal equilibrium is almost indistinguishable from the canon-
ical ensemble with the temperature $T_A(\lambda)$ that is determined 
from the entanglement von Neumann entropy and the energy 
of the subsystem. This implies that the reduced density ma-
trix operator of the subsystem is almost identical to the Gibbs 
state, i.e., thermodynamic density matrix operator, with tem-
perature $T_A(\lambda)$. This is further supported by two simple but 
nontrivial examples, for which one can show analytically that 
the two density matrix operators are exactly the same with 
temperature $T_A(\lambda)$.

Once we accept that the reduced density matrix opera-
tor $\hat{\rho}_A^{\text{red}}(\lambda)$ represents a thermodynamic density matrix op-
erator that describes a statistical ensemble of subsystem $A$ 
at thermodynamic temperature $T_A(\lambda)$, our scheme provides 
an alternative way to calculate finite-temperature properties 
based on pure ground-state quantum-mechanical calculations, 
as demonstrated in Sec. III C. Our scheme is similar to those 
based on purification [49–53] (see Appendix C), but has sev-
eral advantages. For example, a parallel calculation with re-
spect to different temperatures is possible merely by calcu-
lating the ground states $|\Psi_0(\lambda)\rangle$ with different values of $\lambda$ in-
dependently, and no imaginary-time-evolution-type calcula-
tions, which apply $\exp(\beta H_{\lambda}) \otimes I_B$ to some states, are required. 
However, it is not straightforward to have a desired “tempera-
ture” because $T_A(\lambda)$ is not an input parameter but is evaluated 
from the entanglement von Neumann entropy and the energy, 
similarly to microcanonical ensemble methods [23, 54, 55].

In order to have quantitative agreement between the entan-
glement von Neumann entropy $S_A$ and the thermodynamic en-
tropy $S_A$, the entanglement von Neumann entropy $S_A$ should 
be obey the volume law, instead of the area law, because the ther-
modynamic entropy $S_A$ is an extensive quantity. This implies 
that the subsystem $B$ should be at least as large as the sub-
system $A$, i.e., $N_B \geq N_A$. The lower bound $N_B = N_A$ or 
equivalently $N = N_A + N_B = 2N_A$, is in fact consistent with 
the system size that is required for the purification of a mixed state $\hat{\rho}_A^{\text{red}}$.

Technically, the doubling of the system size $N_A$ for a pure 
ground state calculation becomes immediately intractable with 
increasing $N_A$ by the exact diagonalization method sim-
ply because of the exponential increase of computational cost 
with respect to the system size. The density matrix renor-
malization group (DMRG) method [56] might be a choice of 
methods for overcoming this difficulty especially for 1D 
systems. However, since the entanglement von Neumann en-
tropy should obey the volume law, a large amount of com-
putational resource may be required in DMRG calculations 
to obtain accurate results even for 1D systems. Another possi-
bility would be quantum computation for many-body systems, 
for which a quantum algorithm to compute the entanglement 
spectrum [57] can be used.

Although the fidelity $F$ of the two density matrix operators 
is found to be close to 1, the largest deviation from 1 occurs 
at some particular $T_A(\lambda)$, around which the finite size effect 
seems to be the largest (see Fig. 6). Therefore, it is desirable 
to examine the finite size effect more systematically. The ex-
tension of the present study to other systems such as larger 
spins or interacting fermionic systems is also highly interest-
ing to understand under what conditions thermal equilibrium 
can emerge in a subsystem of a pure ground state by quan-
turn entanglement. These studies are certainly beyond the 
currently available computational power and are left for fu-
ture work. Finally, we note that for testing and extending the 
present study, not only numerical calculations, but rather ex-
periments for cold atom systems [38, 58] would be promising.

