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Intensive temperature and quantum correlations for refined quantum measurements

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Abstract – We consider the concept of temperature in a setting beyond the standard thermodynamics prescriptions. Namely, rather than restricting to standard coarse-grained measurements, we consider observers able to master any possible quantum measurement —a scenario that might be relevant at nanoscopic scales. In this setting, we focus on quantum systems of coupled harmonic oscillators and study the question of whether the temperature is an intensive quantity, in the sense that a block of a thermal state can be approximated by an effective thermal state at the same temperature as the whole system. Using the quantum fidelity as figure of merit, we identify instances in which this approximation is not valid, as the block state and the reference thermal state are distinguishable for refined measurements. Actually, there are situations in which this distinguishability even increases with the block size. However, we also show that the two states do become less distinguishable with the block size for coarse-grained measurements —thus recovering the standard picture. We then go further and construct an effective thermal state which provides a good approximation of the block state for any observables and sizes. Finally, we point out the role that entanglement plays in this scenario by showing that, in general, the thermodynamic paradigm of local intensive temperature applies whenever entanglement is not present in the system.

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A characteristic trait of macroscopic matter is the simplicity with which it can be typically described in physical terms. The long-lasting success of thermodynamics is built upon this evidence: few thermodynamic variables are sufficient to effectively describe a piece of matter made of a huge number of particles. The origin of this simplification lies in the fact that macroscopic objects are usually probed by extremely *coarse measurements*. Specifically, macroscopic observations sense only averages and just few properties —namely, thermodynamic variables like entropy or temperature— suffice to describe the system after such averaging [1].

A question arises whether this picture breaks down when the standard requirement of coarse measurements is relaxed and more general measurements —in particular, more *refined measurements*— are at disposal. Of course, the use of refined measurements goes beyond the standard thermodynamic prescriptions. Nonetheless, at

nanoscopic scales, these measurements are foreseeable [2] and this may imply significant deviations from the standard (macroscopic and coarse-grained) thermodynamic scenario. In particular we will consider here quantum systems for which some deviations from thermodynamics have been already explored at small scales [3,4]. Furthermore, a series of recent results suggests that some hypothesis commonly invoked in thermodynamics can be actually relaxed in a quantum setting. This is, for example, the case of subjective lack of knowledge —usually invoked to prove the emergence of the canonical ensemble— which has been shown to be unnecessary [5]. In general there are evidences that thermodynamics principles can be applied to non-standard scenarios, beyond the ones originally envisaged [6].

Here we address these considerations focusing on the concept of temperature. In particular, we test whether the temperature is an intensive quantity by taking into

account both coarse- and refined-measurement scenarios. In fact, considering a quantum setting, previous results have shown that the temperature may not be intensive at small scales —where coarse measurements more evidently show their inadequacy— resulting in the fact that subparts of thermal states may no longer be described as thermal states with the same global temperature as the whole system [6]. However, the role of measurements in this context has not been taken into account in detail. In addition, the mechanism that originates this departure from the standard thermodynamic behaviour is still unclear. In analogy with the case of classical systems, one might expect that the energy balance between subparts of the system should be the main responsible for it. However, we show that this is not the case and that other mechanisms play a major role.

In order to tackle the foregoing questions, we consider quantum systems consisting of coupled harmonic oscillators in a thermal state¹. We study the distinguishability between a block of harmonic oscillators and a reference thermal block at the same temperature as the whole system. We first provide instances in which the temperature is no longer intensive, in the sense that under refined measurements the state of the block can be distinguished from the reference thermal state. Contrary to the intuition stemming from the standard setting of coarse-grained measurements, the breakdown of intensiveness is more easily observed for larger systems. Second, despite this first result, we see how the standard thermodynamic situation (where the state of the block and the reference thermal state do become more indistinguishable for larger systems) is recovered for coarse-grained observables. Third, we show that for any type of observables it is possible to define an appropriate effective thermal state approximating the block state, even for small sizes.

