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

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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 \( \beta \), 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 \( \delta E \) 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 \cite{1,2,3}. 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.

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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 in-
creased 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 [7, 8, 9, 6]. These techniques have already been applied for a new type of
scanning microscopy, using a temperature sensor [10,11], that shows resolutions below 100nm.
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 \( dim \), com-
posed of identical elementary \( n \)-level subsystems. We form \( n_G \) identical groups of \( N \) sub-
systems 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
\[
H = \sum_j h_{\text{loc}}(j) + h_{\text{int}}(j, j + 1),
\]
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]:
\[
h_{\text{loc}}(j) = \frac{n}{2} \sum_\alpha A_\alpha \sigma_\alpha(j)
\]
\[
h_{\text{int}}(j, j + 1) = \frac{n^2}{4} \sum_{\alpha,\beta} C_{\alpha\beta} \sigma_\alpha(j) \sigma_\beta(j + 1)
\]
Here, the \( \sigma_\alpha(j) \) are \( SU(n) \) generators with \( \alpha, \beta = 1, 2, \ldots, n^2 - 1 \), \( n \) being the dimension of
one subsystem. For the \( SU(n) \) generators we adopt the trace relations [12]:
\[
\text{Tr}[\sigma_\alpha(i)] = 0
\]
\[
\text{Tr}[\sigma_\alpha(i) \sigma_\beta(j)] = 2 \frac{\text{dim}}{n} \delta_{ij} \delta_{\alpha\beta}
\]
where the trace (Tr) has to be taken over the whole system of dimension \( \text{dim} \). As a consequence
the trace over one elementary subsystem reads: \( \text{Tr}[\sigma_\alpha(j) \sigma_\beta(j)] = 2 \delta_{\alpha\beta} \). The coefficients in
equation (2) are then given by \( A_\alpha = \text{Tr}(H \sigma_\alpha(i)) / \text{dim} \) and \( C_{\alpha\beta} = \text{Tr}(H \sigma_\alpha(i) \sigma_\beta(i + 1)) / \text{dim} \),
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,
\[
H = H^{(0)}_N + I_N
\]
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,

$$I_N = \sum_i h_{int}(iN, iN+1)$$  \hspace{1cm} (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.

$$H |\mu\rangle = E_\mu |\mu\rangle \quad \text{and} \quad H_N^{(0)} |j_N\rangle = E_{j_N} |j_N\rangle$$  \hspace{1cm} (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 equation (4).

First, consider the identity

$$\sum_\mu (E_\mu - E_{j_N})^2 |\langle j_N|\mu \rangle|^2 = \langle j_N|I_N^2|j_N\rangle$$  \hspace{1cm} (7)

where the left hand side can be interpreted as the mean squared energy distance between a level $E_\mu$ and the energy $E_{j_N}$. The average of equation (7) over all $j_N$ is identical with $I_N^2$, where

$$I_N \equiv \sqrt{\text{Tr}(I_N^2)} \equiv \frac{n}{\sqrt{\text{dim}}} \sqrt{\sum_{\alpha,\beta} C_{\alpha\beta}^2}$$  \hspace{1cm} (8)

Here we have used equation (3).

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

$$\delta E \equiv \sqrt{\sum_\nu \frac{(E_\nu - \bar{E})^2}{\text{dim}}} = \sqrt{\text{Tr}\left[ (H - \bar{E})^2 \right]/\text{dim}} = \sqrt{\frac{n}{2} \sum_{\alpha,\beta} C_{\alpha\beta}^2 + \frac{2}{n} \sum_\alpha A_\alpha^2}$$  \hspace{1cm} (9)

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

$$I_N \leq \frac{1}{\sqrt{N}} \delta E$$  \hspace{1cm} (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 equation (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

$$\langle \mu|\bar{\rho}|\nu \rangle = \frac{e^{-\beta E_\mu}}{Z} \delta_{\mu\nu}$$  \hspace{1cm} (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 \( H^{(0)}_N \) we obtain

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

(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 \( \beta \) 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 equation \((12)\) into a Taylor series around \( E_j \) up to second order,

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

where we have used \( \sum_{\mu} E_{\mu} |\langle j|\mu\rangle|^2 = E_j + (j|I|j) \) and equation \((11)\). The second order term has to be taken into account, since the sum over all energies \( E_{\mu} \) adds up positive and negative contributions for the first order terms but only positive ones for the second order terms. Since \( (j|I|j)^2 \leq (j|I^2|j) \), both correction terms are small if

\[
\beta\sqrt{(j|I^2|j)} \ll 1. \tag{14}
\]

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 \( |E_{\mu} - E_j| > \sqrt{(j|I^2|j)} \) and fixed \( j \). We numerically verified this behavior for a class of systems as shown in figure \(2\). If, on the other hand, the truncation of the sum was not possible, the rhs of equation \((14)\) would contain additional correction terms invalidating a local thermodynamical description.

