Thermal entanglement of Hubbard dimers in the nonextensive statistics

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The thermal entanglement of the Hubbard dimer (two-site Hubbard model) has been studied with the nonextensive statistics. We have calculated the auto-correlation ($O_q$), pair correlation ($L_q$), concurrence ($\Gamma_q$) and conditional entropy ($R_q$) as functions of entropic index $q$ and the temperature $T$. The thermal entanglement is shown to considerably depend on the entropic index. For $q < 1.0$, the threshold temperature where $\Gamma_q$ vanishes or $R_q$ changes its sign is more increased and the entanglement may survive at higher temperatures than for $q = 1.0$. Relations among $L_q$, $\Gamma_q$ and $R_q$ are investigated. The physical meaning of the entropic index $q$ is discussed with the microcanonical and superstatistical approaches. The nonextensive statistics is applied also to Heisenberg dimers.

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1. Introduction

Quantum entanglement is one of the most intriguing subjects in quantum information theory, and it has been investigated from various viewpoints in the last decade (for a review, see Refs. [1,2], and the related references therein). Quantum entanglement is expected to play an essential role as a resource in quantum communication and information processing. Many studies have been made on quantum entanglement with quantum spin models [3–11] and fermion systems [12–27] to clarify both its qualitative and quantitative aspects. The interface between the quantum information and statistical mechanics has been considerably investigated in recent years. It has been shown that entanglement of two neighboring sites shows a sharp peak either near or at the critical point where the phase transition takes place [5–7,14]. This suggests an intimate relation between quantum entanglement and quantum phase transition [2,19,21,20,26].

These studies mentioned above have been made within the Boltzmann–Gibbs statistics (BGS). In the past several years, there is an increased interest in the nonextensive statistics (NES), which was initially proposed by Tsallis [28–30]. This is because the standard method based on the BGS cannot properly deal with nonextensive systems where the physical quantities such as the energy and/or entropy of the $N$-body system are not proportional to $N$. The nonextensivity has been realized in the three typical systems: (1) systems with long-range interactions, (2) small-scale systems with fluctuations of temperatures or energy dissipations, and (3) multi-fractal systems [31]. For example, in a gravitating system with long-range interaction, which is a typical case (1), the specific heat becomes negative [32]. A cluster of 147 sodium atoms, which belongs to the case (2), has been reported to show the negative specific heat [33].

The generalized entropy (referred to as the Tsallis entropy) proposed by Tsallis [28,30] is given by, with $\text{Tr} \hat{\rho} = 1$:

$$S_q = k \left( \frac{\text{Tr} \hat{\rho}^q - 1}{1 - q} \right),$$

where $k$ is a positive constant, $\hat{\rho}$ the density matrix, $\text{Tr}$ the trace and $q$ the entropic index. In the limit of $q \to 1$, Eq. (1) reduces to the von Neumann form,

$$S_1 = -k \text{Tr} \ln \hat{\rho},$$

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where $\text{Tr} \  \hat{\rho} = 1$. We will set $k = k_B$ ($k_B$: the Boltzmann constant) when we discuss the thermodynamical entropy. The nonextensivity (non-additivity) in the Tsallis entropy is explained as follows. For a system consisting of two independent subsystems $A$ and $B$ with the density matrices, $\hat{\rho}(A)$ and $\hat{\rho}(B)$, the density matrix of the total system is described by $\hat{\rho}(A, B) = \hat{\rho}(A) \otimes \hat{\rho}(B)$ from which the Tsallis entropy is given by

$$S_q(A, B) = S_q(A) + S_q(B) + \left(1 - q\right) \frac{1}{k_B} S_q(A)S_q(B), \quad (3)$$

$S_q(\eta)$ denoting the entropy of the subsystem $\eta$ ($=A, B$). Eq. (3) shows that the entropy is additive for $q = 1$ and non-additive for $q \neq 1$. The quantity $(q - 1)$ expresses the measure of nonextensivity. The NES has been applied to a wide class of subjects such as physics, chemistry, and biology [34,35].

Small–scale systems belong to nonextensive systems as mentioned above. It is necessary to take into account the effect of nonextensivity, when we study the properties of quantum information of qubits, which have been mainly investigated within the BGS [12–27]. In recent years, the NES has been applied to the study on quantum information [36–53]. It has been shown that the non-additive Tsallis entropy yields a better measure for the separability criterion of entanglement than the additive von Neumann entropy [36,37,40,53]. Ref. [39] discusses an NES generalization of the von Neumann mutual information which is shown to strongly depend on the entropic index $q$. The above list of applications of the NES to quantum information is not complete; relevant references are presented in Refs. [34,35,53].

It is worthwhile to apply the NES to the Hubbard model [54], which is a typical model for strongly correlated fermion systems and which has been widely adopted for a study on quantum information [12–27]. Despite the simplicity of the model, however, it is very difficult to obtain its exact solution except for some limited cases. In order to obtain a reasonable solution, various approximate methods have been proposed and developed. The Hubbard model provides us with a good qualitative description for many interesting phenomena such as electron correlation, magnetism, superconductivity and quantum entanglement. We may employ a finite-size Hubbard model to obtain an analytical, exact solution. The Hubbard dimer (two-site Hubbard model) has been adopted as a simple model which can be analytically solved. Although the Hubbard dimer seems to be a toy model, it has played an important role as a model of qubits in the theory of quantum information [14,15,18].

In our previous papers [55–58], we applied the NES to Hubbard dimers for investigating the effects of nonextensivity on their thermodynamical and magnetic properties, bearing small-size systems in mind. It is interesting to examine the effect of nonextensivity on the properties of the quantum entanglement of two qubits [2] described by the Hubbard dimer within the NES, which is the main purpose of the present paper. Among various quantities expressing thermal entanglement, we have calculated the pair correlation, concurrence [59,60] and conditional entropy [61,62]. As will be shown in our study, the entropic index $q$ has considerable effects on the properties of thermal entanglement which may be improved by nonextensivity. The concurrence of the Hubbard dimer has been discussed within the BGS [14,15,18]. The generalization of the conditional entropy to the NES has been proposed in Refs. [40,45]. This is the first systematic study on the thermal entanglement of nonextensive fermion systems as far as we are aware of.

The paper is organized as follows. In Section 2, after briefly reviewing the maximum-entropy method (MEM) in the NES [28], we derive the density matrix to obtain auto-correlation and pair correlation, concurrence and conditional entropy. In Section 3, we present model calculations of relevant quantities as functions of the entropic index $q$ and the temperature $T$. In Section 4, we make a comparison among the pair correlation, concurrence and conditional entropy. Effects of magnetic field and interatomic interactions in the adopted model are investigated. The physical meaning of the entropic index $q$ is discussed with the use of the microcanonical approach (MCA) [63–67] and superstatistical approach (SSA) [68–70]. Section 5 is devoted to our conclusion.

2. Formulations

2.1. Hubbard dimers

We consider the extended Hubbard dimer whose Hamiltonian is given by

$$\hat{H} = -t \sum_\sigma (a_{\sigma}^{-\dagger} a_{\sigma} + a_{\sigma}^{\dagger} a_{\sigma}^{-\dagger}) + U \sum_{j=1}^2 n_{j\uparrow} n_{j\downarrow} + V_1 \sum_\sigma n_{1\sigma} n_{2\sigma} + V_2 \sum_\sigma n_{1\sigma} n_{2-\sigma} + \mu_B B \sum_{j=1}^2 (n_{j\uparrow} - n_{j\downarrow}), \quad (4)$$

where $n_{\sigma} = a_{\sigma}^{\dagger} a_{\sigma}$, $a_{\sigma}$ denotes the annihilation operator of an electron with spin $\sigma$ (= $\uparrow, \downarrow$) on a site $j$ (= 1, 2), $t$ the hopping integral, $U$ the intraatomic interaction between electrons with opposite spin, $V_1$ ($V_2$) the interatomic Coulomb interaction between the same (opposite) spin, $\mu_B$ the Bohr magneton and $B$ an applied magnetic field. By using the standard basis for the half-filled case with two electrons given by

$$|\Psi_1\rangle = |\uparrow\downarrow\rangle |0\rangle_2, \quad |\Psi_2\rangle = |0\rangle_1 |\uparrow\downarrow\rangle_2, \quad |\Psi_3\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2,$$

$$|\Psi_4\rangle = |\downarrow\rangle_1 |\uparrow\rangle_2, \quad |\Psi_5\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2, \quad |\Psi_6\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2.$$
we obtain the Hamiltonian matrix,

\[
H = \begin{pmatrix}
U & 0 & -t & -t & 0 & 0 \\
0 & U & -t & -t & 0 & 0 \\
-t & -t & V_2 & 0 & 0 & 0 \\
-t & -t & 0 & V_2 & 0 & 0 \\
0 & 0 & 0 & 0 & V_1 - 2\mu_\beta B & 0 \\
0 & 0 & 0 & 0 & 0 & V_1 + 2\mu_\beta B
\end{pmatrix}.
\]

