On Which Length Scales Can Temperature Exist in Quantum Systems?

Michael Hartmann\textsuperscript{1,2}, Günter Mahler\textsuperscript{2} and Ortwin Hess\textsuperscript{3}

\textsuperscript{1}Institute of Technical Physics, DLR-Stuttgart, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany
\textsuperscript{2}Institute of Theoretical Physics I, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany
\textsuperscript{3}School of Electronics \& Physical Sciences, University of Surrey, Guildford, GU2 7XH, United Kingdom

We consider a regular chain of elementary quantum systems with nearest neighbor interactions and assume that the total system is in a canonical state with temperature $T$. We analyze under what condition the state factors into a product of canonical density matrices with respect to groups of $n$ subsystems each, and when these groups have the same temperature $T$. While in classical mechanics the validity of this procedure only depends on the size of the groups $n$, in quantum mechanics the minimum group size $n_{\text{min}}$ also depends on the temperature $T$! As examples, we apply our analysis to different types of Heisenberg spin chains.

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Thermodynamics is among the most successfully and extensively applied theoretical concepts in physics. Notwithstanding, the various limits of its applicability are not fully understood.\textsuperscript{2,7,8}

Of particular interest is its microscopic limit. Down to which length scales can its standard concepts meaningfully be defined and employed?

Besides its general importance, this question has become increasingly relevant recently since amazing progress in the synthesis and processing of materials with structures on nanometer length scales has created a demand for better understanding of thermal properties of nanoscale devices, individual nanostructures and nanostructured materials.\textsuperscript{1} Experimental techniques have improved to such an extent that the measurement of thermodynamic quantities like temperature with a spatial resolution on the nanometer scale seems within reach.\textsuperscript{5,4}

To provide a basis for the interpretation of present day and future experiments in nanoscale physics and technology and to obtain a better understanding of the limits of thermodynamics, it is thus indispensable to clarify the applicability of thermodynamical concepts on small length scales starting from the most fundamental theory at hand, i.e. quantum mechanics. In this context, one question appears to be particularly important and interesting: Can temperature be meaningfully defined on nanometer length scales?

The existence of thermodynamical quantities, i.e. the existence of the thermodynamical limit strongly depends on the correlations between the considered parts of a system.\textsuperscript{6} With increasing size, the volume of a region in space grows faster than its surface. Thus effective interactions between two regions, provided they are short ranged, become less relevant as the sizes of the regions increase.\textsuperscript{5,9} The scaling of interactions between parts of a system compared to the energy contained in the parts themselves thus sets a minimal length scale on which correlations are still small enough to permit the definition of local temperatures. It is the aim of this letter to study this connection quantitatively.

For this purpose, the applied definition of temperature becomes crucial. We define local temperature to exist if the respective part of the system is in a canonical state. Besides its motivation from statistical mechanics, there are also rather practical arguments for this definition.

The canonical distribution is an exponentially decaying function of energy characterized by one single parameter.\textsuperscript{11} This implies that there is a one-to-one mapping between temperature and the expectation values of observables, by which temperature is usually measured.\textsuperscript{15}

Furthermore, the product of this distribution times the density of states, which is typically a strongly growing function of energy\textsuperscript{10} for large systems, forms a pronounced peak and thus physical quantities like energy have “sharp” values.

Based on the above arguments and noting that a quantum description becomes imperative at nanoscopic scales, the following approach appears to be reasonable: Consider a large homogeneous quantum system, brought into a thermal state via interaction with its environment, divide this system into subgroups and analyze for what subgroup-size the concept of temperature is still applicable.

Recently, spin chains have been subject of extensive studies in condensed matter physics. We therefore study various types of Heisenberg chains with respect to our present purpose.

We consider a homogeneous (i.e. translation invariant) chain of elementary quantum subsystems with nearest neighbor interactions. The Hamiltonian of our system is thus of the form

$$H = \sum_i H_i + I_{i,i+1},$$

where the index $i$ labels the elementary subsystems. $H_i$ is the Hamiltonian of subsystem $i$ and $I_{i,i+1}$ the interaction between subsystem $i$ and $i+1$. We assume periodic boundary conditions.

