Temperature gradients in equilibrium: small microcanonical systems in an external field

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We consider the statistical mechanics of a small gaseous system subject to a constant external field. As is well known, in the canonical ensemble the system i) obeys a barometric formula for the density profile and ii) the kinetic temperature is independent of height, even when the system is small. We show here that in the microcanonical ensemble the kinetic temperature of the particles affected by the field is not constant with height, but that rather, generally speaking, it decreases with a gradient of order $1/N$. Even more, if we have a mixture of two species, one which is influenced by the field and the other which is not, we find that the two species’ kinetic temperatures are generally different, even at the same height. These facts are shown in detail by studying a simple mechanical model: a Lorentz Gas where particles and spinning disks interact and the particles are subjected to a constant external force. In the microcanonical ensemble, the kinetic temperature of the particles is indeed found to vary with height; the disks’ kinetic temperature, on the other hand, is height-independent, and thus, differs from that of the particles with which they interact.

Keywords: definition of temperature, ensemble dependence, small systems, Lorentz Gas

I. INTRODUCTION

When considering small many-body systems one can expect ensemble-dependence on the thermodynamic quantities. In most cases, it is not until the thermodynamic limit is reached that the difference between statistical ensembles disappears. For finite systems, however, differences between the different statistical ensembles may be both significant and rather intriguing. Although

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this has been known ever since the early stages of statistical mechanics, the small-system-regime where ensemble dependences matter has only become relevant to experiments and/or applications during the last decades. Indeed, the microscopic and mesoscopic scales are becoming more important due to technological advances e.g., in nanosystems, as well as by the broadening scope of physics toward phenomena from other disciplines of science, such as molecular chemistry, micromechanics and biological systems. Thus, it may be interesting to review and study the basic properties of simple realistic models in this regime.

In this paper we study the equilibrium properties of a gas under the influence of a constant external field. In the canonical ensemble the system will display a barometric, that is, exponential, dependence of the density on height; whereas the temperature, which in the canonical ensemble can always be computed from the mean kinetic energy of the particles, is independent of height. Our aim is to look at the way in which these facts are modified when considering a simple, yet realistic, isolated system. The system we shall study is the so-called Spinning Lorentz Gas (SLG) – whose transport properties have been presented in [4, 5]. The SLG is simply the Lorentz gas in which the circular scatterers are allowed to rotate and exchange energy with the scattered particles; the system is described in Section II. This model has been shown to have realistic transport properties: specifically, it displays normal transport (Fourier’s and Fick’ laws hold) and it is well described by the hypothesis of Local Thermal Equilibrium. It also shows coupled mass and energy transport and satisfies Onsager’s reciprocity relations. The SLG is thus a very simple interacting particle model with reasonably realistic properties. Its merit in this paper is that its equilibrium statistics can be solved exactly.

In what follows we study an isolated (microcanonical) SLG with a constant external field acting on the particles. We find in Section IV that with this setup the particles reach a non uniform density profile resembling the barometric formula (we note, parenthetically, that the usual Lorentz gas model [6] does not reach such a barometric profile under the effect of an external field). We show there that the kinetic temperature of the particles varies with the height in the system, while the kinetic temperature of the scatterers is constant. We show as well that the kinetic temperature of the scatterers also differs slightly from the proper temperature, calculated from the derivative of the entropy with respect to energy. These effects disappear, of course, in the thermodynamic limit. These results highlight the fact that when a finite and closed system is in equilibrium (in the microcanonical ensemble), the question of how to identify the local temperature must be answered carefully, as kinetic temperature gradients can be present in the system in equilibrium. We have also performed molecular dynamics simulations of this system to verify our results. We have found
that indeed, the kinetic temperature of the particles varies according to their height in the system, whereas that of the scatterers is constant as predicted; however, since the applied field affects the ergodicity properties of the system, microcanonical Monte Carlo simulations were also performed. Next we argue in Section IV that such temperature gradients occur rather generally. From a historical point of view, it may be of interest to note that the height dependence of temperature in systems under the influence of gravity was already stated by Loschmidt [7]. His results strongly exaggerate the effect, however, and do not adequately consider interactions.

