

Finite temperature quantum condensations in the space of states: general proof

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Abstract

We formalize and prove the extension to finite temperature of a class of quantum phase transitions, acting as condensations in the space of states, recently introduced and discussed at zero temperature (Ostilli and Presilla 2021 *J. Phys. A: Math. Theor.* **54** 055005). In details, we find that if, for a quantum system at canonical thermal equilibrium, one can find a partition of its Hilbert space \mathcal{H} into two subspaces, $\mathcal{H}_{\text{cond}}$ and $\mathcal{H}_{\text{norm}}$, such that, in the thermodynamic limit, $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \rightarrow 0$ and the free energies of the system restricted to these subspaces cross each other for some value of the Hamiltonian parameters, then, the system undergoes a first-order quantum phase transition driven by those parameters. The proof is based on an exact probabilistic representation of quantum dynamics at an imaginary time identified with the inverse temperature of the system. We also show that the critical surface has universal features at high and low temperatures.

Keywords: quantum phase transitions, finite temperature, condensation in the space of states, general proof, Grover model

(Some figures may appear in colour only in the online journal)

1. Introduction

The expression ‘quantum phase transitions’ (QPTs) [1–6] usually refers to phase transitions occurring at zero temperature ($T = 0$): in contrast to classical phase transitions, which are driven by the temperature, QPTs are meant to be driven by varying some Hamiltonian parameter of the system. Such a definition, however, might be a bit misleading. In more precise

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terms, one should say that a QPT is characterized by the existence of a singularity taking place at $T = 0$ in correspondence of some value of the Hamiltonian parameters, the quantum critical point (QCP). Here, the quantum nature of the singularity is implicit in the $T = 0$ limit, however, this more precise definition of QPT does not prevent the phase transition, still purely quantum, to exist also for $T > 0$ via the emergence of a critical line separating the two involved phases. Actually, $T = 0$ represents just an ideal limit and understanding the finite temperature counterpart of any QPT is crucially important. However, such a task, in general, represents a quite challenging issue, from both the theoretical and experimental viewpoints since, above zero temperature, quantum and thermal fluctuations compete in an intricate manner.

In this work, we present a comprehensive and rigorous approach to a large class of first-order QPTs at finite temperature. An heuristic derivation of this approach as well as some relevant applications, have been recently presented in [7] while, in the present work, we mainly focus on the proof of the specific thermodynamic inequalities at the base of our general method. In the resulting phase diagram of these first-order QPTs, the critical line emerging from the QCP establishes a region at finite T , which we call ‘condensed’, where the order parameter remains rigidly invariant. In other words, within the condensed region, the system behaves like if it were frozen at $T = 0$; thermal fluctuations do not affect the system. This feature turns out to be particularly appealing for applications to quantum computing protocols aimed at finding the ground state (GS) by using low but finite temperatures, the GS of the condensed phase being the solution of some combinatorial problem of interest, possibly hard [8–10].

The class of the first-order QPTs we are dealing with was first introduced and analyzed at $T = 0$ in a previous work, where it was found that the mechanism of the phase transition consists in a condensation in the space of states [11]. Let us consider a system described by the Hamiltonian

$$H = \Gamma K + V, \quad (1)$$

where K and V are two noncommuting Hermitian operators, K being dimensionless, and Γ a parameter with energy dimensions. If we represent H in the eigenbasis of V , it is natural to call V ‘potential operator’, K ‘hopping operator’, and Γ hopping parameter. We stress however that V is completely arbitrary and can involve any kind of particle-interactions. We will use Γ as the control parameter of the supposed QPT. Since phase transitions occur in the thermodynamic limit (TDL), we need a fair competition between K and V in this limit. If H describes a system of N particles, we assume that the eigenvalues of K and V both scale linearly with N , whereas $\Gamma = O(1)$. A relevant family of models to bear in mind concerns qubits based systems. For these systems, the space of states \mathcal{H} can be identified with the space spanned by the $\dim \mathcal{H} = 2^N$ spin states indicated by $|\mathbf{n}\rangle = |n_1\rangle|n_2\rangle \dots |n_N\rangle$, where $|n_i\rangle = |\pm\rangle$ is an eigenstate of the Pauli matrix σ_i^z relative to the qubit $i = 1, \dots, N$, N being the number of qubits. The potential V is a diagonal operator in the states $|\mathbf{n}\rangle$, namely, $V = \sum_{\mathbf{n}} V_{\mathbf{n}} |\mathbf{n}\rangle \langle \mathbf{n}|$. The hopping operator K is chosen as the sum of single-flip operators $K = -\sum_{i=1}^N \sigma_i^x$. A paradigmatic example of this family of systems is provided by the Grover Hamiltonian, which emulates a benchmark model for quantum search [12–16], where $V_{\mathbf{n}} = -JN\delta_{\mathbf{n},\mathbf{n}_1}$, with $J = O(1) > 0$, and \mathbf{n}_1 represents the target of a totally unstructured (worst case scenario) search. In contrast, structured searches correspond to potentials having a smooth minimum around the target and, therefore, benefit from the application of gradient-descent based methods like, e.g. in the Ising model where, however, the corresponding QPTs are second-order.

In [11] we have proven the following general result at $T = 0$. If we can find a partition of the space of states \mathcal{H} of the system into two subspaces, $\mathcal{H} = \mathcal{H}_{\text{cond}} \oplus \mathcal{H}_{\text{norm}}$, such that, in the TDL, $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \rightarrow 0$ and the GS energies of H restricted to these subspaces cross each other at a finite value of Γ , then the system undergoes a first-order QPT driven by this parameter.

Condensed and *normal*, the names attributed to the two subspaces, were motivated by the vanishing of the dimension of $\mathcal{H}_{\text{cond}}$ relatively to that of \mathcal{H} in the TDL with the consequence that the QPT realizes as a condensation in the space of states⁴. Condensation QPTs seem ubiquitous. Besides qubits based systems, they emerge also in fermionic systems: as we have recently shown, the renowned Wigner crystallization belongs to this class of QPTs [17].

As mentioned, the extension of these quantum condensations to finite temperature has already been presented in the [7], where the phase diagrams at finite T were obtained by simply replacing the crossing between the GS energies restricted to the *condensed* and *normal* subspaces, with the crossing of the corresponding restricted free energies. However, while this generalization at finite T sounds completely natural and physically appealing, it remains an heuristic argument. It is the aim of the present work to provide a rigorous proof. Whereas the proof for the $T=0$ case was obtained via an algebraic-functional approach [11], the present proof for the finite temperature case, which includes the $T=0$ as special limit, is based on an exact probabilistic representation (EPR) of the quantum dynamics on lattices introduced some years ago [18]. In contrast to the algebraic-functional approach, the probabilistic representation of the quantum dynamics has also the advantage to provide a clear physical picture. As we will see in detail, linking the imaginary time to the inverse temperature, we are able to analyze the Gibbs equilibrium at finite temperature by following trajectories of the system that evolve for a corresponding finite time and see how the condensations in the space of states are a consequence of the different crossing rates that exist for traversing the cond/norm boundary in the two directions, one being extensive in the system size, $O(N)$, the other being $o(N)$. In this work, we also show that the critical surface has universal features at high and low temperatures: in the former case it becomes proportional to the potential coupling, while in the latter case it acquires an infinite slope at the QCP.

The paper is organized as follows. Sections 2–4 are devoted to the formal definition of the *condensed* and *normal* subspaces and to a summary of the $T=0$ formulas, while the main result at finite T and its proof are provided in sections 5 and 8, respectively, sections 6 and 7 being devoted, in this order, to a proof of the above mentioned universal features and to an application to the Grover model as an exactly solvable example. Finally, in section 9 we discuss the equivalence between the $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \rightarrow 0$ condition with the above mentioned boundary crossing-rate difference.

2. Normal and condensed subspaces

We start by defining a proper partition of the space of states. Consider a system with Hamiltonian (1), and let $\{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}}$ be a complete orthonormal set of eigenstates of V , *the configurations*: $V|\mathbf{n}_k\rangle = V_k|\mathbf{n}_k\rangle$, $k = 1, \dots, \dim \mathcal{H}$. We assume ordered potential values $V_1 \leq \dots \leq V_{\dim \mathcal{H}}$. For a system of N qubits, for instance, the set of the configurations may correspond to the set of $\dim \mathcal{H} = 2^N$ product states of N spins along some direction, as stated above. For other physical systems composed by N_p particles moving in a lattice of N sites, the filling N_p/N will be assumed to be fixed in the TDL, and the set of the configurations correspond to all possible ways to accommodate the N_p particles in the N sites according to the fermionic or bosonic nature of the particles. In other words, a configuration $|\mathbf{n}_k\rangle$ represents the collective positions

⁴ It is worth to emphasize that, although the condensation that we describe is reminiscent of the Bose–Einstein condensation, the latter is a condensation in the momentum space, which applies to ideal gases and in which the space of states is made by the eigenstates of a single-particle Hamiltonian. On the other hand, we deal with interacting particles and our space of states is made by many-particle states.

of the N_p indistinguishable particles in the case of fermions and bosons, or the collective orientations of the $N_p = N$ distinguishable qubits thought fixed at N different spatial positions. At any rate, there is no limitation in the definition of the set of the configurations defining the space of states as $\mathcal{H} = \text{span}\{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}}$ and our general result applies in each abstract or physical case, without the need of considering separately the nature of the particles involved, as done for other phase transitions [19].

