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Minimal length scales for the existence of local temperature

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We review a recent approach to determine the minimal spatial length scales on which local temperature exists. After mentioning an experiment where such considerations are of relevance, we first discuss the precise definition of the existence of local temperature and its physical relevance. The approach to calculate the length scales in question considers homogenous chains of particles with nearest-neighbour interactions. The entire chain is assumed to be in a thermal equilibrium state and it is analysed when such an equilibrium state at the same time exists for a local part of it. The result yields estimates for real materials, the liability of which is discussed in the sequel. We finally consider a possibility to detect the existence or non-existence of a local thermal state in experiment.

1. Introduction

Large systems in an equilibrium state may, despite their very large number of degrees of freedom, be characterized by only very few quantities. For example, an ideal gas is described by the simple 'thermal equation of state' $pV = nk_BT$, where p is the pressure of the gas, V its volume, n the number of particles it contains, T its temperature and k_B Boltzmann's constant. In physics, one refers to this kind of description as a thermodynamical description.

How can such an extremely reduced description be justified? The reason why a thermodynamical description works so well for equilibrium states is that, with increasing number of particles in a system, a dominant part of microstates have the same macroscopic properties. Microstate refers here to a description where all degrees of freedom are specified. As a result, thermodynamical behaviour becomes 'typical'.

In a more mathematical language this fact is called the existence of the Thermodynamic Limit, which merely means that intensive quantities such as the energy per particle approach a limiting value that no longer depends on the detailed configuration of the system as its size increases. For example, the energy per particle of a very large piece of solid no longer depends on whether this piece is lying on a table or is immersed in a bucket full of water, provided it is in an equilibrium state, i.e. has the same temperature as its surroundings.

Obviously, in the Thermodynamic Limit, the difference between particles inside the solid and those on the surface, which interact with the surroundings, becomes negligible. That is why the size of the solid is important. Let us assume the solid had the shape of a sphere and the density of the particles was uniform within it. Since the surface of a sphere with radius r is $4\pi r^2$ and its volume is $(4\pi/3)r^3$, the ratio of particles sitting on the surface over the total number scales as $1/r$ and thus becomes negligible as r goes to infinity. Such a type of scaling applies not only to spheres but also to more general geometries.

To analyse the existence of *local* temperatures, small parts of large systems are of interest. These parts do inevitably interact with their surrounding. For short-range

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interactions between the constituent particles, again, only those particles sitting on the boundary of the considered part interact with the environment. Thus, the described scaling properties immediately give rise to the following question[†]: How large do parts of those systems have to be to permit a local thermodynamical description, i.e. a thermodynamical description of the part alone?

For a long time, the problem, besides being fundamental, may have been of purely academic interest, since thermodynamics was only used to describe macroscopic systems, where deviations from the Thermodynamic Limit may safely be neglected. However, with the advent of nanotechnology, the microscopic limit of the applicability of thermodynamics became relevant for the interpretation of experiments and may in the near future even have technological importance.

In recent years, amazing progress in the synthesis and processing of materials with structures on nanometer length scales has been made [1 – 4]. 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 [5 – 7]. 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?

Why should we care about the non-existence of local temperature? There are at least three situations for which this possibility needs special attention: one obvious scenario refers to the limit of spatial resolution on which a temperature profile could be defined. However, a spatially varying temperature calls for non-equilibrium—a complication which we will exclude here. A second application concerns partitions on the nanoscale: if a modular system in thermal equilibrium is partitioned into two pieces, say, the two pieces need no longer be in a canonical state, let alone have the same local temperature. Finally, local physical properties may show different behaviour depending on whether the local state is thermal or not.

The existence of thermodynamical quantities, i.e. the existence of the Thermodynamic Limit, strongly depends on the correlations between the considered parts of a system. As mentioned above, with increasing diameter, 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. This scaling behaviour is used to show that correlations between a region and its environment become negligible in the limit of infinite region size and that therefore the Thermodynamic Limit exists [8 – 10].

To explore the minimal region size needed for the application of thermodynamical concepts, situations far away from the Thermodynamic Limit should be analysed. On the other hand, effective correlations between the considered parts need to be small enough [11,12].

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. Here we review an approach to study this connection quantitatively [13,14].

2. Motivation: a thermal nanoscale experiment

In recent years, there has been substantial progress in the fabrication and operating of material with structure on nanoscopic scales and nanoscale devices. In this context, several experiments, that study thermal properties, have been done. We describe here, as an example, one experiment that nicely shows where the existence or non-existence of local temperature becomes relevant [15].

The experiment studies heat conduction across a carbon nanotube. A sketch of the setup is given in figure 1. Two, otherwise thermally well isolated islands are connected through a carbon nanotube of a few μm length. One island is heated by an electric current that runs through a coil with the resistance R_h. This island is thus at a 'hot' temperature T_h. Heat can flow across the nanotube to the other island, which is at a lower temperature T_s. This temperature in turn is measured by another coil, the resistance of which R_s, depends on temperature. Figure 2 shows a picture of this setup.
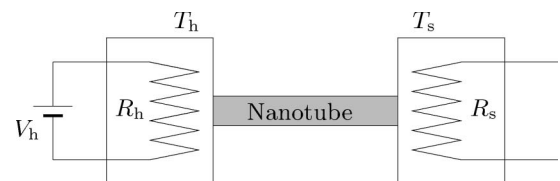

Figure 1. Setup of the experiment. Two, otherwise thermally well isolated, islands are connected by a carbon nanotube. The left island is heated by an electric current running through the coil with resistance R_h and thus maintained at the temperature T_h. The temperature of the right island is measured via the temperature-dependent resistance R_s.

[†]Since the present treatment considers interactions of a small part of a large system with its surroundings, its results are not mere finite size effects as for small isolated systems.
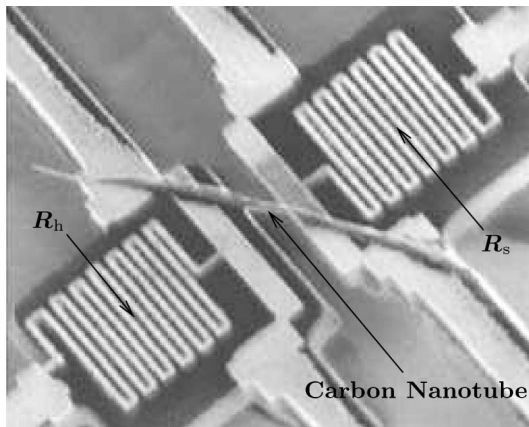
Figure 2. Picture of the setup. The heated island is in the lower left corner and the island where the temperature is measured in the upper right corner. Both are connected by a single carbon nanotube. (With permission from A. Majumdar, Nanoengineering Laboratory, University of California, Berkeley.)