II. BAROMETRIC LORENTZ GAS

In the barometric SLG, $N$ non-interacting particles of mass $m$ move in a plane under the action of a constant applied force field of strength $E$. The particles can exchange energy with $M$ disk scatterers which rotate freely, with their centers fixed in a (finite horizon) triangular lattice. At the walls on either end of the system (see figure II) particles are reflected elastically, while the vertical coordinate $y$ has periodic boundary conditions. The energy of the system is given by

$$H = \sum_{i=1}^{N} \left( \frac{m}{2} v_i^2 + qE x_i \right) + \frac{\Theta}{2} \sum_{i=1}^{M} \omega_j^2,$$

(1)

where $v_i = p_i/m$ is the velocity of a particle with coordinate $x_i$, and $\omega_j$ is the angular velocity of the $j^{th}$ scatterering disk, which have moment of inertia $\Theta$. Interactions in the SLG result from reversible, energy conserving collisions between particles and disks. The collision rules are given by

$$v'_n = -v_n, \quad v'_n = v_n - \frac{2\eta}{1+\eta} (v_n - R\omega),$$

$$R\omega' = R\omega + \frac{2}{1+\eta} (v_n - R\omega),$$

(2)

where $v_{n,s}$ are normal and tangential components of the particle’s velocity with respect to disk surface, $R$ is the disk radius and $\eta \equiv \Theta/mR^2$ is the dimensionless parameter that controls the fraction of total energy exchanged between the disk and the particle [4].

Finally, note that this system has two different confining mechanisms: on the one hand the field limits effectively the particles in a finite region, on the other, there exists a finite box of size $L$. In general the case in which $L \to \infty$ is significantly easier, and we shall occasionally sketch the derivations in that case.
III. DEFINITION OF TEMPERATURE

Classically, in the microcanonical ensemble, up to an additive constant one has the following expression for the entropy $S(E)$ as a function of the energy $E$

$$S(E) = k_B \ln \Omega(E) = k_B \ln \int_{\Gamma} d^N \vec{p} d^N \vec{q} \delta \left[ E - H(\vec{p}, \vec{q}) \right]$$

(3)

where $\Gamma$ is the phase space of the system and $H$ is its Hamiltonian. The temperature is then given by

$$\frac{1}{k_B T_M} = \frac{\partial S(E)}{\partial E}$$

(4)

Here $T_M$ stands for the microcanonical temperature as defined by (4). If $H$ is of the form $\sum \frac{p_i^2}{2m_i} + V(q_1, \ldots)$, as it is in our case, it is readily shown that

$$\frac{1}{k_B T_M} = \left( \frac{dN}{2} - 1 \right) \left\langle K^{-1} \right\rangle$$

(5)

where $K$ stands for the total kinetic energy of the system, $d$ is the dimensionality of ambient space and $N$ is the number of particles. In contrast, in the canonical ensemble, one has the relation

$$k_B T_C = \frac{2}{dN} \left\langle K \right\rangle,$$

(6)

which we will refer to as the kinetic temperature. If the distribution of $K$ is strongly peaked at one value, as usually happens for large systems, both definitions (5) and (6) will coincide. This is a special instance of ensemble equivalence in the thermodynamic limit, and is to be expected on general grounds except for special cases \[9–11\]. On the other hand, the two definitions of temperature will generally differ in finite systems. Nevertheless, since the system we consider can be thought of as being made up of subsystems in contact with each other, it seems reasonable that the “local temperature” could be identified with the average kinetic energy of particles at each position. In a sense, the main message of this paper is precisely that such intuition is altogether untenable, at least in the microcanonical ensemble if one considers terms of order $1/N$.