Let $\dim \mathcal{H}_{\text{cond}}$ be an integer with $1 \leq \dim \mathcal{H}_{\text{cond}} < \dim \mathcal{H}$ and let us consider a partition of the set of the configurations as $\{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}} = \{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}_{\text{cond}}} \cup \{|\mathbf{n}_k\rangle\}_{k=\dim \mathcal{H}_{\text{cond}}+1}^{\dim \mathcal{H}}$. In the Hilbert space of the system, $\mathcal{H} = \text{span}\{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}}$, which is equipped with standard complex scalar product $\langle u|v\rangle$, the above partition induces a decomposition of \mathcal{H} as the direct sum of two mutually orthogonal subspaces, denoted condensed and normal:

$$\mathcal{H} = \mathcal{H}_{\text{cond}} \oplus \mathcal{H}_{\text{norm}}, \tag{2}$$

where

$$\mathcal{H}_{\text{cond}} = \text{span}\{|\mathbf{n}_k\rangle\}_{k=1}^{\dim \mathcal{H}_{\text{cond}}}, \tag{3}$$

$$\mathcal{H}_{\text{norm}} = \text{span}\{|\mathbf{n}_k\rangle\}_{k=\dim \mathcal{H}_{\text{cond}}+1}^{\dim \mathcal{H}} = \mathcal{H}_{\text{cond}}^\perp. \tag{4}$$

Correspondingly, we define

$$E = \inf_{|u\rangle \in \mathcal{H}} \frac{\langle u|H|u\rangle}{\langle u|u\rangle}, \tag{5}$$

$$E_{\text{cond}} = \inf_{|u\rangle \in \mathcal{H}_{\text{cond}}} \frac{\langle u|H|u\rangle}{\langle u|u\rangle}, \tag{6}$$

$$E_{\text{norm}} = \inf_{|u\rangle \in \mathcal{H}_{\text{norm}}} \frac{\langle u|H|u\rangle}{\langle u|u\rangle}, \tag{7}$$

which are the GS eigenvalues, respectively, of H and of H restricted to the condensed and normal subspaces. According to the scaling properties assumed for K and V , we have that E , E_{cond} and E_{norm} increase linearly with N (at least in the TDL).

3. QPTs at $T = 0$

The Hilbert space dimension $\dim \mathcal{H}$ generally diverges exponentially with N , while the dimension $\dim \mathcal{H}_{\text{cond}}$, may or may not be a growing function of N . In [11] we have shown that:

$$\text{if} \quad \lim_{N \rightarrow \infty} \frac{\dim \mathcal{H}_{\text{cond}}}{\dim \mathcal{H}} = 0, \tag{8}$$

$$\text{then} \quad \lim_{N \rightarrow \infty} \frac{E}{N} = \lim_{N \rightarrow \infty} \min \left\{ \frac{E_{\text{cond}}}{N}, \frac{E_{\text{norm}}}{N} \right\}. \tag{9}$$

For finite sizes, up to corrections $O(1)$, equation (9) reads

$$E \simeq \begin{cases} E_{\text{cond}}, & \text{if } E_{\text{cond}} < E_{\text{norm}}, \\ E_{\text{norm}}, & \text{if } E_{\text{norm}} < E_{\text{cond}}. \end{cases} \tag{10}$$

As a consequence of equation (9), by varying one or more parameters of the Hamiltonian H , we obtain a QPT, necessarily of first order, whenever a crossing takes place between E_{cond} and E_{norm} . In the TDL, the space of states splits at the QCP (or, more generally, at the quantum critical surface) defined by

$$\lim_{N \rightarrow \infty} \frac{E_{\text{cond}}}{N} = \lim_{N \rightarrow \infty} \frac{E_{\text{norm}}}{N}, \tag{11}$$

and, in correspondence with equation (10), for the GS $|E\rangle$ we have either $|E\rangle \in \mathcal{H}_{\text{cond}}$ or $|E\rangle \in \mathcal{H}_{\text{norm}}$.

In order to have a QPT, apart from the necessary condition (8), $\dim \mathcal{H}_{\text{cond}}$ should also be chosen in such a way that equation (11) admits a finite solution [17]. As a general criteria, $\mathcal{H}_{\text{cond}}$ should be not too small and not too large so that neither of the two restrictions of H , to $\mathcal{H}_{\text{cond}}$ and to $\mathcal{H}_{\text{norm}}$, have a QPT. In other words, we want that, in the TDL, E_{cond}/N and E_{norm}/N remain both analytic functions of the Hamiltonian parameters, whereas E/N becomes non-analytic at the QCP [17].

4. Order parameter at $T = 0$

The interpretation of the above class of QPTs in terms of a condensation in the space of states holds in general, even when $\mathcal{H}_{\text{cond}}$ contains many eigenstates of V [17]. At zero temperature, the probability for the condensed subspace to be occupied is

$$p_{\text{cond}} = \sum_{|\mathbf{n}_k\rangle \in \mathcal{H}_{\text{cond}}} |\langle \mathbf{n}_k | E \rangle|^2. \tag{12}$$

On the other hand, in the TDL, since it is either $|E\rangle \in \mathcal{H}_{\text{cond}}$ or $|E\rangle \in \mathcal{H}_{\text{norm}}$, we find either $p = 1$ or $p = 0$, respectively (we assume $|E\rangle$ normalized). In other words, p_{cond} represents an order parameter of these first-order QPTs.

We stress that condensation QPTs are intrinsically first-order, for they can be driven by using even one single Hamiltonian parameter. In contrast, as for the classical case, jumps of the order parameter can result when crossing the coexistence line of two different phases that originate from the critical point of a second-order QPT. Notice that, for such a scenario to take place at zero temperature, one needs that the Hamiltonian depends on at least two independent parameters (think to the 1d Ising model in the presence of both a transverse and a longitudinal magnetic field [20, 21]).

5. Finite temperature quantum condensations

Our aim is to extend the above class of condensation QPTs to finite temperature. We suppose that the system, in contact with a heat bath, is at canonical equilibrium at temperature $T = 1/(k_B\beta)$, i.e. it is in the state described by the Gibbs density matrix operator $\rho = e^{-\beta H} / \text{tr} e^{-\beta H}$.

Analogously to the $T = 0$ case, we proceed by defining the Gibbs free energies associated to the spaces \mathcal{H} , $\mathcal{H}_{\text{cond}}$, $\mathcal{H}_{\text{norm}}$,

$$e^{-\beta F} = \text{tr} e^{-\beta H} = \sum_{|\mathbf{n}\rangle \in \mathcal{H}} \langle \mathbf{n} | e^{-\beta H} | \mathbf{n} \rangle, \tag{13}$$

$$e^{-\beta F_{\text{cond}}} = \text{tr}_{\text{cond}} e^{-\beta H_{\text{cond}}} = \sum_{|\mathbf{n}\rangle \in \mathcal{H}_{\text{cond}}} \langle \mathbf{n} | e^{-\beta H_{\text{cond}}} | \mathbf{n} \rangle, \tag{14}$$

$$e^{-\beta F_{\text{norm}}} = \text{tr}_{\text{norm}} e^{-\beta H_{\text{norm}}} = \sum_{|\mathbf{n}\rangle \in \mathcal{H}_{\text{norm}}} \langle \mathbf{n} | e^{-\beta H_{\text{norm}}} | \mathbf{n} \rangle, \tag{15}$$

where H_{cond} and H_{norm} are the restrictions of H to the condensed and normal subspaces⁵. Note that $H_{\text{cond}} + H_{\text{norm}} \neq H$. It is natural to investigate whether equation (9) can be generalized

⁵ In the representation of the eigenstates of V , H_{cond} corresponds to a null matrix except for the block $\langle \mathbf{n}_k | H_{\text{cond}} | \mathbf{n}_{k'} \rangle = \langle \mathbf{n}_k | H | \mathbf{n}_{k'} \rangle$, $k, k' = 1, \dots, M_{\text{cond}}$. Analogously, H_{norm} corresponds to a null matrix except for the block $\langle \mathbf{n}_k | H_{\text{norm}} | \mathbf{n}_{k'} \rangle = \langle \mathbf{n}_k | H | \mathbf{n}_{k'} \rangle$, $k, k' = M_{\text{cond}} + 1, \dots, M$.

to finite temperature just by substituting the energies $E, E_{\text{cond}}, E_{\text{norm}}$ with the free energies $F, F_{\text{cond}}, F_{\text{norm}}$, which scale linearly with N too.