At what point is the existence or non-existence of local temperatures of relevance for the interpretation of this experiment? We know that there is an electric current in the coil of the heated island. This current constantly delivers thermal energy to the island. This energy is transported across the nanotube to the other island, where we observe that the temperature T_s rises. We thus know that the nanotube connects a hot spot T_h to a cold spot T_s. This directly gives rise to the following questions: How hot is the nanotube in between? Can we meaningfully talk at all about the temperature of any part of the nanotube? The answer to these two questions would clarify whether and in what sense a temperature profile (see figure 3) could exist for the present setup.

While a temperature profile can obviously be defined and measured in a macroscopic version of the present experiment, say two buckets of water at different temperatures and connected via an iron bar, its existence, possible resolution and measurability are completely unclear for the nanoscopic version.

To address this question, we first discuss how to define the existence of local temperature in the next section.

3. What is temperature?

Temperature is one of the central quantities in thermodynamics and Statistical Mechanics. Let us note here that it is not a direct observable; it is not represented by an operator in quantum mechanics (see section 8). There exist two standard ways to define it.
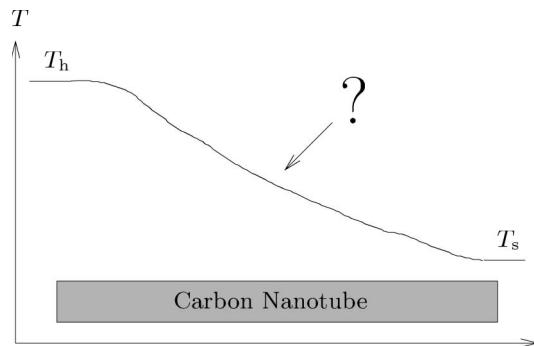

Figure 3. The question of whether a temperature profile exists for the nanotube in the present setup is not clarified.

3.1 Definition in thermodynamics

The thermodynamical definition is purely empirical. Thermodynamics itself is an empirical theory on systems whose macroscopic physics can be sufficiently characterized by a set of a few variables like volume, energy and the number of particles, for example. The values of these variables are called a macro state [16]. A system is said to be in equilibrium if its macro state is stationary for given constraints. As a consequence of this definition, an equilibrium state depends on the applied constraints, e.g. whether the volume or the energy is kept constant, etc. An important, special case of constraints is a bipartite (or multipartite) system with a fixed total energy, where the parts may exchange energy among themselves. The parts are then said to be in thermal equilibrium. In thermodynamics, temperature is defined by the following property.

3.1.1. Definition. Two systems that can exchange energy and are in thermal equilibrium have the same temperature.

To fix a temperature scale, a reference system is needed. The simplest choice for this reference system is the ideal gas (see section 1), where temperature may be defined by

$$T \equiv \frac{pV}{nk_B}. \tag{1}$$

Of course, the above definition is unambiguous only if the states of thermal equilibrium form a one-dimensional manifold [16]. Only then, a single parameter is sufficient for their characterization. This parameter is the temperature T.

3.2 Definition in statistical mechanics

In statistical mechanics, temperature is defined via the derivative of the entropy S with respect to the internal

energy $\bar{E}$. In quantum mechanics the entropy can be defined according to von Neumann as

$$S \equiv -k_{\mathrm{B}} \mathrm{Tr}\, \hat{\rho} \ln \hat{\rho}. \qquad (2)$$

It is a measure of the amount of possible pure states the system could be in. With this definition, entropy always exists, but shows its standard properties, e.g. extensivity, only in the Thermodynamic Limit [9].

In statistical mechanics, an equilibrium state is defined to be the state with the maximal entropy, that is the state with the maximal amount of accessible pure states.

For systems that interact with their surrounding, such that they can exchange energy with it but have a fixed expectation value for the energy, the equilibrium state is a so-called canonical state, described by a density matrix of the form

$$\hat{\rho} = \frac{\exp(-\beta\hat{H})}{Z}, \qquad (3)$$

where the partition sum Z normalizes $\hat{\rho}$ such that $\mathrm{Tr}\, \hat{\rho} = 1$.

In quantum mechanics the internal energy is given by the expectation value of the energy,

$$\bar{E} \equiv \mathrm{Tr}\, \hat{\rho}\hat{H}, \qquad (4)$$

where the Hamiltonian is the energy operator of the isolated system at hand. It does not contain any interactions of the system with its environment. The internal energy is therefore a property of the system itself, it only depends on the state of the system and not on the state of the environment.

Temperature is then defined by

$$\frac{1}{T} \equiv \frac{\partial S}{\partial \bar{E}}, \qquad (5)$$

which in turn exists as long as the entropy S is a function of the internal energy $\bar{E}$. However, the notion of temperature, as defined in equation (5), just like entropy shows its characteristic thermodynamical properties (see above) only for equilibrium states [9,16,17].

3.3 *Local temperature*

Local temperature is, by definition, the temperature of a part of a larger system. Hence, this subsystem is not isolated but can exchange energy with its surrounding. On the other hand, we limit our considerations to cases without particle exchange. Hence, the following convention appears to be reasonable.

3.3.1. Definition. Local temperature exists if the considered part of the system is in a canonical state.

Note: while a local state can always uniquely be defined by tracing out the rest of the system, this definition calls, in addition, for the (approximate) existence of some local spectrum.

Besides being based on statistical mechanics there are further practical reasons for this definition: the canonical distribution is an exponentially decaying function of energy characterized by one single parameter, temperature. This implies that there is a one-to-one mapping between temperature and the expectation values of observables by which it is usually measured. Temperature measurements via different observables thus yield the same result, contrary to distributions with several parameters.

This is a basic property of systems that can be characterized by thermodynamic description. The temperature, if it exists, describes a system in a sufficiently complete way such that several properties of it can be predicted if one only knows its temperature (see also section 8).

Why does the distribution need to be exponentially decaying? In large systems with a modular structure, the density of states is a strongly growing function of energy [17]. The product of the density of states times an exponentially decaying distribution of occupation probabilities will thus form a strongly pronounced peak at the internal energy $\bar{E}$ (see figure 4).

If the distribution was not exponentially decaying, the product of the density of states times the distribution would not have a pronounced peak and thus physical quantities like energy could not have 'sharp' values.
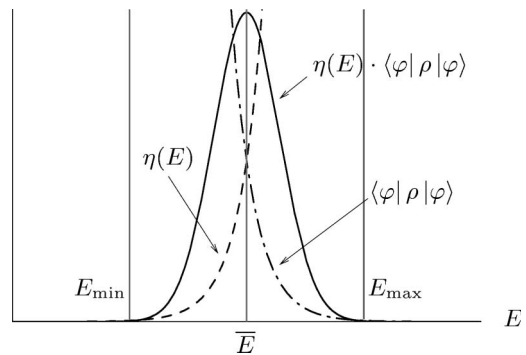

Figure 4. The product of the density of states $\eta(E)$ times the occupation probabilities $\langle\varphi|\rho|\varphi\rangle$ forms a strongly pronounced peak at $\mathrm{E} = \bar{E}$.

