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Entanglement of a microcanonical ensemble

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Abstract

We replace time-averaged entanglement by ensemble-averaged entanglement and derive a simple expression for the latter. We show how to calculate the ensemble average for a two-spin system and for the Jaynes–Cummings model. In both cases the time-dependent entanglement is known as well so that one can verify that the time average coincides with the ensemble average.

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1. Introduction

The entanglement of particles is in principle a time-dependent quantity. This time dependence has been analysed recently in chaotic systems [1], in experimental spectra of triatomic molecules [2] and in Rydberg atoms [3]. Time-dependent entanglement has been studied in theoretical models, such as the Dicke model [4], a model of coupled kicked tops [5], the Harper Hamiltonian [6], a dimer model [7] and Bose–Einstein condensates [8]. In these papers, the notions of time-averaged entanglement and ensemble-averaged entanglement have been shown to be useful in monitoring phase transitions, although the generality of this relationship has been questioned, see e.g. [3].

In addition, time-averaged and ensemble-averaged entanglements are conserved quantities of quantum microcanonical ensembles [9]. As such they are of interest in the study of closed systems. This context is suited to discuss the relation between both concepts, and is the starting point of the present paper.

The entanglement of formation of a pure state is taken here to be defined as the von Neumann entropy of the reduced density matrix. Often, the von Neumann entropy is replaced by the linear entropy because the latter can be computed more easily. After this modification, it still satisfies the criteria [10] that a measure of entanglement should satisfy. A further justification for using the linear entropy is found in [11].

The definition using linear entropy has been used for a theoretical study of entanglement in multi-qubit systems [12] and to link entanglement to spatial delocalization [13]. The

entanglement dynamics of scattering electrons was studied in [14]. In the present paper the use of the linear entropy is essential to obtain simple results.

For the sake of completeness, and to fix notations, the definitions of entanglement of pure and of mixed states are reproduced in the following section. Section 3 introduces the entanglement of microcanonical ensembles of wavefunctions. The main result is announced in section 4. The proof is found in the appendix. It is followed by a section devoted to the complications that arise when the state of the system has additional symmetries. In sections 6 and 7 the main result is applied to a system of two interacting spins. Section 8 deals with the Jaynes–Cummings model. For this model the time-dependent entanglement is known so that it can be compared with the ensemble average. A short discussion follows in section 9.

2. Definition of entanglement

Consider two independent subsystems, labelled A and B. With each normalized wavefunction ψ of the combined system corresponds to a reduced density matrix ρ_A of the subsystem labelled A. The latter is defined by the relation

$$\text{Tr}_A \rho_A X = \langle \psi | X \otimes \mathbb{I} | \psi \rangle \quad \text{for all } X. \quad (1)$$

The entanglement of ψ is then equal to the von Neumann entropy of ρ_A . For technical reasons we replace this entropy by the linear entropy. The general definition of entanglement is

$$\mathcal{E}_A(\psi) = S_f(\rho_A) \equiv \text{Tr}_A \rho_A f(\rho_A), \quad (2)$$

with $f(x) = -\ln x$ in the von Neumann case, and $f(x) = 1 - x$ in the case of the linear entropy.

If ψ is of the product form $\psi = \psi_A \otimes \psi_B$, then ρ_A is a one-dimensional projection operator. Hence, the entanglement vanishes. A similar definition holds for ρ_B and for \mathcal{E}_B . The entanglements $\mathcal{E}_A(\psi)$ and $\mathcal{E}_B(\psi)$ are equal [15]. To see this, select a basis u_m in subsystem A and a basis v_p in subsystem B, so that

$$\psi = \sum_n \sqrt{p_n} u_n \otimes v_n. \quad (3)$$

This is possible by means of the Schmidt construction. Then ρ_A and ρ_B are diagonal, with eigenvalues p_n and with entropy equal to $\sum_n p_n f(p_n)$.

Often, the state of the system is not described by a wavefunction ψ but by a density matrix ρ . Such a density matrix can be written into the form

$$\rho = \sum_n p_n |\psi_n\rangle \langle \psi_n|, \quad (4)$$

with $p_n \geq 0$, $\sum_n p_n = 1$ and with ψ_n normalized wavefunctions. Then the entanglement of ρ has been defined [16] as the minimum of the average entanglement

$$\mathcal{E}(\rho) = \min \sum_n p_n \mathcal{E}_A(\psi_n), \quad (5)$$

where the minimum is taken over all possible ways to write (4).

3. Definition of mean entanglement of a microcanonical ensemble

The mean entanglement, which is studied in the present paper, is *not* the average (5), but rather the average over a microcanonical ensemble, as introduced in [9].