Six eigenvalues of the system are given by [15,71]

\[
\epsilon_i = \frac{1}{2}(U + V_2 - D), \quad \frac{1}{2}(U + V_2 + D), \quad U, \quad V_2, \quad V_1 - 2\mu_\beta B, \quad V_1 + 2\mu_\beta B \quad \text{for } i = 1 \text{ to } 6,
\]

and the corresponding eigenvectors are given by

\[
|\Phi_1\rangle = \frac{\sin \theta}{\sqrt{2}} (|\uparrow \downarrow \rangle_1|0\rangle_2 + |0\rangle_1|\uparrow \downarrow \rangle_2) + \frac{\cos \theta}{\sqrt{2}} (|\uparrow \rangle_1|\downarrow \rangle_2 + |\downarrow \rangle_1|\uparrow \rangle_2),
\]

\[
|\Phi_2\rangle = \frac{\cos \theta}{\sqrt{2}} (|\uparrow \downarrow \rangle_1|0\rangle_2 + |0\rangle_1|\uparrow \downarrow \rangle_2) - \frac{\sin \theta}{\sqrt{2}} (|\uparrow \rangle_1|\downarrow \rangle_2 + |\downarrow \rangle_1|\uparrow \rangle_2),
\]

\[
|\Phi_3\rangle = \frac{1}{\sqrt{2}} (|\uparrow \rangle_1|\downarrow \rangle_2 - |\downarrow \rangle_1|\uparrow \rangle_2),
\]

\[
|\Phi_4\rangle = \frac{1}{\sqrt{2}} (|\uparrow \rangle_1|\downarrow \rangle_2 - |\downarrow \rangle_1|\uparrow \rangle_2),
\]

\[
|\Phi_5\rangle = |\uparrow \rangle_1|\uparrow \rangle_2,
\]

\[
|\Phi_6\rangle = |\downarrow \rangle_1|\downarrow \rangle_2,
\]

where

\[
\tan \theta = \frac{4t}{U - V_2 + D},
\]

\[
D = \sqrt{(U - V_2)^2 + 16t^2}.
\]

For \(t/U \ll 1\) with \(V_1 = V_2 = B = 0\), we obtain

\[
\epsilon_1 = -\frac{4t^2}{U}, \quad \epsilon_2 = U + \frac{4t^2}{U}, \quad \epsilon_3 = U, \quad \epsilon_4 = \epsilon_5 = \epsilon_6 = 0,
\]

\[
\sin^2 \theta = \frac{4t^2}{U^2}, \quad \cos^2 \theta = 1 - \frac{4t^2}{U^2},
\]

where \(\epsilon_1\) is the lowest eigenstate for \(U > 0\).

The partition function in the BGS is given by

\[
Z_{BG} = Z_1 = \text{Tr} \, e^{-\beta H} = \sum_i e^{-\beta \epsilon_i} = 2e^{-\beta(U+V_2)/2} \cosh \left( \frac{\beta D}{2} \right) + e^{-\beta U} + e^{-\beta V_2} + 2e^{-\beta V_1} \cosh(2\beta \mu_\beta B),
\]

where \(\beta = 1/k_B T\). From Eq. (16) we can obtain various thermodynamical quantities of the system.

2.2. Maximum-entropy method in the NES

We will study the Hubbard dimer given by Eq. (4) within the NES, where the probability distribution function (PDF) or the density matrix is evaluated by the MEM for the Tsallis entropy. At the moment there are four MEMs in the NES: (a) original method [28], (b) un-normalized method [29], (c) normalized method [30], and (d) optimal Lagrange multiplier (OLM) method [72]. The four MEMs are compared in Ref. [31]. Among the four MEMs, (c) normalized MEM and (d) OLM–MEM with the \(q\)-average have been widely adopted for a study of nonextensive systems, because they are believed to be more superior than (a) original MEM [28] and (b) un-normalized MEM [29,31] with the normal average. Recent papers [73–75], however, have pointed out that thermodynamical quantities obtained by the \(q\)-average are unstable for a small change in the PDF, whereas those obtained by the normal average are stable [76]. The stability of the \(q\)-average is currently controversial [73, 75–78]. Although (c) normalized MEM [30] with the \(q\)-average was adopted in our previous papers [55–58,79], we have
employed in the present study, (a) original MEM with the normal average [28,73]. In Appendix A, thermodynamical quantities of the entropy, specific heat and susceptibility calculated by (a) original MEM [28,73] with the normal average are summarized and compared to the previous ones obtained by (c) normalized MEM [30] with the \( q \)-average [55–58,79]. In Appendix B the NES with (a) original MEM [28,73] is applied also to Heisenberg dimers.

Imposing the two constraints given by

\[
\text{Tr} (\hat{\rho}_q) = 1, \tag{17}
\]

\[
\text{Tr}(\hat{\rho}_q \hat{H}) = \langle \hat{H} \rangle_q = E_q, \tag{18}
\]

we obtain the density matrix given by

\[
\hat{\rho}_q = \frac{1}{X_q} \text{Exp}_q[-\beta(H - E_q)], \tag{19}
\]

with

\[
X_q = \text{Tr} \text{Exp}_q[-\beta(H - E_q)], \tag{20}
\]

where \( \langle \cdot \rangle_q \) expresses the average over \( \hat{\rho}_q \), \( \beta \) the inverse of the temperature and \( \text{Exp}_q(x) \) is defined by [73]

\[
\text{Exp}_q(x) = [1 + (1 - 1/q)x]^{1/(q-1)}, \tag{21}
\]

with \( [y]_+ = \max(y, 0) \). Note that \( \text{Exp}_q(x) \) is different from the conventional \( q \)-exponential function \( \exp_q(x) \) defined by [28]

\[
\exp_q(x) = [1 + (1 - q)x]^{1/(1-q)}. \tag{22}
\]

The two \( q \)-exponential functions, \( \text{Exp}_q(x) \) and \( \exp_q(x) \), have the relation [73]:

\[
\exp_q(x) = \text{Exp}_{2-q}(2 - q)x, \quad \text{Exp}_q(x) = \exp_{2-q}(x/q). \tag{23}
\]

Both \( \text{Exp}_q(x) \) and \( \exp_q(x) \) reduce to the exponential function \( \exp(x) \) in the limit of \( q \to 1.0 \).

### 2.3. Auto-correlation and pair correlation

For the Hubbard dimer under consideration, we obtain

\[
\hat{\rho}_q = \frac{1}{X_q} \sum_i w_i |\Phi_i\rangle \langle \Phi_i|, \tag{24}
\]

\[
E_q = \frac{1}{X_q} \sum_i w_i e_i, \tag{25}
\]

\[
X_q = \sum_i w_i, \tag{26}
\]

where

\[
w_i = \text{Exp}_q[-\beta(e_i - E_q)]. \tag{27}
\]

The energy \( E_q \) in Eq. (25) includes the partition function \( X_q \) which is expressed in terms of \( E_q \) in Eq. (27). Then \( E_q \) and \( X_q \) are self-consistently determined by Eqs. (25)–(27) for given \( q \) and \( \beta \).