4. General theory for the existence of local temperature

After having introduced and discussed the conception, when temperature is defined to exist locally, we now turn to describe the approach to analyse its existence.

Since temperature is defined to exist locally, i.e. for a given part of the system we consider, if the respective part is in a thermal equilibrium state, it is defined to exist on a certain length scale, if all possible partitions of the corresponding size are simultaneously in an equilibrium state.

This requirement for the local equilibrium states in the parts to exist at the same time needs some further discussion: for a given temperature profile, it should not make a difference whether the profile is scanned by one single thermometer, which is moved in small steps across the sample, or whether the profile is measured by several thermometers simultaneously, which are located at small distances to each other.

For systems which are globally in a non-equilibrium state it is very difficult to decide under what conditions equilibrium states show up locally [18] and only very few exact results are known [19]. Nonetheless, whenever local equilibrium exists, the macroscopic temperature gradient is small ($\delta T/T \ll 1$). Here, we restrict ourselves to systems which are in a global equilibrium state (3)[†]. In these situations, subunits of the total system are in an equilibrium state whenever their effective interaction is weak enough and correlations between them are small so that the global thermal state approximately factorizes into a product of local thermal states.

Whenever the macroscopic temperature gradient is small ($\delta T/T \ll 1$), one would expect the results to be applicable even for situations with only local equilibrium but non-equilibrium on the global scale.

To explore how local temperature can exist, that is how small the respective part may be, one needs to look at parts of different sizes. The idea behind this approach is the scaling behaviour which ensures the existence of the Thermodynamic Limit (see section 1) [9,10].

We consider systems that are composed of elementary subsystems with short-range interaction, for simplicity say nearest-neighbour interaction. If then n adjoining subsystems form a part, the energy of the part is n times the average energy per subsystem and is thus expected to grow as the size of the part, n. Since the subsystems only interact with their nearest neighbours, two adjacent parts interact via the two subsystems at the respective boundaries, only. As a consequence, the effective coupling between two parts is independent of the part size n and thus becomes less relevant compared to the energy contained in the parts as their size increases (figure 5).

[†]One can imagine that the system has been brought into thermal contact with an even larger bath and has, in this way, relaxed into its thermal state. However, the way the system has reached its state is not relevant for our considerations.
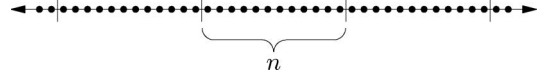

Figure 5. Groups of n adjoining subsystems are formed.

4.1 *The model*

As models we consider here homogeneous (i.e. translation invariant) systems with nearest-neighbour interactions which we divide into identical parts. The Hamiltonian of the system thus reads

$$H = \sum_i H_i + I_{i,i+1}, \qquad (6)$$

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

Now N_G groups of n subsystems each (index $i \to (\mu - 1) n + j$, $\mu = 1, \ldots, N_G, j = 1, \ldots, n$), are formed and the Hamiltonian is split into two parts,

$$H = H_0 + I, \qquad (7)$$

where H_0 is the sum of the Hamiltonians of the isolated groups,

$$H_0 = \sum_{\mu=1}^{N_G} \mathcal{H}_\mu, \qquad (8)$$

with

$$\mathcal{H}_\mu = \sum_{j=1}^{n} H_{n(\mu-1)+j} + \sum_{j=1}^{n-1} I_{n(\mu-1)+j,n(\mu-1)+j+1},$$

and I contains the interaction terms of each group with its neighbour group,

$$I = \sum_{\mu=1}^{N_G} I_{\mu n,\mu n+1}. \qquad (9)$$

The eigenstates $|a\rangle$ of the Hamiltonian H_0, $H_0|a\rangle = E_a|a\rangle$, are products of group eigenstates of the individual groups,

$$|a\rangle = \prod_{\mu=1}^{N_G} \otimes |a_\mu\rangle, \quad \text{with } \mathcal{H}_\mu|a_\mu\rangle = E_\mu|a_\mu\rangle, \qquad (10)$$

where E_μ is the energy of one subgroup only and $E_a = \sum_{\mu=1}^{N_G} E_\mu$.

4.2 Thermal state in the product basis

To test whether a part $H_{\mu 0}$ is in a thermal state, we have to calculate its reduced density matrix by tracing out the rest of the system. This trace can only be performed in the basis formed by the states $|a\rangle$, (10). We thus have to write the global equilibrium state (3) in this basis. Denoting the eigenstates and eigenenergies of the global Hamiltonian with Greek indices, $|\varphi\rangle$, $|\psi\rangle$ and E_φ, E_ψ, the global equilibrium state $\hat{\rho}$ reads

$$\langle\varphi|\hat{\rho}|\psi\rangle = \frac{e^{-\beta E_\varphi}}{Z}\delta_{\varphi\psi} \qquad (11)$$

in the global eigenbasis and the diagonal elements in the product basis are

$$\langle a|\hat{\rho}|a\rangle = \int_{E_0}^{E_1} w_a(E)\frac{e^{-\beta E}}{Z}\,\mathrm{d}E, \qquad (12)$$

where the original sum Σ_φ has been replaced by an integral over the energy.

$w_a(E)$ is the probability to obtain an energy value between E and $E+\Delta E$ if the total energy H is measured for a system in the state $|a\rangle$, i.e.

$$w_a(E) = \frac{1}{\Delta E}\sum_{\{|\varphi\rangle:E\leq E_\varphi<E+\Delta E\}}|\langle a|\varphi\rangle|^2, \qquad (13)$$

where the sum runs over all states $|\varphi\rangle$ with energy eigenvalues E_φ in the respective energy range and ΔE is small. E_0 is the energy of the ground state and E_1 the upper limit of the spectrum, which should be taken to be infinite if the spectrum does not have an upper bound.

We thus have to know the distributions $w_a(E)$ in order to be able to compute the reduced density matrices of the groups and to test whether they are of canonical form.

Fortunately, one can indeed show that there exists a quantum central limit theorem for many particle systems with nearest-neighbour interactions [20,21]. Therefore, in the limit of infinitely many groups, w_a takes on the following form:

$$\lim_{N_G\to\infty} w_a(E) = \frac{1}{\sqrt{2\pi}\Delta_a}\exp\left(-\frac{(E-\bar{E}_a)^2}{2\Delta_a^2}\right), \qquad (14)$$

where $\bar{E}_a$, the expectation value of H in the state $|a\rangle$, and Δ_a^2, its variance, read

$$\bar{E}_a \equiv \langle a|H|a\rangle, \qquad (15)$$

$$\text{and } \Delta_a^2 \equiv \langle a|H^2|a\rangle - \langle a|H|a\rangle^2. \qquad (16)$$

Note here that the limit of infinite number of groups is taken while the size of each individual group remains finite.