We now form $N_G$ groups of $n$ subsystems each (index $i \rightarrow (\mu - 1)n + j; \mu = 1, \ldots, N_G; j = 1, \ldots, n$) and split

\textsuperscript{*}E-mail address: michael.hartmann@dlr.de
this Hamiltonian into two parts,

\[ H = H_0 + I, \]  

(2)

where \( H_0 \) is the sum of the Hamiltonians of the isolated groups,

\[
H_0 = \sum_{\mu = 1}^{N_G} (H_\mu - I_{\mu_\mu \mu n + 1}) \quad \text{with}
\]

\[
H_\mu = \sum_{j = 1}^n \left( H_n(\mu - 1) + j + I_n(\mu - 1) + j, n(\mu - 1) + j + 1 \right)
\]

(3)

and \( I \) contains the interaction terms of each group with its neighbor group,

\[
I = \sum_{\mu = 1}^{N_G} I_{\mu_\mu \mu n + 1}.
\]

(4)

The eigenstates of the group Hamiltonian \( H_0 \) are products of group eigenstates,

\[
H_0 |\alpha\rangle = E_\alpha |\alpha\rangle \quad \text{with} \quad |\alpha\rangle = \prod_{\mu = 1}^{N_G} |a_\mu\rangle,
\]

(5)

where \( (H_\mu - I_{\mu_\mu \mu n + 1})|a_\mu\rangle = E_\mu|a_\mu\rangle \), \( E_\mu \) is the energy of one subgroup only and \( E_\alpha = \sum_{\mu = 1}^{N_G} E_\mu \).

We assume that the total system is in a thermal state,

\[
\hat{\rho} = \frac{e^{-\beta H}}{Z},
\]

(6)

where \( Z \) is the partition sum and \( \beta = (k_B T)^{-1} \) the inverse temperature with Boltzmann’s constant \( k_B \) and temperature \( T \).

For our purpose, we need to know the representation of \( \hat{\rho} \) in the basis formed by the product states \( |\alpha\rangle \). The diagonal elements \( \langle a|\hat{\rho}|a\rangle \) are the expectation values of \( \hat{\rho} \) in the states \( |a\rangle \),

\[
\langle a|\hat{\rho}|a\rangle = \int_{E_0}^{E_1} w_a(E) \frac{e^{-\beta E}}{Z} dE,
\]

(7)

where \( w_a(E) \) is the probability density of the occurrence of the energy eigenvalue \( E \) in the state \( |a\rangle \). \( E_0 \) is the energy of the ground state and \( E_1 \) the upper limit of the spectrum. For systems with an energy spectrum that does not have an upper bound, the limit \( E_1 \to \infty \) should be taken.

One can show that a quantum central limit theorem exists for the present model\(^{12,14}\) and that \( w_a(E) \) thus converges to a Gaussian normal distribution in the limit of infinite number of groups \( N_G \),

\[
\lim_{N_G \to \infty} w_a(E) = \frac{1}{\sqrt{2\pi} \Delta_a} \exp\left(-\frac{(E - E_a - \varepsilon_a)^2}{2 \Delta_a^2}\right),
\]

(8)

where the quantities \( \varepsilon_a \) and \( \Delta_a \) are defined by

\[
\varepsilon_a = \langle a|H|a\rangle - E_a \quad \text{and} \quad \Delta_a^2 = \langle a|H^2|a\rangle - \langle a|H|a\rangle^2.
\]

(9, 10)

\( \varepsilon_a \) is the difference between the energy expectation value of the distribution \( w_a(E) \) and the energy \( E_a \), while \( \Delta_a^2 \) is the variance of the energy \( E \) for the distribution \( w_a(E) \). Note that \( \varepsilon_a \) has a classical counterpart while \( \Delta_a^2 \) is purely quantum mechanical. It appears because the commutator \([H, H_0]\) is nonzero, and the distribution \( w_a(E) \) therefore has nonzero width.

The rigorous proof of eq. (8) is given in\(^{12}\) and based on the following two assumptions: The energy of each group \( H_\mu \) as defined in eq. (3) is bounded, i. e.

\[
\langle \chi|H_\mu|\chi\rangle \leq C
\]

(11)

for all normalized states \( |\chi\rangle \) and some constant \( C \), and

\[
\langle a|H^2|a\rangle - \langle a|H|a\rangle^2 \geq N_G C'
\]

(12)

for some constant \( C' > 0 \).