For any partition $\mathcal{H} = \mathcal{H}_{\text{cond}} \oplus \mathcal{H}_{\text{norm}}$, we will prove that (X stands for either cond or norm and Y for its complement)

$$1 \leq \frac{\langle \mathbf{n} | e^{-\beta H} | \mathbf{n} \rangle}{\langle \mathbf{n} | e^{-\beta H_X} | \mathbf{n} \rangle} \leq e^{\beta \Gamma \min\{A_X^{(\text{out})}, A_Y^{(\text{out})}\}}, \quad |\mathbf{n}\rangle \in \mathcal{H}_X, \quad (16)$$

$$F \leq \min\{F_{\text{cond}}, F_{\text{norm}}\}, \quad (17)$$

$$F \geq \min\{F_{\text{cond}}, F_{\text{norm}}\} - \min\{A_{\text{cond}}^{(\text{out})}, A_{\text{norm}}^{(\text{out})}\} \Gamma, \quad (18)$$

where $A_X^{(\text{out})} = \sup_{|\mathbf{n}\rangle \in \mathcal{H}_X} \sum_{|\mathbf{n}'\rangle \in \mathcal{H}_Y} |\langle \mathbf{n} | K | \mathbf{n}' \rangle|$ represents the maximum number of outgoing links (nonzero matrix elements of K) from \mathcal{H}_X to \mathcal{H}_Y . The product $\min\{A_X^{(\text{out})}, A_Y^{(\text{out})}\} \Gamma$ determines approximately the rate of convergence to 1 of the probability for crossing the boundary between \mathcal{H}_X and \mathcal{H}_Y along the quantum dynamics at imaginary times (see section 8). In the Grover model, e.g. $A_{\text{norm}}^{(\text{out})} = 1$ while $A_{\text{cond}}^{(\text{out})} = N$. As we show in section 9, the important point is that, in most of the systems of interest, the conditions $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \rightarrow 0$ and $A_{\text{norm}}^{(\text{out})} / N \rightarrow 0$ are equivalent and, under any of these conditions, equations (17) and (18), up to a term $o(N)$, provide the natural generalization of equation (10)

$$F \simeq \begin{cases} F_{\text{cond}}, & \text{if } F_{\text{cond}} < F_{\text{norm}}, \\ F_{\text{norm}}, & \text{if } F_{\text{norm}} < F_{\text{cond}}. \end{cases} \quad (19)$$

Equation (19) extends the $T=0$ QPT to finite temperature. The crossing between F_{cond} and F_{norm} gives rise to a first order phase transition controlled by Hamiltonian parameters and temperature, the equation for the critical surface being

$$\lim_{N \rightarrow \infty} \frac{F_{\text{cond}}}{N} = \lim_{N \rightarrow \infty} \frac{F_{\text{norm}}}{N}. \quad (20)$$

Hereafter, we assume $\min\{A_{\text{cond}}^{(\text{out})}, A_{\text{norm}}^{(\text{out})}\} = A_{\text{norm}}^{(\text{out})}$.

The probability for the condensed subspace to be occupied represents an order parameter also at finite temperature and the phase transition can be interpreted as a condensation in the space of states. In fact, due to equation (16)

$$p_{\text{cond}} = \sum_{|\mathbf{n}\rangle \in \mathcal{H}_{\text{cond}}} \langle \mathbf{n} | \rho | \mathbf{n} \rangle \simeq \frac{1}{1 + e^{-\beta(F_{\text{norm}} - F_{\text{cond}})}}, \quad (21)$$

where the equality holds in the TDL with $p_{\text{cond}} = 1$ in the condensed phase $F_{\text{cond}} < F_{\text{norm}}$ and $p_{\text{cond}} = 0$ in the normal one $F_{\text{norm}} < F_{\text{cond}}$. At the critical surface separating the two phases we have $p_{\text{cond}} = 1/2$.

Equations (17) and (18) are easily derived from equation (16). Before giving the proof of equation (16), we illustrate some universal features of the finite temperature condensations and the application of our findings to the Grover model.

6. Universal features of the critical surface

We recall that standard canonical thermodynamics relations such as $F = U - TS$, U being the internal energy and $S = -\partial F / \partial T$ the entropy, apply also to the quantum case. Suppose that the potential V in the Hamiltonian (1) depends on a single parameter, say J , having energy dimensions: $V = J\tilde{V}$, \tilde{V} being dimensionless. In this case, keeping fixed the kinetic parameter Γ , the equation for the critical surface (20) determines the critical temperature as a function

of J : $T = T(J)$. The critical temperature $T(J)$ is the $N \rightarrow \infty$ limit of the ‘finite size critical temperature’ $T_N(J)$ determined by the finite size analogous of equation (20). Under the mild assumption that $T_N(J)$ converges uniformly to $T(J)$ we are allowed to exchange the order of limits $N \rightarrow \infty$ with $J \rightarrow \infty$ and also to exchange the order of the limit $N \rightarrow \infty$ with the derivative d/dJ . In the following, we shall make use of these properties to establish two universal features of the critical temperature: at large potential values, $J \rightarrow \infty$, and at the QCP, $J \rightarrow J_c$. In both cases the starting point is equation (20) at finite size rewritten as

$$T_N(J) = \frac{U_{\text{norm}} - U_{\text{cond}}}{S_{\text{norm}} - S_{\text{cond}}}. \quad (22)$$

Let us consider the limit $J \rightarrow \infty$. Here, all the eigenvalues of H , as well as all the eigenvalues of the restrictions of H to the normal and condensed subspaces, become proportional to J . As a consequence, the internal energies U_{norm} and U_{cond} become also proportional to J . It follows that $U_{\text{norm}} - U_{\text{cond}} = \alpha NJ$, where α is a constant independent of J . On the other hand, for the entropy (of the whole space and, similarly, of the restrictions), we have

$$S = k_B \log \left(\text{tr} e^{-\beta_N(J)H} \right) + \frac{U}{T_N(J)}. \quad (23)$$

From equation (23) we see that, by assuming $T_N(J) = \gamma J$, where γ is a finite positive constant, in the limit $J \rightarrow \infty$, the entropy (of the whole space and, similarly, of the restrictions) becomes independent of J . On combining this fact with equation (22) we see that, in the limit $J \rightarrow \infty$, $T_N(J) = \gamma J$ is solution of equation (22). Finally, in the TDL, taking into account that S_{norm} must be extensive (S_{cond} could be extensive or not), we get the value of γ as follows

$$\gamma = \lim_{J \rightarrow \infty} \frac{T(J)}{J} = \lim_{J \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{U_{\text{norm}} - U_{\text{cond}}}{J(S_{\text{norm}} - S_{\text{cond}})}. \quad (24)$$

Let us now consider the limit $J \rightarrow J_c$. By using $\partial F/\partial T = -S$, and, similarly, for the restrictions to the subspaces, we can evaluate the total derivative of equation (20) with respect to J as

$$\frac{\partial(F_{\text{norm}} - F_{\text{cond}})}{\partial J} - (S_{\text{norm}} - S_{\text{cond}}) \frac{\partial T_N(J)}{\partial J} = 0, \quad (25)$$

which provides

$$\frac{\partial T_N(J)}{\partial J} = \frac{\partial(F_{\text{norm}} - F_{\text{cond}})}{\partial J} \frac{1}{S_{\text{norm}} - S_{\text{cond}}}. \quad (26)$$

Again we observe that the free energies and, at any finite T , also the entropies, are extensive quantities. This implies that, for any finite T , the TDL of equation (26) is finite. However, since $J \rightarrow J_c$ implies $T \rightarrow 0$, disregarding cases like spin-glass models, the entropy density of the system as well as of its restrictions tend to zero in the TDL. Let us assume that, for $J = J_c$, in the TDL we have $\partial(E_{\text{norm}}/N - E_{\text{cond}}/N)/\partial J \neq 0$. From equation (26) we conclude that

$$\lim_{J \rightarrow J_c} \frac{\partial T(J)}{\partial J} = \lim_{J \rightarrow J_c} \lim_{N \rightarrow \infty} \frac{\partial T_N(J)}{\partial J} = +\infty. \quad (27)$$

We can show that equation (27) holds true also when, for $J = J_c$, in the TDL we have $\partial(E_{\text{norm}}/N - E_{\text{cond}}/N)/\partial J = 0$ but $\partial^2(E_{\text{norm}}/N - E_{\text{cond}}/N)/\partial J^2 \neq 0$ and possibly infinite. The argument is based on the assumption that, in the limit $T \rightarrow 0$, the specific heat of the two restrictions tend to 0 faster than T , or else that $\partial^2(E_{\text{norm}}/N - E_{\text{cond}}/N)/\partial J^2 \rightarrow \infty$ in the TDL, as indeed occurs in many cases of interest.

Clearly, what actually matters is the ratio J/Γ . In fact, by using the same arguments we can equivalently rewrite equation (24) as $\gamma = \lim_{J/\Gamma \rightarrow \infty} T(J)/J$ or else, if the potential parameter J is kept constant and Γ is varied, as $\gamma = \lim_{\Gamma/J \rightarrow 0} T(\Gamma)/J$ and, similarly, we can rewrite equation (27) as $\lim_{\Gamma \rightarrow \Gamma_c} \partial T(\Gamma)/\partial \Gamma = +\infty$, where $T(\Gamma)$ is the critical temperature in the limit $N \rightarrow \infty$ and Γ_c provides the QCP. As we shall see in the next section, the constant γ can be easily evaluated in the exactly solvable Grover model where $\gamma = 1/(k_B \log 2)$.