For the theorem to hold, two further conditions have to be met: the energy of each group including its interactions with the neighbouring group has to be bounded and the variance Δ_a^2 has to grow faster than $N_G C$ for some positive constant C. In scenarios where the energy spectrum of each elementary subsystem has an upper limit, such as spins, the first condition is met *a priori*. For subsystems with an infinite energy spectrum, such as harmonic oscillators, the present analysis is restricted to states where the energy of every group, including the interactions with its neighbour groups, is bounded. Thus, the considerations do not apply to product states $|a\rangle$, for which all the energy is located in only one group or only a small number of groups. The number of such states is vanishingly small compared to the number of all product states.

The expectation value of the entire Hamiltonian H in the state $|a\rangle$, $\bar{E}_a$, is the sum of the energy eigenvalue of the isolated groups E_a and a term that contains the interactions,

$$\bar{E}_a = E_a + \varepsilon_a. \qquad (17)$$

Therefore, the two quantities ε_a and Δ_a^2 can also be expressed in terms of the interaction (see equation (7)) only,

$$\varepsilon_a = \langle a|I|a\rangle, \qquad (18)$$

$$\text{and } \Delta_a^2 = \langle a|I^2|a\rangle - \langle a|I|a\rangle^2, \qquad (19)$$

meaning that ε_a is the expectation value and Δ_a^2 the squared width of the interactions in the state $|a\rangle$. Note that ε_a has a classical counterpart while Δ_a^2 is purely quantum mechanical. It appears because the commutator $[H, H_0]$ is non-zero, and the distribution $w_a(E)$ therefore has non-zero width.

Applying equation (14) to calculate the integral in equation (12) yields, for $N_G \gg 1$,

$$\langle a|\hat{\rho}|a\rangle = \frac{1}{Z}\exp\left(-\beta(E_a+\varepsilon_a)+\frac{\beta^2\Delta_a^2}{2}\right)$$
$$\times\frac{1}{2}\left[\mathrm{erfc}\left(\frac{E_0-E_a-\varepsilon_a+\beta\Delta_a^2}{\sqrt{2}\Delta_a}\right)\right.$$
$$\left.-\mathrm{erfc}\left(\frac{E_1-E_a-\varepsilon_a+\beta\Delta_a^2}{\sqrt{2}\Delta_a}\right)\right], \qquad (20)$$

where $\mathrm{erfc}(x)$ is the conjugate Gaussian error function [22]. The second error function appears only 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 the arguments of the conjugate error functions grow proportional to $\sqrt{N_G}$ or stronger, therefore the

asymptotic expansion of the latter [22] may be used for $N_G \gg 1$.

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 Gaussian distributions 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.

4.3 *Conditions for local thermal states*

We now test under what conditions the density matrix $\hat{\rho}$ may be approximated by a product of canonical density matrices with temperature β_{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 if they were canonical their product would be of the form $\langle a|\hat{\rho}|a\rangle \propto \exp(-\beta_{loc}E_a)$ We thus have to verify whether the logarithm of the r.h.s. of equation (20) is a linear function of the energy E_a defined in equation (10) and below,

$$\ln(\langle a|\hat{\rho}|a\rangle) \approx -\beta_{loc}E_a + c, \qquad (21)$$

where β_{loc} and c are constants.

Applying the asymptotic expansion of the conjugate error function to (20) shows that equation (21) can only be true for

$$\frac{E_a + \varepsilon_a - E_0}{\sqrt{N_G}\Delta_a} > \beta \frac{\Delta_a^2}{\sqrt{N_G}\Delta_a}, \qquad (22)$$

$$\text{and} \; -\varepsilon_a + \frac{\beta}{2}\Delta_a^2 \approx c_1 E_a + c_2, \qquad (23)$$

where c_1 and c_2 are constants. These two conditions constitute the general result of this section.

Note that ε_a and Δ_a^2 need not be functions of E_a and therefore in general cannot be expanded in a Taylor series.

Temperature becomes intensive, if the constant c_1 vanishes,

$$|c_1| \ll 1 \Rightarrow \beta_{loc} = \beta. \qquad (24)$$

Even if this was not the case, temperature might still exist locally.

For the existence of local temperature, one should only require that the diagonal elements (12) are canonically distributed in an appropriate energy range, $E_{min} \leq E_a \leq E_{max}$. As described in the previous section, the density of states $\eta(E)$ is, for large modular systems, an exponentially growing

function of energy and its product with the exponentially decaying canonical distribution $\langle \varphi|\rho|\varphi\rangle$ forms a strongly pronounced peak at the expectation value of the global energy $\bar{E}$ (see figure 4).

If the diagonal elements (12) are canonically distributed in an energy range, that is centered at this peak and is large enough to entirely cover it, all observables with non-vanishing matrix elements in that range show the same behaviour as for a true canonical distribution. Observables which are not of that kind are in general not of interest. If one considers for example 1 kg of iron at 300 K with an average energy of roughly 130 kJ, one is usually not interested in the processes that take place at energies of 0.1 kJ or 10^5 kJ.

Therefore, a pertinent and 'safe' choice for the energy range $E_{min} \leq E_a \leq E_{max}$ should be

$$E_{min} = \max([E_a]_{min}, (1/\alpha)\bar{E} + E_0),$$
$$E_{max} = \min([E_a]_{max}, \alpha\bar{E} + E_0), \qquad (25)$$

where $\alpha \gg 1$ and $\bar{E}$ will in general depend on the global temperature β. In equation (25), $[E_\mu]_{min}$ and $[E_\mu]_{max}$ denote the minimal and maximal values E_μ can take.

Figure 6 shows the logarithm of equation (20) and the logarithm of a canonical distribution with the same β for the example of a harmonic chain. The actual density matrix is more mixed than the canonical one. In the interval between the two vertical lines, both criteria (22) and (23) are satisfied. For $E < E_{low}$ (22) is violated and (23) for $E > E_{high}$. To allow for a description by means of canonical density matrices, the group size needs to be chosen such that $E_{low} < E_{min}$ and $E_{high} > E_{max}$.