We first consider auto-\( \langle O_q \rangle \) and pair correlations \( \langle l_q \rangle \) defined by

\[
O_q = 1 - \sum_{j=1}^2 \langle n_j n_j \rangle_q, \tag{28}
\]

\[
l_q = \sum_{\sigma} \langle n_{1\sigma} n_{2\sigma} - n_{1\sigma} n_{2-\sigma} \rangle_q. \tag{29}
\]

When we employ the relations given by

\[
\sum_{j=1}^2 \langle n_j n_j \rangle_q = \left\langle \frac{\partial H}{\partial U} \right\rangle_q, \tag{30}
\]

\[
\sum_{\sigma} \langle n_{1\sigma} n_{2\sigma} \rangle_q = \left\langle \frac{\partial H}{\partial V_1} \right\rangle_q, \tag{31}
\]

\[
\sum_{\sigma} \langle n_{1\sigma} n_{2-\sigma} \rangle_q = \left\langle \frac{\partial H}{\partial V_2} \right\rangle_q \tag{32}
\]
Eqs. (28) and (29) become
\[ O_q = 1 - \frac{\partial H}{\partial U} \bigg|_q, \] (33)
\[ L_q = \frac{\partial H}{\partial V_1} \bigg|_q - \frac{\partial H}{\partial V_2} \bigg|_q. \] (34)

We may evaluate \( \partial H/\partial \theta \big|_q \) with \( \theta = U, V_1, \) and \( V_2 \) as follows. Taking the derivative of \( X_q \) in Eq. (20) with respect to \( \theta \), we obtain
\[ \frac{\partial X_q}{\partial \theta} = -\beta \text{ Tr} \left\{ (\text{Exp}_q[-\beta(H - E_q)]) \left( \frac{\partial H}{\partial \theta} - \frac{\partial E_q}{\partial \theta} \right) \right\}, \] (35)
\[ = -\beta X_q \left( \frac{\partial H}{\partial \theta} \bigg|_q - \frac{\partial E_q}{\partial \theta} \right), \] (36)
which leads to
\[ \left( \frac{\partial H}{\partial \theta} \right) \bigg|_q = \frac{\partial E_q}{\partial \theta} - \frac{1}{\beta X_q} \frac{\partial X_q}{\partial \theta}. \] (37)

From Eqs. (25)-(27), self-consistent equations for \( \partial E_q/\partial \theta \) and \( \partial X_q/\partial \theta \) are given by
\[ \frac{\partial E_q}{\partial \theta} = a_{11} \frac{\partial E_q}{\partial \theta} + a_{12} \frac{\partial X_q}{\partial \theta} + c_{1q}, \] (38)
\[ \frac{\partial X_q}{\partial \theta} = a_{21} \frac{\partial E_q}{\partial \theta} + a_{22} \frac{\partial X_q}{\partial \theta} + c_{2q}, \] (39)
with
\[ c_{2q} = -\beta \sum_i w_i \left( \frac{\partial \epsilon_i}{\partial \theta} \right), \] (40)
where an explicit expression for \( c_{1q} \) is not necessary (see below). Solving Eqs. (38)-(40) with respect to \( \partial E_q/\partial \theta \) and \( \partial X_q/\partial \theta \) and substituting them into Eq. (37), we obtain
\[ \left( \frac{\partial H}{\partial \theta} \right) \bigg|_q = -\frac{c_{2q}}{a_{21}} = \frac{1}{X_q} \sum_i w_i \left( \frac{\partial \epsilon_i}{\partial \theta} \right). \] (41)

Simple calculations with the use of Eqs. (5) and (41) lead to
\[ \left( \frac{\partial H}{\partial U} \right) \bigg|_q = \frac{1}{X_q} \left[ \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) w_1 + \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) w_2 + w_3 \right], \] (42)
\[ \left( \frac{\partial H}{\partial V_1} \right) \bigg|_q = \frac{1}{X_q} (w_5 + w_6), \] (43)
\[ \left( \frac{\partial H}{\partial V_2} \right) \bigg|_q = \frac{1}{X_q} \left[ \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) w_1 + \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) w_2 + w_4 \right]. \] (44)

Substituting Eqs. (42)-(44) into Eqs. (33) and (34), we finally obtain
\[ O_q = 1 - \frac{1}{X_q} \left[ \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) w_1 + \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) w_2 + w_3 \right], \] (45)
\[ L_q = \frac{1}{X_q} \left[ w_5 + w_6 - \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) w_1 - \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) w_2 - w_4 \right]. \] (46)

In the limit of \( q \to 1 \), Eqs. (45) and (46) reduce to
\[ O_1 = 1 - \frac{1}{Z} \left[ \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) e^{-\beta \epsilon_1} + \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) e^{-\beta \epsilon_2} + e^{-\beta \epsilon_3} \right], \] (47)
\[ L_1 = \frac{1}{Z} \left[ e^{-\beta \epsilon_5} + e^{-\beta \epsilon_6} - \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right) e^{-\beta \epsilon_1} - \frac{1}{2} \left( 1 - \frac{U - V_2}{D} \right) e^{-\beta \epsilon_2} - e^{-\beta \epsilon_4} \right]. \] (48)
In the limit of $T = 0$, the auto-correlation in the BGS and NES is given by

\[ O_q = -L_q = \frac{1}{2} \left( 1 + \frac{U - V_2}{D} \right), \quad (49) \]

\[
= \left\{ \begin{array}{ll}
\frac{1}{2} & \text{for } (U - V_2)/t = 0, \\
1 & \text{for } (U - V_2)/t \to \infty.
\end{array} \right. \quad (50)
\]

2.4. Concurrence

The concurrence $\Gamma$ has been proposed as a measure of entanglement for systems of two qubits [59,60]. It is defined with eigenvalues $\lambda_1^2 \geq \cdots \geq \lambda_4^2$ for the positive Hermitian matrix $\hat{R} = \sqrt{\hat{\rho}} \sqrt{\hat{\rho}}$ by [59,60]

\[ \Gamma = \max(\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0), \quad (51) \]

where $\tilde{\rho} = (\sigma^x \otimes \sigma^y) \rho^* (\sigma^y \otimes \sigma^x)$ and $^*$ denotes the complex conjugate. The entanglement of formation $E_F$ [80] is expressed in terms of $\Gamma$ by

\[ E_F = -\sum_{\xi = \pm} \left( 1 + \frac{\xi \sqrt{1 - \Gamma^2}}{2} \right) \log_2 \left( 1 + \frac{\xi \sqrt{1 - \Gamma^2}}{2} \right). \quad (52) \]

For a pair of qubits of the Hubbard dimer, the concurrence is given by [14,15]

\[ \Gamma = \max \left( \left\langle \sum_{\sigma} \left( a_{1\sigma}^\dagger a_{2\sigma} \right) - \sum_{\sigma} \left( n_{1\sigma} n_{2\sigma} \right), 0 \right\rangle \right). \quad (53) \]

where the bracket $\langle \cdot \rangle$ means the average over the density matrix. It is straightforward to generalize the method of Ref. [15] to the NES, in which the $q$-dependent concurrence $\Gamma_q$ is given by

\[ \Gamma_q = \max \left( \left\langle \sum_{\sigma} \left( a_{1\sigma}^\dagger a_{2\sigma} \right)_q - \sum_{\sigma} \left( n_{1\sigma} n_{2\sigma} \right)_q, 0 \right\rangle \right). \quad (54) \]

\[
= \max \left( \frac{1}{2} \left\langle \frac{\partial H}{\partial t} \right\rangle_q - \left\langle \frac{\partial H}{\partial V_1} \right\rangle_q, 0 \right). \quad (55) \]

In deriving Eq. (55), we employ the relations given by Eq. (31) and by

\[ \sum_{\sigma} \left( a_{1\sigma}^\dagger a_{2\sigma} + a_{2\sigma}^\dagger a_{1\sigma} \right)_q = -\left\langle \frac{\partial H}{\partial t} \right\rangle_q. \quad (56) \]

By using Eqs. (5) and (41) with $\theta = t$, we may calculate $\langle \partial H/\partial t \rangle_q$.

\[ \left\langle \frac{\partial H}{\partial t} \right\rangle_q = -\frac{8t}{X_q D} (w_1 - w_2). \quad (57) \]

Substituting Eqs. (43) and (57) into Eq. (55), we obtain

\[ \Gamma_q = \frac{1}{X_q} \max \left[ \left( \frac{4t}{D} \right) \left| (w_1 - w_2) - (w_5 + w_6), 0 \right| \right]. \quad (58) \]

In the limit of $T = 0$, $\Gamma_q$ in both the NES and BGS is given by

\[ \Gamma_q = \frac{4t}{D}, \quad (59) \]

\[
= \left\{ \begin{array}{ll}
1 & \text{for } (U - V_2)/t = 0, \\
0 & \text{for } (U - V_2)/t \to \infty.
\end{array} \right. \quad (60) \]

In the limit of $q = 1.0$, Eq. (58) reduces to

\[ \Gamma_q = \frac{1}{Z_t} \max \left[ \left( \frac{4t}{D} \right) \left| (e^{-\beta e_1} - e^{-\beta e_2}) - (e^{-\beta e_5} + e^{-\beta e_6}), 0 \right| \right]. \quad (61) \]

which is in agreement with the result of Ref. [15]. By increasing the temperature, the concurrence is decreased and vanishes above the threshold temperature, as will be shown in Section 3.2.
2.5. Conditional entropy

The conditional entropy for subsystems A and B in the NES is expressed by [40,45]

\[
S_q(A|B) = \frac{S_q(A, B) - S_q(B)}{1 + (1 - q)S_q(B)/k_B},
\]

with

\[
S_q(A, B) = k_B \frac{\text{Tr}[\rho_q(A, B)]^q - 1}{1 - q},
\]

\[
S_q(B) = k_B \frac{\text{Tr}[\rho_q(B)]^q - 1}{1 - q},
\]

\[
\hat{\rho}_q(B) = \text{Tr}_A \hat{\rho}_q(A, B),
\]

where Tr_A stands for the partial trace over the state A and \(\hat{\rho}_q(B)\) denotes the marginal density operator. In the limit of \(q \to 1\), \(S_q(A|B)\) reduces to the von Neumann conditional entropy, \(S_1(A|B) = S_1(A, B) - S_1(B)\), whose properties have been discussed in Refs. [61,62]. In independent subsystems A and B where the relation: \(\hat{\rho}(A, B) = \hat{\rho}(A) \otimes \hat{\rho}(B)\) holds, Eqs. (3) and (62) lead to \(S_q(A|B) = S_q(A)\) [40,45].

