

Scaling behavior of interactions in a modular quantum system and the existence of local temperature

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(received 19 June 2003; accepted in final form 15 December 2003)

PACS. 05.30.-d – Quantum statistical mechanics.

PACS. 05.70.Ce – Thermodynamic functions and equations of state.

PACS. 65.80.+n – Thermal properties of small particles, nanocrystals, nanotubes.

Abstract. – We consider a quantum system of fixed size consisting of a regular chain of n -level subsystems, where n is finite. Forming groups of N subsystems each, we show that the strength of interaction between the groups scales with $N^{-1/2}$. As a consequence, if the total system is in a thermal state with inverse temperature β , a sufficient condition for subgroups of size N to be approximately in a thermal state with the same temperature is $\sqrt{N} \gg \beta \delta E$, where δE is the width of the occupied level spectrum of the total system. These scaling properties indicate on what scale local temperatures may be meaningfully defined as intensive variables. This question is particularly relevant for non-equilibrium scenarios such as heat conduction, etc.

Introduction. – Thermodynamics has successfully been applied to the description of macroscopic systems since more than a century. For that reason this theory enjoys widespread acceptance. Nevertheless, its microscopic foundation is, in most cases, not well understood.

The theory of thermodynamics is based on the notions of extensive and conjugate intensive thermodynamic variables. The existence of the thermodynamical limit in a mathematical sense has been shown for many fundamental cases [1–3]. The standard proofs are based on the idea that, as the spatial extension increases, the surface of a region in space grows slower than its volume. If the interaction potential is short-ranged enough, one can show that the “effective” interactions between one region and another become negligible in the limit of infinite size, implying extensivity.

However, the scaling behavior of the interactions with the size of those regions has, to our knowledge, not been studied in any detail yet. While it has been shown that they vanish in the thermodynamical limit, it remains unclear what happens in situations that are in some sense only close to this limit. There is not even a precise understanding of what “close” means in that case.

For standard applications of thermodynamics, this might not pose any serious problem since the number of particles within any region is so large that deviations from infinite systems may safely be neglected. Nevertheless, the differences should become important when the considered regions are significantly smaller. It is here where a quantum approach becomes imperative [4].

The applicability of thermodynamical concepts to mesoscopic or even microscopic systems has intensively been discussed in recent years [5], since nano-scale physics has attracted increased attention [6]. Due to the advance of experimental techniques, the measurement of thermodynamic quantities like temperature with a spatial resolution on the nanometer scale seems within reach [6–9]. These techniques have already been applied for a new type of scanning microscopy, using a temperature sensor [10, 11], that shows resolutions below 100 nm. An important question thus arises [6]: Down to what spatial scale does a meaningful notion of temperature exist at all?

In this paper we consider a quantum system of fixed Hilbert-space dimension dim , composed of identical elementary n -level subsystems. We form n_G identical groups of N subsystems each ($dim = n^{n_G N}$) and show that the interaction strength between the groups scales inversely proportional to \sqrt{N} . Based on this scaling relation and assuming the total system to be in a thermal state, we analyse for what group size N a thermodynamical description of the individual group is appropriate. The results are confirmed by numerical studies for a chain of 8 spins. For this chain, partitions into two 4-spin-groups, four 2-spin-groups and eight single spins are considered.

Scaling law. – We consider a chain of identical n -level systems with identical nearest-neighbour interactions. The Hamiltonian of such a linear chain may be written as

$$H = \sum_j h_{\text{loc}}(j) + h_{\text{int}}(j, j+1), \quad (1)$$

where the index j labels the elementary subsystems. The local terms $h_{\text{loc}}(j)$ and the nearest-neighbour interactions $h_{\text{int}}(j, j+1)$ have the form [12]:

$$\begin{aligned} h_{\text{loc}}(j) &= \frac{n}{2} \sum_{\alpha} A_{\alpha} \sigma_{\alpha}(j), \\ h_{\text{int}}(j, j+1) &= \frac{n^2}{4} \sum_{\alpha, \beta} C_{\alpha\beta} \sigma_{\alpha}(j) \sigma_{\beta}(j+1). \end{aligned} \quad (2)$$