7. The Grover model as an exactly solvable paradigmatic example

7.1. The case $T=0$

Here $V_1 = -JN$, with $J > 0$, and $V_k = 0$, for $k = 2, 3, \dots, \dim \mathcal{H} = 2^N$. We can assume $\dim \mathcal{H}_{\text{cond}} = 1$ independent of N . We find $|E_{\text{cond}}\rangle = |\mathbf{n}_1\rangle$ and $E_{\text{cond}} = V_1$. Up to a correction $O(N/\dim \mathcal{H})$, we also have $E_{\text{norm}} = -\Gamma N$ [11]. Therefore equation (10) becomes

$$E \simeq \begin{cases} -JN, & \text{if } \Gamma < \Gamma_c, \\ -\Gamma N, & \text{if } \Gamma > \Gamma_c, \end{cases} \quad (28)$$

where the QCP, Γ_c , is determined by equation (11), namely, $\Gamma_c = J$. For $\Gamma > \Gamma_c$ the GS of the model coincides with the GS of the hopping operator K , while for $\Gamma < \Gamma_c$ the system stays locked in the configuration $|\mathbf{n}_1\rangle$. We thus have a QPT that corresponds to a condensation in the space of states.

7.2. The general case $T \geq 0$

Since $\dim \mathcal{H}_{\text{cond}} = 1$, we have $-\beta F_{\text{cond}} = -\beta V_1$ with $V_1 = -JN$. Up to corrections exponentially small in N , the free energy of the normal subspace coincides with that of the hopping operator K whose levels are $-\Gamma(N - 2j)$, $j = 0, \dots, N$, and have degeneracy $N!/(j!(N-j)!)$,

$$e^{-\beta F_{\text{norm}}} = \text{tr} e^{-\beta K} = \sum_{j=0}^N \binom{N}{j} e^{-\beta(-\Gamma(N-2j))}, \quad (29)$$

which provides $-\beta F_{\text{norm}} = N \log(2 \cosh(\beta \Gamma))$. The critical surface defined by equation (20) is thus given by $\log(2 \cosh(\beta \Gamma)) = \beta J$ (a result also found in [16] via approximate methods) which can be solved to explicitly provide $\Gamma_c = \Gamma_c(T)$ ⁶,

$$\Gamma_c(T) = J + k_B T \log \left(\frac{1}{2} + \sqrt{\frac{1}{4} - e^{-2J/(k_B T)}} \right). \quad (30)$$

Note that equation (30) is defined only for $k_B T \leq J/\log 2$ and for $T \rightarrow 0^+$ returns the already analyzed $T=0$ QPT. A parametric plot of $(\Gamma_c(T), T)$ is shown in figure 1. The shaded area is the condensed phase. No condensed phase is possible for $\Gamma > \Gamma_c(0) = J$ (point of minimal entropy). For $0 \leq \Gamma \leq \Gamma_c(0)$ the condensed phase extends to the finite temperature $T_c(\Gamma)$ obtained inverting equation (30). No condensed phase is possible for $T > T_c(0) = J/(k_B \log 2)$ (point of maximal entropy).

Thermodynamics follows easily: internal energies $U_{\text{cond}} = -JN$ and $U_{\text{norm}} = -\Gamma N \tanh(\beta \Gamma)$; entropies $S_{\text{cond}} = 0$ and $S_{\text{norm}} = N k_B [\log(2 \cosh(\beta \Gamma)) - \beta \Gamma \tanh(\beta \Gamma)]$; specific heats

⁶ On posing $x = e^{\beta \Gamma}$, we are left with the reciprocal equation $\log(x + x^{-1}) = \beta J$ that can, in turn, be transformed into a quadratic equation for x having two real and positive roots: one with $x > 1$, which corresponds to a positive Γ (equation (30)), and the other one with $x < 1$, which corresponds to a negative Γ .

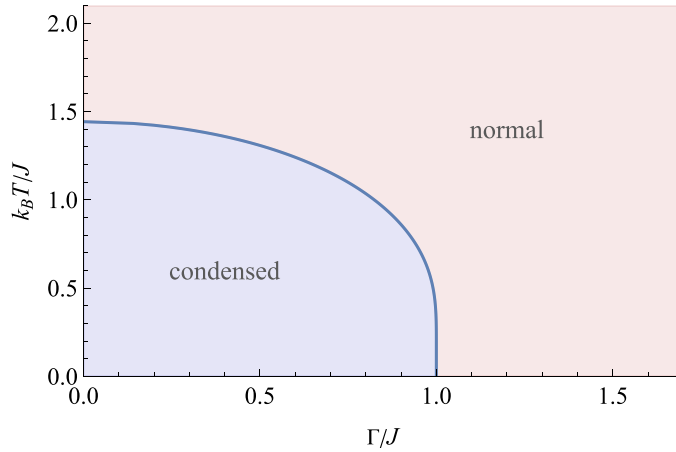


Figure 1. Phase diagram for the Grover model at thermal equilibrium, the solid line separating the two phases is drawn according to equation (30).

$c_{\text{cond}} = 0$ and $c_{\text{norm}} = k_B (\beta\Gamma / \cosh(\beta\Gamma))^2$. Notice that, whereas the free energy F is always continuous in T , the internal energy U , the entropy S , and the specific heat c , are all discontinuous along any curve that crosses the critical surface, except for $T \rightarrow 0$. This in particular implies a non-null latent heat proportional to the entropy of the normal phase: $U_{\text{norm}} - U_{\text{cond}}|_{T=T_c} = k_B T_c S_{\text{norm}}|_{T=T_c}$. This latent heat represents the minimal amount of energy to be subtracted from the system in order to bring it from the normal to the condensed phase.

8. Proof of equation (16)

In the following, we prove the lower and upper bounds of equation (16). The starting point is the EPR of the quantum evolution introduced in [18]. According to this EPR, at imaginary time t , to be identified here with the inverse temperature β , we have ($\hbar = 1$)

$$\langle \mathbf{n} | e^{-Ht} | \mathbf{n}_0 \rangle = \mathbb{E} \left(\mathcal{M}_{\mathbf{n}_0}^{[0,t]} \delta_{\mathbf{n}_{N_t}, \mathbf{n}} \right), \quad (31)$$

where $\mathbb{E}(\cdot)$ is the probabilistic expectation over the continuous time Markov chain of configurations $\mathbf{n}_0, \mathbf{n}_{s_1}, \dots, \mathbf{n}_{s_{N_t}}$ (hereafter, named trajectory) defined by the transition matrix

$$P_{\mathbf{n}, \mathbf{n}'} = \frac{|\langle \mathbf{n} | \mathbf{K} | \mathbf{n}' \rangle|}{A(\mathbf{n})}, \quad A(\mathbf{n}) = \sum_{\mathbf{n}'} |\langle \mathbf{n} | \mathbf{K} | \mathbf{n}' \rangle|, \quad (32)$$

and the sequence of jumping times s_1, s_2, \dots, s_{N_t} obtained from the Poissonian conditional probability density

$$P(s_k | s_{k-1}) = e^{-\Gamma A(\mathbf{n}_{s_{k-1}})(s_k - s_{k-1})} \Gamma A(\mathbf{n}_{s_{k-1}}). \quad (33)$$

N_t being the number of jumps occurred along the trajectory before the time t . Note that hereafter with the term *configuration* we may indicate the eigenstate of V , $|\mathbf{n}\rangle$, or the set of indices \mathbf{n} which define such state. The integer $A(\mathbf{n})$ is called the number of links, or degree, of \mathbf{n} and represents the number of non null off-diagonal matrix elements $\langle \mathbf{n} | H | \mathbf{n}' \rangle$. Starting from the configuration \mathbf{n}_0 at time $s_0 = 0$, we draw a configuration \mathbf{n}_{s_1} with probability $P_{\mathbf{n}_0, \mathbf{n}_{s_1}}$ at time s_1 drawn with probability density $P(s_1 | s_0)$, then we draw a configuration \mathbf{n}_{s_2} with probability

$P_{n_{s_1}, n_{s_2}}$ at time s_2 drawn with probability density $P(s_2|s_1)$, and so on until we reach the configuration \mathbf{n}_{N_t} at time s_{N_t} such that $s_{N_t+1} > t$ ⁷. The stochastic functional $\mathcal{M}_{n_0}^{[0,t]}$ is then defined as

$$\mathcal{M}_{n_0}^{[0,t]} = e^{\sum_{k=0}^{N_t-1} [\Gamma A(\mathbf{n}_{s_k}) - V(\mathbf{n}_{s_k})](s_{k+1} - s_k)} e^{[\Gamma A(\mathbf{n}_{s_{N_t}}) - V(\mathbf{n}_{s_{N_t}})](t - s_{N_t})}. \quad (34)$$

Whereas a more general formulation of the EPR is possible [18], that presented above holds in the statistically manageable case in which no sign problem arises, e.g. when $\langle \mathbf{n} | K | \mathbf{n}' \rangle \leq 0$ for any \mathbf{n}, \mathbf{n}' . We assume to be in this class of ‘bosonic’ systems. In particular, for qubit systems K is the sum of single flip operators, for which $\langle \mathbf{n} | K | \mathbf{n}' \rangle = 0, -1$. If the whole set of configurations is connected by K , as we assume, the Markov chain is ergodic with invariant measure $\pi_n = A(\mathbf{n}) / \sum_{n'} A(\mathbf{n}')$. For example, in qubit systems as the Grover model, the degree of the configurations is constant, $A(\mathbf{n}) = N$, and $\pi_n = 1 / \dim \mathcal{H}$.