For a model of the class considered here, the two conditions (22) and (23) must both be satisfied. In the following sections, these fundamental criteria will be applied to a concrete model.
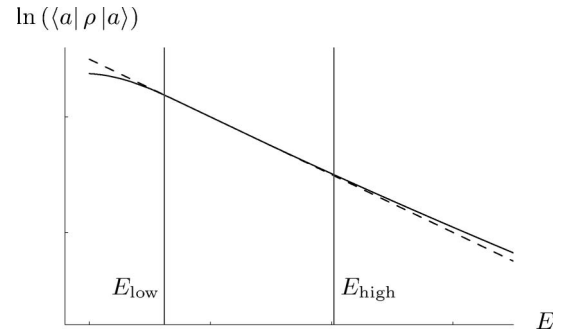

Figure 6. In $(\langle a|\rho|a\rangle)$ for ρ as in equation (20) (solid line) and a canonical density matrix ρ (dashed line) for a harmonic chain.

5. Harmonic chain

We consider a harmonic chain of $N_G \cdot n$ particles of mass m and spring constant $\sqrt{m}\omega_0$ [13,23]. In this case, the respective terms in the Hamiltonian (6) read

$$H_i = \frac{m}{2}p_i^2 + \frac{m}{2}\omega_0^2 q_i^2, \tag{26}$$

$$I_{i,i+1} = -m\omega_0^2 q_i q_{i+1}, \tag{27}$$

where p_i is the momentum of the particle at site i and q_i the displacement from its equilibrium position $i \cdot a_0$ with a_0 being the distance between neighbouring particles at equilibrium. We divide the chain into N_G groups of n particles each and thus get a partition of the type considered in section 4.

The Hamiltonian of each group is diagonalized by a Fourier transform and the definition of creation and annihilation operators $a_k^\dagger$ and a_k for the Fourier modes [14]. In this way we get

$$E_a = \sum_{\mu=1}^{N_G} E_\mu, \quad \text{with } E_\mu = \sum_k \omega_k \left(n_k^a(\mu) + \frac{1}{2}\right), \tag{28}$$

where $k = \pi l/(a_0(n+1))$ $(l = 1, 2, \ldots, n)$ and the frequencies ω_k are given by $\omega_k^2 = 4\omega_0^2 \sin^2(ka_0/2)$. $n_k^a(\mu)$ is the occupation number of mode k of group μ in the state $|a\rangle$. We choose units where $\hbar = 1$. Let us first verify that the central limit theorem (14) applies to this model, i.e. that the required assumptions (given below equation (16)) are met.

To see that Δ_a^2 grows faster than $N_G C$ $(C > 0)$, one needs to express the group interaction $V(q_{\mu n}, q_{\mu n+1})$ in terms of $a_k^\dagger$ and a_k; this yields $\Delta_a^2 = \sum_{\mu=1}^{N_G} \Delta_\mu^2$, where $\Delta_\mu^2 > 0$, implying that the assumption is met.

Since the spectrum of every single oscillator is infinite, the requirement that the energy per group should be bounded can only be satisfied for states for which the energy of the system is distributed among a relevant fraction of the groups. As discussed in section 4, states where this is not the case constitute only a negligible fraction of all product states $|a\rangle$.

The expectation values of the group interactions (equation (18)) vanish, $\varepsilon_a = 0$, while the widths Δ_μ^2 according to equation (16) depend on the occupation numbers $n_k(\mu)$ and therefore on the energies E_μ. To analyse conditions (22) and (23), one makes use of the continuum or Debye approximation [24], requiring $n \gg 1$, $a_0 \ll l$, where $l = na_0$, and the length of the chain to be finite. As will become clear below, the resulting minimal group sizes n_{min} are larger than 10^3 for all temperatures and the application of the Debye approximation is well justified.

Using this approximation we now have $\omega_k = vk$ with the constant velocity of sound $v = \omega_0 a_0$ and the width of the group interaction reads

$$\Delta_\mu^2 = \frac{4}{n^2} E_\mu E_{\mu+1}, \tag{29}$$

where $n + 1 \approx n$ has been used.

The relevant energy scale is introduced by the thermal expectation value of the entire chain

$$\bar{E} = E_0 + N_G n k_B \Theta \left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} \frac{x}{e^x - 1} dx, \tag{30}$$

and the ground state energy E_0 is given by

$$E_0 = N_G n k_B \Theta \left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} \frac{x}{2} dx = \frac{N_G n k_B \Theta}{4}, \tag{31}$$

where Θ is the Debye temperature [24].

Inserting equations (30) and (31) into equations (22) and (23), taking into account (25), one can now calculate the minimal n for given α, Θ and T. In doing so, one needs to introduce another accuracy parameter δ, which, for the r.h.s. of equation (23), quantifies how much smaller terms quadratic and higher order in E_a are compared to the zero order and linear ones. More precisely, δ is the ratio of the higher order terms to the (at most) linear ones.

Figure 7 shows n_{min} for $\alpha = 10$ and $\delta = 0.01$ as a function of T/Θ.

For high (low) temperatures n_{min} can be estimated by

$$n_{min} \approx \begin{cases} \dfrac{2\alpha}{\delta}, & \text{for } T > \Theta, \\[2ex] \dfrac{3\alpha}{2\pi^2}\dfrac{\Theta^3}{T^3}, & \text{for } T < \Theta. \end{cases} \tag{32}$$
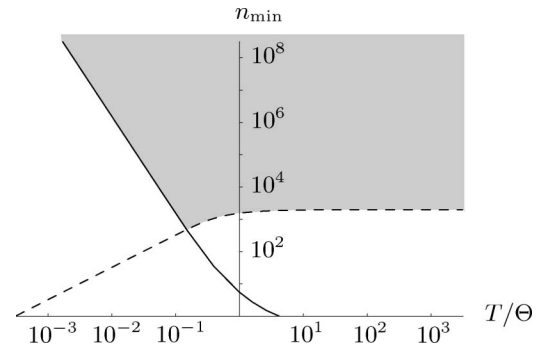

Figure 7. n_{min} as a function of T/Θ for a harmonic chain as determined by equation (22) (solid line) and as determined by equation (23) (dashed line) for $\alpha = 10$ and $\delta = 0.01$. Local temperature exists in the shaded region.

In addition, local temperatures are equal to the global one whenever they exist, $\beta_{loc} = \beta$, implying that temperature is intensive (see equation (24)).

In the following section the results obtained above will be applied to real materials.

6. Estimates for real materials

Thermal properties of insulating solids can successfully be described by harmonic lattice models. Probably the best known example of such a successful modeling is the correct prediction of the temperature dependence of the specific heat based on the Debye theory [24]. Therefore, one would expect the present approach to also give reasonable estimates for real materials.

We thus take the results obtained in section 5 for the harmonic chain and insert the corresponding parameters, in particular the Debye temperature which can be found tabulated [24]. One obtains a length scale by multiplying n_{min} by the corresponding lattice constant. The minimal length scale on which intensive temperatures exist in insulating solids should thus be given by

$$l_{min} = n_{min} a_0, \tag{33}$$

where a_0 is the lattice constant, the distance between neighbouring atoms.

