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Stability of PPT in equilibrium states

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Abstract

We use simple spectral perturbation theory to show that the positive partial transpose property is stable under bounded perturbations of the Hamiltonian, for equilibrium states in infinite dimensions. The result holds provided the temperature is high enough, or equivalently, provided the perturbation is small enough.

Key words: entanglement, thermal equilibrium, positive partial transpose, Peres–Horodecki criterion, Dyson series expansion

1. Introduction

The positive partial transposition (PPT), or Peres–Horodecki criterion, gives a necessary condition for a density matrix ρ of a bipartite quantum system SB ("system-bath") to be separable. Namely, if ρ is separable, then the partial transpose (relative to either subsystem, say B), $T_\mathrm{B}[\rho]$ is a positive operator [1, 2]. Equivalently, if ρ is not PPT, then it must be inseparable, also called entangled. If the dimension of the subsystem Hilbert spaces are two or three, then the converse statement is also correct [2]. However, in dimension $\geqslant 4$, there are states, which are PPT and yet entangled [3]. In this situation, the entanglement is called bound. It is called so since one cannot extract from such a state, pure singlet (entangled) states, which would be needed as a resource for quantum information purposes. In contrast, if it is possible to extract (by LOCC protocols) from an entangled mixed state (or many copies thereof), pairs of particles in a pure singlet state, then the mixed state is said to have "distillable" entanglement [4]. The corresponding state is said to be distillable. It is shown in ref. [5] (for finite-dimensional systems) that if a state is PPT, then it is not distillable. The converse is not true in dimension 3 or higher, though. Any possible entanglement in a PPT state is bound. For qubits (dimension 2), it was shown in ref. [6] that any entangled state is distillable. However, in higher dimensions, there are entangled states with bound entanglement, as shown in ref. [7].

A great feature of the PPT criterion is that in principle, it is easy to apply. To verify that a given density matrix ρ of a bipartite system is entangled, one "simply" has to check that the partial transpose $T_\mathrm{B}[\rho]$ is not a positive operator. We are addressing the following question here:

Suppose a density matrix ρ_0 is PPT, and consider a modified density matrix $\rho = \rho_0 + \rho'$, where ρ' is a perturbation operator. Under what conditions is ρ still PPT?

To investigate the question, we first note that since ρ is hermitian (= self-adjoint), then so is $T_\mathrm{B}[\rho]$ (see also eq. (26) below). Thus, $T_\mathrm{B}[\rho] \geqslant 0$ if and only if all the eigenvalues of $T_\mathrm{B}[\rho]$ are non-negative. The partial trace is a linear operation, $T_\mathrm{B}[\rho] = T_\mathrm{B}[\rho_0] + T_\mathrm{B}[\rho']$. Basic perturbation theory [8] tells us that the eigenvalues of $T_\mathrm{B}[\rho]$ lie within a neighbourhood of the size $\|T_\mathrm{B}[\rho']\|_\infty$ (operator norm of the perturbation) of the eigenvalues of $T_\mathrm{B}[\rho_0]$. Since ρ_0 is PPT, we know that $T_\mathrm{B}[\rho_0] \geqslant 0$. If $T_\mathrm{B}[\rho_0]$ has a lowest eigenvalue $\lambda_0 > 0$, then for $\|T_\mathrm{B}[\rho']\|_\infty < \lambda_0$, the spectrum of $T_\mathrm{B}[\rho]$ is guaranteed to be $\geqslant 0$, which means that ρ is PPT.

This straightforward approach breaks down as soon as the dimension is infinite. The reason is that ρ_0 and hence $T_\mathrm{B}[\rho_0]$ are Hilbert–Schmidt operators (c.f. eq. (25)). In particular, $T_\mathrm{B}[\rho_0]$ is a compact operator and therefore, in the infinite-dimensional case, its eigenvalues must accumulate at the origin. Consequently, no matter how small we take $\|T_\mathrm{B}[\rho']\|_\infty$, the simple argument given above does not work.

We show in this paper how one can modify the simple perturbation argument for equilibrium states, where the perturbation is a bounded interaction term V in the Hamiltonian,

$$\rho_0 = \frac{e^{-\beta H_0}}{\mathrm{Tr} e^{-\beta H_0}}, \quad \rho = \frac{e^{-\beta(H_0+V)}}{\mathrm{Tr} e^{-\beta(H_0+V)}} \tag{1}$$

with

$$H_0 = H_\mathrm{A} \otimes \mathbb{1}_\mathrm{B} + \mathbb{1}_\mathrm{A} \otimes H_\mathrm{B}$$

Thermal states form the cornerstone of equilibrium statistical mechanics. Examining their quantum properties, one of which is measured by entanglement, is an important question. That said, the equilibrium setup eq. (1) is mathematically quite general. Indeed, any faithful density matrix[1] ρ_0 can be written in the form $\rho_0 = e^{-H_0}/\mathrm{Tr} e^{-H_0}$ for some Hermitian (self-adjoint) H_0, and similarly for ρ. Our approach is applica-

[1] A density matrix is called faithful if zero is not one of its eigenvalues.