As said, the origin of the deviation from intensiveness relies on the capacity to perform refined measurements. The fact that larger systems exhibit larger deviations reveals that the energy balance between subparts of the system does not play a significant role. On the other hand we will relate this deviation with the presence of correlations in the system. Specifically, we show that the presence of genuine quantum correlations is related to the departure from the intensive behaviour: when quantum entanglement is significantly present, the temperature ceases to be intensive for refined measurements; vice versa, for vanishing entanglement the thermodynamic paradigm of intensive temperature applies for *any* possible measurements.

Our approach to this problem stems from concepts and methods proper of quantum information theory [7], for a twofold reason. First, as said, we assess the intensiveness of

¹Let us stress that we consider systems that have already undergone thermalization, possibly via weak coupling with a thermal environment. We are not addressing the thermalization dynamics leading to the thermal state of the oscillators and our approach is static in this sense.

temperature by considering the distinguishability between a region of the system and a thermal state. For this purpose we use the quantum fidelity, a quantum information concept that quantifies the distinguishability between two states given *any* possible measurement. Second, in order to investigate the origin of the non-intensive behaviour of temperature, we distinguish quantum from classical correlations. This requires the use of entanglement quantifiers, since correlation functions commonly considered in condensed-matter theory are not sensitive to this distinction.

Local states and temperature. — Let us consider a system S composed of a macroscopic number of elementary constituents that —after having thermalized with a proper environment— lies in a canonical state. The interactions among the system are described by the Hamiltonian H . Following refs. [4,6,8], we adopt here the following notion of *local intensiveness*: given S at temperature T , we say that the temperature is locally intensive when the block B can be described by a canonical state at the same temperature T . More specifically, the system state is given by $\Omega(\beta) = \exp[-\beta H]/Z$, where β is the inverse temperature, and Z the partition function. The actual state of the block is thus given by

$$\rho_B(\beta) = \text{Tr}_R \Omega(\beta) = \text{Tr}_R(\exp[-\beta H]/Z), \quad (1)$$

where the trace is over the rest of the system. We say that the temperature is intensive when $\rho_B(\beta) \approx \Omega'_B(\beta)$, being $\Omega'_B(\beta)$ a thermal state for the block,

$$\Omega'_B(\beta) = \exp[-\beta H'_B]/Z', \quad (2)$$

where H'_B is an effective Hamiltonian acting only on B .

Clearly, H'_B cannot be left arbitrary. Here we introduce a generic procedure to identify a proper block Hamiltonian. In particular, we impose the following requirements to H'_B : (R_1) it is temperature independent; (R_2) it gives rise to an intensive behaviour for high temperatures. Requirement (R_1) is motivated by the fact that if H'_B was free to change with β the problem would lose relevance. In fact, any state ρ can be trivially written as $\rho = e^{-\beta H}/Z$ with arbitrary β for a proper H . Concerning (R_2), it is motivated by the physical request of recovering the standard intensive behaviour for high temperatures. The choice of these two requirements, a part from the mentioned physical motivations, turns out to have sensible benefits *a posteriori*. In fact, we will see that this procedure singles out a unique Hamiltonian H'_B which, in turn, coincides with the quantized version of the classical Hamiltonian associated to the classical analogue of our quantum system. Let us stress that here we consider these two requirements for a specific family of Hamiltonian systems. However, the procedure can be applied more in general (see also ref. [8]).

In what follows, we quantify the degree of temperature intensiveness by the distinguishability between

the two quantum states, $\rho_B(\beta)$ and $\Omega'_B(\beta)$, under any possible measurement. This concept is captured by the quantum fidelity [9], defined for two generic states σ_1 and σ_2 as $F[\sigma_1, \sigma_2] = \text{Tr} [\sqrt{\sigma_1 \sigma_2 \sqrt{\sigma_1}}]^{1/2}$. Recall that the fidelity is unity only when two states are identical, and a given amount of fidelity gives the distance between the two set of data obtained from the measurement that—among all possible measurements—distinguishes at best the two considered states. We introduce then the intensive fidelity

$$F_I(\beta) = F[\rho_B(\beta), \Omega'_B(\beta)], \quad (3)$$

which decreases as temperature loses its intensive character and approaches unity when it is intensive. In the latter case, no measurement—no matter how refined—can distinguish the state of the block from a thermal one.