ACKNOWLEDGMENTS

The authors would like to thank Tomonori Shirakawa and 
Hiroaki Matsueda for valuable discussions. Parts of nu-
merical simulations have been done on the HOKUSAII 
supercomputer at RIKEN (Project ID: G20015). This work 
was supported by Grant-in-Aid for Research Activity start-up 
(No. JP19K23433) and Grant-in-Aid for Scientific Research 
(B) (No. JP18H01183) from MEXT, Japan.

Appendix A: Relative entropy

1. Definition

For density matrix operators $\hat{\rho}_0$ and $\hat{\rho}_1$, the relative entropy 
$D(\hat{\rho}_1|\hat{\rho}_0)$ is defined as [59–61]

$$D(\hat{\rho}_1|\hat{\rho}_0) = \text{Tr}[\hat{\rho}_1 \ln \hat{\rho}_1] - \text{Tr}[\hat{\rho}_1 \ln \hat{\rho}_0] \geq 0.$$  \hspace{1cm} \text{(A1)}

The equality is satisfied if and only if $\hat{\rho}_1 = \hat{\rho}_0$. In terms of the 
etanglement entropy $S(\hat{\rho}) = -\text{Tr}[\hat{\rho} \ln \hat{\rho}]$, the relative entropy 
can be rewritten as

$$D(\hat{\rho}_1|\hat{\rho}_0) = -\text{Tr}[(\hat{\rho}_1 - \hat{\rho}_0) \ln \hat{\rho}_0] - [S(\hat{\rho}_1) - S(\hat{\rho}_0)].$$  \hspace{1cm} \text{(A2)}
For convenience, let us simply write the relative entropy as $\lambda$ parametrized by $\Delta$. The Taylor expansion of $D(\Delta)\lambda$ vanishes. Moreover, the first derivative vanishes at $D(\Delta)\lambda(0)$, for comparison.

$$D(\Delta)\lambda \equiv D(\hat{\rho}(\lambda + \Delta)|\hat{\rho}(\lambda)).$$

The Taylor expansion of $D(\Delta)\lambda$ around $\Delta\lambda = 0$ is

$$D(\Delta)\lambda = D(\Delta)\lambda(0) + \frac{dD(\Delta)\lambda}{d\Delta}\bigg|_{\Delta\lambda = 0} \Delta\lambda + O\left(\left(\Delta\lambda\right)^2\right).$$

Since $D(\Delta)\lambda(0) = 0$, the first term in the right hand side of Eq. (A4) vanishes. Moreover, the first derivative vanishes at $\Delta\lambda = 0$, i.e.,

$$\frac{dD(\Delta)\lambda}{d\Delta}\bigg|_{\Delta\lambda = 0} = 0.$$  

This can be shown by substituting the Taylor expansion $\hat{\rho}(\lambda + \Delta\lambda) = \hat{\rho}(\lambda) + \frac{d\hat{\rho}(\lambda)}{d\lambda}\Delta\lambda + O\left(\left(\Delta\lambda\right)^2\right)$ into Eq. (A2) and using $\text{Tr}\left[\frac{d}{d\lambda}\hat{\rho}(\lambda)\right] = \frac{d}{d\lambda}\text{Tr}[\hat{\rho}(\lambda)] = 0$. Since $D(\Delta)\lambda(\lambda > 0)$ for $\Delta\lambda \neq 0$, the vanishing of the first derivative in Eq. (A5) implies that $D(\Delta)\lambda$ is differentiable at $\Delta\lambda = 0$ (see Fig. 8), as discussed in Ref. [47]. We thus find that