Regarding subsystems A and B as sites 1 and 2 in the Hubbard dimer under consideration, we may obtain the marginal density operator given by

\[
\hat{\rho}_q(1) = \text{Tr}_2 \hat{\rho}_q(1, 2)
\]

\[
= \frac{1}{X_q} (g_1|0_1⟩|0_1⟩ + g_2|↑_1⟩|↑_1⟩ + g_3|↓_1⟩|↓_1⟩ + g_4|↑_1⟩|↓_1⟩),
\]

with

\[
g_1 = g_4 = \frac{1}{2} (w_1 \sin^2 \theta + w_2 \cos^2 \theta + w_3),
\]

\[
g_2 = \frac{1}{2} (w_1 \cos^2 \theta + w_2 \sin^2 \theta + w_4 + 2w_5),
\]

\[
g_3 = \frac{1}{2} (w_1 \cos^2 \theta + w_2 \sin^2 \theta + w_4 + 2w_6),
\]

where \(\hat{\rho}_q(1, 2) = \hat{\rho}_q\) given by Eq. (24). From Eqs. (62)-(69), the conditional entropy is given by

\[
R_q \equiv S_q(1|2) = S_q(2|1) = \frac{k_B}{1 - q} \left( \frac{c_q}{d_q} - 1 \right),
\]

where

\[
c_q = \text{Tr}(\hat{\rho}_q^0) = \frac{1}{X_q} \sum_i w_i^q = X_q^{1-q},
\]

\[
d_q = \text{Tr}_1[\hat{\rho}_q(1)|^q = \frac{1}{X_q} (g_1^q + g_2^q + g_3^q + g_4^q).
\]

When \(\epsilon_i\) is the lowest eigenstate at \(T = 0.0\), we obtain \(w_i/X_q = 1.0\) and \(w_i/X_q = 0.0\) for \(i \neq 1\), which lead to

\[
\hat{\rho}_q(1, 2) = |\Phi_1⟩⟨\Phi_1|,
\]

\[
\hat{\rho}_q(1) = \left( \frac{\cos^2 \theta}{2} \right) (|↑⟩|↑⟩|1⟩) (|↓⟩|↓⟩|1⟩) + \left( \frac{\sin^2 \theta}{2} \right) (|0⟩|0⟩|1⟩ + |↑⟩|↓⟩|1⟩),
\]

\[
= \begin{cases} 
\frac{1}{4} (|0⟩|0⟩|1⟩ + |↑⟩ |1⟩ + |↓⟩|1⟩) & \text{for } U/t \to 0, \\
\frac{1}{2} (|↑⟩|↑⟩|1⟩ + |↓⟩|↓⟩|1⟩) & \text{for } U/t \to \infty.
\end{cases}
\]

By using Eqs. (70)-(72) and (74), we obtain the conditional entropy given by

\[
R_q = \frac{k_B}{1 - q} \left[ \frac{2^{q-1}}{(\cos^2 \theta + \sin^2 \theta)} - 1 \right],
\]

\[
= \begin{cases} 
\frac{4^{q-1} - 1}{(1 - q)} & \text{for } U/t \to 0, \\
\frac{k_B}{1 - q} (2^{q-1} - 1) & \text{for } U/t \to \infty.
\end{cases}
\]
Fig. 1. (Color online) (a) Temperature dependences of various correlations for $U/t = 5.0$ with $q = 0.6$ (solid curves) and 1.0 (dashed curves).

For $q = 1.0$ with $t/U \ll 1.0$ and $V_1 = V_2 = B = 0$, calculations using Eqs. (14) and (15) yield

$$\frac{g_1}{X_1} = \frac{g_4}{X_1} = \frac{2t^2}{U^2} \left( 1 - 3e^{-4q^2/U} \right),$$

$$\frac{g_2}{X_1} = \frac{g_3}{X_1} = \left( 1 - \frac{2t^2}{U^2} \right) \left( 1 - 3e^{-4q^2/U} \right) + 3e^{-4q^2/U},$$

from which the conditional entropy is given by

$$R_1 = S_1(1, 2) - S_1(1),$$

with

$$S_1(1, 2) = 3k_B \left( 1 + \frac{4\beta t^2}{U} \right) e^{-4\beta t^2/U},$$

$$S_1(1) = k_B \left( \ln 2 + \frac{4t^2}{U^2} \right) \left[ 1 - \ln \left( \frac{4t^2}{U^2} \right) - 6e^{-4q^2/U} \right].$$

At $T = 0.0$, Eqs. (80)–(82) yield $R_1 = -k_B \ln 2$ where the negative $R_1$ expresses the quantum correlation [61,62]. By rising the temperature, the conditional entropy is increased and changes its sign from negative to positive because of a contribution of the classical correlation, as will be shown in Section 3.3.

3. Model calculations

3.1. Auto-correlation and pair correlation

We have performed numerical calculations, solving self-consistent equations for $E_q$ and $X_q$ given by Eqs. (25)–(27), by using the Newton–Raphson method with $V_1 = V_2 = B = 0$ otherwise noticed. Fig. 1 shows the temperature dependences of various correlations given by Eqs. (30)–(32) and (56) for $U/t = 5.0$ with $q = 0.6$ and 1.0. By increasing the temperature, $\sum_{\sigma} \langle n_{1\sigma} n_{2\sigma} \rangle_q$ is increased while both $\sum_{\sigma} \langle n_{1\sigma} n_{2-\sigma} \rangle_q$ and $\sum_{\sigma} \langle a_{1\sigma} a_{2\sigma} + a_{1\sigma} a_{1\sigma} \rangle_q$ are decreased. In contrast, $\sum_{\sigma=1}^2 \langle n_{1\sigma} n_{j\sigma} \rangle_q$ is almost temperature independent. Temperature dependences of correlations for $q = 0.6$ are less significant than those for $q = 1.0$. These $q$ and $T$ dependences of correlations shown in Fig. 1 reflect on those of $O_q$, $L_q$, $\Gamma_q$ and $R_q$, as will be shown in the following.

Fig. 2(a) and (b) show the temperature dependence of the auto-correlation ($O_q$) for $U/t = 0.0$ and 5.0, respectively, with $q = 0.6, 0.8, 1.0$ and 1.2. The magnitude of spin correlation is given by $\langle s_1 \cdot s_2 \rangle_q = (3/4)O_q$. At $T = 0.0$, $O_q$ is 0.5 and 0.89 for $U/t = 0.0$ and 5.0, respectively, independently of $q$. $O_q$ for $U/t = 0.0$ is increased with increasing temperature. For $U/t = 5.0$, $O_q$ is once increased with rising $T$, but it is decreased at higher temperatures after showing the maximum.

Temperature dependences of pair correlation ($-L_q$) for $U/t = 0.0$ and 5.0 are shown in Fig. 2(c) and (d), respectively, with $q = 0.6, 0.8, 1.0$ and 1.2. At $T = 0.0$, we obtain $L_q = -0.5$ and $-0.89$ for $U/t = 0.0$ and 5.0, respectively, independently of $q$; the negative sign of $L_q$ stands for antiferromagnetic correlations for adopted parameters of $V_1 = V_2 = B = 0.0$. When the temperature is increased, magnitude of $L_q$ is monotonously decreased. We note that $-L_q$ for $q < 1.0$ is larger than that for $q = 1.0$ at $k_BT/t \geq 0.3$, which expresses the intrigue effect of nonextensivity on the pair correlation.
Fig. 2. (Color online) Temperature dependences of auto-correlation ($O_q$) for (a) $U/t = 0.0$ and (b) $U/t = 5.0$, pair correlation ($-L_q$) for (c) $U/t = 0.0$, (d) $U/t = 5.0$, concurrence ($\Gamma_q$) for (e) $U/t = 0.0$ and (f) $U/t = 5.0$, and the conditional entropy ($R_q$) for (g) $U/t = 0.0$ and (h) $U/t = 5.0$ with $q = 0.6$ (solid curves), 0.8 (dotted curves), 1.0 (dashed curves) and 1.2 (chain curves).