Let us indicate by $\widehat{\mathcal{H}} = \{\mathbf{n}_k\}_{k=1}^{\dim \mathcal{H}_{\text{cond}}}$ ($\widetilde{\mathcal{H}} = \{\mathbf{n}_k\}_{k=\dim \mathcal{H}_{\text{cond}}+1}^{\dim \mathcal{H}}$) the set of configurations defining the states in $\mathcal{H}_{\text{cond}}$ ($\mathcal{H}_{\text{norm}}$). A generic configuration of $\widehat{\mathcal{H}}$ ($\widetilde{\mathcal{H}}$) will be indicated by $\widehat{\mathbf{n}}$ ($\widetilde{\mathbf{n}}$). For any configuration $\mathbf{n} = \widehat{\mathbf{n}}$ or $\mathbf{n} = \widetilde{\mathbf{n}}$ we can always split its degree as

$$A(\mathbf{n}) = A^{(\text{in})}(\mathbf{n}) + A^{(\text{out})}(\mathbf{n}), \quad (35)$$

where $A^{(\text{in})}(\mathbf{n})$ and $A^{(\text{out})}(\mathbf{n})$ represent the number of links connecting \mathbf{n} with configurations inside or outside its membership subset, $\widehat{\mathcal{H}}$ or $\widetilde{\mathcal{H}}$ ⁸.

Consider trajectories beginning and ending at a configuration $\widetilde{\mathbf{n}}$ of $\widetilde{\mathcal{H}}$. Introducing the random variable $K_t = 0, 1, 2, \dots$ counting the number of times the Markov chain transits through-out $\widetilde{\mathcal{H}}$ in the interval $[0, t)$, we decompose the expectation as a sum of two constrained expectations as follows

$$\langle \widetilde{\mathbf{n}} | e^{-Ht} | \widetilde{\mathbf{n}} \rangle = \mathbb{E} \left(\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}}; K_t = 0 \right) + \mathbb{E} \left(\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}}; K_t \geq 1 \right). \quad (36)$$

Consider the term $K_t = 0$. Each trajectory contributing to this event is characterized by a sequence of N_t jumping times s_1, s_2, \dots, s_{N_t} extracted along a sequence of configurations $\widetilde{\mathbf{n}}, \widetilde{\mathbf{n}}_1, \widetilde{\mathbf{n}}_2, \dots, \widetilde{\mathbf{n}}_{N_t}$. Hence, regardless of any other detail, such a trajectory is realized if none of the associated out links jump, which occurs with probability $\exp\{-\Gamma[A^{(\text{out})}(\widetilde{\mathbf{n}})s_1 + A^{(\text{out})}(\widetilde{\mathbf{n}}_1)(s_2 - s_1) + \dots + A^{(\text{out})}(\widetilde{\mathbf{n}}_{N_t-1})(s_{N_t} - s_{N_t-1}) + A^{(\text{out})}(\widetilde{\mathbf{n}}_{N_t})(t - s_{N_t})]\}$. On the other hand, equation (34) shows that along the same trajectory the hopping term provides the weight $\exp\{\Gamma[A(\widetilde{\mathbf{n}})s_1 + A(\widetilde{\mathbf{n}}_1)(s_2 - s_1) + \dots + A(\widetilde{\mathbf{n}}_{N_t-1})(s_{N_t} - s_{N_t-1}) + A(\widetilde{\mathbf{n}}_{N_t})(t - s_{N_t})]\}$. By using $A(\widetilde{\mathbf{n}}) - A^{(\text{out})}(\widetilde{\mathbf{n}}) = A^{(\text{in})}(\widetilde{\mathbf{n}})$, we obtain

$$\begin{aligned} \mathbb{E} \left(\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}}; K_t = 0 \right) &= \mathbb{E} \left(\widetilde{\mathcal{M}}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}} \right) \\ &= \langle \widetilde{\mathbf{n}} | e^{-H_{\text{norm}}t} | \widetilde{\mathbf{n}} \rangle, \end{aligned} \quad (37)$$

where $\widetilde{\mathcal{M}}_{\widetilde{\mathbf{n}}}^{[0,t]}$ is the stochastic functional defined in terms of H_{norm} ⁹ and equation (31) has been used again (now applied to the system governed by H_{norm}) to get the second equality. Since $\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} > 0$, equations (36) and (37) give

$$\langle \widetilde{\mathbf{n}} | e^{-Ht} | \widetilde{\mathbf{n}} \rangle \geq \langle \widetilde{\mathbf{n}} | e^{-H_{\text{norm}}t} | \widetilde{\mathbf{n}} \rangle. \quad (38)$$

⁷ Note that the Poisson processes associated to each jump are defined left continuous [18], as a consequence, the configuration \mathbf{n}_{N_t} is the one realized by the Markov chain just before the final time t .

⁸ Note that $A^{(\text{in})}(\widehat{\mathbf{n}})$ and $A^{(\text{in})}(\widetilde{\mathbf{n}})$ represent the number of non-null off-diagonal matrix elements $\langle \widehat{\mathbf{n}} | H_{\text{cond}} | \widehat{\mathbf{n}}' \rangle$ and $\langle \widetilde{\mathbf{n}} | H_{\text{norm}} | \widetilde{\mathbf{n}}' \rangle$, respectively.

⁹ See footnote 8.

Considering trajectories beginning and ending at a configuration $\widehat{\mathbf{n}}$ of $\widehat{\mathcal{H}}$, we get a similar relation with $\widetilde{\mathbf{n}} \rightarrow \widehat{\mathbf{n}}$ and $H_{\text{norm}} \rightarrow H_{\text{cond}}$. This completes the proof of the first inequality in equation (16).

Proving the second inequality of (16) requires the analysis of the term $K_t \geq 1$ in equation (36), which is quite more involved. We have

$$\mathbb{E} \left(\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}}; K_t \geq 1 \right) = \sum_{\xi} \mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]}(\xi) \mathbb{P}_t(\widetilde{\mathbf{n}} \xrightarrow{\xi} \widetilde{\mathbf{n}}; K_t \geq 1), \quad (39)$$

where the sum runs over the ‘space-time’ trajectories ξ , and $\mathbb{P}_t(\widetilde{\mathbf{n}} \xrightarrow{\xi} \widetilde{\mathbf{n}}; K_t \geq 1)$ stands for the probability that, starting from $\widetilde{\mathbf{n}}$, ξ ends in $\widetilde{\mathbf{n}}$ by transiting throughout $\widehat{\mathcal{H}}$ at least once within the time t . Apart from K_t , each ξ has a probability obtained via the sequence of jumping links and jumping times according to equations (32) and (33). If $A(\mathbf{n}) = N$ is constant, which happens in many qubit systems, the trajectories have no preferential directions and, therefore, no correlation with the random variable K_t (in particular, trajectories visiting the same number of configurations and corresponding jumping times have the same probability). In more general systems, due to the condition (8), the correlations with K_t become negligible in the TDL. We then have

$$\begin{aligned} \mathbb{E} \left(\mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]} \delta_{n_{N_t}, \widetilde{\mathbf{n}}}; K_t \geq 1 \right) &\simeq \sum_{\xi} \mathcal{M}_{\widetilde{\mathbf{n}}}^{[0,t]}(\xi) \mathbb{P}_t(\widetilde{\mathbf{n}} \xrightarrow{\xi} \widetilde{\mathbf{n}}) \mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1) \\ &= \langle \widetilde{\mathbf{n}} | e^{-Ht} | \widetilde{\mathbf{n}} \rangle \mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1), \end{aligned} \quad (40)$$

where $\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1)$ stands for the total probability that, within the time t and starting from a given configuration $\widetilde{\mathbf{n}}$, the system transits through $\widehat{\mathcal{H}}$ at least once. It is clear that, given N , $\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1) \rightarrow 1$ for $t \rightarrow \infty$. However, we are interested in the other order of limits and, actually, here t must be kept finite while extrapolating the TDL. In fact, we want a bound for $\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1)$ in the TDL. We have

$$\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1) \leq 1 - \mathbb{P}_t(\widetilde{\mathbf{n}}; K_t = 0). \quad (41)$$