If conditions (11) and (12) are met, eq. (7) can be computed for \( N_G \gg 1;^{13} \)

\[
\langle a|\hat{\rho}|a\rangle = \frac{1}{2Z} \exp\left(-\beta y_a + \frac{\Delta_a^2}{2}\right) \left[ \text{erfc}\left(\frac{E_0 - y_a + \beta \Delta_a^2}{\sqrt{2} \Delta_a}\right) - \text{erfc}\left(\frac{E_1 - y_a + \beta \Delta_a^2}{\sqrt{2} \Delta_a}\right) \right]
\]

(13)

where \( y_a = E_a + \varepsilon_a \) and \( \text{erfc}(x) \) is the conjugate Gaussian error function.\(^{16}\) The second error function in (13) only appears if the energy is bounded and the integration extends from the energy of the ground state \( E_0 \) to the upper limit of the spectrum \( E_1 \).

Note that \( y_a \) is a sum of \( N_G \) terms and that \( \Delta_a \) fulfills eq. (12). The arguments of the conjugate error functions thus grow proportional to \( \sqrt{N_G} \) or stronger. If these arguments divided by \( \sqrt{N_G} \) are finite (different from zero), the asymptotic expansion of the error function\(^{16}\) may thus be used for \( N_G \gg 1: \text{erfc}(x) \to \exp\left(-x^2\right) / (\sqrt{\pi x}) \) for \( x \to \infty \) and \( \text{erfc}(x) \to 2 + (\exp\left(-x^2\right)) / (\sqrt{\pi x}) \) for \( x \to -\infty \). Inserting this approximation into eq. (13) and using \( E_0 < y_a < E_1 \) shows that the second conjugate error function, which contains the upper limit of the energy spectrum, can always be neglected compared to the first, which contains the ground state energy.

The off diagonal elements \( \langle a|\hat{\rho}|b\rangle \) vanish for \( |E_a - E_b| > \Delta_a + \Delta_b \) because the overlap of the two distributions of conditional probabilities becomes negligible. For \( |E_a - E_b| < \Delta_a + \Delta_b \), the transformation involves an integral over frequencies and thus these terms are significantly smaller than the entries on the diagonal.

We now test under what conditions the density matrix \( \hat{\rho} \) may be approximated by a product of canonical density matrices with temperature \( \beta_{\text{loc}} \) for each subgroup \( \mu = 1, 2, \ldots, N_G \). Since the trace of a matrix is invariant under basis transformations, it is sufficient to verify the correct energy dependence of the product density matrix. If we assume periodic boundary conditions, all reduced density matrices are equal and their product is of the form \( \langle a|\hat{\rho}|a\rangle \propto \exp(-\beta_{\text{loc}} E_a) \). We thus have to verify whether the logarithm of rhs of eq. (13) is a linear function of the energy \( E_a \),

\[
\ln \langle (a|\hat{\rho}|a) \rangle \approx -\beta_{\text{loc}} E_a + c,
\]

(14)

where \( \beta_{\text{loc}} \) and \( c \) are constants.

We exclude negative temperatures (\( \beta > 0 \)). Eq. (14)
can only be true for
\[ \frac{E_a + \varepsilon_a - E_0}{\sqrt{N_G} \Delta_a} > \beta \frac{\Delta^2_a}{\sqrt{N_G} \Delta_a}, \]
(15)
as can be seen from eqs. (13) and the asymptotic expansion of the error function. To satisfy (14), \( \varepsilon_a \) and \( \Delta^2_a \) furthermore have to be of the following form:
\[ -\varepsilon_a + \frac{\beta}{2} \Delta^2_a \approx c_1 E_a + c_2 \]
(16)
where \( c_1 \) and \( c_2 \) are constants. Note that \( \varepsilon_a \) and \( \Delta^2_a \) need not be functions of \( E_a \) and therefore in general cannot be expanded in a Taylor series.