Let be given a density matrix ρ , which is diagonal in the orthonormal basis of wavefunctions ψ_n , with eigenvalues $p_n : \rho\psi_n = p_n\psi_n$. Associated with this diagonal density matrix is an ensemble of wavefunctions of the form

$$\psi = \sum_n \sqrt{p_n} e^{i\chi_n} \psi_n, \tag{6}$$

where χ_n are arbitrary phase factors. The ensemble average of the entanglement is then denoted $\bar{\mathcal{E}}$ and is given by

$$\bar{\mathcal{E}} = \left\langle \mathcal{E}_A \left(\sum_n \sqrt{p_n} e^{i\chi_n} \psi_n \right) \right\rangle_\chi, \tag{7}$$

where the average over χ is obtained by integrating over all phase factors χ_n from 0 to 2π , normalized by dividing by a factor 2π . Note that the ensemble average (7) does not depend on the chosen subsystem because $\mathcal{E}_A(\psi) = \mathcal{E}_B(\psi)$ for all ψ .

The ensemble (6) can be obtained by starting from a single wavefunction ψ , in combination with the quantum mechanical time evolution. The Hamiltonian H is the generator of the unitary time evolution

$$\psi_t = U(t)\psi \quad \text{with} \quad U(t) = e^{-i\hbar^{-1}tH}. \tag{8}$$

The time average of the entanglement $\mathcal{E}_A(\psi)$ is then defined by

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathcal{E}_A(\psi_t). \tag{9}$$

Assume now that the Hamiltonian is diagonal in the basis of wavefunctions ψ_n , with eigenvalues ϵ_n . Then one has

$$\psi_t = \sum_n \lambda_n e^{-i\hbar^{-1}\epsilon_n t} \psi_n \tag{10}$$

and hence

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathcal{E}_A \left(\sum_n \lambda_n e^{-i\hbar^{-1}\epsilon_n t} \psi_n \right). \tag{11}$$

The wavefunctions ψ_t belong to the ensemble (6) with $p_n = |\lambda_n|^2$. If the conditions of the classical ergodic theorem hold then the time average (11) coincides with the ensemble average (7)—see [9]. But even when the classical ergodic theorem does not hold, one can continue to use the ensemble average instead of the time average because experimentally the slightest perturbation may restore ergodicity.

4. Main result

Let be given an ensemble of wavefunctions of the form (6). With each of the basis vectors ψ_n is associated a couple of reduced density matrices ρ_A and ρ_B . For convenience, these will be denoted by σ_n and τ_n . Introduce the density matrices σ and τ , defined by

$$\sigma = \sum_n p_n \sigma_n \quad \text{and} \quad \tau = \sum_n p_n \tau_n. \tag{12}$$

In some sense, σ is the ensemble average of ρ_A , τ is the ensemble average of ρ_B .

Our main result is now that the mean entanglement, defined by (7), using the linear entropy S_1 , can be written as

$$\bar{\mathcal{E}} = S_1(\sigma) + S_1(\tau) - \Delta, \tag{13}$$

where Δ is a contribution common to both $S_1(\sigma)$ and $S_1(\tau)$. It is given by

$$\Delta = 1 - \sum_m p_m^2 \text{Tr}_A \sigma_m^2 = 1 - \sum_m p_m^2 \text{Tr}_B \tau_m^2. \quad (14)$$

The proof of this relation is given in the appendix.

The applications of (13) are explored in later sections.

5. Degeneracies

The ensemble (6) is uniquely defined by the density operator ρ in the case that the eigenvalues p_n of ρ are two-by-two distinct. Then the eigenfunctions ψ_n are unique up to a phase factor. However, if some of the eigenvalues p_n coincide then the orthonormal basis is non-unique. In particular, if a non-zero eigenvalue p_n is degenerate then different choices of orthonormal wavefunctions may influence the value of $\bar{\mathcal{E}}$. This shows that $\bar{\mathcal{E}}$ is the average entanglement of the ensemble and is not suitable as a definition of the entanglement of ρ .

A similar question is whether the entanglement of the ensemble can be used as the definition of the mean entanglement of the wavefunction ψ . Consider the situation that some of the eigenvalues ϵ_n of the Hamiltonian H are degenerate. Then the basis of wavefunctions ψ_n , which diagonalizes H , is not uniquely defined (up to phase factors). In that case the wavefunction ψ should not be decomposed into an arbitrary diagonalizing orthonormal basis. Rather, it should be projected onto the invariant subspaces of H . This determines in a unique way an orthonormal basis which then can be used to form the ensemble associated with ψ . An example of the degenerate case is given below.