ble to any such ρ_0 and ρ. In this work, we express the perturbation $\rho_0 \mapsto \rho$ as an interaction term V in the Hamiltonian because this is physically intuitive. Our main idea is to use the Dyson expansion to write

$$e^{-\beta(H_0+V)} = e^{-\beta H_0/2}\,[\mathbb{1} + \mathcal{O}(V)]\,e^{-\beta H_0/2} \tag{2}$$

where $\mathcal{O}(V)$ is an operator that vanishes for $V = 0$. PPT for ρ will then follow provided $T_B[\mathcal{O}(V)]$ is small enough such that

$$\mathbb{1} + T_B[\mathcal{O}(V)] \geq 0$$

By factoring out the operators $e^{-\beta H_0/2}$ in eq. (2), we remove the problem of eigenvalues accumulating at the origin, as the unperturbed density matrix is effectively replaced by the operator $\mathbb{1}$ now, whose spectrum $\{1\}$ is separated from the origin. The detailed control of $\mathcal{O}(V)$ leading to the wanted bounds involves the size of V as well as the inverse temperature β. We assume a bound on the Hilbert–Schmidt norm of the imaginary time-evolved interaction operator. Namely, we assume that there are constants a, b, and $s_* > 0$ such that for all $0 \leq s \leq s_*$, we have the bound

$$\| e^{-sH_0} V e^{sH_0} \|_2 \leq a e^{bs}$$

We then show in Theorem 2.2 that for large enough temperature $\beta \leq \max\{\beta_*, s_*\}$, the perturbed state ρ is PPT. The upper bound β_* on β depends on the constants a and b. If a is small (say V contains an overall small coupling constant) then $\beta_* \sim \ln(1/a)$. So the smaller a is, the larger we can take β (the smaller we can take the actual temperature T=$1/\beta$) for the result to hold. Conversely, if the coupling V is not small (a sizeable), then the temperature has to be higher for the validity of our derivation.

Literature. The question of separability of thermal equilibrium states has a rich history. Entanglement is a measure for the degree of their "quantumness". Intuitively, it is expected that a quantum to classical transition happens at high temperature T, that is, entanglement disappears for large T. From a quantum information point of view, this means that only cool enough materials may be used as a quantum resource.

Many works deal with spin (qubit) chains in equilibrium. They analyze how two-qubit entanglement along the chain depends on various parameters [9–18], in particular finding temperature bounds which guarantee entanglement or separability. In this situation, one can conveniently use concurrence to quanitfy entanglement. An analysis for two spins of arbitrary length (where concurrence cannot be used as an entanglement measure) was carried out in ref. [19]. In that work, the validity of the PPT criterion was linked to properties of the spin correlators. More generally, it was shown in refs. [20, 21] that for finite-dimensional systems, thermal states with respect to *any* Hamiltonian are separable at high enough temperature $T \geqslant T_c$, for some critical T_c, and that any interval $I \subset (0, T_c)$ contains a T' such that the equilibrium state at temperature T' is entangled. A general topological argument, which again works for finite-dimensional systems, was presented in ref. [22]. Then the equilibrium density matrix at infinite temperature $T \to \infty$ is proportional to the identity matrix, which is a product state (under any bi-partition of the total system), and it is contained in a "ball" (topological neighbourhood) of separable states. As the equilibrium density matrix depends continuously on the inverse temperature $\beta = 1/T$, the infinite temperature density matrix cannot be transformed into an entangled density matrix by an infinitesimal change of β away from $\beta = 0$. Hence, there must be a critical temperature T_c so that for $T > T_c$, the state is separable.

In all the works above, entanglement between finite-dimensional systems is studied. The advantage of our method is that it is very simple and works in infinite dimensions. However, we only show that the PPT property holds at high enough temperatures, and this gives only partial information on the entanglement. Namely, we do not settle the question of bound entanglement; our results presented here does not show whether there exists entanglement in the regime where PPT is satisfied. In this sense, our results are more modest than many of the ones cited above. The presence of bound entanglement in thermal spin states (finite dimensions) was derived in refs. [23, 24]. The authors of ref. [25] consider the thermal states of a closed chain of harmonic oscillators and find an explicit expression for the logartihmic negativity. This allows them to discuss entanglement properties for this specific infinite-dimensional system. Based on this work, the existence of bound entanglement in the same system was shown in ref. [26]. A more general approach exhibiting bound entanglement for infinite-dimensional systems would be valuable.

Finally, it is interesting to note that there are models where entanglement survives "at all temperatures". This was shown to hold for a mirror in thermal equilibrium interacting with an electromagnetic field mode in a coherent state [27].

2. PPT criterion and main result

We start out by defining the notions involved in the PPT criterion and state that criterion below in Theorem 2.2.

Let $\mathcal{H}$ be a separable Hilbert space, $dim\mathcal{H} \leq \infty$. Our main focus will be on the infinite-dimensional case (but our results are valid also in finite dimensions, of course). The norm of a vector $|\psi\rangle \in \mathcal{H}$ is given by $\| \,|\psi\rangle\, \| = \sqrt{\langle\psi|\psi\rangle}$, where $\langle\cdot|\cdot\rangle$ is the inner product of $\mathcal{H}$. Let $\mathcal{B}(\mathcal{H})$ denote the set of all bounded linear operators on $\mathcal{H}$. We use the following three norms of operators $X \in \mathcal{B}(\mathcal{H})$:

$$\| X\|_\infty = \sup_{|\psi\rangle\in\mathcal{H}, \||\psi\rangle\|=1} \| X|\psi\rangle \|, \;\; \| X \|_2 = \left(\mathrm{Tr}\,|X|^2\right)^{1/2}, \;\; \| X\|_1 = \mathrm{Tr}|X|$$