IV. MICROCANONICAL CALCULATION

The statistics in the microcanonical ensemble are given by

$$\rho_E(\vec{p}_i, \omega_i; x_i, y_i, \phi_i) := \frac{1}{\Omega_{N,M}(E)} \delta \left[ E - H(\vec{p}_i, \omega_i; x_i, y_i, \phi_i) \right]$$

(7)
FIG. 1: The geometric setting of our SLG system: in the closed slab of length $L$ the array of $M$ rotors is set in a (finite horizon) triangular lattice so that $N$ particles (in dots) cannot enter and leave an hexagonal cell surrounding each disc without having at least one scattering collision. Particles are reflected elastically by walls at $x = 0$ and $x = L$; the vertical coordinate is periodic. Two cells are the minimum width of the slab in order to avoid consecutive collisions with the same disk. The field strength $E$ is constant along the slab.

where $\Omega_{M,N}(E)$ is the microcanonical partition function, with the dependencies on $E$, $M$ and $N$ explicitly displayed

$$\Omega_{N,M}(E) = \int d^{2N}p \, d^{N}x \, d^{N}y \, d^{M}\omega \, \delta [E - H(\vec{p}_i, \omega_j; x_i, y_i, \phi_j)]$$

(8)

and the Hamiltonian we consider is given by

$$H(\vec{p}_i, \omega_j; x_i, y_i, \phi_j) = \sum_{i=1}^{N} \frac{p_{i}^2}{2m} + \frac{1}{2\Theta} \sum_{i=1}^{M} \omega_{i}^2 + qE \sum_{i=1}^{N} x_{i}$$

(9)

What we want to compute is the kinetic temperature at $x_0$. That is, we want to know the average kinetic energy of a particle, given that its position is in the infinitesimal interval $[x_0, x_0 + dx_0]$. The local kinetic temperature is expressed as

$$k_B T(x_0) = \int dp_x \, dp_y \, \frac{p_x^2 + p_y^2}{2m} \rho(\vec{p}|x_0),$$

(10)

where $\rho(\vec{p}|x_0)$ is the momentum distribution conditional to the particle position being $x_0$. This conditional probability is, of course, normalized, i.e.

$$\int d^2\vec{p}_0 \, \rho(\vec{p}_0|x_0) = 1,$$

(11)

it follows, then, that if $\rho(p_0|x_0)$ is known up to an arbitrary multiplicative constant which is independent of $p_0$, then it is in fact fully known since (11) determines this constant. Thus, we may without loss of information discard any multiplicative constant that is independent of $p_0$. Denoting
by \( \propto \) the equality of two expressions up to such a constant we have

\[
\rho(\vec{p}_0|x_0) \propto \int d^{2N} p \, d^N x \, d^N y \, d^M \omega \, \rho_E(\vec{p}_i, \omega_i; x_i, y_i, \phi_i) \times \\
\times \sum_{j=1}^{N} \delta(\vec{p}_j - \vec{p}_0) \delta(x_j - x_0).
\]  

(12)

Thus

\[
\rho(\vec{p}_0|x_0) \propto \Omega_{N-1,M} \left( E - q\mathcal{E}x_0 - \frac{p_0^2}{2m} \right)
\]  

(13)

To proceed we must calculate \( \Omega_{N,M}(E) \). In the case \( L \to \infty \), an entirely straightforward scaling argument shows that

\[
\Omega_{N,M}(E) \propto E^{2N+M/2-1}
\]  

(14)

From which the kinetic temperature in this limit, \( (22) \), can be readily derived. We proceed directly to the general case, which is slightly more involved: consider the Laplace transform

\[
\hat{\Omega}_{N,M}(z) = \int_0^\infty e^{-zE} \Omega_{N,M}(E) dE
\]  

(15)

or, explicitly:

\[
\hat{\Omega}_{N,M}(z) = \int_{-\infty}^{\infty} d^2 p \int_0^L d^N x \int_0^W d^N y \int_{-\infty}^{\infty} d^M \omega \exp \left[ -z \left( \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2\mathcal{E}} \sum_{i=1}^{M} \omega_i^2 + q\mathcal{E} \sum_{i=1}^{N} x_i \right) \right]
\]  