3.2. Concurrence

Fig. 2(e) and (f) show temperature dependences of the concurrence ($\Gamma_q$) for $U/t = 0.0$ and 5.0, respectively, with $q = 0.6$, 0.8, 1.0 and 1.2. At $T = 0.0$, $\Gamma_q = 1.0$ and 0.63 for $U/t = 1.0$ and 5.0, respectively, independently of $q$. By increasing the temperature, $\Gamma_q$ is more slowly decreased for smaller $q$. $\Gamma_q$ vanishes above the threshold temperature $T_{\Gamma}$ which is implicitly determined by

$$T_{\Gamma} = \ldots$$
Fig. 3. (Color online) $q$ dependences of threshold temperatures of $T_{F}$ (the solid curve) and $T_{R}$ (the dashed curve) for $U/t = 5.0$, the inset showing $T_{R}$ against $T_{F}$.

Fig. 4. (Color online) (a) $\Gamma_{q}$ as a function of $-L_{q}$ and (b) $\Gamma_{q}$ as a function of $-R_{q}$ with $q = 0.6$ (solid curves) and 1.0 (dashed curves), the result of $U/t = 5.0$ in (a) for $q = 0.6$ being indistinguishable from that for $q = 1.0$.

The $q$ dependence of $T_{R}$ is plotted by the dashed curve in Fig. 3, which shows that $T_{R}$ is increased with decreasing $q$ below unity. $T_{R}$ is correlated with $T_{F}$ as shown in the inset of Fig. 4, although $T_{R}$ does not agree with $T_{F}$.

We note in Fig. 2(a)–(h) that temperature dependences of $O_{q}$, $L_{q}$, $\Gamma_{q}$ and $R_{q}$ become more significant with increasing $q$, which is consistent with the more significant temperature dependences in the specific heat ($C_{q}$) and susceptibility ($\chi_{q}$) shown in Appendix A (Fig. 6).

4. Discussion

4.1. Relations among $L_{q}$, $\Gamma_{q}$ and $R_{q}$

It is interesting to investigate the relations among $L_{q}$, $\Gamma_{q}$ and $R_{q}$. In Fig. 4(a), $\Gamma_{q}$ for $U/t = 0.0$ and 5.0 with $q = 0.6$ and 1.0 are plotted as a function of $-L_{q}$, which shows a linear relation: $\Gamma_{q} \approx a(−L_{q}) − b \ (a, b > 0)$. This linear relation between $\Gamma_{q}$...
and \( -L_q \) shown in Fig. 4(a) is realized in the parametric plot of \( -L_q(T) \) versus \( \Gamma_q(T) \) with fixed model parameters. However, it does not hold between \( -L_q \) and \( \Gamma_q \) when the model parameters are changed. This fact is easily realized when we compared Eq. (50) with Eq. (60), which shows that with increasing \( U \), \( |L_q| \) is increased but \( \Gamma_q \) is decreased. In Fig. 4(b), \( \Gamma_q \) for \( U/t = 0.0 \) and 5.0 with \( q = 0.6 \) and 1.0 is plotted as a function of \( -R_q \), which shows the correlation between \( \Gamma_q \) and \( R_q \). We note in Fig. 4(a) and (b) that \( L_q \), \( \Gamma_q \) and \( R_q \) are correlated although the precise relations among them are not clear.

4.2. Effect of magnetic field and interatomic interactions

We have so far assumed \( V_1 = V_2 = B = 0.0 \) for which the lowest eigenvalue of \( \epsilon_1 \) leads to the singlet ground state. If \( V_1 \), \( V_2 \) and/or \( B \) are, however, introduced, the triplet state may be the ground state. The critical condition for the singlet–triplet transition is given by \( \epsilon_1 = \epsilon_S \), i.e.,

\[
\mu_B B = \frac{1}{4} \left( 2V_1 - V_2 - U + \sqrt{(U - V_2)^2 + 16t^2} \right). \tag{85}
\]

Fig. 5 shows temperature dependences of \( \Gamma_q \) for \( q = 1.0 \) (dashed curves) and \( q = 0.6 \) (solid curves) when \( B \) is changed with \( U/t = 5.0 \) and \( V_1 = V_2 = 0.0 \), for which Eq. (85) yields the critical field given by \( \mu_B B_c/t = 0.351 \). The triplet state becomes the ground state for \( B > B_c \), where the pair correlation and marginal entropy are positive (\( L_q > 0 \), \( R_q > 0 \)) and the concurrence vanishes (\( \Gamma_q = 0 \)).

Similarly, when we introduce \( V_1 \) and/or \( V_2 \) which satisfy Eq. (85), the triplet state becomes the ground state even if \( B = 0 \). In the triplet state, we obtain \( L_q > 0 \), \( R_q > 0 \) and \( \Gamma_q = 0 \). The effect of interatomic interactions on energy, entropy and specific heat of the Hubbard dimer in the singlet state has been investigated within the NES [71].

4.3. Physical meaning of the entropic index

The entropic index \( q \) is conventionally regarded as a parameter which is determined by a fitting of the \( q \)-exponential distribution to experimental data except for some cases where \( q \) may be determined in a microscopic way [31]. We will briefly discuss the physical meaning of the entropic index in a small system coupled to finite bath for which \( q \) is theoretically derived with the use of the MCA [63–67] and SSA [68–70].

(1) MCA

We consider a microcanonical ensemble consisting of a system and a bath with energies of \( E_S \) and \( E_B \), respectively (\( E = E_S + E_B \) is conserved). Available states for the system with energy between \( E_S \) and \( E_S + \Delta E_S \) are given by [63,65]

\[
\rho(E_S) \Delta E_S = \frac{\Omega_1(E_S) \Omega_2(E - E_S)}{\Omega_{1+2}(E)} \Delta E_S, \tag{86}
\]

where \( \Omega_\eta(E) \) denotes the structure function expressing the number of states with energy \( E \) in \( \eta (= S, B \) and \( S + B \). We assume that the structure function is given by [63,65]

\[
\Omega_\eta(E) = K m_\eta E^{m_\eta - 1}, \tag{87}
\]

where \( K \) is a constant and \( m_\eta \) the degree of freedom of variables in \( \eta \). Eq. (87) is justified for \( d \)-dimensional \( N \)-body ideal gases and harmonic oscillators, for which \( m = dN/2 \) and \( dN \), respectively. For \( E_S \ll E_B \) and \( m_S \ll m_B \), Eqs. (86) and (87)
lead to the PDF given by [63,65]

\[
p(E_S) \propto \left( 1 - \frac{E_S}{E} \right)^{m_B} ,
\]

\[
\propto \text{Exp}_q(-q\beta E_S) ,
\]

with

\[
q = 1 + \frac{1}{m_B} ,
\]

\[
\beta = \frac{1}{(q - 1)E} ,
\]

where \( \text{Exp}_q(x) \) denotes the \( q \)-exponential function given by Eq. (21). Eq. (89) corresponds to the PDF obtained in the normal average. In the case of \( m_B \to \infty \), Eq. (88) reduces to

\[
p(E_S) \propto e^{-\beta E_S} ,
\]

with

\[
\beta = \frac{m_B}{E} = \frac{1}{k_B T} .
\]
The specific heat of the bath is shown to be given by [64]
\[ C_v = \frac{dE_h}{dT} \propto \frac{1}{q-1}. \] (94)

Eqs. (89), (90), (92) and (94) imply that for finite bath, the PDF is given by the q-exponential function whereas for infinite bath \((C_v = \infty)\), the PDF is given by the exponential function. A similar analysis has been made within the microcanonical approach in Refs. [66,67].