6. Two-spin example

The simplest example is that of two quantum spins, each described by Pauli spin matrices and a Hamiltonian H which is diagonal in the basis of wavefunctions:

$$\begin{aligned} \psi_1 &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\ \psi_2 &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \\ \psi_3 &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ \psi_4 &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \end{aligned} \quad (15)$$

We assume that the energy levels are non-degenerate. Their actual value is not needed.

The reduced density matrices σ_m and τ_m , corresponding with ψ_m , are all equal to $\frac{1}{2}\mathbb{I}$. Hence, also the averages σ and τ are equal to $\frac{1}{2}\mathbb{I}$. As a consequence, the linear entropies $S_1(\sigma)$ and $S_1(\tau)$ both equal $1/2$. However, the common part Δ depends on the choice of the wavefunction ψ . One finds

$$\Delta = 1 - \sum_m p_m^2 \text{Tr}_A \sigma_m^2 = 1 - \frac{1}{2} \sum_m p_m^2. \quad (16)$$

The final result for the mean entanglement of ψ is therefore

$$\bar{\mathcal{E}} = \frac{1}{2} + \frac{1}{2} - \left(1 - \frac{1}{2} \sum_m p_m^2\right) = \frac{1}{2} \sum_m p_m^2. \quad (17)$$

Note that this result lies between $1/4$ and $1/2$.

It is possible but tedious to verify by explicit calculation that the mean entanglement (17) coincides with the time average of $\mathcal{E}_A(\psi_t)$, as it should be.

7. Degenerate two-spin example

Consider a two-spin system with energy $-\epsilon$ for anti-parallel spins and $+\epsilon$ for parallel spins. This is a degenerate limit of the previous example. The ensemble, generated by an arbitrary ψ , now contains two free phase factors instead of four. It consists of all wavefunctions of the form

$$e^{i\chi_1} \lambda_1 \psi_1 + e^{i\chi_2} \lambda_2 \psi_2, \quad (18)$$

with χ_1 and χ_2 arbitrary, and with $\lambda_1 \psi_1, \lambda_2 \psi_2$ given by

$$\begin{aligned} \lambda_1 \psi_1 &= |\uparrow\downarrow\rangle\langle\uparrow\downarrow|\psi\rangle + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\psi\rangle \\ \lambda_2 \psi_2 &= |\uparrow\uparrow\rangle\langle\uparrow\uparrow|\psi\rangle + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\psi\rangle. \end{aligned} \quad (19)$$

The coefficients λ_1 and λ_2 are chosen in such a way that ψ_1 and ψ_2 are normalized. The reduced density matrices are found to be

$$\begin{aligned} p_1 \sigma_1 &= \begin{pmatrix} p_{+-} & 0 \\ 0 & p_{-+} \end{pmatrix} \\ p_2 \sigma_2 &= \begin{pmatrix} p_{++} & 0 \\ 0 & p_{--} \end{pmatrix}, \end{aligned} \quad (20)$$

with $p_{+-} = |\langle\uparrow\downarrow|\psi\rangle|^2$ and similar definitions for p_{-+}, p_{++} and p_{--} . Similar expressions hold for τ_1 and τ_2 :

$$\begin{aligned} p_1 \tau_1 &= \begin{pmatrix} p_{-+} & 0 \\ 0 & p_{+-} \end{pmatrix} \\ p_2 \tau_2 &= \begin{pmatrix} p_{++} & 0 \\ 0 & p_{--} \end{pmatrix}. \end{aligned} \quad (21)$$

The mean entanglement can now be calculated using (13). The result is

$$\bar{\mathcal{E}} = 2p_{++}p_{--} + 2p_{+-}p_{-+}. \quad (22)$$

In the notation of the previous section this becomes

$$\bar{\mathcal{E}} = \frac{1}{2}(p_1 - p_2)^2 + \frac{1}{2}(p_3 - p_4)^2, \quad (23)$$

which is less than (17) by the term $-p_1 p_2 - p_3 p_4$.

8. The Jaynes–Cummings model

The Jaynes–Cummings model [17, 18] describes a two-level system interacting with a harmonic oscillator. The latter represents a single mode of the electromagnetic field in a cavity. The model has been studied extensively.

The Hamiltonian of the model reads

$$H = \hbar\omega a^\dagger a + \frac{1}{2}\hbar\omega_0 \sigma_z + \hbar\kappa(a^\dagger \sigma_- + a \sigma_+), \quad (24)$$

with a^\dagger and a creation and annihilation operators of the harmonic oscillator, and with the Pauli matrices σ_z and σ_\pm describing the two-level system.