From now on, we will say that the temperature undergoes a breakdown of intensiveness whenever $F_I(\beta)$ is significantly lower than unity. As said, this means that an observer able to perform refined measurements can detect that the actual state of block B is not a thermal state at the same temperature as the whole system S . However, this by no means implies that the temperature ceases to be intensive for standard thermodynamic measurements—an undisputed property that clearly remains valid under the prescriptions of thermodynamics. Let us also stress here that the fidelity is a very sensitive measure, in the sense that apparently small differences between two states can lead to very low values of the fidelity². This, rather than being a misbehaviour, is just a consequence of the fact that fidelity quantifies the distinguishability of two states under any possible measurement.

Harmonic systems. – In this work we focus on quantum harmonic systems (see fig. 1) composed of n_S interacting oscillators defined by position and momentum operators q_i and p_i , respectively ($i = 1, \dots, n_S$). Introducing the vector $X = (q_1, \dots, q_{n_S}, p_1, \dots, p_{n_S})$, the Hamiltonian $H = X(V \oplus \mathbb{1}_S)X^T$ describes the system, with $\mathbb{1}_S$ denoting the $n_S \times n_S$ identity matrix. Here the ground and thermal states are Gaussian, thus permitting the use of powerful methods—developed in the context of quantum information theory—for the calculation of fidelity [10] and quantum correlations [11]. The Hamiltonian H models a variety of physical systems, ranging from vibrational degrees of freedom in crystal lattices and ion traps to the free scalar Klein-Gordon field on a lattice [12]. Besides, being exactly solvable³, these models are a standard testbed in quantum thermodynamics [3,4,6].

²For example, consider two product states composed of a huge number of spins 1/2 which differ only in one spin (e.g., $|\uparrow, \dots, \uparrow, \downarrow\rangle$ and $|\uparrow, \dots, \uparrow, \uparrow\rangle$). The fidelity between these states is zero (they are perfectly distinguishable), despite being almost identical in a coarse sense.

³The generalization of our analysis to non-integrable systems is outside the scope of the present investigation and could be the subject of future studies.

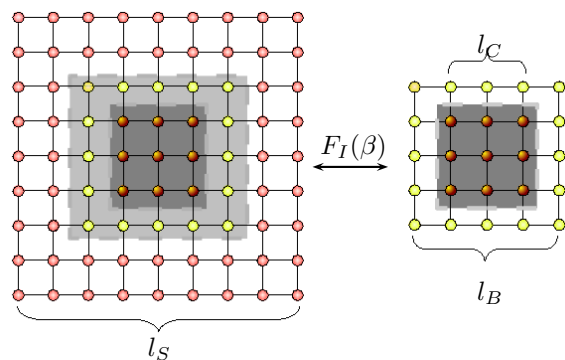


Fig. 1: (Colour on-line) Schematic representation of a two-dimensional harmonic lattice composed of $n_S = l_S \times l_S$ oscillators set up in a thermal state. The reduced state of a distinguished block of it (light plus dark-grey region), composed of $n_B = l_B \times l_B$ oscillators, is compared to a thermal state of a $l_B \times l_B$ -oscillator system, as in the right panel, via the fidelity $F_I(\beta)$ (see text). The cores of the two systems, both composed of $n_C = l_C \times l_C$ oscillators (dark-grey regions), are also shown.