Since n_{min} has been calculated for a one-dimensional model the results we obtain here should be valid for one-dimensional or at least quasi-one-dimensional structures of the respective materials. Let us consider two examples.

Silicon is used in many branches of technology. In its crystalline form, it has a Debye temperature of $\Theta \approx 645$ K and its lattice constant is $a_0 \approx 2.4$ Å. Using these parameters, figure 8 shows the minimal length scale on which temperature can exist in a one-dimensional silicon wire as a function of global temperature. Here, the accuracy
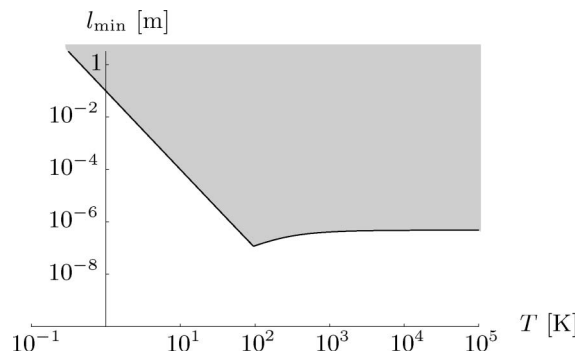
parameters α (see equation (25)) and δ (see below equation (31)) are chosen to be $\alpha = 10$ and $\delta = 0.01$. Local temperature exists in the shaded area.

Recently, carbon has been investigated for the fabrication of nano-structured devices [25,26]. In particular, we consider carbon nanotubes here, which are widely used in nano-technological experiments. Carbon nanotubes have diameters of only a few nanometers. Measurements of their specific heat have shown that their thermal properties can be accurately modeled with one-dimensional harmonic chains [27]. The presented results can thus be expected to be accurately applicable to them. Carbon nanotubes have a Debye temperature of $\Theta \approx 1100$ K and a lattice constant of $a_0 \approx 1.4$ Å.

Figure 9 shows the minimal length scale on which temperature can exist in a carbon nanotube as a function of global temperature. It provides a good estimate of the maximal accuracy with which temperature profiles in such tubes can be meaningfully discussed [1]. Again, the accuracy parameters α and δ are chosen to be $\alpha = 10$ and $\delta = 0.01$. Local temperature exists in the shaded area.

Of course the validity of the harmonic lattice model will eventually break down at high but finite temperatures. The estimates drawn from the considered approach, in particular the results presented in figures 8 and 9, will then no longer apply.

7. Discussion of the length scale results

The length scales one obtains here are, in particular for low temperatures, surprisingly large. One might thus wonder whether the approach really captures the relevant physics. Let us therefore discuss some possible limitations.

Firstly, one may argue that taking the limit of an infinite number of groups, as required for the central limit theorem, will not correspond to physically relevant situations.
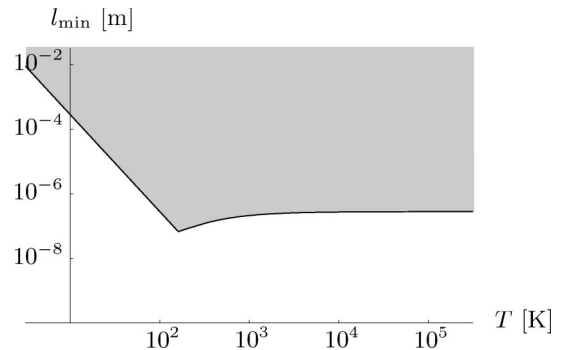
Fugure 8. l_{min} as a function of temperature T for crystalline silicon. $a_0 \approx 2.4$ Å, $\Theta \approx 645$ k, accuracy parameters $\alpha = 10$ and $\delta = 0.01$. Local temperature exists in the shaded area.

Figure 9. l_{min} as a function of temperature T for a carbon nanotube. $a_0 \approx 1.4$ Å, $\Theta \approx 1100$ K, accuracy parameters $\alpha = 10$ and $\delta = 0.01$. Local temperature exists in the shaded area.

However, having in mind that we intended to analyse when a small part of a larger system can be in a thermal state, taking this limit should be well justified.

Secondly, only one-dimensional models were considered. A real physical system, even if it is of a very prolate shape, is always three dimensional. A generalization of the approach to those models is thus of high interest. However, let us stress here that the general conditions (22) and (23) apply to systems of arbitrary dimension, it is only the application to specific models which needs to be generalized.

Furthermore, the harmonic chain is an exactly diagonalizable model, which means that no phonon scattering occurs. The purely harmonic model, for example, does not predict any expansion or shrinking of the material caused by heating or cooling. It is therefore possible that the harmonic model may fail to give reliable results for our present investigation. In particular at low temperatures, entanglement [28–30] plays an important role and this effect can be highly nonlinear.

Finally, one might speculate whether the length scales could significantly change if the assumption of a global equilibrium state was relaxed. This possibility of course exists, nonetheless one would expect the estimates to still apply as long as temperature gradients are small. Imagine there are two baths attached to the ends of the considered harmonic chain of section 5. If both baths have the same temperature, the chain is in a 'global' equilibrium state and the present results are applicable. If one now continuously increased the temperature of one bath, the density matrix of the chain would also change continuously. Hence, the minimal group sizes would also change continuously and the present results should still be good estimates, at least for small temperature gradients.

To clarify whether the above findings are in agreement or in conflict with experiments, their measurability needs to be considered in more detail. We proceed to do this in the next section.

8. Consequences for measurements

In this section we give some examples of possible experimental consequences of the local breakdown of the temperature concept at small length scales, i.e. of the fact that the respective individual subsystems or even subgroups do not reach a canonical state.

8.1 *Standard temperature measurements*

Temperature is always measured indirectly via observables, which, in quantum mechanics, are represented by Hermitian operators. Usually, one is interested in measuring the temperature of a system in a stationary state. The chosen observable should therefore be a conserved quantity, i.e. its

operator should commute with the Hamiltonian of the system.

For example, a conventional technique is to bring the piece of matter, the temperature T of which is to be measured, in thermal contact with a box of an ideal gas and to measure the pressure p of the gas, which is related to its temperature by $nk_B T = pV$ (see section 1). Since the gas is in thermal equilibrium with the considered piece of matter, both substances have the same temperature. A measurement of p for constant V allows us to infer the global temperature T of the piece of matter.

One might wonder whether a small (possibly even nanoscopic) thermometer [5], which is locally coupled to one subsystem of the large chain considered in section 4, is capable of measuring a local temperature or whether the measurement would show any indications of a possible local breakdown of temperature.