where $|X| = \sqrt{X^\dagger X}$ and $X^\dagger$ denotes the adjoint of X. The norms are also called the operator norm ($\|X\|_\infty$), the Hilbert–Schmidt norm ($\|X\|_2$) and the trace norm ($\|X\|_1$). The inequalities $\|X\|_\infty \leq \|X\|_j$, $j = 1$ and 2 are well known. We denote by $\mathcal{T}_2(\mathcal{H})$ all bounded operators X such that $\|X\|_2 < \infty$. These are called the Hilbert–Schmidt operators. $\mathcal{T}_2(\mathcal{H})$ is Hilbert space when equipped with the inner product $\langle X, Y\rangle = \mathrm{Tr}(X^\dagger Y)$. The collection of all trace class operators in $\mathcal{H}$ (operators with finite trace norm) is denoted by $\mathcal{T}_1(\mathcal{H})$. It is a Banach space under the trace norm. Hilbert–Schmidt and trace class operators are compact operators.

Let $\{|e_n\rangle\}_{n\geqslant 1}$ be a fixed orthonormal basis of $\mathcal{H}$, and let $X \in \mathcal{B}(\mathcal{H})$. We define a new operator $T[X] \in \mathcal{B}(\mathcal{H})$ by the relation

$$\langle e_m|T[X]e_n\rangle = \langle e_n|Xe_m\rangle$$

The new operator $T[X]$ is called the *transpose of* X. Of course, $T[X]$ depends on the choice of the basis $\{|e_n\rangle\}_{n\geqslant 1}$. One can show that $\|T[X]\|_\infty = \|X\|_\infty$, so T is a linear isometry on $\mathcal{B}(\mathcal{H})$ and moreover, $T^2 = \mathbb{1}$.

An operator $X \in \mathcal{B}(\mathcal{H})$ is said to be *positive*, written $X \geqslant 0$, if $\langle\psi|X\psi\rangle \geqslant 0$ for all $|\psi\rangle \in \mathcal{H}$. We have the following equivalence: $X \geqslant 0$ if and only if $X = X^\dagger$ and the spectrum of X satisfies spec(X)$\subset[0, \infty)$. A *density matrix* is an operator $\rho \in \mathcal{T}_1(\mathcal{H})$ such that $\rho \geqslant 0$ and $\mathrm{Tr}\rho = 1$.

Composite quantum systems are described by tensor products of Hilbert spaces. Let $\mathcal{H}_\mathrm{A}$ and $\mathcal{H}_\mathrm{B}$ be two separable Hilbert spaces and set

$$\mathcal{H}_\mathrm{AB} = \mathcal{H}_\mathrm{A} \otimes \mathcal{H}_\mathrm{B}$$

We say that a density matrix ρ on the bipartite Hilbert space $\mathcal{H}_\mathrm{AB}$ is *separable* if it can be approximated in trace norm by a convex combination of product states [28, 29].[2] That is, ρ is separable if for $n \in \mathbb{N}$, there are density matrices ρ_n^A and ρ_n^B on $\mathcal{H}_\mathrm{A}$ and $\mathcal{H}_\mathrm{B}$, respectively, and probabilities $0 \leq p_n \leq 1$ and $\sum_{n\geqslant 1} p_n = 1$, such that

$$\rho = \sum_{n\geq 1} p_n\, \rho_n^\mathrm{A} \otimes \rho_n^\mathrm{B} \tag{3}$$

where the series converges in the $\|\cdot\|_1$ norm of $\mathcal{B}(\mathcal{H}_\mathrm{AB})$. If ρ is not separable, then it is called *entangled*. Equivalently, the term inseparable is used in ref. [5]. An extraordinarily useful criterion to check that a state is entangled is the PPT criterion, given in Theorem 2.1 below. Before stating it, we define the notion of partial transposition.

The *partial transposition* is the operation $\mathbb{1} \otimes T$ acting on $\mathcal{B}(\mathcal{H}_\mathrm{AB}) = \mathcal{B}(\mathcal{H}_\mathrm{A}) \otimes \mathcal{B}(\mathcal{H}_\mathrm{B})$, where T is the transposition operator on $\mathcal{B}(\mathcal{H}_\mathrm{B})$, relative to a fixed basis of $\mathcal{H}_\mathrm{B}$, as introduced above. For $X \in \mathcal{B}(\mathcal{H}_\mathrm{AB})$, the operator $(\mathbb{1} \otimes T)X$ is called the *partial transpose* of X, also denoted by

$$T_\mathrm{B}[X] = (\mathbb{1} \otimes T)X$$

A density matrix ρ on $\mathcal{H}_\mathrm{A} \otimes \mathcal{H}_\mathrm{B}$ satisfying $T_\mathrm{B}[\rho] \geqslant 0$ is said to be PPT. The following result is the famous PPT, or Peres–Horodecki criterion for separability, which originated in refs. [1, 2].

Theorem 2.1 (PPT criterion) Let ρ be a density matrix on the bipartite Hilbert space $\mathcal{H} = \mathcal{H}_\mathrm{A} \otimes \mathcal{H}_\mathrm{B}$. If ρ is separable, then ρ is PPT.

[2] The word “separable” is used for states and, in a different context, for Hilbert spaces—a separable Hilbert space is one that has a countable orthonormal basis. In the original paper [28], separable states are called *classically correlated* states.