(2) SSA

In the superstatistics [68–70], it is assumed that properties of a given system may be expressed by a superposition over the spatially and/or temporarily fluctuating intensive parameter \(i.e., \) the inverse temperature \([68–70]\). Since the PDF of the equilibrium state \(i\) with the inverse temperature \(\beta (=1/k_BT)\) is given by \(e^{-\beta q}/Z_i(\beta)\), the PDF averaged over fluctuating \(\beta\)-variable is assumed to be given by [68–70]
\[ p_i = \int_0^\infty \frac{e^{-\beta \epsilon_i}}{Z_i(\beta)} f(\beta) d\beta, \] (95)

with
\[ f(\beta) = \frac{1}{\Gamma(n/2)} \left( \frac{n}{2\beta_0} \right)^{n/2} \beta^{n/2-1} e^{-n\beta/2\beta_0}. \] (96)

Here \(\Gamma(x)\) is the gamma function and \(f(\beta)\) denotes the \(\chi^2\)-distribution with rank \(n\) which expresses the distribution of sum of squares of \(n\) random normal variables with zero mean and unit variance [69]. Average and variance of \(\beta\) are given by \((\beta) \equiv \beta_0\) and \(((\beta^2) \equiv \beta_0^2)/(2\beta_0) = 2/n\). When adopting the type-A superstatistics in which the \(\beta\) dependence in \(Z_i(\beta)\) is neglected [70], we obtain (with \(n = n_5\)),
\[ p_i \propto \left( 1 + \frac{2\beta_0}{n_5} \right)^{-n_5/2}, \] (97)

which is rewritten as
\[ p_i \propto \text{Exp}_q(-q\beta_0 \epsilon_i), \] (98)

with
\[ q = 1 - \frac{2}{n_5}. \] (99)

Eq. (98) is in conformity with the normal average PDF.

It has been shown by a detailed microscopic calculation that the distribution of the inverse temperature of a system containing independent \(n\) particles coupled to a bath characterized by a fixed inverse temperature of \(\beta\), is given by [81]
\[ f_I(\beta) = \frac{\bar{\beta}}{\Gamma(n/2)} \left( \frac{n\bar{\beta}}{2} \right)^{n/2} \beta^{-n/2-2} e^{-n\beta/2\bar{\beta}}. \] (100)

Eq. (100) expresses the inverse-gamma distribution, and its profile is similar to that of the gamma-distribution given by Eq. (96) for large \(n\) [81]. Unfortunately, we cannot obtain an analytic expression for the PDF averaged over \(f_I(\beta)\) by using Eq. (95) with \(f(\beta) \rightarrow f_I(\beta)\). Nevertheless the calculation of Ref. [81] justifies the concept of the superstatistics.

5. Conclusion

We have calculated various quantities of quantum entanglement such as auto-\((O_q)\) and pair correlations \((L_q)\), concurrence \((\Gamma_q)\) and conditional entropy \((R_q)\) of the half-filled Hubbard dimer as functions of the entropic index and the temperature within the framework of the NES [28]. It has been shown that the properties of \(O_q, L_q, \Gamma_q\) and \(R_q\) are considerably modified by nonextensivity. In particular, for \(q < 1.0\), the thermal entanglement may be survive at higher temperatures than that for \(q = 1.0\), because the threshold temperature where \(\Gamma_q\) vanishes \((T_G)\) or \(R_q\) changes its sign \((\bar{T}_q)\) is more raised for a larger \((1 - q)\) (Fig. 3). The three measures of \(L_q, \Gamma_q\) and \(R_q\) for thermal entanglement are correlated with each other although the precise relations among them are not clear.

The NES has a wider applicability than the BGS, which corresponds to the \(q = 1.0\) limit of the NES. We note that the PDF in the MCA given by Eq. (89) is equivalent to that in the SSA given by Eqs. (98). There is, however, distinct differences in their expressions of \(q\) (Eqs. (90) and (99)) [82–84]:
\[ q = \begin{cases} 
1 + \frac{1}{m_b} & \geq 1.0 \text{ in the MCA}, \\
1 - \frac{2}{n_5} & \leq 1.0 \text{ in the SSA}.
\end{cases} \] (101)
The entropic index in the MCA is expressed in terms of the bulk parameter \((m_B)\) while that in the SSA is given in terms of the system one \((n_S)\). Furthermore, the conceivable value of \(q\) in the MCA is different from that in the SSA. In this respect, we have not obtained a unified physical interpretation of the entropic index at the moment. Nevertheless, Eq. (101) shows that the entropic index \(q\) may be related with the size of the system and/or bath and that nonextensivity may be realized in such a small-scale system. It might be interesting to perform experiments by changing the size of the system and/or bath, in order to examine the possibility that nonextensivity reflects on the thermal entanglement of two-qubit Hubbard dimer. Such experimental studies might clarify the role of nonextensivity in small systems and provide valuable insight on the validity of the MCA and SSA.

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**Appendix A. Thermodynamical quantities of the Hubbard dimers with the original MEM**

A.1. Energy and entropy

When the energy \(E_q\) and partition function \(X_q\) are obtained by solving Eqs. (25)-(27) for given \(q\) and \(\beta\), the Tsallis entropy given by Eq. (1) may be calculated as

\[
S_q = k_B \left( \frac{c_q - 1}{1 - q} \right),
\]

with

\[
c_q = \text{Tr}(\hat{\rho}_q^q) = \frac{1}{X_q} \sum_i w_i^q = X_q^{1-q}.
\]

A.2. Specific heat

The specific heat is given by [55, 56]

\[
C_q = \left( \frac{\partial E_q}{\partial T} \right) \left( \frac{\partial E_q}{\partial \beta} \right),
\]

where \(\partial E_q/\partial \beta\) may be determined by simultaneous equations given by

\[
\begin{align*}
\frac{\partial E_q}{\partial \beta} &= a_{11} \frac{\partial E_q}{\partial \beta} + a_{12} \frac{\partial X_q}{\partial \beta} + b_1, \\
\frac{\partial X_q}{\partial \beta} &= a_{21} \frac{\partial E_q}{\partial \beta} + a_{22} \frac{\partial X_q}{\partial \beta} + b_2,
\end{align*}
\]

with

\[
\begin{align*}
a_{11} &= \frac{\beta}{q X_q} \sum_i w_i^{2-q}\epsilon_i, & a_{12} &= -\frac{E_q}{X_q}, & a_{21} &= \beta X_q, & a_{22} &= 0, \\
b_1 &= -\frac{1}{q X_q} \sum_i w_i^{2-q}\epsilon_i(\epsilon_i - E_q), & b_2 &= 0.
\end{align*}
\]

Eqs. (A.4)-(A.6) are derived from Eqs. (25)-(27). Solving Eqs. (A.4)-(A.6) for \(\partial E_q/\partial \beta\), we obtain

\[
C_q = -\frac{b_1}{k_B T^2} \frac{1}{1 - a_{11} - a_{12} a_{21}}.
\]

In the limit of \(q = 1.0\), \(C_q\) becomes

\[
C_1 = \left( \frac{1}{k_B T^2} \right) \langle (\epsilon_i^2)_{1} - (\epsilon_i)_{1}^2 \rangle.
\]

A.3. Susceptibility

The paramagnetic spin susceptibility \(\chi_q\) is given by [55, 56]
\[ \chi_q = -\frac{E_q^{(2)}}{\beta X_q} + \frac{1}{\beta X_q} X_q^{(2)}, \]  
(A.9)

where \( E_q^{(2)} = \frac{\partial^2 E_q}{\partial B^2} \bigg|_{B=0} \) and \( X_q^{(2)} = \frac{\partial^2 X_q}{\partial B^2} \bigg|_{B=0} \). From Eqs. (25)–(27), we obtain the simultaneous equations for \( E_q^{(2)} = \frac{\partial^2 E_q}{\partial B^2} \bigg|_{B=0} \) and \( X_q^{(2)} = \frac{\partial^2 X_q}{\partial B^2} \bigg|_{B=0} \).

\[ E_q^{(2)} = a_{11} E_q^{(2)} + a_{12} X_q^{(2)} + f_1, \]  
(A.10)

\[ X_q^{(2)} = a_{21} E_q^{(2)} + a_{22} X_q^{(2)} + f_2, \]  
(A.11)

with

\[ f_2 = \frac{\beta^2}{q} \sum_i w_i^{2-q} \mu_i^2. \]  
(A.12)

From Eqs. (A.9)–(A.12), we obtain

\[ \chi_q = \frac{f_2}{a_{21}} = \frac{\beta}{q X_q} \sum_i w_i^{2-q} \mu_i^2, \]  
(A.13)

which does not include \( f_1 \). In the limit of \( q = 1.0 \), the spin susceptibility is given by

\[ \chi_1 = \frac{\beta}{Z_1} \sum_i e^{-\beta \epsilon_i} \mu_i^2. \]  
(A.14)