(16)

where \( L \) is the length of the system in the \( x \)-direction and \( W \) is the length in the periodic \( y \)-direction. The advantage of this expression is, of course, that the integrals are separable and can be evaluated. Again omitting irrelevant constants, we have:

\[
\hat{\Omega}_{N,M}(z) \propto z^{-2N-M/2} \left( 1 - e^{-zq\mathcal{E}L} \right)^N.
\]  

(17)

In order to state the final results more expeditiously, we first define a function \( \Phi_N(\nu|x) \) as follows:

\[
\Phi_N(\nu|x) = \sum_{n=0}^{N} \binom{N}{n} (-1)^n(x-n)^\nu \Theta(x-n),
\]  

(18)

where \( \Theta(x) \) is the step function.

It is now readily seen that, by inverting (17), we obtain

\[
\Omega_{N,M}(E) \propto (q\mathcal{E}L)^{2N+M/2-1} \Phi_N \left( 2N + M/2 - 1 \middle| \frac{E}{q\mathcal{E}L} \right).
\]  

(19)
We can now calculate $\rho(p_0|x_0)$ explicitly:

$$\rho(p_0|x_0) = \left( \frac{2N + M/2 - 2}{2\pi m qE_L} \right) \frac{\Phi_{N-1} \left( \frac{E-qE_Lp_0/(2m)}{qE_L} \right)}{\Phi_{N-1} \left( \frac{E-qE_Lx_0}{qE_L} \right)}$$

(20)

Thus, the kinetic temperature as a function of position $x_0$ is given by

$$k_B T(x_0) = \left( \frac{qE_L}{2N + M/2 - 1} \right) \frac{\Phi_{N-1} \left( \frac{E-qE_Lx_0}{qE_L} \right)}{\Phi_{N-1} \left( \frac{E-qE_L}{qE_L} \right)}$$

(21)

We observe in (21) that for finite values of $N$ and $M$, if the temperature $T(x)$ is defined as the local average of the kinetic energy of the particles, then such temperature is not constant as a function of $x$. The limiting behaviors of the above expression are relatively easy to evaluate. First we consider the case in which the system size grows to infinity: when $qE_L > E$ then the step functions are zero for all value of $x_0$, except for the term $n = 0$. Thus, in this limit we have

$$k_B T(x_0) = \frac{(E - qE_Lx_0)}{2N + M/2 - 1}. \Theta(E - qE_Lx_0). \quad (22)$$

It is amusing to note that this may be an outrageous limit: if the field is earth's gravity, for example, to achieve the desired limit we need heights larger than those that would be reached if we allocate all the energy of the system as the gravitational potential energy of a single particle. If we consider that molecular masses are of the order of $10^{-25}$ kg, energies corresponding to temperatures of a few degrees Kelvin correspond to heights of hundreds of meters even for systems consisting of a few molecules.

The limit in which the field vanishes $NqE_L/E \rightarrow 0$, can be calculated using the fact that

$$\sum_{m=0}^{M} \frac{M!}{m!(M-m)!} (-1)^m m^n = (-1)^M \begin{cases} 
0 & \text{if } n < M; \\
M! & \text{if } n = M; \\
M(M+1)!/2 & \text{if } n = M+1; \\
\vdots & \text{if } n \geq M+1;
\end{cases}$$

(23)

Then, in this limit, the kinetic temperature of the particles becomes

$$k_B T(x_0) = \frac{E}{N + M/2} \left[ 1 - \frac{qE_N L}{E} \left( 1 - \frac{(L-x_0)}{NL} \right) + \cdots \right]; \quad (NqE_L/E \rightarrow 0) \quad (24)$$

where we have kept terms to leading order in the strength of the field only to highlight the first order at which the dependence on the position $x_0$ appears.
We can make an entirely similar computation for the disks, where now we want to calculate $g(w_j)$, the probability that the $j^{th}$ scatterer has angular velocity $w_j$,

$$g(w_j) \propto \Omega_{N,M-1} \left( E - \frac{\Theta w_j^2}{2} \right)$$  \hspace{1cm} (25)