As discussed in the introduction, deriving the PPT property using perturbation theory is not immediate, in the infinite-dimensional setting. However, for perturbations stemming from an interaction term in the Hamiltonian of an uncoupled bipartite equilibrium state, one can still use simple perturbation theory to infer the PPT property. Let the Hamiltonian of a bipartite system, with Hilbert space $\mathcal{H}_\mathrm{A} \otimes \mathcal{H}_\mathrm{B}$, be given by

$$H_\mathrm{AB} = H_0 + V \tag{4}$$

$$H_0 = H_\mathrm{A} + H_\mathrm{B} \tag{5}$$

where $H_\mathrm{A} \equiv H_\mathrm{A} \otimes \mathbb{1}_\mathrm{B}$ and $H_\mathrm{B} \equiv \mathbb{1}_\mathrm{A} \otimes H_\mathrm{B}$ are individual (hermitian) Hamiltonians and V is a hermitian interaction operator. It is assumed that for $\beta > 0$,[3]

$$\mathrm{Tr}_\mathrm{AB}\, e^{-\beta H_0} < \infty, \quad \mathrm{Tr}_\mathrm{AB}\, e^{-\beta H_\mathrm{AB}} < \infty \tag{6}$$

The equilibrium state at inverse temperature β is the Gibbs state with density matrix

$$\rho_\beta = \frac{e^{-\beta H_\mathrm{AB}}}{\mathrm{Tr}\, e^{-\beta H_\mathrm{AB}}} \tag{7}$$

To carry out a rigorous proof, we make the following assumption: There are constants $s_* > 0$ and $a, b \geqslant 0$ such that for $0 \leq s \leq s_*$,

$$\|\, e^{-sH_0} V e^{sH_0} \|_2 \leq a e^{bs} \tag{8}$$

Our main result is

Theorem 2.2 Suppose β is small enough,

$$0 < \beta \leq \max\{s_*, \beta_*\}, \quad \text{where} \quad \beta_* \equiv \frac{2}{b}\ln\left[1 + \frac{b}{a}\frac{\ln 2}{2}\right] \tag{9}$$

Then the equilibrium state ρ_β, eq. (7), is PPT.

The theorem says that if the temperature $1/\beta$ is large enough, then the coupled equilibrium state ρ_β is PPT.

Discussion of Theorem 2.2

(D1) Weak coupling versus low temperature. In the case where the interaction operator carries an overall coupling constant λ, that is $H = H_0 + \lambda V$, the constant a in eq. (8) is multiplied by $|\lambda|$. So the upper bound β_* in Theorem 2.2 is

$$\beta_* = \frac{2}{b}\ln\left[1 + \frac{1}{|\lambda|}\frac{b}{a}\frac{\ln 2}{2}\right]$$

[3] If $dim\mathcal{H}_\mathrm{A,B} < \infty$, then eq. (6) is automatically true. If $dim\mathcal{H}_\mathrm{AB} = \infty$, then $\mathrm{Tr}\, e^{-\beta H} < \infty$ (for $H = H_0$ or $H = H_{AB}$) is the same as saying that all the eigenvalues $\lambda_n > 0$ of $e^{-\beta H}$ are finitely degenerate and satisfy $\sum_n \lambda_n < \infty$; in particular, $\lambda_n \to 0$ as $n \to \infty$. Modulo a global additive shift, the energy spectrum of H is given by $E_n = -\frac{1}{\beta}\ln(\lambda_n)$, and so $E_n \to \infty$, that is, H must be unbounded.

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For fixed a, b we have $\beta_* \sim \ln|\lambda|^{-1}$ for small λ. This means that taking low enough temperatures (β large enough) is equivalent to taking the coupling λ small, for the condition of Theorem 2.2 to hold.

(D2) Examples for the validity of eq. (8)

(*i*) If $dim\mathcal{H}_\mathrm{A}$, $dim\mathcal{H}_\mathrm{B} < \infty$, then we can take $a = \|V\|_2$ and $b = \|H_0\|_\infty$. (Note, by a simple translation in energy, which does not affect the equilibrium state, we can always assume that $H_0 \geqslant 0$.) As a concrete example, we consider two interacting qubits A and B, with

$$H_\mathrm{A} = \frac{1}{2}\omega_\mathrm{A}\sigma_z,\ \ H_\mathrm{B} = \frac{1}{2}\omega_\mathrm{B}\sigma_z,\ \ V = \lambda\sigma_x \otimes \sigma_x$$

where $\omega_\mathrm{A}, \omega_\mathrm{B} > 0$ and $\lambda \in \mathbb{R}$ are constants and σ_x, σ_z are Pauli matrices, with $\sigma_x = |-\rangle\langle+|+|+\rangle\langle-|$. Then,

$$e^{-sH_0}Ve^{sH_0} = \lambda\left(e^{-s\omega_\mathrm{A}}|+\rangle\langle-| + e^{s\omega_\mathrm{A}}|-\rangle\langle+|\right) \otimes \left(e^{-s\omega_\mathrm{B}}|+\rangle\langle-| + e^{s\omega_\mathrm{B}}|-\rangle\langle+|\right)$$

and one calculates

$$\|\,e^{-sH_0}Ve^{sH_0}\|_2 = 2\lambda\sqrt{\cosh(2s\omega_\mathrm{A})\cosh(2s\omega_\mathrm{B})} \leq 2\lambda e^{s(\omega_\mathrm{A}+\omega_\mathrm{B})}$$

Thus, eq. (8) is satisfied for all $s \geqslant 0$ with $a = 2\lambda$ and $b = \omega_\mathrm{A} + \omega_\mathrm{B}$.