A.4. Model calculations

Fig. 6 shows temperature dependences of the calculated entropy, specific heat and susceptibility. Temperature dependences of the entropy \( S_q \) for \( U/t = 0.0 \) and 5.0 are plotted in Fig. 6(a) and (d), respectively, with \( q = 0.6, 0.8, 1.0 \) and 1.2. For a larger \( U \) value, \( S_q \) is more quickly increased at low temperatures. This is because the energy difference between the ground state \( (\epsilon_1) \) and the first excited state \( (\epsilon_4) \) becomes smaller when the strength of \( U \) is more increased. With increasing \( q \), the saturation value of \( S_q \) at higher temperatures becomes smaller. Temperature dependences of specific heat \( C_q \) for \( U/t = 0.0 \) and 5.0 are plotted in Fig. 6(b) and (e), respectively, for various \( q \) values. Fig. 6(c) and (f) show temperature dependences of the susceptibility \( \chi_q \) for \( U/t = 0.0 \) and 5.0, respectively, with \( q = 0.6, 0.8, 1.0 \) and 1.2. We note that temperature dependences of \( C_q \) and \( \chi_q \) at low temperatures for \( q = 1.2 \) are more significant than those for \( q = 1.0 \) whereas those for \( q = 0.8 \) is less significant than those of \( q = 1.0 \): temperature dependences of \( C_q \) and \( \chi_q \) become more significant with increasing \( q \). In contrast, \( S_q \) is increased with increasing \( q \). These behaviors are understood as follows. The \( q \)- and \( T \)-dependent thermodynamical quantity \( Q_q(T) \) may be expand at \( q = 1.0 \),

\[ Q_q(T) = \sum_{k=0}^{\infty} \frac{(q-1)^k}{k!} Q_q^{(k)}(T), \]  
(A.15)

\[ \simeq Q_1(T) + (q-1)Q_1^{(1)}(T) + \cdots, \]  
(A.16)

where \( Q_1^{(k)}(T) = \frac{\partial^k Q_1(T)}{\partial q^k} \bigg|_{q=1} \). Actual analytical evaluation of \( Q_1^{(1)}(T) \) is tedious because it involves self-consistent calculations as discussed in preceding subsections. Our model calculations show that \( Q_1^{(1)}(T) > 0 \) for \( C_q \) and \( \chi_q \) whereas \( Q_1^{(1)}(T) < 0 \) for \( S_q \) at low temperatures. The characteristic temperature dependences in thermodynamical quantities depend on the entropic index \( q \). When comparing these results with the counterparts obtained in our previous study [55] using the normalized MEM with \( q \)-average [30], we realize that both results approximately have the \( q \leftrightarrow 1/q \) symmetry; for example, results of \( q = 0.6 \) in Fig. 6 are similar to those of \( q = 1.5 \) in Figs. 2, 3 and 4 of Refs. [55, 79].

Appendix B. Heisenberg dimers with the original MEM

It is well known that the Hubbard dimer with \( U/t \gg 1 \) (with \( V_1 = V_2 = 0 \)) is equivalent to the Heisenberg dimer with the superexchange interaction of \( J_{se} \sim -t^2/U \). It is worthwhile to apply the NES with the original MEM [28, 73] to a Heisenberg dimer given by \( s = 1/2 \)

\[ H = -J s_1 \cdot s_2 - g \mu_B B (s_{1z} + s_{2z}), \]  
(B.1)

where the exchange interaction \( J \) is positive (negative) for ferromagnetic (antiferromagnetic) coupling. \( g (=2) \) denotes the \( g \)-factor, \( \mu_B \) the Bohr magneton, and \( B \) an applied magnetic field. Four eigenvalues of \( H \) are given by

\[ \epsilon_i = \frac{3J}{4} - \frac{J}{4} \pm \frac{J}{4} - g \mu_B B, -\frac{J}{4} + g \mu_B B \quad \text{for } i = 1, 2, 3 \text{ and } 4, \]  
(B.2)
and corresponding eigenvectors are given by

\[ |\Phi_1\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2), \] (B.3)

\[ |\Phi_2\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2), \] (B.4)

\[ |\Phi_3\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2, \] (B.5)

\[ |\Phi_4\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2. \] (B.6)

When \( B = 0 \), \( |\Phi_3\rangle \) and \( |\Phi_4\rangle \) may be alternatively expressed by

\[ |\Phi_3\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\uparrow\rangle_2 - |\downarrow\rangle_1 |\downarrow\rangle_2), \] (B.7)

\[ |\Phi_4\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\uparrow\rangle_2 + |\downarrow\rangle_1 |\downarrow\rangle_2). \] (B.8)

Eqs. (B.3), (B.4), (B.7) and (B.8) form the Bell basis.

In the BGS the partition function is given by

\[ Z_{BG} = Z_1 = e^{-\frac{3bJ}{4} + e^{\frac{6bJ}{4}} \left[ 1 + 2 \cosh (2\beta \mu B) \right]}, \] (B.9)

from which various thermodynamical quantities are easily calculated. The susceptibility is, for example, given by

\[ \chi_{BG} = \left( \frac{\mu^2}{k_B T} \right) \left( \frac{8}{3 + e^{-\beta J}} \right). \] (B.10)

The calculation for the Heisenberg dimer within the NES goes parallel to that for the Hubbard dimer with the use of four eigenvalues given by Eq. (B.2). The average energy and partition function are expressed by

\[ E_q = \frac{1}{X_q} \sum_i w_i \epsilon_i, \] (B.11)

\[ X_q = \sum_i w_i, \] (B.12)

with

\[ w_i = \text{Exp}_q \left[ -\beta (\epsilon_i - E_q) \right]. \] (B.13)

The pair correlation function \( (L_q) \) is defined by

\[ \left( \frac{3}{4} \right) L_q = \langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle_q, \] (B.14)

\[ = - \left( \frac{\partial H}{\partial J} \right)_q, \] (B.15)

\[ = \frac{1}{X_q} \sum_i w_i^q \left( -\frac{\partial \epsilon_i}{\partial J} \right), \] (B.16)

which yields (with \( B = 0.0 \) hereafter)

\[ L_q = \frac{1}{X_q} \left\{ \left( \text{Exp}_q \left[ -\beta \left( -\frac{3J}{4} - E_q \right) \right] \right)^q - \left( \text{Exp}_q \left[ -\beta \left( \frac{3J}{4} - E_q \right) \right] \right)^q \right\}. \] (B.17)

For \( q = 1.0 \) with \( B = 0 \), Eq. (B.17) reduces to

\[ L_1 = \frac{1}{Z_1} \left( e^{\frac{6bJ}{4}} - e^{-\frac{6bJ}{4}} \right). \] (B.18)

The concurrence for \( J < 0 \) is given by

\[ \Gamma_q = \frac{1}{X_q} \max \left[ 2w_1 - \sum_i w_i, 0 \right]. \] (B.19)
For $q = 1.0$ and $B = 0$, Eq. (B.19) becomes

$$\Gamma_q = \frac{1}{Z_1} \max \left[ |e^{-3\beta J_4} - 3e^{\beta J_4}|, 0 \right].$$  \hfill (B.20)

which is in agreement with the result of Ref. [3].

By using the marginal density matrix given by

$$\hat{\rho}_q(1) = \frac{1}{2} \left( |\uparrow \rangle \langle \uparrow |_1 + |\downarrow \rangle \langle \downarrow |_1 \right),$$  \hfill (B.21)

we obtain the conditional entropy [40],

$$R_q = k_B \left[ \frac{(2^{q-1} - q^1 - q)}{(1 - q)} \right].$$  \hfill (B.22)