We first derive the effective Hamiltonian H'_B for the block by imposing the requirements (R₁) and (R₂) introduced above. Being Gaussian, the states $\Omega(\beta)$ are completely described by their covariance matrix $\gamma(\beta)$. The elements of the latter are defined as $\gamma(\beta)_{kl} = \text{Re}(\text{Tr}\{\Omega(\beta)[X_k - \bar{X}_k][X_l - \bar{X}_l]\})$, where $\bar{X}_k = \text{Tr}\{\Omega(\beta)X_k\}$. The explicit expression of $\gamma(\beta)$ is

$$\gamma(\beta) = [V^{-1/2}W(\beta) \oplus [V^{1/2}W(\beta)]], \quad (4)$$

where $W(\beta) = \mathbb{1}_S + 2[\exp(\beta V^{1/2}) - \mathbb{1}_S]^{-1}$. The high-temperature limit of $\gamma(\beta \rightarrow 0)$ is given by $\frac{2}{\beta}[V^{-1} \oplus \mathbb{1}_S]$. From the latter one can easily obtain the high-temperature limit of the block covariance matrix, denoted as $\gamma_B(\beta \rightarrow 0)$. Let us recast V as a block matrix,

$$V = \begin{pmatrix} V_B & V_{BR} \\ V_{BR}^T & V_R \end{pmatrix}, \quad (5)$$

where V_B (V_R) refers to the block (rest) and V_{BR} to the interaction between B and R . In this notation $\gamma_B(\beta \rightarrow 0) = \frac{2}{\beta}[V'^{-1} \oplus \mathbb{1}_B]$, where we introduce an effective potential matrix $V' = V_B - V_{BR}V_R^{-1}V_{BR}^T$. The unique choice of the effective Hamiltonian H'_B of the block is $H'_B = X_B(V' \oplus \mathbb{1}_B)X_B^T$, where X_B denotes the operators referring to the block, which satisfies both requirements (R1) and (R2).

Before proceeding further, let us consider the classical analogue of the quantum systems under consideration. This helps in clarifying our approach for the choice of H'_B and in singling out the genuine quantum aspects responsible for the intensiveness breakdown. Let us denote with H_c the classical version of the Hamiltonian H , where the positions and momenta in X are classical phase space coordinates. At thermal equilibrium, the system is described by a Boltzmann-Gibbs distribution

$P(X) = e^{-\beta H_c}/Z$. The distribution of the block $P_B(X_B)$ is obtained after integrating $P(X)$ over the oscillators in R . This results in the distribution $P_B(X_B) = e^{-\beta H'_{B,c}}/Z'$, where $H'_{B,c} = X_B(V' \oplus \mathbb{1}_B)X_B^T$ and the potential matrix turns out to coincide with V' introduced above. Indeed, this further clarifies the physical meaning of H'_B , since it can be interpreted as the quantized version of $H'_{B,c}$. Notice that since $V' \neq V_B$ the oscillators of the block are subjected to a renormalization of their bare frequency, a well-known effect in open systems [13]. Remarkably, the expression of $P_B(X_B)$ shows that the temperature is always intensive in classical harmonic systems (for any block size, temperature, and coupling). This fact already suggests that any possible deviation from intensiveness in quantum harmonic systems should have a genuine quantum origin.

In what follows, we focus on one- and two-dimensional harmonic lattices endowed with periodic boundary conditions and composed of n_S oscillators interacting with their nearest neighbours. The potential matrix for 1D systems can be expressed as a $n_S \times n_S$ circulant matrix of the form $V_1 = \text{circ}\{1, -c, 0, \dots, 0, -c\}$. For 2D systems, composed of $n_S = l_S \times l_S$ oscillators (see fig. 1), one has instead a block-circulant matrix:

$$V_2 = \text{circ}\{V_1, -c\mathbb{1}_{l_S}, 0_{l_S}, \dots, 0_{l_S}, -c\mathbb{1}_{l_S}\}. \quad (6)$$

where V_1 , $\mathbb{1}_{l_S}$, and 0_{l_S} are in turn $l_S \times l_S$ matrices. The coupling parameter c belongs to $[0, 1/2^d)$, where $d = 1, 2$ is the dimension, and the system is critical at zero temperature for $c \rightarrow 1/2^d$.