(*ii*) Denote the energy spectrum of H_0 by E_j, $j \geqslant 1$ (labelled in increasing order). We consider interaction operators V having the following property: Starting from any E_j, V only makes transitions to finitely many levels $E_{j\pm\ell}$, where $\ell \in \{0, 1, \ldots, L_j\}$ for some $L_j \geqslant 0$. Written in matrix form, V is then a matrix whose non-zero entries on row j lie within a neighbourhood of size L_j around the diagonal entry,

$$V = \begin{pmatrix} *\,*\,* & & & & & \\ \ *\,*\,*\,* & & & & & \\ \ \ *\,* & & & & & \\ \ *\,*\,*\,* & & & & & \\ & & \ddots & & & \\ & & * \ \ *\,* & & & \\ & & & *\,*\,* \ \ * & & \\ & & & & \ddots & \end{pmatrix} \tag{10}$$

In other words,

$$V = \sum_{j\geq 1}\sum_{\ell=1}^{L_j} V_{j,j+\ell}\,|\phi_j\rangle\langle\phi_{j+\ell}| + \mathrm{h.c.} \tag{11}$$

where $V_{j,k} = \langle\phi_j|V\phi_k\rangle$. Then one easily sees that

$$\|\,e^{-sH_0}Ve^{sH_0}\|_2 \leq 2\sum_{j\geq 1}\sum_{\ell=1}^{L_j} e^{|s||E_j - E_{j+\ell}|}|V_{j,j+\ell}|$$

So, we have the bound eq. (8) for all $s \geqslant 0$, with

$$a = 2\sum_{j\geq 1}\sum_{\ell=1}^{L_j}|V_{j,j+\ell}|, \quad b = \sup_{j\geq 1}\max_{1\leq\ell\leq L_j}|E_j - E_{j+\ell}| \tag{12}$$

For a to be finite, we need $V_{j,\,j+\ell} \to 0$ with increasing j, meaning that the interaction has a high energy cut-off. This is a physically reasonable condition.

As an explicit example, we consider the Jaynes–Cummings type Hamiltonian describing an atom (two level system) interacting with a radiation mode (harmonic oscillator), described by the Hamiltonian

$$H_\mathrm{A} = \omega\sigma_z,\ \ H_\mathrm{B} = \Omega a^\dagger a,\ \ V = \chi_E\left(\sigma_+ \otimes a + \sigma_- \otimes a^\dagger\right)\chi_E \tag{13}$$

Here, ω, $\Omega > 0$, and $\sigma_\pm$ are the raising and lowering operators of the atom. The χ_E is an energy cut-off, namely, the projection operator onto the eigenspace of $H_0 = H_\mathrm{A} + H_\mathrm{B}$ associated to eigenvalues $\leq E$, where $E > 0$ is any fixed number. Consider for simplicity of the presentation that $\omega < \frac{1}{2}\Omega$. Then, the eigenvalues of H_0, denoted in increasing order as $E_1 < E_2 < E_3 < \cdots$, are given by $E_{2n} = (n-1)\Omega + \omega$ and $E_{2n+1} = n\Omega - \omega$. The associated eigenvectors are $|\psi_{2n}\rangle = |+, n-1\rangle$ and $|\psi_{2n+1}\rangle = |-, n\rangle$, where $\pm$ in the ket refers to the ground and excited state of the atom and n in the ket refers to the level of excitation of the oscillator. One readily checks that the interaction operator V can only make transitions $E_k \to E_\ell$ with $|k - \ell| \leq 2$. In other words, $L_j = 2$ in the above language. As the interaction operator V is essentially proportional to the square root of the oscillator number operator, we have $|V_{j,j+\ell}| \leq 2\sqrt{j+\ell}$. Using this in eq. (12) yields the bounds $a \leq 8\sum_{j=1}^{J_E}\sqrt{j+2}$ and $b \leq \Omega$, where J_E is the largest integer satisfying $E_{J_E} \leq E$. It is interesting to note that for the Jaynes–Cummings model eq. (13) *without* the cut-off χ_E, the equilibrium state is not separable for *any* (non-zero) temperature, as was shown in ref. [30].

(*iii*) A popular open system is an oscillator (system a, $a^\dagger$) interacting with N other oscillators (bath b_j, $b_j^\dagger$) through the Hamiltonian

$$H' = H_0 + \sum_{j=1}^{N}\left(g_j a^\dagger b_j + \mathrm{h.c.}\right), \quad H_0 = \omega_0 a^\dagger a + \sum_{j=1}^{N}\omega_j b_j^\dagger b_j \tag{14}$$

where ω_0, $\omega_j > 0$, and the $g_j \in \mathbb{C}$ are coupling coefficients. A related model is the *spin Boson* model (with finitely many oscillators) and its generalizations, in which the system oscillator is replaced by a finite L-level system. Our method applies to that model as well. The interaction in eq. (14) is not a bounded operator, so Theorem 2.2 does not apply without modifications.