In the basis \( |j\rangle \), the off-diagonal elements of the density matrix \( \sum_{\mu} |j|\mu\rangle \langle \mu|j'\rangle \exp(-\beta E_{\mu}) \) vanish for \( |E_j - E_{j'}| > 2\bar{T} \) because \( |\langle j|\mu\rangle \langle \mu|j'\rangle| \approx 0 \). When \( |E_j - E_{j'}| < 2\bar{T} \), one can use the same approximation as for the diagonal terms, where now the zero 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 equations \((11)\) and \((14)\) we thus conclude that the condition

\[
\sqrt{N} \gg \beta \delta E. \tag{15}
\]

is sufficient to allow for an approximate local thermodynamical description for a group size \( N \).

In equation \((15)\) we have used that \( \bar{T} \) is the arithmetic mean of all \( (j|I^2|j) \): these are positive quantities and therefore \( \beta\bar{T} \ll 1 \) implies \( \beta\sqrt{(j|I^2|j)} \ll 1 \) 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

\[
H = \frac{\Delta E}{2} \sum_{j=1}^{8} \sigma_z(j) + \lambda \sum_{j=1}^{8} \sum_{\alpha=1}^{3} c_{\alpha\beta} \sigma_\alpha(j) \sigma_\beta(j+1) \tag{16}
\]

Without loss of generality, we restrict the local part to terms in \( \sigma_z \) only; different local terms would merely imply a rotation of the coordinate system. Periodic boundary conditions are
chosen, \( \sigma_\alpha(9) = \sigma_\alpha(1) \). \( \lambda \) is a scaling factor for the interactions and the \( \sigma_\alpha (\alpha = 1, 2, 3) \) are the Pauli matrices. In the following all energies (i.e. \( \lambda, \beta^{-1} \)) will be taken to be in terms of \( \Delta E \).

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 \( \delta E \) to be \( \approx 5\lambda \). Therefore, from equation (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 equation (1). The partitions are: two 4-spin-chains, four 2-spin-chains and eight single spins. For the inverse temperature of the total system \( \beta \) we consider the values \( \beta \lambda = 0.1, 0.2, 0.3, 0.4 \) which implies \( 2.5 \leq \sqrt{N}/(\beta \lambda) \leq 20 \). For the scaling behavior of the interaction, equation (10). In figure 1 we have plotted the ratio \( \sqrt{\delta E} \) (see equations (8) and (9)) for all three partitions. For each realisation 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, equation (10). In figure 1 we have plotted the distribution \( w_j(\mu) \eta(E_\mu - E_j) \) for all three partitions. For each \( j \) we have plotted the distribution \( w_j(\mu) \eta(E_\mu - E_j) \) versus \( x = (E_\mu - E_j)/\sqrt{\langle |j|^2 \rangle} \) 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 \( |E_\mu - E_j| > \sqrt{\langle |j|^2 \rangle} \), the functions \( 0.25 \exp(-\beta |E_\mu - E_j|) = 0.25 \exp(-0.5 |x|) \), taking \( \beta \sqrt{\langle |j|^2 \rangle} = 0.5 < 1 \). 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.

**Fig. 1** – The ratio of the average interaction strength and the level spreading \( \sqrt{\delta E} \) (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 \( x = (E_\mu - E_j)/\sqrt{\langle |j|^2 \rangle} \). The lines \( 0.25 \exp(-0.5 |x|) \) are shown for comparison.

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

\[
\hat{\rho} = \prod_{j=1}^{n_\lambda} \rho_{G^\lambda(j)}
\]

where \( \rho_{G^\lambda(j)} \) is of the same form as in equation (11) but only for one subgroup. As a measure
for the distance we use
\[ \text{dist}(\rho, \bar{\rho}) = \sqrt{\text{Tr}[(\rho - \bar{\rho})^2]} \] (18)

The result is shown in figure 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 equation (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 \( \beta' \). The spectral temperature is the sum of all these \( \beta' \) weighted by the occupation probability \( p_i \) of the excited level \( E_i \):

\[ \beta_{\text{spec}} \equiv -\sum_{i>0} \frac{p_i \ln(p_i) - \ln(p_0)}{E_i - E_0} \] (19)

Such a \( \beta_{\text{spec}} \) can be defined for any state and coincides with the thermodynamical \( \beta \) for a canonical state. Since periodic boundary conditions were assumed, all subgroups of the same size \( N \) have the same temperature. In figure 4, the ratios between \( \beta_{\text{spec}} \) defined by equation (19) and the inverse temperature of the total system \( \beta \) are plotted versus 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 $\sqrt{N} \gg \beta \delta E$.

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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