Intensiveness breakdown for refined quantum measurements. – We have now introduced all the ingredients needed to study the behaviour of the intensive fidelity (3). The dependence of $F_I(\beta)$ on the block size is plotted in figs. 2(a) and (b), for 1D and 2D systems, respectively. Notice first that there are parameters for which $F_I(\beta)$ is very close to unity: the block is there well approximated by a thermal state even when refined measurements are available. This means that, in these cases, the thermodynamic paradigm of local intensive temperature applies, even beyond the standard thermodynamics setting. However, there are also parameters for which the intensive fidelity is significantly smaller than unity. Actually, an interesting behaviour emerges: the fidelity either stays constant (1D) or drops (2D) as the block gets larger, contrary to what considerations on the energy balance between subparts of the system would suggest. In particular, for 2D systems the fidelity may drop to zero in the limit of macroscopically large blocks, despite the interactions at the boundary of the block being negligible with respect to the ones in its bulk. That is, an observer able to master all possible measurements will detect the failure of temperature intensiveness easier for larger systems.

Clearly, the energy balance between subparts of the system cannot be responsible for this counterintuitive

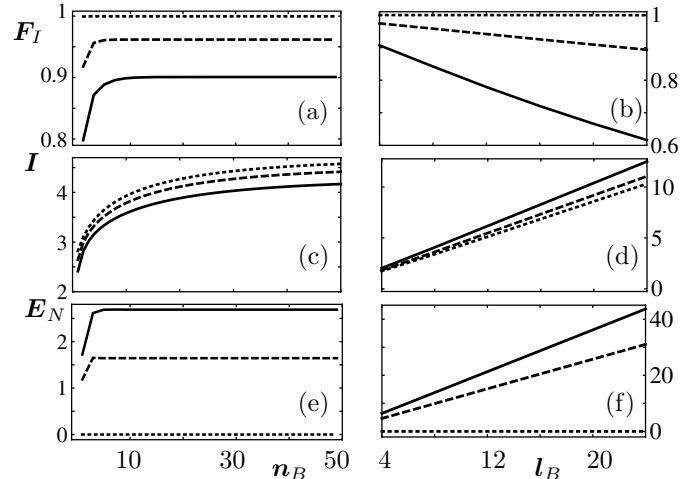


Fig. 2: Left panels: from top to bottom: fidelity $F_I(\beta)$, mutual information $I(\beta)$, and negativity of entanglement $E_N(\beta)$ for 1D systems as a function of the block size n_B (the system is composed of $n_S = 400$ oscillators and the coupling is $c = 0.4999$). Right panels: from top to bottom: $F_I(\beta)$, $I(\beta)$, and $E_N(\beta)$ for 2D systems as a function of l_B ($n_B = l_B \times l_B$, $n_S = 4n_B$, $c = 0.24$). In all panels, the inverse temperature is $\beta = 1, 5, 10$ for the dotted, dashed, and solid lines, respectively. Note that all the plotted quantities follow an area law.

result. In particular, the standard thermodynamic argument to show the intensiveness of temperature (or, equivalently, the extensiveness of the entropy) invokes the fact that the interaction at the border between B and R becomes negligible, for large block sizes, with respect to the energy of B and R [14]. However, in the refined-measurement setting adopted here, this border effect may still be—and in fact happens to be—relevant. More specifically, correlations are responsible for this result. Recall that in the considered systems, the correlations between B and R follow an *area law*: when increasing B , correlations saturate for 1D systems—since the boundary between B and R stays constant—while they change linearly with l_B for 2D systems. This is precisely the same behaviour observed for the intensive fidelity. The crucial point identified here is that $F_I(\beta)$ is such a highly sensitive quantity that detects boundary effects (see footnote ²).