A prerequisite for the above gas thermometer to work properly is that the thermometer does not significantly perturb the system. For our class of models this means that the thermometer system should only be weakly coupled to the respective subsystem of the chain and that it should be significantly smaller than the latter. These two requirements ensure that the energy exchange between system and thermometer would not significantly alter the energy contained in the system. Therefore, this measurement scenario can be accurately modeled as follows.

Let the thermometer be represented by a single spin, which is locally coupled to a harmonic chain, say. Since the coupling is assumed to be weak and the chain is assumed to be very large and in a thermal state, the present scenario can accurately be modeled with a master equation approach [31]. However, it is a well-known result of such system bath models that the reduced density matrix of the spin relaxes into a canonical state with the temperature being equal to the global temperature of the harmonic chain (i.e. the bath). The spin (thermometer) thus measures the global temperature of the total chain, even for perfectly local coupling.

As long as the chain is in a global equilibrium state, a temperature measurement of this type thus does not have any spatial resolution at all. It is only capable of measuring the global temperature of the chain. No local temperatures can be measured or any signatures of their breakdown be detected.

This conclusion obviously no longer holds for scenarios with only local but no global equilibrium. Macroscopic temperature profiles are routinely measured with the standard technique described above. Whether such measurements of temperature profiles are still possible for much smaller systems and what their maximally possible spatial resolution is in that case should be subject to further investigation.

According to the above considerations, one might think that the question of local temperatures for systems in global

equilibrium was an irrelevant issue since it has no observable consequences. This, however, is not the case. In the following we turn to discuss an example of such measurable consequences of the local breakdown of the concept of temperature.

8.2 *Non-thermal local properties*

We now turn to observables of the object (chain) itself, which could be used to infer local temperatures T_{loc}, i.e. temperatures of subsystems, provided the subsystems are in a canonical state. On the other hand, if the respective subsystems are not in a canonical state, this fact should then modify the measurement results for those observables.

The minimal group sizes calculated in section 4 depend on the global temperature and on the strength of the interactions between neighbouring subsystems. Furthermore, local temperatures can even exist for single subsystems if these are finite dimensional. In the limiting case of infinite temperature, the density matrix of a chain of finite-dimensional subsystems is proportional to the identity matrix and thus has the same form in every basis including the product basis, which in turn implies that local temperature would then exist for single subsystems [14]. For systems composed of finite-dimensional subsystems, local temperatures thus exist for single subsystems at relatively low global temperatures if the coupling is weak, while they do not if the coupling is strong.

Pertinent systems for which such effects could easily by studied are magnetic materials [32]. These can in many cases be described by spin lattice or spin chain models. Since, as we will see below, the properties of single spins can be inferred from measurements of even macroscopic magnetic observables, those materials thus allow the study of the existence of temperature, as defined by the existence of a canonical state, on the most local scale possible, i.e. for single spins.

For a spin-1/2 system, it is always possible to assign a Boltzmann factor and thus a local temperature to the ratio of the occupation probability of the higher and lower level. Here we consider a homogeneous chain of spin-1 particles interacting with their nearest neighbours. For the interactions, one assumes a Heisenberg model. The Hamiltonian of this system reads [33]:

$$H = B \sum_{j=1}^{n} \sigma_j^z + J \sum_{j=1}^{n} \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z, \quad (34)$$

where σ_j^x, σ_j^y and σ_j^z are the spin-1 matrices, B is an applied magnetic field, J the coupling and n the number of spins. The coupling J is taken to be positive, $J > 0$. The spins thus tend to align anti-parallelly and the material is anti-ferromagnetic. The local Hamiltonian of subsystem j is $H_j = B\sigma_j^z$. The system has periodic boundary conditions

and is thus translation invariant. As in the previous sections, the entire system (34) is assumed to be in a thermal state (see equation (3)).

As an example of an experiment, we will now consider two different magnetic observables of a spin-1 system with the Hamiltonian (34). The first observable is the magnetization in the direction of the applied field[†], m_z, which is here defined to be the total magnetic moment per particle:

$$m_z \equiv \frac{1}{n} \left\langle \sum_{j=1}^{n} \sigma_j^z \right\rangle, \quad (35)$$

where $\langle \mathcal{O} \rangle$ is the expectation value of the operator $\mathcal{O}$, i.e. $\langle \mathcal{O} \rangle = \mathrm{Tr}(\rho \mathcal{O})$. In the translation invariant state ρ, the reduced density matrices of all individual spins are equal, and the magnetization (35) can be written as

$$m_z = \langle \sigma_k^z \rangle, \quad (36)$$

for any $k = 1, 2, \ldots, n$. The magnetization, although defined macroscopically, is thus actually a property of a single spin, i.e. a strictly local property.

As a second observable one can choose the occupation probability, p, of the $s_z = 0$ level (averaged over all spins),

$$p = \frac{1}{n} \left\langle \sum_{j=1}^{n} |0_j\rangle \langle 0_j| \right\rangle. \quad (37)$$

Similar to m_z according to equation (36), p may be written as

$$p = \langle |0_k\rangle \langle 0_k| \rangle, \quad (38)$$

for any $k = 1, 2, \ldots, n$ and is thus also strictly local.

Now, if each single spin was in a canonical state with temperature T_{loc}, m_z and p would both have to be monotonic functions of T_{loc}. In this case, T_{loc} could, after calibration, be inferred from measurements of m_z or p, respectively. Note that m_z is proportional to the local energy, the average energy of one subsystem.

Figure 10 shows m_z and p as a function of the global temperature T for a spin-1 chain of four particles with the Hamiltonian (34) for weak interactions, $J = 0.1 \times B$. Both quantities are monotonic functions of each other.

The situation changes drastically when the spins are strongly coupled. In this case the concept of temperature breaks down locally due to correlations of each single spin with its environment.

Figure 11 shows m_z and p as a function of temperature T for a spin-1 chain of four particles with the Hamiltonian (34) for strong interactions $J = 2 \times B$. Both quantities are

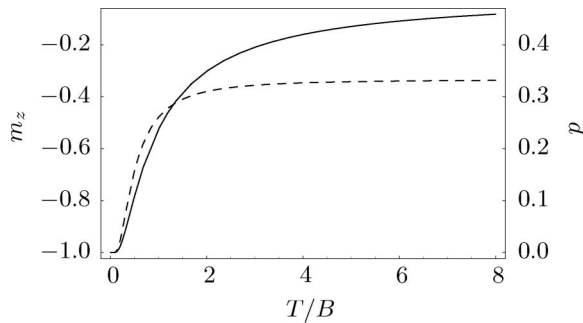[†]The two other components of the magnetization vanish for symmetry reasons.