One way to make the interaction bounded is to exclude processes involving energies beyond some cut-off $\Omega > 0$. This amounts to setting

$$V = \chi_{H_0\leq\Omega}\left(\sum_{j=1}^{N} g_j a^\dagger b_j + \mathrm{h.c.}\right)\chi_{H_0\leq\Omega} \tag{15}$$

where $\chi_{H_0\le\Omega}$ is the spectral projection of H_0 onto the eigenspaces with spectral values contained in the interval [0, Ω]. We then consider the Hamiltonian

$$H = H_0 + V$$

where H_0 and V are given in eqs. (14) and (15), respectively. We show in Section 3.2 that

$$\| e^{-sH_0} V e^{sH_0} \|_2 \le 2 \| g\|_2 \sqrt{N} (\Omega/\omega_{\min} + 1)^{(N+3)/2} e^{|s|\Delta\omega} \tag{16}$$

where

$$\omega_{\min} = \min_{0\le j\le N} \omega_j, \quad \Delta\omega = \max_{1\le j\le N} |\omega_0 - \omega_j|, \quad \| g \|_2 = \left(\sum_{j=1}^{N} |g_j|^2\right)^{1/2}$$

The condition eq. (8) holds with

$$a = 2 \| g\|_2 \sqrt{N} (\Omega/\omega_{\min} + 1)^{(N+3)/2}, \quad b = \Delta\omega$$

The presence of low-lying modes ($\omega_{\min}$ small) increases the value of a, and hence diminishes β_*, eq. (9). This means that if some of the oscillators have low frequencies, then the temperature $1/\beta$ must be chosen large in order for Theorem 2.2 to hold.

3. Proofs

3.1. Proof of Theorem 2.2

Using the Dyson series, we have

$$e^{-\beta H_{AB}} = [\mathbb{1} + D(\beta)]\, e^{-\beta H_0} \tag{17}$$

with

$$D(\beta) = \sum_{n\ge1} \int_0^\beta ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\; V(s_n) \cdots V(s_2) V(s_1) \tag{18}$$

and where

$$V(s) = e^{-sH_0} V e^{sH_0} \tag{19}$$

Under the condition eq. (8), the series eq. (18) converges in the Hilbert–Schmidt norm and

$$\begin{aligned}\| D(\beta) \|_2 &\le \sum_{n\ge1} a^n \int_0^\beta ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\; e^{b(s_1+\ldots+s_n)} \\ &= \sum_{n\ge1} \frac{a^n}{n!} \left[\int_0^\beta e^{bs} ds\right]^n = \exp\left[a \frac{e^{\beta b}-1}{b}\right] - 1\end{aligned} \tag{20}$$

We use eq. (17) to arrive at

$$\begin{aligned} e^{-\beta H_{AB}} &= \left[e^{-\beta H_{AB}/2}\right]^\dagger e^{-\beta H_{AB}/2} \\ &= e^{-\beta H_0/2} \left[\mathbb{1} + D(\beta/2)^\dagger\right] [\mathbb{1} + D(\beta/2)]\, e^{-\beta H_0/2} \\ &= e^{-\beta H_0/2} [\mathbb{1} + F(\beta)]\, e^{-\beta H_0/2} \end{aligned} \tag{21}$$

where

$$F(\beta) = D(\beta/2)^\dagger + D(\beta/2) + D(\beta/2)^\dagger D(\beta/2) \tag{22}$$

For any Hilbert–Schmidt operator X, we have

$$\| X^\dagger \|_2 = \| X \|_2 \quad \text{and} \quad \| X^\dagger X \|_2 \le \| X \|_2 \| X \|_\infty \le \| X \|_2^2$$

Hence, it follows from eqs. (20) and (22) that

$$\| F(\beta) \|_2 \le \| D(\beta/2) \|_2 (2 + \| D(\beta/2) \|_2) \le \exp\left[2a \frac{e^{\beta b/2}-1}{b}\right] - 1 \tag{23}$$

Denote by T_B the linear operator acting on operators of $\mathcal{H}_{AB}$, which takes the partial transpose of the system B. More precisely, let $|e_k\rangle$ and $|f_\ell\rangle$ be orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, and let X be a bounded linear operator acting on $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. Then, $T_B[X]$ is the linear operator on $\mathcal{H}_{AB}$, defined by its matrix elements

$$\langle e_k \otimes f_\ell | T_B[X] | e_m \otimes f_n \rangle = \langle e_k \otimes f_n | X | e_m \otimes f_\ell \rangle \tag{24}$$

The map T_B depends on the choice of the basis of $\mathcal{H}_B$—which we consider to be arbitrary, but fixed. The map T_B generally does not preserve the $\| \cdot \|_\infty$ norm of operators, but it leaves the Hilbert–Schmidt norm invariant,[4]

$$\| T_B[X] \|_2 = \| X \|_2, \quad X \in \mathcal{T}_2(\mathcal{H}_{AB}) \tag{25}$$

Moreover, we have

$$(T_B[X])^\dagger = T_B\left[X^\dagger\right] \tag{26}$$

So, if X is hermitian, then so is $T_B[X]$ and vice versa.