Let $|g\rangle$ and $|e\rangle$ denote the ground state, respectively the excited state of the two-level system. Let $|n\rangle$, $n = 0, 1, \dots$ denote the eigenstates of the harmonic oscillator. The eigenstates of the Jaynes–Cummings Hamiltonian are explicitly known, see e.g. [19]. An orthonormal basis of eigenfunctions is given by

$$\begin{aligned}\psi_0 &= |g\rangle \otimes |0\rangle \\ \psi_{1,n} &= \cos(\theta_n)|g\rangle \otimes |n+1\rangle + \sin(\theta_n)|e\rangle \otimes |n\rangle \\ \psi_{2,n} &= -\sin(\theta_n)|g\rangle \otimes |n+1\rangle + \cos(\theta_n)|e\rangle \otimes |n\rangle.\end{aligned}\tag{25}$$

The angles θ_n , $n = 0, 1, 2, \dots$ follow from the relation

$$\tan \theta_n = \kappa \frac{\sqrt{n+1}}{\frac{1}{2}(\omega - \omega_0) + \lambda_n},\tag{26}$$

with

$$\lambda_n = \sqrt{\frac{1}{4}(\omega - \omega_0)^2 + \kappa^2(n+1)}.\tag{27}$$

The time dependence of the reduced density matrix can be calculated explicitly if the initial state is a product state with the two-level system in the excited state and the harmonic oscillator is in the n th eigenstate, see e.g. [19]. The result for the reduced state of the two-level system is

$$\rho_A(t) = W_n(t)|g\rangle\langle g| + (1 - W_n(t))|e\rangle\langle e|,\tag{28}$$

with

$$W_n(t) = 2\gamma_n \sin^2(t\kappa\sqrt{n+1}),\tag{29}$$

and with

$$\gamma_n = \frac{1}{2} \sin^2(2\theta_n).\tag{30}$$

The linear entanglement is therefore

$$\mathcal{E}_A(\psi_t) = 1 - W_n^2(t) - (1 - W_n(t))^2.\tag{31}$$

The time average equals

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = 2\gamma_n - 3\gamma_n^2.\tag{32}$$

It is straightforward to calculate the reduced density matrices for the eigenfunctions of the model. The result is

$$\sigma_0 = |0\rangle\langle 0|,\tag{33}$$

$$\sigma_{1,n} = \cos^2 \theta_n |n+1\rangle\langle n+1| + \sin^2 \theta_n |n\rangle\langle n|,\tag{34}$$

$$\sigma_{2,n} = \sin^2 \theta_n |n+1\rangle\langle n+1| + \cos^2 \theta_n |n\rangle\langle n|,\tag{35}$$

$$\tau_0 = |g\rangle\langle g|,\tag{36}$$

$$\tau_{1,n} = \cos^2 \theta_n |g\rangle\langle g| + \sin^2 \theta_n |e\rangle\langle e|,\tag{37}$$

$$\tau_{2,n} = \sin^2 \theta_n |g\rangle\langle g| + \cos^2 \theta_n |e\rangle\langle e|.\tag{38}$$

Hence, it is straightforward to evaluate the mean entanglement $\bar{\mathcal{E}}$ for an arbitrary wavefunction ψ . However, we did not succeed to rewrite the resulting expression in a simple and transparent way.

In the case that ψ is of the product form

$$\psi = |e\rangle \otimes |n\rangle = \sin(\theta_n)\psi_{1,n} + \cos(\theta_n)\psi_{2,n}, \tag{39}$$

one obtains

$$\begin{aligned} \sigma &= \sin^2(\theta_n)\sigma_{1,n} + \cos^2(\theta_n)\sigma_{2,n} \\ &= \gamma_n|n+1\rangle\langle n+1| + (1-\gamma_n)|n\rangle\langle n| \\ \tau &= \sin^2(\theta_n)\tau_{1,n} + \cos^2(\theta_n)\tau_{2,n} \\ &= \gamma_n|g\rangle\langle g| + (1-\gamma_n)|e\rangle\langle e| \\ \Delta &= 1 - \sin^4(\theta_n) \text{Tr}_B \tau_{1,n}^2 - \cos^4(\theta_n) \text{Tr}_B \tau_{2,n}^2 \\ &= 1 - (1-\gamma_n)^2. \end{aligned} \tag{40}$$

This leads to the result

$$\bar{\mathcal{E}} = 2\gamma_n - 3\gamma_n^2, \tag{41}$$

which is identical with the time-averaged result (32).