To ensure that the density matrix of each subgroup \( \mu \) is approximately canonical, one needs to satisfy (16) for each subgroup \( \mu \) separately:
\[ \frac{\varepsilon_{\mu-1} + \varepsilon_{\mu}}{\frac{\beta}{4} \Delta^2_{\mu-1} + \Delta^2_{\mu}} \approx c_1 E_{\mu} + c_2 \]
where \( \varepsilon_{\mu} = \langle a | I_{\mu}^{\mu+\mu+1} | a \rangle \) with \( \varepsilon_a = \sum_{\mu=1}^{N_G} \varepsilon_{\mu} \),
\[ \Delta^2_{\mu} = \langle a | H^2 | a \rangle - \langle a | H_{\mu} | a \rangle^2 \] and \( \Delta^2_{\mu-1} = \sum_{\nu \neq \mu=1}^{\mu-1} \langle a | H_{\nu-1} H_{\nu} + H_{\nu} H_{\nu-1} | a \rangle - 2 \langle a | H_{\mu-1} | a \rangle \langle a | H_{\mu} | a \rangle \).

Temperature becomes intensive, if the constant \( c_1 \) vanishes,
\[ |c_1| \ll 1 \Rightarrow \beta_{\text{loc}} = \beta. \]
(18)
If this was not the case, temperature would not be intensive, although it might exist locally.

It is sufficient to satisfy conditions (15) and (17) for an adequate energy range \( E_{\text{min}} \leq E_{\mu} \leq E_{\text{max}} \) only. For systems composed of a large number of subsystems, the density of states is typically a rapidly growing function of energy.\(^{10}\) If the total system is in a thermal state, occupation probabilities decay exponentially with energy. The product of these two functions is thus sharply peaked at the expectation value of the energy \( \bar{E} \) of the total system \( \bar{E} + E_0 = \text{Tr}(H \hat{\rho}) \), with \( E_0 \) being the ground state energy. Therefore a pertinent and "safe" choice for \( E_{\text{min}} \) and \( E_{\text{max}} \) is
\[ E_{\text{min}} = \max \left( |E_\mu|_{\text{min}}, \frac{\bar{E}}{\alpha N_G} + \frac{E_0}{N_G} \right) \]
\[ E_{\text{max}} = \min \left( |E_\mu|_{\text{max}}, \alpha \frac{\bar{E}}{N_G} + \frac{E_0}{N_G} \right) \]
(19)
where \( \alpha \gg 1 \) and \( \bar{E} \) will in general depend on the global temperature. In eq. (19), \( |E_\mu|_{\text{min}} \) and \( |E_\mu|_{\text{max}} \) denote the minimal and maximal values \( E_\mu \) can take on.

For a model obeying eqs. (11) and (12), the two conditions (15) and (17), which constitute the general result of this letter, must both be satisfied. These fundamental criteria will now be applied to a concrete example.

We now consider the Heisenberg-model of a spin chain in a transverse field. The Hamiltonian reads\(^{17,18}\)
\[ H_i = B \sigma_i^z; \quad I_{i,i+1} = J (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) \]
(20)
where \( \sigma_i^x, \sigma_i^y \) and \( \sigma_i^z \) are the Pauli matrices. \( B \) is the magnetic field and \( J \) the coupling parameter. We will always assume \( B > 0 \).

We partition the chain into \( N_G \) groups of \( n \) adjacent spins, as considered above, and numerically analyze eqs. (15) and (17) by exact diagonalization of the groups. In doing so, we apply the approximation \( \Delta^2_a \ll \Delta^2_{\mu} \). Since \( \Delta^2_\mu = \sum_{\nu=\mu-1}^{\mu+1} |a | I_{\nu-1} I_\nu + I_\nu I_{\nu-1} | a \rangle - 2 \langle a | I_{\mu-1} | a \rangle \langle a | I_{\nu} | a \rangle \), only \( \sigma^x \otimes \sigma^x \) terms contribute and, among those, only terms which are products of one diagonal element and one off-diagonal element of the two \( \sigma^x \). \( \Delta^2_a \) thus contains much more terms, which, in addition, are all positive.

The conditions for the central limit theorem are met for almost all states \( | a \rangle \) of the present model: Condition (11) is fulfilled because the Hamiltonian of a single spin has finite dimension. The numerics shows that for almost all states, \( \Delta^2_\mu \) is a finite positive number, which implies that condition (12) is satisfied.

For single spins, a local temperature can always be defined by assigning a Boltzmann factor to the occupation probabilities of the upper and lower level. This local temperature, however, is not equal to the global one.

For groups of more than one spin, neither \( \varepsilon_{\mu} \) nor \( \Delta^2_{\mu} \) can be approximated by linear functions of \( E_{\mu} \). Therefore local temperature can only exists if the rhs of eq. (17) is a constant. As a direct consequence, temperature is intensive, \( \beta_{\text{loc}} = \beta \).