In order to confirm the foregoing intuition, we compare the core of the block and the core of the reference thermal state by tracing out few boundary layers of the two states (see fig. 1 for 2D systems with core composed of $n_C = l_C \times l_C$ oscillators). The resulting fidelity is indistinguishable from unity, as shown in fig. 3. We can also see that all the deviation from intensiveness resides in the shell surrounding the core. This observation has two operational consequences. First, the actual state and the reference thermal state become more indistinguishable when increasing the size for standard coarse-grained measurements. Consider, for instance, the internal energy

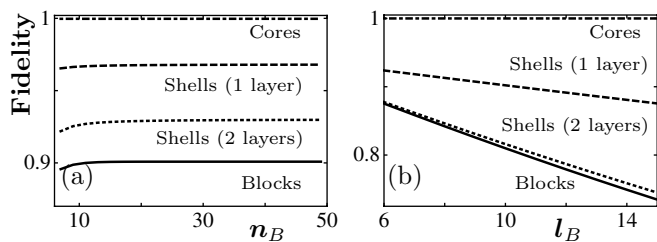


Fig. 3: Right and left panels correspond to 1D and 2D systems, respectively. From bottom to top: fidelities between the distinguished block $\rho_B(\beta)$ and the reference thermal state $\Omega_B(\beta)$, their shells (composed of two and one layer), and their cores (with $n_C = n_B - 2$ for 1D and $l_C = l_B - 2$ for 2D). We set $\beta = 10$ in both panels and other parameters as in fig. 2.

$U = \langle H \rangle$. For large systems, both $\text{Tr}(\rho_B H)$ and $\text{Tr}(\Omega_B H)$ are approximately equal and given by the value of U at the core. Clearly, the same reasoning can be applied to any observable consisting of averages of local observables. Second, it is possible to define an effective thermal state for any size and observable. It suffices to consider a thermal state for a slightly bigger system, $B + \varepsilon$, and trace out the shell ε to take into account boundary effects. That is, the resulting thermal state for the block reads

$$\tilde{\Omega}_B(\beta) = \text{Tr}_\varepsilon \Omega_{B+\varepsilon}(\beta). \quad (7)$$

As shown in fig. 3, the fidelity between the actual state and this effective thermal state is always very close to unity. This approximation works remarkably well even for small sizes, near criticality and for all observables.

Quantum and classical correlations. – The previous analysis points out the key role that correlations play for an intensive behaviour of the temperature. Note that, as the system is mixed, both classical and quantum correlations can coexist. Our last goal is to identify which correlations are responsible for the breakdown of temperature intensiveness.

The analysis on classical harmonic systems already suggested that classical correlations should play no role. Another intuition pointing at the relevance of quantum correlations stems from the following argument. Consider a generic quantum system and two extreme cases, zero and infinite temperature. In the latter case, the system is factorized and maximally mixed, as well as any block of it: the temperature is intensive. For zero temperature, instead, two situations might occur (provided the ground state is pure; *i.e.*, any possible degeneracy has been broken): either the ground state is entangled, thus enforcing non-zero entropy and non-zero temperature for any block, or it is factorized and any block is pure. Thus, for these two extreme cases we have that only in the absence of entanglement the temperature is intensive.

To address the origin of the intensiveness breakdown quantitatively, let us consider both the total correlations, given by the mutual information $I(\beta)$, and a form of

genuinely quantum correlations, given by the entanglement negativity $E_N(\beta)$ [12]. We have calculated $I(\beta)$ and $E_N(\beta)$ in the B vs. R partition. In figs. 2(c), (d), (e) and (f) we can see that both quantities follow an area law, as expected [12]. There is, however, an important difference: while $I(\beta)$ takes finite values in the limit of infinite temperature [15], $E_N(\beta)$ drops to zero. That is, while total correlations are present even in situations where the intensive fidelity is nearly unity, our calculations indicate a much better agreement between the presence of entanglement and intensiveness breakdown.