References

[1] M.A. Nielsen, L.I. Chuang, Quantum Computation and Quantum Information, Cambridge Univ. Press, Cambridge, 2000.
[2] L. Amico, R. Osterich, V. Vedral, Rev. Modern Phys. 80 (2008) 517.
[3] M.C. Arnesen, S. Bose, V. Vedral, Phys. Rev. Lett. 87 (2001) 017901.
[4] X. Wang, Phys. Rev. A 64 (2001) 012313.
[5] A. Osterloh, L. Amico, G. Falci, R. Fazio, Nature 416 (2002) 608.
[6] T.J. Osborne, M.A. Nielsen, Phys. Rev. A 66 (2002) 032110.
[7] G. Vidal, J.I. Latorre, E. Rico, A. Kitaev, Phys. Rev. Lett. 90 (2003) 227902.
[8] S.-J. Gu, H.-L. Lin, Y.-Q. Li, Phys. Rev. A 68 (2003) 042330.
[9] Y. Chen, P. Zanardi, F.C. Zhang, New J. Phys. 8 (2006) 97.
[10] S.-J. Gu, C-P. Sun, H.-Q. Lin, J. Phys. A: Math. Theor. 41 (2008) 025002.
[11] N.-L. Chan, J.-P. Cao, D. Yang, S.-J. Gu, J. Phys. A: Math. Theor. 40 (2007) 12143.
[12] J. Schliemann, D. Loss, A.H. MacDonald, Phys. Rev. B 63 (2001) 085311.
[13] P. Zanardi, Phys. Rev. A 65 (2002) 042101.
[14] Shu-Sa Deng, Shi-Jian Gu, You-Quan Li, Hai-Qing Lin, Phys. Rev. Lett. 93 (2004) 086402.
[15] Shu-Sa Deng, Shi-Jian Gu, Hai-Qing Lin, Chin. Phys. Lett. 22 (2005) 804.
[16] Shu-Sa Deng, Shi-Jian Gu, Hai-Qing Lin, Phys. Rev. B 74 (2006) 045103.
[17] D. Larsson, H. Johannesson, Phys. Rev. Lett. 95 (2005) 196406.
[18] M.R. Dowling, A.C. Doherty, H.M. Wiseman, Phys. Rev. A 73 (2006) 052323.
[19] D. Larsson, H. Johannahs, Phys. Rev. A 73 (2006) 042320.
[20] L.-A. Wu, M.S. Sarandy, H.J. Chang, Phys. Rev. A 68 (2003) 042335.
[21] A. Anfossi, P. Giorda, A. Montorsi, Phys. Rev. B 75 (2007) 165106.
[22] A. Ramšak, M. Čapek, Phys. Status Solidi B 246 (2009) 1006.
[23] A. Ramšak, M. Čapek, T. Rejec, Phys. Rev. Lett. 100 (2008) 070403.
[24] A.M.C. Souza, F.A.G. Almeida, Phys. Rev. A 79 (2009) 052337.
[25] L.D. Carr, M.I. Wall, D.G. Schirmert, R.C. Brown, E.J. Williams, C.W. Clark, Phys. Rev. A 81 (2010) 013613.
[26] J.P. Caro, W.Y. Franc, L.D. Amico, Phys. Rev. A 81 (2010) 053212.
[27] C. Tsallis, J. Stat. Phys. 52 (1988) 479.
[28] E.M.F. Curado, C. Tsallis, J. Phys. A 24 (1991) L69, 25 (1992) 1019.
[29] C. Tsallis, R.S. Mendes, AA.R. Plastino, Physica A 261 (1998) 534.
[30] C. Tsallis, Physica D 193 (2004) 3.
[31] T. Padmanabhan, Phys. Rep. 188 (1990) 285.
[32] M. Schmidt, R. Kusche, T. Hippler, J. Donges, W. Kronmüller, B. von Issendorff, H. Haberland, Phys. Rev. Lett. 86 (2001) 1191.
[33] C. Tsallis, Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World, Springer, New York, 2009.
[34] Lists of many applications of the nonextensive statistics are available at URL: http://tsallis.cat.cbpf.br/biblio.htm.
[35] A.K. Rajagopal, Phys. Rev. A 60 (1999) 4338.
[36] S. Abe, A.K. Rajagopal, Phys. Rev. A 60 (1999) 3461.
[37] A.K. Rajagopal, S. Abe, Phys. Rev. Lett. 83 (1999) 1711.
[38] A. Vidiella-Barranco, Phys. Lett. A 260 (1999) 315.
[39] A. Vidiella-Barranco, Phys. Lett. A 260 (1999) 325.
[40] S. Abe, A.K. Rajagopal, Phys. Rev. Lett. 91 (2001) 126001.
[41] S. Abe, A.K. Rajagopal, Physica A 289 (2001) 157.
[42] A. Vidiella-Barranco, H. Moya-Cessa, Phys. Lett. A 279 (2001) 156.
[43] C. Tsallis, S. Lloyd, M. Baranger, Phys. Rev. A 63 (2001) 042104.
[44] C. Tsallis, P.W. Lamberti, D. Prato, Physica A 295 (2001) 158.
[45] S. Abe, Physica A 306 (2002) 316.
[46] S. Abe, A.K. Rajagopal, Phys. Rev. A 65 (2002) 052323.
[47] C. Tsallis, D. Prato, C. Anteneodo, Eur. Phys. J. B 29 (2002) 605.
[48] A.K. Rajagopal, R.W. Rendell, Phys. Rev. A 66 (2002) 012104.
[49] J. Bätte, M. Casas, A.R. Plastino, A. Plastino, J. Phys. A: Math. Gen. 35 (2002) 10311.
[50] F.C. Alcaraz, C. Tsallis, Phys. Lett. A 301 (2002) 105.
[51] S. Abe, Phys. Rev. A 68 (2003) 022302.
[52] J. Bätte, M. Casas, A.R. Plastino, A. Plastino, Eur. Phys. J. B 35 (2003) 391.
[53] A.K. Rajagopal, R.W. Rendell, Eur. Phys. J. B 22 (2004) 531.
[54] J. Hubbard, Proc. R. Soc. Lond. Ser. A 281 (1964) 401.
[55] H. Hasegawa, Bull. Tokyo Gakugei Univ. Sci. IV 57 (2005) 75. arXiv:cond-mat/0408669.
[56] H. Hasegawa, Physica A 351 (2005) 273.
[57] H. Hasegawa, Progr. Theoret. Phys. 162 (2006) 70.
[58] H. Hasegawa, Progr. Mater. Sci. 52 (2007) 333.
[59] S. Hill, W.K. Wootters, Phys. Rev. Lett. 78 (1997) 5022.
[60] W.K. Wootters, Phys. Rev. Lett. 80 (1998) 2245.
[61] N.J. Cerf, C. Adami, Phys. Rev. Lett. 79 (1997) 5194.
[62] N.J. Cerf, C. Adami, Phys. Rev. A 60 (1999) 893.
[63] A.R. Plastino, A. Plastino, Physica A 193 (1994) 193.
[64] M.P. Almeida, Physica A 300 (2001) 424.
[65] F.Q. Potiguar, U.M.S. Costa, Physica A 321 (2003) 482.
[66] A.K. Aringazin, M.I. Mazhitov, Physica A 325 (2003) 409.
[67] R.S. Johal, A. Planes, E. Vives, Phys. Rev. E 68 (2003) 056113.
[68] G. Wilk, Z. Wlodarczyk, Phys. Rev. Lett. 84 (2000) 2770.
[69] C. Beck, Phys. Rev. Lett. 87 (2001) 180601.
[70] E.G.D. Cohen, Physica D 193 (2004) 35.
[71] F.A.R. Navarro, J.J.V. Flores, arXiv:0912.5386.
[72] S. Martinez, F. Nicolas, F. Pennini, A. Plastino, Physica A 286 (2000) 489.
[73] S. Abe, Phys. Rev. E 79 (2009) 041116.
[74] S. Abe, J. Stat. Mech. (2009) P07027.
[75] J.F. Lutsko, J.P. Boon, P. Grosfils, Europhys. Lett. 86 (2009) 40005.
[76] R. Hanel, S. Thurner, C. Tsallis, Europhys. Lett. 85 (2009) 20005.
[77] H. Hasegawa, J. Math. Phys. 51 (2010) 093301.
[78] H. Hasegawa, Phys. Rev. E 82 (2010) 031138.
[79] The result of the OLM-MEM [72] is equivalent to that of the normalized MEM [30] with the Lagrange multiplier of $\beta = c_q / k_B T$ (method B in Ref. [55]) where $c_q = \text{Tr}(\hat{\rho}_q)^{q'}$.
[80] C.H. Bennett, D.P. DiVincenzo, J.A. Smolin, W.K. Wootters, Phys. Rev. A 54 (1996) 3824.
[81] H. Touchette, in: M. Gellmann, C. Tsallis (Eds.), Nonextensive Entropy-Interdisciplinary Applications, Oxford Univ. Press, 2002, p. 159.
[82] When Eqs. (88) and (97) are expressed such that they are in conformity with the $q$-average PDF [Eq. (22)], we obtain $q = 1 / m_B \leq 1.0$ in the MCA while $q = 1 / 2 n_S \geq 1.0$ in the SSA, which is different from Eq. (101).
[83] It should be noted that the $q$-exponential function adopted in Refs. [64,65] is defined by $e^q_x = (1 + (q' - 1)x)^{(q'-1)^{-1}}$ for $q' > 1$, which is different from that given by Eq. (22) proposed in Ref. [28]. The relation between $q'$ and $q$ is $q' = 1 + 1 - q$.
[84] Ref. [66] claimed that Eqs. (50) and (99) are equivalent if we read $m_B = n_B / 2$, which is misleading because $q = 1 + 1 / m_B$ in Eq. (90) while $q = 1 + 2 / n_B$ in Eq. (99).