$$D(\Delta)\lambda = O\left(\left(\Delta\lambda\right)^2\right).$$

Appendix B: Effective temperature in subsystem $B$

In Sec. III, we have found excellent agreement between statistical-mechanical quantities such as the thermodynamic entropy $S_A(\beta)$ and the internal energy $E_A(\beta)$ for an isolated subsystem $A$ and quantum-mechanical quantities such as the entanglement von Neumann entropy $S_A(\lambda)$ and the energy $E_A(\lambda)$ of a partitioned subsystem $A$ for a ground state of the whole system $A + B$, provided that the thermodynamic temperature $T = 1/\beta$ in the former is set properly to the effective temperature $T_A(\lambda)$ determined in the latter. A natural question is now how the effective temperature $T_B(\lambda)$ of the subsystem $B$ behaves. Here, $1/T_B(\lambda)$ is defined as in Eq. (21) but with the energy $E_B(\lambda)$ of the subsystem $B$ instead of $E_A(\lambda)$ of the subsystem $A$ [note that $S_B(\lambda) = S_A(\lambda)$]. Because of the interaction term $\hat{V}_{AB}(\lambda)$, there exists quantum entanglement between subsystems $A$ and $B$. This is different from the case discussed in Sec. V A 2, where no interactions are assumed between subsystems $X$ and $Y$, and hence $T_A(\lambda) = T_B(\lambda)$ is expected in general.

Figure 9 shows the effective temperature $T_B(\lambda)/J_B$ of subsystem $B$ as a function of $T_A(\lambda)/J_A$ for the three different lattices studied in Sec. III. We find that $T_A(\lambda)/J_A \approx T_B(\lambda)/J_B$ even for $J_B/J_A \neq 1$. Apparently, this relation is somewhat similar to the common temperature condition in thermodynamics, which is a consequence of the equilibrium between two subsystems. However, the important distinction is that here the microscopic energy scales $J_A$ and $J_B$ of subsystems $A$ and $B$, respectively, which are absent in thermodynamics, enters in the relation. Moreover, the relatively simple relation between $T_A(\lambda)$ and $T_B(\lambda)$ found here might be due to our setting of the Hamiltonian where $\hat{H}_B = (J_B/J_A)\hat{H}_A$. Finally, we note that the same relation is exactly satisfied in the two analytical examples discussed in Sec. IV.

Appendix C: Thermofield-double-like state

In terms of the Schmidt decomposition of the ground-state wavefunction $|\Psi_0(\lambda)\rangle$, the assumption in Eq. (104) along with Eq. (107) can be rephrased as

$$|\Psi_0(\lambda)\rangle = \sum_{n=1}^{D_A} \frac{e^{-B_n(\lambda)\epsilon_n^A/2}}{\sqrt{Z_A(\lambda_B)}} |\psi_n^A\rangle_A |g_n\rangle_B,$$

where $|\psi_n^A\rangle_A$ is the $n$th eigenstate of $\hat{H}_A$ with its eigenvalue $\epsilon_n^A$ and $|g_n\rangle_B$ is an orthonormal basis set of subsystem $B$. The purification of $\hat{\rho}_A^\text{red}(\lambda)$ in Eq. (C1) resembles to the thermofield double state [39]. Indeed, if the subsystem $B$ is selected to be equivalent to the subsystem $A$, the right hand side in Eq. (C1) should reproduce the thermofield double state for the subsystem $A$ at temperature $1/J_A(\lambda)$. 

\begin{figure}[h]
\centering
\includegraphics{figure8}
\caption{Schematic figure of the relative entropy $D(\Delta)\lambda = D(\hat{\rho}(\lambda + \Delta\lambda)|\hat{\rho}(\lambda))$ for small $|\Delta\lambda|$ (red thick line), showing that $D(\Delta)\lambda(0) = 0$ and $dD(\Delta)\lambda(0)/d\lambda = 0$. Blue dashed line indicates a function proportional to $(\Delta\lambda)^2$, for comparison.}
\end{figure}
FIG. 9. The effective temperature $T_B(\lambda)/J_B$ of subsystem $B$ as a function of the effective temperature $T_A(\lambda)/J_A$ of subsystem $A$ for the spin-1/2 antiferromagnetic Heisenberg model in (a) the two coupled 1D chains (i.e., two-leg ladder), (b) the two coupled 2D square lattice (i.e., bilayer square lattice), and (c) the two coupled 2D triangular lattice (i.e., bilayer triangular lattice) with $N_A = N_B = 8$.

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