Notice that $\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t = 0)$ represents the probability to remain in $\widetilde{\mathcal{H}}$ during the time t and it does not coincide with the complement of $\mathbb{P}_t(\widetilde{\mathbf{n}}; K_t \geq 1)$. In fact, by definition, if $K_t \geq 1$, K_t counts how many times a trajectory that starts from $\widetilde{\mathcal{H}}$, transits through $\widehat{\mathcal{H}}$, and eventually goes back to $\widetilde{\mathcal{H}}$, while the complement of the event $K_t \geq 1$ contains also all the trajectories that, starting from $\widetilde{\mathcal{H}}$, transit through $\widehat{\mathcal{H}}$ a certain number of times but eventually do not terminate in $\widetilde{\mathcal{H}}$. Let $\widetilde{\partial}$ be the boundary set between $\widetilde{\mathcal{H}}$ and $\widehat{\mathcal{H}}$ belonging to $\widetilde{\mathcal{H}}$:

$$\widetilde{\partial} = \left\{ \widetilde{\mathbf{n}} \in \widetilde{\mathcal{H}} : \exists \widehat{\mathbf{n}} \in \widehat{\mathcal{H}} \text{ such that } \langle \widetilde{\mathbf{n}} | K | \widehat{\mathbf{n}} \rangle \neq 0 \right\}. \quad (42)$$

Clearly, $\widetilde{\partial}$ represents the set of configurations having the smallest probability of remaining in $\widetilde{\mathcal{H}}$ and such a probability corresponds to the event where no jump occurs through the outgoing links of these boundary configurations. Therefore, according to equation (33) and to the definition (35) we have

$$\begin{aligned} \mathbb{P}_t(\widetilde{\mathbf{n}}; K_t = 0) &\geq \inf_{\widetilde{\mathbf{n}} \in \widetilde{\partial}} \mathbb{P}_t(\widetilde{\mathbf{n}}; K_t = 0) \\ &= \inf_{\widetilde{\mathbf{n}} \in \widetilde{\partial}} e^{-\Gamma A^{(\text{out})}(\widetilde{\mathbf{n}})t} \\ &= e^{-\sup_{\widetilde{\mathbf{n}} \in \widetilde{\partial}} \Gamma A^{(\text{out})}(\widetilde{\mathbf{n}})t}. \end{aligned} \quad (43)$$

In conclusion, we have

$$\sup_{\tilde{\mathbf{n}}} \mathbb{P}_t(\tilde{\mathbf{n}}; K_t \geq 1) \leq 1 - e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\partial}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t}. \quad (44)$$

Equation (44) shows that the probability we are interested in has an upper bound that still goes to 1 exponentially in the TDL, but with a rate that is not extensive in N , in fact, $A^{(\text{out})}(\tilde{\mathbf{n}})$ is not extensive in N . Typically, in qubit systems $A^{(\text{out})}(\tilde{\mathbf{n}})$ is $O(1)$, but for our aims it could be also $o(N)$, as it occurs in system of fermions or hard-core bosons. Combining equations (36), (37) and (40), and then equation (44), we obtain

$$\langle \tilde{\mathbf{n}} | e^{-Ht} | \tilde{\mathbf{n}} \rangle \leq \langle \tilde{\mathbf{n}} | e^{-H_{\text{norm}}t} | \tilde{\mathbf{n}} \rangle + \langle \tilde{\mathbf{n}} | e^{-Ht} | \tilde{\mathbf{n}} \rangle \left(1 - e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\partial}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t} \right), \quad (45)$$

or

$$\langle \tilde{\mathbf{n}} | e^{-Ht} | \tilde{\mathbf{n}} \rangle \leq \langle \tilde{\mathbf{n}} | e^{-H_{\text{norm}}t} | \tilde{\mathbf{n}} \rangle e^{\sup_{\tilde{\mathbf{n}} \in \tilde{\partial}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t}, \quad (46)$$

Since $\sup_{\tilde{\mathbf{n}} \in \tilde{\partial}} A^{(\text{out})}(\tilde{\mathbf{n}}) = A_{\text{norm}}^{(\text{out})}$ and we assumed $A_{\text{norm}}^{(\text{out})} < A_{\text{cond}}^{(\text{out})}$, the second inequality in equation (16) is proven for $X = \text{norm}$.

To prove the second inequality in equation (16) for $X = \text{cond}$, we have to proceed in a slightly different way. Notice, in fact, that the analogous of equation (44) for the set $\tilde{\mathcal{H}}$ also holds, but it is of little use because, in general, whereas $A^{(\text{out})}(\tilde{\mathbf{n}})$ is not extensive in N , $A^{(\text{out})}(\hat{\mathbf{n}})$ can be extensive in N . In fact, this is just the case of the Grover model previously analyzed, as well as the case of regular qubit systems. Therefore, we avoid using equation (44) for $\tilde{\mathcal{H}}$ directly. The main idea here is that, due to the fact that $\tilde{\mathcal{H}}$ is a small portion of the whole set of configurations, the probability for a trajectory starting from $\tilde{\mathcal{H}}$ to reach $\tilde{\mathcal{H}}$, approaches 1 exponentially (in both t and N) with a large rate, but once it is in $\tilde{\mathcal{H}}$, the probability that it goes back to $\tilde{\mathcal{H}}$ approaches 1 with the same identical small rate of equation (44). Let us make concrete this idea by explicitly taking into account just one jump into $\tilde{\mathcal{H}}$ as follows

$$\begin{aligned} \sup_{\hat{\mathbf{n}}} \mathbb{P}_t(\hat{\mathbf{n}}; L_t \geq 1) &= \sup_{\hat{\mathbf{n}} \in \hat{\partial}} \mathbb{P}_t(\hat{\mathbf{n}}; L_t \geq 1) \\ &\simeq \sup_{\hat{\mathbf{n}} \in \hat{\partial}} \sum_{\tilde{\mathbf{n}} \in \mathcal{A}^{(\text{out})}(\hat{\mathbf{n}})} \int_0^t ds \Gamma e^{-\Gamma A(\hat{\mathbf{n}})s} \mathbb{P}_t(\tilde{\mathbf{n}}; Q_{t-s} \geq 1) \end{aligned} \quad (47)$$

where L_t and $\hat{\partial}$ are the analogous of K_t and $\tilde{\partial}$ for $\hat{\mathcal{H}}$, $\mathcal{A}^{(\text{out})}(\hat{\mathbf{n}})$ is the set of configurations in $\tilde{\mathcal{H}}$ which are first neighbors of $\hat{\mathbf{n}}$ (whose number is $A^{(\text{out})}(\hat{\mathbf{n}})$), s is a random time at which a jump toward one configuration $\tilde{\mathbf{n}} \in \mathcal{A}^{(\text{out})}(\hat{\mathbf{n}}) \subset \tilde{\partial}$ takes place, and Q_t counts the number of times the trajectory that starts from $\tilde{\mathcal{H}}$ leaves $\tilde{\mathcal{H}}$ by ending in $\tilde{\mathcal{H}}$ within the time interval $[0, t)$. Equation (47) holds approximately because we have neglected the trajectories that, starting from $\tilde{\partial}$, reach for the first time $\tilde{\mathcal{H}}$ by using more than one jump within the time interval $[0, t)$. However, due to the condition (8), such extra contributions become negligible in the TDL. Note that the analogous of equation (41) holds also for the random variable Q_t , namely,

$$\mathbb{P}_t(\tilde{\mathbf{n}}; Q_t \geq 1) \leq 1 - \mathbb{P}_t(\tilde{\mathbf{n}}; K_t = 0). \quad (48)$$

Therefore, we can now use equation (44) and get

$$\begin{aligned}
& \sum_{\tilde{\mathbf{n}} \in \mathcal{A}^{(\text{out})}(\hat{\mathbf{n}})} \int_0^t ds \Gamma e^{-\Gamma A(\hat{\mathbf{n}})s} \left(1 - e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})(t-s)} \right) \\
&= \frac{A^{(\text{out})}(\hat{\mathbf{n}})}{A(\hat{\mathbf{n}})} \left(1 - e^{-\Gamma A(\hat{\mathbf{n}})t} \right) \\
&\quad - A^{(\text{out})}(\hat{\mathbf{n}}) e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t} \frac{\left(1 - e^{-\Gamma [A(\hat{\mathbf{n}}) - \sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} A^{(\text{out})}(\tilde{\mathbf{n}})]t} \right)}{A(\hat{\mathbf{n}}) - \sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} A^{(\text{out})}(\tilde{\mathbf{n}})} \\
&\leq \frac{A^{(\text{out})}(\hat{\mathbf{n}})}{A(\hat{\mathbf{n}})} - \frac{A^{(\text{out})}(\hat{\mathbf{n}}) e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t}}{A(\hat{\mathbf{n}}) - \sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} A^{(\text{out})}(\tilde{\mathbf{n}})} \\
&\leq 1 - e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t}, \tag{49}
\end{aligned}$$

where, for the last inequality, we have used $A(\hat{\mathbf{n}}) \geq A^{(\text{out})}(\hat{\mathbf{n}})$, valid for any configuration. In conclusion, also for the configurations in $\tilde{\mathcal{H}}$ we have

$$\sup_{\hat{\mathbf{n}}} \mathbb{P}_t(\hat{\mathbf{n}}; L_t \geq 1) \leq 1 - e^{-\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} \Gamma A^{(\text{out})}(\tilde{\mathbf{n}})t}. \tag{50}$$

Equations (44) and (50) show that what matters is always the smallest border crossing-rate determined by $\sup_{\tilde{\mathbf{n}} \in \tilde{\delta}} A^{(\text{out})}(\tilde{\mathbf{n}})$. This concludes the proof of equation (16).