Here, the $\sigma_{\alpha}(j)$ are $SU(n)$ generators with $\alpha, \beta = 1, 2, \dots, n^2 - 1$, n being the dimension of one subsystem. For the $SU(n)$ generators we adopt the trace relations [12]:

$$\begin{aligned} \text{Tr}[\sigma_{\alpha}(i)] &= 0, \\ \text{Tr}[\sigma_{\alpha}(i) \sigma_{\beta}(j)] &= 2 \frac{dim}{n} \delta_{ij} \delta_{\alpha\beta}, \end{aligned} \quad (3)$$

where the trace (Tr) has to be taken over the whole system of dimension dim . As a consequence, the trace over one elementary subsystem reads: $\text{Tr}_j[\sigma_{\alpha}(j) \sigma_{\beta}(j)] = 2\delta_{\alpha\beta}$. The coefficients in eq. (2) are then given by $A_{\alpha} = \text{Tr}(H \sigma_{\alpha}(i))/dim$ and $C_{\alpha\beta} = \text{Tr}(H \sigma_{\alpha}(i) \sigma_{\beta}(i+1))/dim$, respectively, and taken to be independent of i . We assume periodic boundary conditions and H to be traceless.

If we now form n_G groups of N subsystems each, we can split the Hamiltonian H into two parts,

$$H = H_N^{(0)} + I_N, \quad (4)$$

where $H_N^{(0)}$ is the sum of the Hamiltonians of the individual groups and I_N describes the interaction between each group and its nearest neighbour,

$$I_N = \sum_i h_{\text{int}}(iN, iN + 1). \tag{5}$$

We label the eigenstates of the total Hamiltonian H and its energies by Greek indices and eigenstates and energies of the group Hamiltonian $H_N^{(0)}$ by Latin indices, *i.e.*

$$H|\mu\rangle = E_\mu|\mu\rangle \quad \text{and} \quad H_N^{(0)}|j_N\rangle = E_{j_N}|j_N\rangle. \tag{6}$$

Obviously, the $|j_N\rangle$ are simply products of group eigenstates. We now proceed to compare two characteristic quantities of the system according to eq. (4).

First, consider the identity

$$\sum_\mu (E_\mu - E_{j_N})^2 |\langle j_N | \mu \rangle|^2 = \langle j_N | I_N^2 | j_N \rangle, \tag{7}$$

where the left-hand side can be interpreted as the mean-squared energy distance between a level E_μ and the energy E_{j_N} . The average of eq. (7) over all j_N is identical with \bar{I}_N^2 , where

$$\bar{I}_N \equiv \sqrt{\frac{\text{Tr}(I_N^2)}{\text{dim}}} = \frac{n}{2} \sqrt{n_G \sum_{\alpha,\beta} C_{\alpha\beta}^2}. \tag{8}$$

Here we have used eq. (3).

The second quantity of interest is the width of the distribution of the energy levels of the total system $\overline{\delta E}$ around the mean energy $\bar{E} = \text{Tr}(H)/\text{dim} = 0$:

$$\overline{\delta E} \equiv \sqrt{\sum_\nu \frac{(E_\nu - \bar{E})^2}{\text{dim}}} = \sqrt{\frac{\text{Tr}[(H - \bar{E})^2]}{\text{dim}}} = \sqrt{N} \frac{n}{2} \sqrt{n_G \left(\sum_{\alpha,\beta} C_{\alpha\beta}^2 + \frac{2}{n} \sum_\alpha A_\alpha^2 \right)}. \tag{9}$$

Here we have again used eq. (3). Combining eqs. (8) and (9), we get the following scaling law:

$$\bar{I}_N \leq \frac{1}{\sqrt{N}} \overline{\delta E}. \tag{10}$$

Note that this law is a property of the Hamiltonian (1) and does not depend on the state of the system. The equality sign applies, if the local terms vanish, $A_\alpha = 0$. Equation (10) does not depend on the convention used in eq. (3), since normalisations cancel. It is straightforward to see that the same scaling law holds for a three-dimensional lattice with cubes of N^3 subsystems as the subgroups.

Relation (10) has been derived here for a perfectly homogenous system. However, it is evident by means of stationary perturbation theory that it still holds approximately for systems with small disorder.