9. Discussion

The calculation of the time dependence of the entanglement of a quantum system is a hard problem. The average over time is more accessible because it can be replaced by an ensemble average. This is in particular so when the entanglement is defined using the linear entropy instead of the von Neumann entropy of the reduced density matrix, because in that case there exists a simple expression for the mean entanglement—see (13). We have used this expression in a two-spin system and in the Jaynes–Cummings model. For these systems it is feasible to calculate both the averages over time and over the ensemble of wavefunctions. The results of the two calculations coincide, as it should be.

We have pointed out that a systematic degeneracy of the energy levels of the Hamiltonian due to the presence of a symmetry influences the choice of the ensemble of wavefunctions, used in the calculation of the average entanglement. In the example of the two-spin system the additional symmetry leads to a reduction of the entanglement.

Finally, let us note that the use of the linear entropy is rather essential in our paper. It is of course possible as well to define the ensemble average of the entanglement, based on the von Neumann entropy. It is however unlikely that a simple formula like (13) exists in that case.

Appendix

Here, the proof of (13) is given. From definition (7) follows, assuming a linear entropy,

$$\bar{\mathcal{E}} = 1 - \langle \text{Tr}_A \rho_A^2(\chi) \rangle_\chi, \tag{A.1}$$

with $\rho_A(\chi)$ defined by

$$\begin{aligned} \text{Tr}_A \rho_A(\chi) X &= \left\langle \sum_m \sqrt{p_m} e^{i\chi_m} \psi_m \left| X \otimes \mathbb{I} \right| \sum_n \sqrt{p_n} e^{i\chi_n} \psi_n \right\rangle \\ &= \sum_{mn} \sqrt{p_m p_n} e^{-i(\chi_m - \chi_n)} \text{Tr}_A \sigma_{mn} X, \end{aligned} \tag{A.2}$$

with σ_{mn} defined by

$$\mathrm{Tr}_A \sigma_{mn} X = \langle \psi_m | X \otimes \mathbb{I} | \psi_n \rangle. \quad (\text{A.3})$$

Hence, one obtains

$$\begin{aligned} \bar{\mathcal{E}} &= 1 - \left\langle \mathrm{Tr}_A \left(\sum_{mn} \sqrt{p_m p_n} e^{-i(\chi_m - \chi_n)} \sigma_{mn} \right)^2 \right\rangle_X \\ &= 1 - \sum_{mn} \sum_{rs} \sqrt{p_m p_n p_r p_s} \langle e^{-i(\chi_m - \chi_n)} e^{-i(\chi_r - \chi_s)} \rangle_X \mathrm{Tr}_A \sigma_{mn} \sigma_{rs} \\ &= 1 - \sum_{mn} p_m p_n \mathrm{Tr}_A \sigma_{mm} \sigma_{nn} - \sum_{mn} p_m p_n \mathrm{Tr}_A \sigma_{mn} \sigma_{nm} \\ &\quad + \sum_m p_m^2 \mathrm{Tr}_A \sigma_{mm}^2. \end{aligned} \quad (\text{A.4})$$

Now use that $\sigma_{mm} \equiv \sigma_m$ to see that the first two terms yield the contribution $S_1(\sigma)$. The last term is $1 - \Delta$. Hence, it remains to be shown that

$$S_1(\tau) = 1 - \sum_{mn} p_m p_n \mathrm{Tr}_A \sigma_{mn} \sigma_{nm}. \quad (\text{A.5})$$

Choose an orthonormal basis u_r for the subsystem A and an orthonormal basis v_p for the subsystem B. Then one has

$$\sigma_{mn} = \sum_{rsp} [\langle \psi_m | u_s \otimes v_p \rangle \langle u_r \otimes v_p | \psi_n \rangle] |r\rangle \langle s|, \quad (\text{A.6})$$

so that

$$\begin{aligned} \mathrm{Tr}_A \sigma_{mn} \sigma_{nm} &= \sum_{rspq} \langle \psi_m | u_s \otimes v_p \rangle \langle u_r \otimes v_p | \psi_n \rangle \langle \psi_n | u_r \otimes v_q \rangle \langle u_s \otimes v_q | \psi_m \rangle \\ &= \sum_{pq} \langle \psi_m | (\mathbb{I} \otimes |v_p\rangle \langle v_q|) | \psi_m \rangle \langle \psi_n | (\mathbb{I} \otimes |v_q\rangle \langle v_p|) | \psi_n \rangle \\ &= \sum_{pq} \langle v_q | \tau_m | v_p \rangle \langle v_p | \tau_n | v_q \rangle \\ &= \mathrm{Tr}_B \tau_m \tau_n. \end{aligned} \quad (\text{A.7})$$

Relation (A.5) now follows readily.

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