9. Equivalence of the conditions $A_{\text{norm}}^{(\text{out})}/N \rightarrow 0$ and $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$

We have stated that equation (19) are valid under the condition $\sup_{\tilde{\mathbf{n}}} A^{(\text{out})}(\tilde{\mathbf{n}})/N \rightarrow 0$. On the other hand, from [11] we know that equations (19) at $T=0$ are valid under the condition $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$. It is hence important to establish a relation between these two apparently independent conditions.

We recall that the matrix elements of the hopping operator K induce in \mathcal{H} a graph with $\dim \mathcal{H}$ nodes represented by the configurations, where the degree of a configuration \mathbf{n} is given by its number of links $A(\mathbf{n})$. In the following, we shall focus only on regular qubit systems of N qubits so that $\dim \mathcal{H} = 2^N$, and ‘regular’ here means that the hopping operator K is made by the usual sum of N single-flip operators, so that $A(\mathbf{n}) \equiv N$. Note that, since $A(\mathbf{n})/\dim \mathcal{H} \rightarrow 0$, the graph associated to \mathcal{H} is a regular sparse graph [22].

Let us first consider the Grover model. This model is characterized by the fact that there exist only two possible values of the potential, $V = -JN$ e $V = 0$, and that the former is realized by just one configuration (for example the one in which all the spins are up) so that $\dim \mathcal{H}_{\text{cond}} = 1$. For this model we have $A^{(\text{out})}(\tilde{\mathbf{n}}) \leq 1$ and also $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} = 1/2^N \rightarrow 0$. We can generalize the Grover model by allowing the value $V = -JN$ to be $\dim \mathcal{H}_{\text{cond}} > 1$ degenerate provided that we still have $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$. It is clear that, as far as the $\dim \mathcal{H}_{\text{cond}}$ configurations associated to $V = -JN$ are sufficiently separated, we keep having $A^{(\text{out})}(\tilde{\mathbf{n}}) \leq 1$. More precisely, it is easy to see that, as far as the $\dim \mathcal{H}_{\text{cond}}$ configurations associated to $V = -JN$ differ for the values of at least three spins (i.e. in the graph, the configurations of $\tilde{\mathcal{H}}$ are at least three links far apart among each other), we still have $A^{(\text{out})}(\tilde{\mathbf{n}}) \leq 1$ for any $\tilde{\mathbf{n}}$. This condition is illustrated in figure 2. However, it should be clear that the condition $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$ alone in general does not imply the condition $A^{(\text{out})}(\tilde{\mathbf{n}}) = O(1)$. As a counter-example, if we define

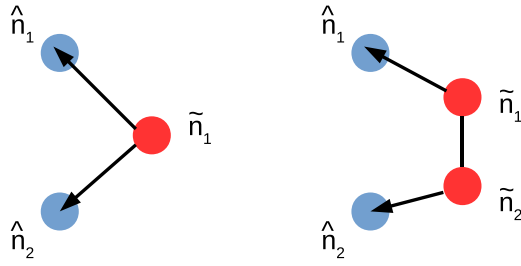


Figure 2. Left panel: an example of two configurations of $\widehat{\mathcal{H}}$ which differ by the status of two spins. In this case there exists a configuration of $\widetilde{\mathcal{H}}$ connected to the two configurations of $\widehat{\mathcal{H}}$. Right panel: an example of two configurations of $\widehat{\mathcal{H}}$ which differ by the status of three spins. In this case there is no configuration of $\widetilde{\mathcal{H}}$ connected directly to both the two configurations of $\widehat{\mathcal{H}}$.

$\widehat{\mathcal{H}}$ as the set of the N configurations first neighbors of a given one, $\widetilde{\mathbf{n}}$, we see that by construction $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \rightarrow 0$ but now $A^{(\text{out})}(\widetilde{\mathbf{n}}) = N$ (indeed, here the $\dim \mathcal{H}_{\text{cond}}$ configurations associated to $V = -JN$ differ for the direction of two spins).

The above counter example, however, is rather nonphysical as it does not take into account how the structure of a physical potential operator V acts on the definition of $\mathcal{H}_{\text{cond}}$. The definition of $\mathcal{H}_{\text{cond}}$ is in principle arbitrary but the most interesting cases are those in which $\mathcal{H}_{\text{cond}}$ is defined directly from the structure of the operator V . The idea is to define $\mathcal{H}_{\text{cond}}$ through the configurations \mathbf{n} having potential levels $V(\mathbf{n}) = \langle \mathbf{n} | V | \mathbf{n} \rangle$ not larger than some threshold value $\max V_{\text{cond}}$, namely, $\widehat{\mathcal{H}} = \{ \mathbf{n} : V(\mathbf{n}) \leq \max V_{\text{cond}} \}$. For given N , if V has some physical origin, $\dim \mathcal{H}_{\text{cond}}$ is expected to be a fast growing function of $\max V_{\text{cond}}$, typically exponential. Notice, however, that this assumption holds true for not too large values of $\max V_{\text{cond}}$, being $\dim \mathcal{H}_{\text{cond}}$ limited by $\dim \mathcal{H}$. In fact, it holds true as far as $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \ll 1$. As a consequence, if $\dim \mathcal{H}_{\text{cond}} / \dim \mathcal{H} \ll 1$, the subgraph induced by K on the set $\widehat{\mathcal{H}}$, can effectively be treated as a regular Cayley tree of size $\dim \mathcal{H}_{\text{cond}}$ and degree N , i.e. a finite graph without loops where each node has degree N , except for its boundary, where the nodes have degree 1. This assumption corresponds to the usual tree-like approximation that holds true locally in many sparse graphs. By contrast, the subgraph induced by K on the set $\widetilde{\mathcal{H}}$ cannot be treated as a tree. In fact, we have to take into account that the total graph induced by K in \mathcal{H} , is a regular graph without an actual boundary; it is not a tree. As a consequence, we see that the complement of any tree in the total graph, and therefore also in the subgraph induced by K on the set $\widetilde{\mathcal{H}}$, cannot be treated as a tree either, see figure 3 for an illustrative example. More precisely, in the graphs associated to \mathcal{H} and $\widetilde{\mathcal{H}}$ there are loops whose shortest length l is of the order $l = \log(\dim \mathcal{H}) / \log(N)$.

As is known, one peculiar feature of the Cayley tree is the fact that its boundary constitutes a finite portion of its total number nodes, see for example [23]. Moreover, we have to take into account the constraint that the total number of outgoing links from $\widehat{\mathcal{H}}$ to $\widetilde{\mathcal{H}}$ must be equal to the total number of outgoing links from $\widetilde{\mathcal{H}}$ to $\widehat{\mathcal{H}}$. By making use of the mean numbers of outgoing links $\overline{A}_{\text{cond}}^{(\text{out})}$ and $\overline{A}_{\text{norm}}^{(\text{out})}$, along the boundaries $\widehat{\partial}$ and $\widetilde{\partial}$, respectively, we have (see figure 4 for an illustrative example)

$$\overline{A}_{\text{cond}}^{(\text{out})} |\widehat{\partial}| = \overline{A}_{\text{norm}}^{(\text{out})} |\widetilde{\partial}|, \tag{51}$$

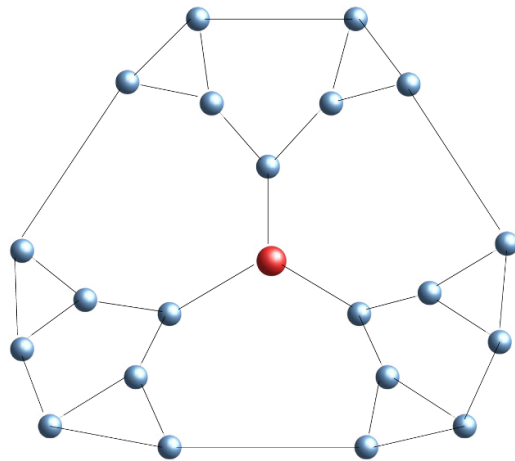


Figure 3. A regular graph of degree $A = 3$ drawn from the perspective of the ‘central’ red node. The subgraphs having a boundary at the distances $l = 1$ or $l = 2$ from the central node, i.e. those obtained by removing all the nodes at distance larger than l as well as all the links emanating from these removed nodes, are Cayley trees of degree $A = 3$ (except for the boundary, where the nodes have degree 1). However, the complements of these subgraphs are not trees. In particular, the complement of the case $l = 2$ is a regular graph of degree 2.