Distributions. – We now use the scaling law (10) to estimate the density matrix elements of the groups of N subsystems assuming that the total system is in a thermal state with the density matrix

$$\langle \mu | \hat{\rho} | \nu \rangle = \frac{e^{-\beta E_\mu}}{Z} \delta_{\mu\nu} \tag{11}$$

in the eigenbasis of H . Here, Z is the partition sum and $\beta = (k_B T)^{-1}$ the inverse temperature. Transforming the density matrix (11) into the eigenbasis of $H_N^{(0)}$, we obtain

$$\langle j|\hat{\rho}|j\rangle = \sum_{\mu} |\langle j|\mu\rangle|^2 \frac{e^{-\beta E_{\mu}}}{Z} = \frac{e^{-\beta E_j}}{Z} \sum_{\mu} |\langle j|\mu\rangle|^2 \exp[-\beta(E_{\mu} - E_j)] \quad (12)$$

(for simplicity we skip the index N from now on).

A thermodynamical description of the groups of N subsystems by canonical density matrices with the same inverse temperature β is appropriate, if $\langle j|\hat{\rho}|j\rangle$ was approximately proportional to $\exp[-\beta E_j]$. Truncating the sum to terms with $\beta|E_{\mu} - E_j| \ll 1$ (which will be motivated below), we can expand the second exponential in the rhs of eq. (12) into a Taylor series around E_j up to second order,

$$\langle j|\hat{\rho}|j\rangle \approx \frac{e^{-\beta E_j}}{Z} \left(1 - \beta \langle j|I|j\rangle + \frac{\beta^2}{2} \langle j|I^2|j\rangle \right), \quad (13)$$

where we have used $\sum_{\mu} E_{\mu} |\langle j|\mu\rangle|^2 = E_j + \langle j|I|j\rangle$ and eq. (7). The second-order term has to be taken into account, since the sum over all energies E_{μ} adds up positive and negative contributions for the first-order terms but only positive ones for the second-order terms. Since $\langle j|I|j\rangle^2 \leq \langle j|I^2|j\rangle$, both correction terms are small if

$$\beta \sqrt{\langle j|I^2|j\rangle} \ll 1. \quad (14)$$

Equation (14) justifies the above truncation if the distribution $w_j(\mu) = |\langle j|\mu\rangle|^2$ times the density of states $\eta(E_{\mu} - E_j)$ decayed faster than $\exp[-\beta|E_{\mu} - E_j|]$ for $|E_{\mu} - E_j| > \sqrt{\langle j|I^2|j\rangle}$ and fixed j . We numerically verified this behavior for a class of systems as shown in fig. 2 below. If, on the other hand, the truncation of the sum was not possible, the rhs of eq. (13) would contain additional correction terms invalidating a local thermodynamical description.

In the basis $|j\rangle$, the off-diagonal elements of the density matrix $\sum_{\mu} \langle j|\mu\rangle \langle \mu|j'\rangle \exp[-\beta E_{\mu}]$ vanish for $|E_j - E_{j'}| > 2\bar{I}$ because $|\langle j|\mu\rangle \langle \mu|j'\rangle| \approx 0$. When $|E_j - E_{j'}| < 2\bar{I}$, one can use the same approximation as for the diagonal terms, where now the zeroth-order term is zero. In the first- and second-order corrections each term of the sum carries a phase and thus these corrections are smaller than for diagonal elements.

Combining eqs. (10) and (14) we thus conclude that the condition

$$\sqrt{N} \gg \beta \bar{\delta E} \quad (15)$$

is sufficient to allow for an approximate local thermodynamical description for a group size N . In eq. (15) we have used that \bar{I}^2 is the arithmetic mean of all $\langle j|I^2|j\rangle$: these are positive quantities and therefore $\beta \bar{I} \ll 1$ implies $\beta \sqrt{\langle j|I^2|j\rangle} \ll 1$ for almost all states $|j\rangle$. Equation (15) is the main result of our paper.

Numerical results. – To test the condition (15) and the approximations involved, we investigate a chain of 8 spins with a Hamiltonian of the form (1) rewritten as

$$H = \frac{\Delta E}{2} \sum_{j=1}^8 \sigma_z(j) + \lambda \sum_{j=1}^8 \sum_{\alpha, \beta=1}^3 c_{\alpha\beta} \sigma_{\alpha}(j) \sigma_{\beta}(j+1). \quad (16)$$

Without loss of generality, we restrict the local part to terms in σ_z only; different local terms would merely imply a rotation of the coordinate system. Periodic boundary conditions are