Finally, in order to get a better picture of this connection, we introduce size-independent quantities. We focus here on 2D systems, but similar results hold true for 1D. Consider the slope α_F of the fidelity decay as a function of the block size: $F_I(\beta) \approx \alpha_F l_B$ (in the case of 1D systems one should consider the fidelity saturation value). This slope gives an assessment of the intensiveness breakdown, since the smaller it is, the more intensive the temperature. This allows us to depict a complete “intensiveness phase diagram” in the c - β plane, by plotting the contours of α_F (see fig. 4(a)). We recognize two regions: for low temperatures and strong coupling the system behaves non-intensively, whereas intensiveness is recovered in the region of high temperatures or weak coupling. A crossover between these two behaviours appears for intermediate β and c .

Following the same procedure for mutual information and entanglement, we introduce the slopes α_I and α_E , respectively, and plot their “phase diagrams” (see figs. 4(b) and (c)). We can see that total correlations play no role in the breakdown of intensiveness, showing no relation with the regions individuated in fig. 4(a). On the other hand, the relation between intensiveness and entanglement is enforced, pointing out the role of genuine quantum correlations in detecting the intensive region. In fact, similar considerations hold true also if we consider other size-independent quantities. For example, the correlation length ξ (given by $\langle q_i q_{i+r} \rangle \propto \exp\{-r/\xi\}$) —extensively studied in condensed-matter systems but unable to distinguish quantum from classical correlations— fails in detecting the intensive region and shows a similar behaviour as the mutual information (see fig. 4(d)). Although we cannot claim that the intensiveness breakdown *strictly* depends on the block negativity, as the contour plots of figs. 4(a) and (c) do not strictly coincide, temperature ceases to be intensive in the regions where entanglement is significantly present. Vice versa, without quantum correlations the thermodynamic paradigm of intensive temperature applies.

In conclusion, we have tested the concept of intensive temperature when the standard thermodynamics prescription of coarse measurement is relaxed and more refined measurements are at disposal. For systems composed of quantum oscillators, we have seen that the thermodynamic paradigm of local intensive temperature applies also to this setting whenever the presence of entanglement in the

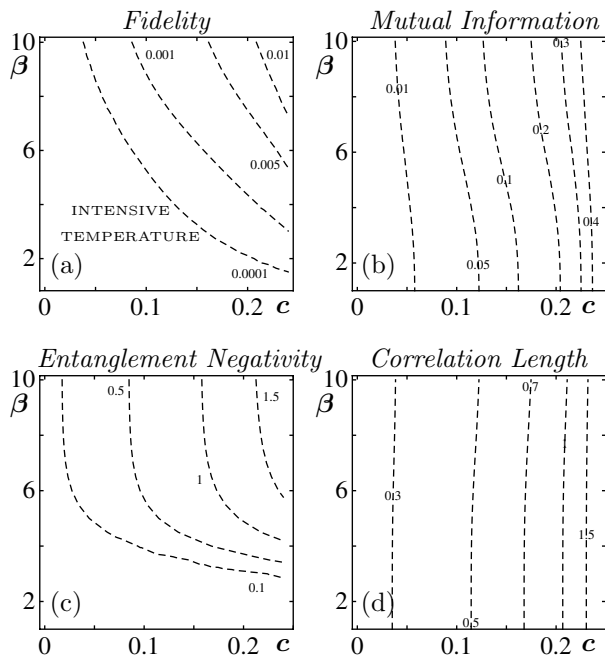


Fig. 4: Contour plots of the following quantities: (a) slope α_F of the fidelity; (b) slope α_I of the mutual information; (c) slope α_E of the negativity of entanglement; (d) two-point correlation length (see text). Panel (a) shows that the temperature is locally intensive for high temperatures or weak coupling. The quantities in the right panels ((b), (d)) —insensitive to the distinction between quantum and classical correlations— are almost temperature independent, thus failing to identify regions where temperature is not intensive. On the other hand, the negativity of entanglement —an indicator of purely quantum correlations— is effective in singling out the loss of intensiveness. The system is a 2D lattice with $n_S = 400$.

system is negligible. This extends the concept of temperature, and assesses its limits of validity, to a scenario beyond the standard one and that might be relevant for future technologies at mesoscopic and nanoscopic scale.

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