Let X_A, Y_A and X_B, Y_B be operators on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and let Z be an operator on $\mathcal{H}_{AB}$. Then, one readily sees that

$$T_B[(X_A \otimes X_B) Z (Y_A \otimes Y_B)] = (X_A \otimes T[Y_B])\, T_B[Z]\, (Y_A \otimes T[X_B])$$

where $T[\,\cdot\,]$ is the transpose in the given, fixed basis of $\mathcal{H}_B$. As $e^{-\beta H_0} = e^{-\beta H_A} \otimes e^{-\beta H_B}$, one obtains by applying T_B to eq. (21) that

$$\begin{aligned} T_B\left[e^{-\beta H_{AB}}\right] = &\left\{e^{-\beta H_A/2} \otimes T\left[e^{-\beta H_B/2}\right]\right\} T_B[\mathbb{1} + F(\beta)] \\ &\times \left\{e^{-\beta H_A/2} \otimes T\left[e^{-\beta H_B/2}\right]\right\} \end{aligned} \tag{27}$$

The operator $e^{-\beta H_A/2} \otimes T\left[e^{-\beta H_B/2}\right]$ is positive and invertible, and it follows from eq. (27) that[5]

$$T_B\left[e^{-\beta H_{AB}}\right] \ge 0 \iff T_B[\mathbb{1} + F(\beta)] \ge 0 \tag{28}$$

[4] To see that eq. (25) holds, one notices that T_B is (hermitian) self-adjoint with respect to the inner product of $\mathcal{T}_2(\mathcal{H}_{AB})$, namely for all $X, Y \in \mathcal{T}_2(\mathcal{H}_{AB})$, we have $\langle T_B[X]|Y\rangle = \langle X|T_B[Y]\rangle$. Then, eq. (25) follows by expressing the norm via the inner product and using that $T_B[T_B[X]] = X$.

[5] The implication $\Longleftarrow$ in eq. (28) is immediate by eq. (27). In infinite dimensions, $\Longrightarrow$ needs to be shown with some care, since even though $Q \equiv e^{-\beta H_A} \otimes T\left[e^{-\beta H_B}\right]$ is a positive and bounded operator, its inverse, $Q^{-1} \equiv e^{\beta H_A} \otimes T\left[e^{\beta H_B}\right]$ is an *unbounded* operator.

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Next, $T_B[\mathbb{1} + F(\beta)] = \mathbb{1} + T_B[F(\beta)]$. As $T_B[F(\beta)]$ is hermitian, the spectrum of $\mathbb{1} + T_B[F(\beta)]$ is real and we have the bound

$$T_B[\mathbb{1} + F(\beta)] \geq \mathbb{1} - \| T_B[F(\beta)] \|_\infty \geq \mathbb{1} - \| T_B[F(\beta)] \|_2 = \mathbb{1} - \| F(\beta) \|_2 \quad (29)$$

Combining this with eq. (23), we obtain

$$T_B[\mathbb{1} + F(\beta)] \geq 2 - \exp\left[2a\frac{e^{\beta b/2} - 1}{b}\right] \quad (30)$$

The right hand side is $\geqslant 0$ provided

$$\beta \leq \frac{2}{b}\ln\left[1 + \frac{b}{a}\frac{\ln 2}{2}\right] \quad (31)$$

It follows that under the condition eq. (31), the operator $T_B\left[e^{-\beta H_{AB}}\right]$ is positive. This completes the proof of Theorem 2.2. □

3.2. Proof of eq. (16)

The eigenvectors of H_0 are $|\mathbf{n}\rangle \equiv |n_0, n_1, \ldots, n_N\rangle$, where $\mathbf{n} = (n_0, n_1, \ldots, n_N)$ and $n_0, n_j \in \mathbb{N}$ are the occupation or excitation numbers of the oscillators. The associated eigenvalues are

$$E(n) = \omega_0 n_0 + \sum_{j=1}^{N} \omega_j n_j$$

We calculate

$$\begin{aligned}\| e^{-sH_0} V e^{sH_0} \|_2^2 &= \mathrm{Tr}\left(e^{-sH_0} V e^{2sH_0} V e^{-sH_0}\right) \\ &= \sum_n e^{-2sE(n)} \langle n|V e^{2sH_0} V|n\rangle \\ &= \sum_{n,m} e^{-2s[E(n)-E(m)]} |\langle n|V|m\rangle|^2 \end{aligned} \quad (32)$$

The operator $a^\dagger b_j$ acts on an eigenstate as $a^\dagger b_j|m\rangle = \sqrt{(m_0+1)m_j}|m'\rangle$, where $\mathbf{m}'$ is obtained form $\mathbf{m}$ by reducing m_j by one and increasing m_0 by one. It follows that $\langle n|a^\dagger b_j|m\rangle = \sqrt{(m_0+1)m_j}\delta_{n_0,m_0+1}\delta_{n_j,m_j-1}\prod_{\ell\neq 0,j}\delta_{n_\ell,m_\ell}$ (Kronecker deltas). Note also that $\chi_{H_0\leq\Omega}|m\rangle = \chi_{E(m)\leq\Omega}|m\rangle$. We then estimate the matrix element as

$$\begin{aligned}|\langle n|V|m\rangle|^2 &\leq \chi_{E(m)\leq\Omega}\ \chi_{E(n)\leq\Omega}\left(\sum_{j=1}^{N}|g_j|\left\{\langle n|a^\dagger b_j|m\rangle + \langle n|ab_j^\dagger|m\rangle\right\}\right)^2 \\ &\leq 2\chi_{E(m)\leq\Omega}\ \chi_{E(n)\leq\Omega}\left(\sum_{j=1}^{N}|g_j|^2\right)\left(\sum_{j=1}^{N}\langle n|a^\dagger b_j|m\rangle^2 + \langle n|ab_j^\dagger|m\rangle^2\right)\end{aligned} \quad (33)$$

where we used the Cauchy–Schwarz inequality for sums and that $(A+B)^2 \leq 2(A^2+B^2)$. Next,