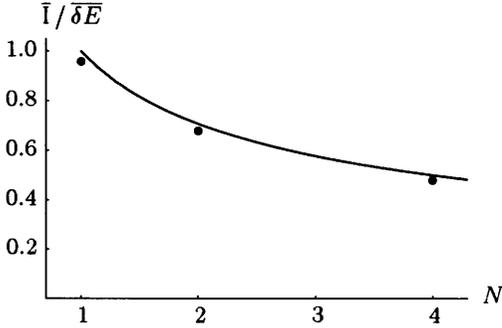


Fig. 1

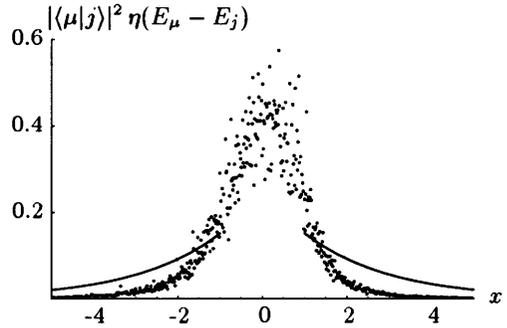


Fig. 2

Fig. 1 – The ratio of the average interaction strength and the level spreading $\bar{I}/\overline{\delta E}$ (dots) as a function of the number of subsystems per group N for $\lambda = \Delta E$. The line shows $1/\sqrt{N}$.

Fig. 2 – The conditional probabilities $|\langle \mu | j \rangle|^2$ weighted with the density of states $\eta(E_\mu)$ as a function of $x = (E_\mu - E_j)/\sqrt{\langle j | I^2 | j \rangle}$. The lines $0.25 \exp[-0.5|x|]$ are shown for comparison.

chosen, $\sigma_\alpha(9) = \sigma_\alpha(1)$. λ is a scaling factor for the interactions and the σ_α ($\alpha = 1, 2, 3$) are the Pauli matrices. In the following all energies (*i.e.* λ, β^{-1}) will be taken to be in terms of ΔE .

For each realisation the matrix elements $c_{\alpha\beta}$ are randomly chosen from the interval $[-1, 1]$ with equal weight. Based on 100 such realisations, we find the average of $\overline{\delta E}$ to be $\approx 5\lambda$. Therefore, from eq. (15), a local thermodynamical description is expected to be appropriate for $\sqrt{N}/(\beta\lambda) \gg 5$.

We consider three different partitions of this system into groups of adjoining subsystems as described in eq. (4). The partitions are: two 4-spin-chains, four 2-spin-chains and eight single spins. For the inverse temperature of the total system β and the interaction strength λ we consider the values $\beta\lambda = 0.1, 0.2, 0.3, 0.4$ which implies $2.5 \leq \sqrt{N}/(\beta\lambda) \leq 20$.

First, we test the scaling behavior of the interaction, eq. (10). In fig. 1 we have plotted the ratio $\bar{I}/\overline{\delta E}$ (see eqs. (8) and (9)) for the three partitions and $1/\sqrt{N}$ for comparison. The result confirms eq. (10). The values are slightly smaller than $1/\sqrt{N}$, which is due to the neglect of the local terms of the Hamiltonian.

Then, we calculate $w_j(\mu)\eta(E_\mu - E_j)$ for all three partitions. For each j we have plotted the distribution $w_j(\mu)\eta(E_\mu - E_j)$ *vs.* $x = (E_\mu - E_j)/\sqrt{\langle j | I^2 | j \rangle}$ thus rescaling its width to unity. Figure 2 shows a superposition of all these plots for one realisation. For comparison we have plotted in the range where $|E_\mu - E_j| > \sqrt{\langle j | I^2 | j \rangle}$, the functions $0.25 \exp[-\beta|E_\mu - E_j|] = 0.25 \exp[-0.5|x|]$, taking $\beta\sqrt{\langle j | I^2 | j \rangle} = 0.5 < 1$. The normalisation 0.25 was deliberately chosen to show that the distribution $w_j(\mu)\eta(E_\mu - E_j)$ indeed decays fast enough in that range. All numerical tests we made showed such a behavior.