Figure 10. m_z (solid line) and p (dashed line) as a function of temperature T for a spin-1 chain of four particles. T is given in units of B and $J = 0.1 \times B$.
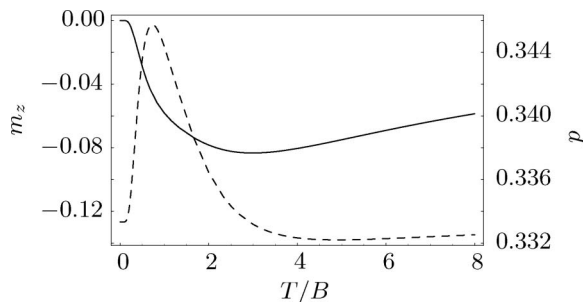

Figure 11. m_z (solid line) and p (dashed line) as a function of temperature T for a spin-1 chain of four particles. T is given in units of B and $J = 2 \times B$.

non-monotonic functions of T and therefore no mapping between m_z and p exists.

How could a local observer determine whether the system he observes, a single spin, is in a thermal state and can therefore be characterized by a temperature? The local observer would need to compare two situations.

In the first situation, the spin is weakly coupled to a larger system, the heat bath. In this situation, the local observer could measure m_z and p as functions of the temperature of the heat bath and would get a result similar to figure 10. This result would not be sensitive to the details of the coupling to the heat bath. The local observer would thus recognize this situation as a particular one and might term it the 'thermal' situation.

The second situation is fundamentally different. The spin is now strongly coupled to its surroundings. If the local observer again measures m_z and p as functions of the temperature of the surroundings, he would get a result like in figure 11.

The observer can tell the difference between both situations, even if he has no access to the global (true) temperature T of the surroundings. In the first case he can construct a mapping from say m_z to p, i.e. $p(m_z)$, or

vice versa, $m_z(p)$; in the second he cannot: there exist, for example, two values of p corresponding to only one value of m_z. Here the concept of a local temperature breaks down at least on the level of individual particles, since temperature measurements via different local observables would contradict each other.

The question of whether and on what scale local temperatures can exist in systems that are in a global equilibrium state is thus indeed physically relevant. The advantage of the concept of temperature is that it allows us to predict various physical properties of the considered system. This is only possible if different properties (expectation values of observables) map one to one on each other as in figure 10. The following example illustrates the situation.

Consider a piece of metal, say a wire. Assume its temperature is measured via its electrical resistance. Why are we interested in this temperature? We are interested in it because it also allows us to predict how the wire behaves with respect to other physical processes. For example, if we know its temperature, we can tell whether the wire is going to melt or not. Effectively, we thus have a mapping of the resistance onto the fact that the wire is going to melt or is not going to melt. In a more mathematical language, we can construct a function: melting as a function of the resistance. Analogously, for the scenario of figure 10, a local observer is able to construct a function $m_z(p)$.

What happens if such functions can no longer be constructed? In this situation, the concept of temperature becomes useless. Assume our wire had such properties. We could still measure its resistance and, if we wished, could assign a 'temperature value' to it. This 'temperature value', however, would be of no further use, since it would not allow us to predict whether the wire is going to melt or not. A situation where such problems really occur is the scenario of figure 11.

8.3 Potential experimental tests

Finally, we address the question of whether the effects described here could be observed in real experiments. Indeed, pertinent experiments are available and have partly already been carried out.

A realization of a quasi-one-dimensional anti-ferromagnetic spin-1 Heisenberg chain is the compound $CsNiCl_3$ [34–36]. Here the coupling is $J \approx 2.3\,\text{meV}$. To achieve a detectable modulation of m_z and p, the spins should be significantly polarized for $T > 0$. Therefore, a sufficiently strong applied magnetic field is needed. For $CsNiCl_3$, a field of roughly 9.8 Tesla would correspond to $J = 4 \times B$.

The magnetization in an applied field can be measured with high precision by means of a SQUID [37]. The occupation probability of the $s_z = 0$ states, on the other hand, is accessible via neutron scattering experiments

[38,39]. The differential cross section for neutron scattering of spin systems is a function of the Fourier transforms of the spin correlation functions [40]. One can thus obtain information about the quantity

$$\frac{1}{n}\sum_r \langle \sigma_r^x(0)\sigma_r^x(0) + \sigma_r^y(0)\sigma_r^y(0)\rangle = 1 + p \qquad (39)$$

from the measurement data. Therefore, p is measurable in neutron scattering experiments.

Such experiments or a combination thereof could thus be used to demonstrate the non-existence of local temperature.

9. Conclusion and outlook

In the present work we have considered the minimal spatial length scales on which local temperature can meaningfully be defined. For large systems in a global equilibrium state, we have reviewed the derivation of two criteria which are valid for quantum many body systems with nearest-neighbour interactions and have discussed the physical relevance of the existence and non-existence of local temperatures.

Some questions related to the microscopic limit of the applicability of thermodynamics have thus been clarified. Nevertheless, some open problems remain and even new ones have appeared in the context of the present approach.

First of all, the generalization of the calculations to scenarios with only local but no global equilibrium is an issue of significant importance. One might expect that the length scales no longer depend on the interactions and the global temperature only, but that the temperature gradient also becomes relevant.

For global non-equilibrium, local temperature measurements of the standard type are very interesting and important issues on their own. As we have discussed here, these measurements have no spatial resolution if the sample is in a global equilibrium state. On the other hand, local temperature measurements with spatial resolution are being done for macroscopic setups and nobody would dare to question their validity. Therefore, the maximal spatial resolution of this kind of measurement is an interesting question and the present understanding of this topic is quite poor.

Future research could also be concerned with new physics that might appear for small entities that are in contact with thermal surroundings, but show non-thermal behaviour due to the breakdown of temperature on the respective scale. One example of this is the observable features discussed in section 8. However, one might think about more surprising phenomena, such as, for example, anomalous pressure fluctuations in very small gas bubbles enclosed in a piece of solid. With respect to future nanotechnologies, such phenomena could equally be harmful or useful, depending on whether one is able to design the devices in a pertinent way.

Finally, possible generalizations of thermodynamics that could apply on even smaller scales are interesting. In the present work, we have considered the microscopic limit of the usual thermal behaviour in quantum systems, i.e. Quantum Thermodynamics [41], where effective interactions among the considered parts are small. One might thus wonder whether only partitions with weak effective couplings can be considered within such a 'universal' description, that does not depend on the details of the microscopic constituents, or whether there exists again an intermediate level of description, not as universal as standard thermodynamics but applicable on smaller scales. Since, in standard thermodynamics, equilibrium states are fully characterized by one single parameter, temperature (see equation (3)), one could, for example, imagine that there exists a class of generalized equilibrium states that require say two or three parameters for their characterization. Some phenomenological attempts in this direction have already been made [42,43]. Nonetheless, justification of these attempts from an underlying theory, i.e. quantum or classical mechanics, is still missing.

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