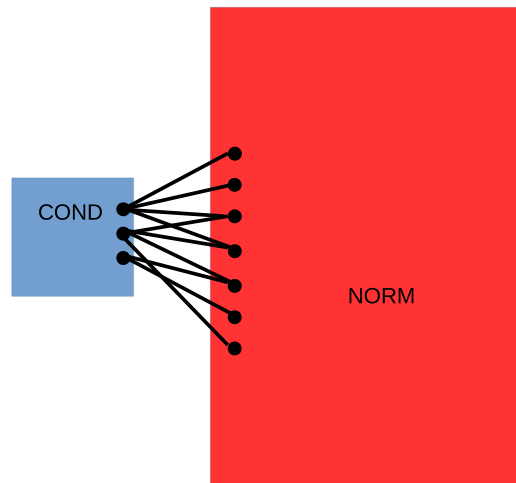


Figure 4. A schematic example of a cond–norm partition where the nodes (configurations) on the two boundaries, $\hat{\partial}$ and $\tilde{\partial}$, are put in evidence near the two adjacent sides. Also the links connecting the two boundaries are put in evidence. The $|\hat{\partial}| = 3$ nodes in $\hat{\partial}$ have degrees 4, 4, 2, while the $|\tilde{\partial}| = 7$ nodes in $\tilde{\partial}$ have degrees 1, 1, 2, 2, 2, 1, 1. We can read the total number of links connecting the two boundaries from cond to norm as $4 + 4 + 2 = 10 = \bar{A}_{\text{cond}}^{(\text{out})} |\hat{\partial}|$, or else from norm to cond as $1 + 1 + 2 + 2 + 2 + 1 + 1 = 10 = \bar{A}_{\text{norm}}^{(\text{out})} |\tilde{\partial}|$, where $\bar{A}_{\text{cond}}^{(\text{out})}$ and $\bar{A}_{\text{norm}}^{(\text{out})}$ are the mean numbers of the outgoing links of the two partitions. In this example we have $\bar{A}_{\text{cond}}^{(\text{out})} = 10/3$ and $\bar{A}_{\text{norm}}^{(\text{out})} = 10/7$.

which, if we call α_{cond} the coefficient providing $|\widehat{\partial}| = \alpha_{\text{cond}} \dim \mathcal{H}_{\text{cond}}$ and use $|\widetilde{\partial}| \leq \dim \mathcal{H} - \dim \mathcal{H}_{\text{cond}}$, gives

$$\overline{A}_{\text{cond}}^{(\text{out})} \alpha_{\text{cond}} \dim \mathcal{H}_{\text{cond}} \leq \overline{A}_{\text{norm}}^{(\text{out})} (\dim \mathcal{H} - \dim \mathcal{H}_{\text{cond}}) \leq \overline{A}_{\text{norm}}^{(\text{out})} \dim \mathcal{H}. \quad (52)$$

For a regular Cayley tree of degree N it is easy to see that $\alpha_{\text{cond}} \rightarrow 1^-$ so that equation (52) gives

$$\frac{\dim \mathcal{H}_{\text{cond}}}{\dim \mathcal{H}} \leq \frac{\overline{A}_{\text{norm}}^{(\text{out})}}{\overline{A}_{\text{cond}}^{(\text{out})}}. \quad (53)$$

Finally, since $\overline{A}_{\text{cond}}^{(\text{out})} = O(N)$, equation (53) proves that the condition $\overline{A}_{\text{norm}}^{(\text{out})}/N \rightarrow 0$ implies the condition $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$.

The above equation (53) is exact but it does not allow to prove the converse. Nevertheless, if we take into account the exponential growth with N of $\dim \mathcal{H}$, holding for most of the systems of interest, equation (53) leads us to make the following ansatz

$$\frac{\overline{A}_{\text{norm}}^{(\text{out})}}{\overline{A}_{\text{cond}}^{(\text{out})}} \sim -1/\log \left(\frac{\dim \mathcal{H}_{\text{cond}}}{\dim \mathcal{H}} \right), \quad (54)$$

which in turn implies that $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$ if and only if $\overline{A}_{\text{norm}}^{(\text{out})}/N \rightarrow 0$.

The ansatz (54) is compatible with equation (53) and is clearly satisfied in the case of the Grover model and its generalizations. To make concrete the ansatz with a more physical example, let us consider the interaction potential of the one-dimensional Ising model with periodic boundary conditions. If we represent the configurations by products of single spin states along the z axis, $|\mathbf{n}\rangle = |\sigma_1^z\rangle \otimes \cdots \otimes |\sigma_N^z\rangle$, with $\sigma_i^z = \pm 1$, $i = 1, \dots, N$, we have

$$\langle \mathbf{n} | V | \mathbf{n} \rangle = V(\mathbf{n}) = -J \sum_{i=1}^N \sigma_i^z \sigma_{i+1}^z. \quad (55)$$

We assume $J > 0$. We are free to define $\widehat{\mathcal{H}}$ (and then $\mathcal{H}_{\text{cond}} = \text{span}\{\widehat{\mathcal{H}}\}$) in several ways, and we want to see to what extent the conditions $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \rightarrow 0$ and $\overline{A}_{\text{norm}}^{(\text{out})}/N \rightarrow 0$ are equivalent. We can start by including in $\widehat{\mathcal{H}}$ the two lowest GSs with all parallel spins. Then we can enlarge $\widehat{\mathcal{H}}$ by including all the states in which one spin is reversed with respect to all the other $N - 1$ parallel ones and so on. Alternatively and more effectively, we can characterize any configuration by the number of cuts q in it, where a cut is present if, reading the sequence of the pointers σ_i^z for example from left to right, we meet an inversion. In terms of q equation (55) reads (we can have at most $N - 1$ number of cuts and we start by considering the two GSs in which all the spins are parallel)

$$V_q = -JN + 2Jq, \quad D(q) = 2 \binom{N-1}{q}, \quad q = 0, \dots, N-1, \quad (56)$$

where $D(q)$ is the number of configurations \mathbf{n} having potential $V(\mathbf{n}) = V_q$. We define $\widehat{\mathcal{H}}$ by introducing a threshold $\max V_{\text{cond}}$ as the maximum allowed potential value of its configurations. If we choose $\max V_{\text{cond}} = V_k$, we have $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}(k)$ with

$$\widehat{\mathcal{H}}(k) = \{\mathbf{n} : V(\mathbf{n}) \leq V_k\}, \quad \dim \mathcal{H}_{\text{cond}} = 2 \sum_{q=0}^k \binom{N-1}{q}. \quad (57)$$

By recalling that $\binom{N}{k}/2^N$ tends, for $N \rightarrow \infty$, to a Dirac delta function centered at $k = N/2$, we see that

$$\frac{\dim \mathcal{H}_{\text{cond}}}{\dim \mathcal{H}} \rightarrow 0 \quad \text{as soon as} \quad \frac{k}{N} < \frac{1}{2}. \quad (58)$$

On the other hand, we can verify that the condition on $A_{\text{norm}}^{(\text{out})}$ is satisfied whenever $k/N < 1/2$ as follows. Given k , let us consider the boundary of $\tilde{\mathcal{H}}$

$$\tilde{\partial} = \{\mathbf{n} : V(\mathbf{n}) = V_{k+1}\}. \quad (59)$$

Given $\tilde{\mathbf{n}} \in \tilde{\partial}$, by inverting one of its spins located at a cut, the cut will be either shifted or removed, leaving the potential unchanged or lowered by $2J$ (and then entering $\hat{\mathcal{H}}$), respectively. It is instructive to consider the two opposite regimes: k very small, and k very large. The former regime occurs when $k \ll N$ as when a few isolated spins are antiparallel to the others. In this case we have $A_{\text{norm}}^{(\text{out})}(\tilde{\mathbf{n}}) = O(k)$. The other regime occurs when there are nearly half spins up and half spins down, i.e. when $k \sim N/2$, where $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} = O(1)$, and here we have $A_{\text{norm}}^{(\text{out})}(\tilde{\mathbf{n}}) = O(N)$. In the intermediate regime we have $A_{\text{norm}}^{(\text{out})}(\tilde{\mathbf{n}}) = o(N)$, i.e. non-extensive. This example shows that the conditions $A_{\text{norm}}^{(\text{out})}/N \rightarrow 0$ and (58) are essentially equivalent and that the ansatz (54) is realized with $\dim \mathcal{H}_{\text{cond}}/\dim \mathcal{H} \sim \exp(k - N)$. However, we warn that, as we have shown in [11], in the case of the Ising model, equation (11) has no solution, whatever k , so that our theory turns out to be not useful in such a case, as it always occurs when the QPT is second-order. Yet, the above picture is very general and can be similarly applied to many models, as in the particularly important case of interacting fermions [17] (where the QPT is first-order). We have directly checked that in all these models the condition $A_{\text{norm}}^{(\text{out})}(\tilde{\mathbf{n}})/N \rightarrow 0$ turns out to be satisfied and that the ansatz (54) holds true.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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