Let us now assume the whole system to be in a thermal state with a reciprocal temperature β and a density matrix according to eq. (11). We calculate the distance between this density matrix and a product of canonical density matrices of the subgroups corresponding to a partition

$$\tilde{\rho} = \prod_{j=1}^{n_G} \otimes \rho_G^{\text{can}}(j), \quad (17)$$

where $\rho_G^{\text{can}}(j)$ is of the same form as in eq. (11) but only for one subgroup. As a measure for

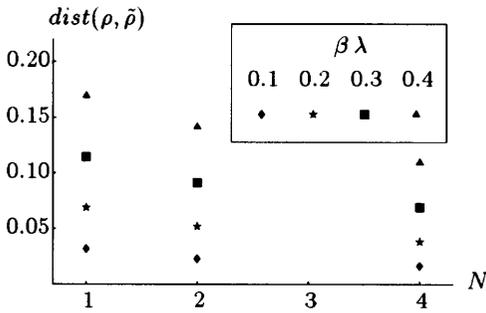


Fig. 3

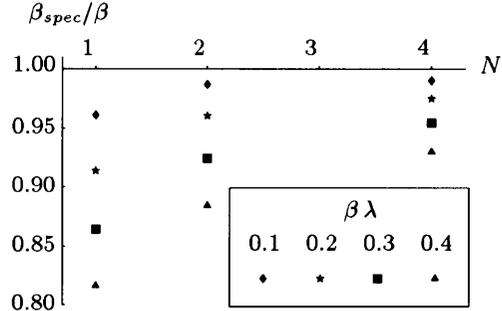


Fig. 4

Fig. 3 – Distance between the density matrix ρ and a product of canonical density matrices of the subgroups corresponding to the selected partition $\tilde{\rho}$. N is the number of subsystems per group.

Fig. 4 – Ratios of the spectral inverse temperatures β_{spec} of the subgroups to the given inverse temperature β of the total system. N is the number of subsystems per group.

the distance we use

$$\text{dist}(\rho, \tilde{\rho}) = \sqrt{\text{Tr}[(\rho - \tilde{\rho})^2]}. \quad (18)$$

The result is shown in fig. 3: The distance between the state of a global and a local thermodynamical description is found to be approximately proportional to $\beta\lambda$ and decreases as the group size N increases. The points with $\sqrt{N}/(\beta\lambda) > 5$, for which our estimates should apply, are below 0.1, which supports eq. (15).

Finally, to further confirm our findings, we calculate a “spectral temperature” of each subgroup in the following way [13]: The canonical density matrix of the whole system is transformed into the product basis (6). To each pair of states formed by an excited energy level E_i and the ground level E_0 of a subgroup, one can then assign a Boltzmann factor with an inverse temperature β' . The spectral temperature is the sum of all these β' weighted by the occupation probability p_i of the excited level E_i :

$$\beta_{\text{spec}} \equiv - \sum_{i>0} \frac{p_i}{1-p_0} \frac{\ln(p_i) - \ln(p_0)}{E_i - E_0}. \quad (19)$$

Such a β_{spec} can be defined for any state and coincides with the thermodynamical β for a canonical state. Since periodic boundary conditions were assumed, all subgroups of the same size N have the same temperature. In fig. 4 the ratios between β_{spec} defined by eq. (19) and the inverse temperature of the total system β are plotted *vs.* group size N . Here the points, which fulfill our criteria, lie above 0.9, which again confirms our results. The spectral temperatures of the subgroups are, in general, higher than the temperature of the total system. This indicates that the state of a subgroup is more mixed than the state of the whole system, which may be due to the entanglement of the subgroups caused by their mutual interaction [14].

Conclusion. – We have studied a modular system of fixed size composed of elementary subsystems with a finite energy spectrum and nearest-neighbour interactions. We have shown that if one forms groups of N subsystems each, the interaction between neighbouring groups scales as $N^{-1/2}$. We have then considered a chain of such interacting subsystems in a global thermal state with canonical density matrix. We have argued that due to the scaling property

of the interaction, the reduced density matrix of each group may be approximated by a canonical one with the same temperature as that of the total density matrix, if $\sqrt{N} \gg \beta \overline{\delta E}$: The temperature becomes an intensive quantity on a coarse-grained size and length-scale only. In the same way, energy becomes more and more extensive as the group size increases.

We have tested this assertion numerically with a chain of 8 interacting spins and find that our predictions are met in spite of the still small size of the total system.

Our studies should be extended to the total system being in a local thermodynamical equilibrium only. Here, heat conduction [6, 15] becomes an interesting problem. For strong coupling, meaningful temperature profiles can be defined with limited resolution only [16].

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We thank M. MICHEL, H. SCHMIDT, M. STOLLSTEIMER, and F. TÖNNER for fruitful discussions.

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