Eq. (15) can be checked directly. To check eq. (17), we need to quantify what "approximately constant" means. We thus use
\[ \beta \left[ \Delta^2_a \right]_{\text{max}} - \left[ \varepsilon_{\mu} \right]_\text{min} \ll \left[ E_\mu \right]_{\text{max}} - \left[ E_\mu \right]_{\text{min}} \]
(21)
where \( [\cdot]_{\text{max}} \) and \( [\cdot]_{\text{min}} \) denote the maximal and minimal value \( x \) takes on in all states \( | a \rangle \). Condition (21) implies, that (17) holds.

By numerical evaluation of eqs. (15) and (21), one can calculate a minimal group size \( n_{\text{min}} \geq 2 \) for each temperature \( T \), where we consider (21) to be satisfied if the lhs is 100 times smaller than the rhs. This corresponds to a tolerable deviation from the canonical distribution of 1%. Figure 1 shows \( n_{\text{min}} \) as a function of \( T \) for antiferromagnetic coupling with strength \( J = B \). Local temperature can exist in the shaded region. As mentioned above, local temperature can always be defined for single spins. For the present coupling strength, however, it is not intensive unless \( T \to \infty \).

Figure 2 shows \( n_{\text{min}} \) as a function of the temperature \( T \) for antiferromagnetic couplings of different strength. Diamonds correspond to \( J = 0.1B \), stars to \( J = 1B \) and squares to \( J = 10B \). The regions, where local temperatures exist are as indicated in figure 1. For single spins, local temperature always exists, but is only intensive for \( J = 0.1B \) and \( T > 2.5B \).

In both plots, only the one of eqs. (15) and (17), which sets the stronger bound enters. For the present parameter range, this is exclusively eq. (17). The results for the ferromagnetic case are approximately the same and are therefore not given separately here.

In summary, we have considered a homogeneous chain of quantum systems with nearest neighbor interactions. We have partitioned the chain into identical groups of \( n \) adjoining subsystems each. Taking the number of such groups to be very large and assuming the total system to
be in a thermal state with temperature $T$ we have found conditions (eqs. (15) and (17)), which ensure that each group is approximately in a thermal state. Furthermore, we have determined when the isolated groups have the same temperature $T$, i.e., when temperature is intensive.

The result shows that, in the quantum regime, these conditions depend on the temperature $T$, contrary to the classical case. The characteristics of the temperature dependence are determined by the width $\Delta_n$ of the distribution of the total energy eigenvalues in a product state and its dependence on the group energies $E_n$. The low temperature behavior, in particular, is related to the fact that $\Delta_n$ has a nonzero minimal value. This fact does not only appear in spin chains but is a general feature of quantum systems composed of interacting particles or subsystems. The commutator $[H, H_0]$ is nonzero and the ground state of the total system is energetically lower than the lowest product state, therefore $\Delta_n$ is nonzero, even at zero temperature.\(^{19}\)

For the models we consider here, the off-diagonal elements of the density operator in the product basis, $\langle a | \hat{\rho} | b \rangle$ ($a \neq b$), are significantly smaller than the diagonal ones, $\langle a | \hat{\rho} | a \rangle$. Our general result, conditions (15) and (17), thus states that the density matrix $\hat{\rho}$ “approximately” factorizes with respect to the considered partition. This implies that the state $\hat{\rho}$ is not entangled with respect to this partition, at least within the chosen accuracy. It would therefore be interesting to see how our result relates to the scaling of entanglement in many particle systems.\(^{20}\)

Unfortunately, our approach only applies to nonzero temperatures. The underlying central limit theorem\(^{12,14}\) is about the weak convergence of the distribution of energy eigenvalues. Weak convergence means that only integrals over energy intervals of nonzero length do converge. We thus cannot make statements about a system in its ground state let alone about the entanglement in that state.

We have then applied the general method to several types of Heisenberg spin chains. For concrete models, the conditions (15) and (17) determine a minimal group size and thus a minimal length scale on which temperature may be defined according to the temperature concept we adopt. Grains of size below this length scale are no more in a thermal state. Thus temperature measurements with a higher resolution should no longer be interpreted in a standard way.

The length scales, calculated in this paper, should also constrain the way one can meaningfully define temperature profiles in non-equilibrium scenarios.\(^{21}\)

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