$$\sum_{j=1}^{N}\langle n|a^\dagger b_j|m\rangle^2 + \langle n|ab_j^\dagger|m\rangle^2 = \sum_{j=1}^{N}(m_0+1)m_j\langle n|m'_j\rangle + m_0(m_j+1)\langle n|m''_j\rangle \leq \sum_{j=1}^{N}(m_0+1)(m_j+1)\left(\delta_{n,m'_j} + \delta_{n,m''_j}\right) \quad (34)$$

where m'_j is $\mathbf{m}$ with m_0 replaced by m_0+1 and m_j replaced by $m_j - 1$ and similarly for m''_j. Here, $\delta_{\mathbf{n},\mathbf{k}}$ takes the value 1 if $\mathbf{n} = \mathbf{k}$ and 0 otherwise. In view of eq. (32), we need to multiply with $e^{-2s[E(\mathbf{n})-E(\mathbf{m})]}$. Either delta function selects values such that $|E(\mathbf{n}) - E(\mathbf{m})| = |\omega_0 - \omega_j|$; one excitation is transferred, and so $e^{-2s[E(n)-E(m)]} \leq e^{2|s||\omega_0-\omega_j|}$. Also, the summation over $\mathbf{n}$ in eq. (32) disappears due to the presence of the delta functions.

We combine eqs. (32)–(34) to obtain

$$\begin{aligned}\| e^{-sH_0}Ve^{sH_0}\|_2^2 &\leq 2\left(\sum_{j=1}^{N}|g_j|^2\right)\sum_{j=1}^{N}e^{2|s||\omega_0-\omega_j|} \\ &\quad\times\sum_{m:E(m)\leq\Omega}(m_0+1)(m_j+1)\sum_{n:E(n)\leq\Omega}\left(\delta_{n,m'_j}+\delta_{n,m''_j}\right) \\ &\leq 4\left(\sum_{j=1}^{N}|g_j|^2\right)\sum_{j=1}^{N}e^{2|s||\omega_0-\omega_j|}\sum_{m:E(m)\leq\Omega}(m_0+1)(m_j+1) \\ &\leq 4\left(\sum_{j=1}^{N}|g_j|^2\right)Ne^{2|s|\Delta\omega}(\Omega/\omega_{\min}+1)^2\sum_{m:E(m)\leq\Omega}1\end{aligned} \quad (35)$$

where $\omega_{\min} = \min_{0\leq j\leq N}\omega_j$ and $\Delta\omega = \max_{1\leq j\leq N}|\omega_0 - \omega_j|$. We have used that in the summation, $\omega_k m_k \leq \Omega$ for all $k = 0, \ldots, N$. An easy (but rough) upper bound for the last sum in

Suppose then that $Y \equiv T_B\left[e^{-\beta H_{AB}}\right] \geq 0$. We want to show that $X \equiv T_B[\mathbb{1} + F(\beta)] \geq 0$. Let P_n be the spectral projection of Q on the subspace where $Q \geqslant 1/n$. Then, $P_nYP_n = P_nQXQP_n$ and, as $Q^{-1}P_n$ is bounded, $Q^{-1}P_nYP_nQ^{-1} = P_nXP_n$. By the positivity of Y, and hence that of $Q^{-1}P_nYP_nQ^{-1}$, we have $\langle f|P_nXP_n|f\rangle \geqslant 0$ for any vector $|f\rangle$. Since $P_n|f\rangle \to |f\rangle$ as $n \to \infty$, it follows that $\langle f|X|f\rangle \geqslant 0$ for any vector $|f\rangle$. Hence $X \geqslant 0$.

eq. (35) is obtained as follows. That sum counts the number of indices $\mathbf{m}$ such that $E(\mathbf{m}) \le \Omega$, and we write it as

$$\sum_{m:E(m)\le\Omega} 1 = \sum_{m_0\ge0}\sum_{m_1\ge0}\cdots\sum_{m_N\ge0}\chi_{\sum_{j=0}^{N}\omega_j m_j\le\Omega}(m)$$

where $\chi_{\sum_{j=0}^{N}\omega_j m_j\le\Omega}(m)$ is the function of $\mathbf{m}$, which equals one if the inequality is satisfied and zero else. In each one of the $N + 1$ sums, we have $\omega_j m_j \le \Omega$, or $m_j \le \Omega/\omega_{\min}$. Let $M = \lfloor \Omega/\omega_{\min} \rfloor$ be the largest integer smaller than or equal to $\Omega/\omega_{\min}$. Hence,

$$\sum_{m:E(m)\le\Omega} 1 = \sum_{m_0=0}^{M}\cdots\sum_{m_N=0}^{M}\chi_{\sum_{j=0}^{N}\omega_j m_j\le\Omega}(m) \le \sum_{m_0=0}^{M}\cdots\sum_{m_N=0}^{M} 1 = \left(\sum_{m=0}^{M} 1\right)^{N+1} = (M+1)^{N+1} \le (\Omega/\omega_{\min}+1)^{N+1}$$

Using this estimate in eq. (35), we conclude that

$$\| e^{-sH_0} V e^{sH_0} \|_2 \le 2\sqrt{N}(\Omega/\omega_{\min}+1)^{(N+3)/2}\left(\sum_{j=1}^{N}|g_j|^2\right)^{1/2} e^{|s|\Delta\omega} \qquad (36)$$

This completes the proof of eq. (16). □

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Data availability

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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The authors declare that there are no competing interests.

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