Using the explicit expression for $\Omega_{N,M}(E)$ and normalizing, one obtains

$$g(w_j) = 2 \left( \frac{\Theta}{2} \right)^{1/2} \frac{\Gamma(2N + M/2)(q\epsilon L)^{-1/2}}{\Gamma(1/2)\Gamma(2N + M/2 - 1/2)} \frac{\Phi_N \left( 2N + M/2 - 3/2, \frac{E - \Theta w_j^2/2}{q\epsilon L} \right)}{\Phi_N \left( 2N + M/2 - 1, \frac{E}{q\epsilon L} \right)}. \hspace{1cm} (26)$$

Thus, for the scatterers, using the mean kinetic energy to define the temperature yields

$$k_B T_S(E) = \frac{q\epsilon L}{2N + M/2} \frac{\Phi_N \left( 2N + M/2, \frac{E}{q\epsilon L} \right)}{\Phi_N \left( 2N + M/2 - 1, \frac{E}{q\epsilon L} \right)}$$  \hspace{1cm} (27)

which, in contrast to (21) is constant throughout the system. In the limit $L \to \infty$, again only the $n = 0$ terms contribute and the above expression becomes:

$$k_B T_S(E) = \frac{E}{2N + M/2}; \hspace{1cm} (28)$$

whereas in the limit $Nq\epsilon L/E \to 0$ one recovers the value

$$k_B T_S(E) = \frac{E}{N + M/2} \hspace{1cm} \text{(} Nq\epsilon L/E \to 0). \hspace{1cm} (29)$$

Of course, in this limit the field $\epsilon$ no longer plays a role and the kinetic temperature of disks (29) and particles (24) tend to the same value.

Finally, to finish muddling the situation, we can calculate the temperature directly from eq. (4),

$$k_B T_M(E) = \frac{q\epsilon L}{2N + M/2 - 1} \frac{\Phi_N \left( 2N + M/2 - 1, \frac{E}{q\epsilon L} \right)}{\Phi_N \left( 2N + M/2 - 2, \frac{E}{q\epsilon L} \right)}$$  \hspace{1cm} (30)

which is a constant of the system, albeit, not equal to the kinetic temperature of the scatterers (27). Expression (30) takes the value

$$k_B T_M(E) = \frac{E}{2N + M/2 - 1}, \hspace{1cm} (31)$$

as $L \to \infty$, which again differs slightly from the value reached by the scatterers (28). This is slightly unexpected: indeed, we might have expected that, since the scatterers are in contact with the particles, these could be assimilated to a “thermal bath”, so that the scatterers would effectively be in the canonical ensemble. This is in fact correct if $N \gg M$ or if $M \gg 1$, but not in general.
On the other hand, in the limit, $Nq\mathcal{E}L/E \rightarrow 0$, from (30) we obtain
\[
k_B T_M(E) = \frac{E}{N + M/2 - 1}, \quad (Nq\mathcal{E}L/E \rightarrow 0).
\]
(32)

This difference is easy to understand, if we realize that the height now drops out as a variable which contributes to equipartition.

Of particular interest is the fact that the disks have a constant kinetic temperature that is \textit{different} from the local kinetic temperature of the particles with which they interact. Further, the global temperature in the system does not coincide with the kinetic temperatures of the components. While these results appear to be quite contrary to the usual notion of equilibrium, they are, in fact, a consequence of the equilibrium statistics in the microcanonical ensemble for finite systems.

In hindsight, the origin of the variation of the kinetic energy with the height of the particles in system is easy to understand: The presence of the applied field implies that potential energy is required for particles to reach certain height. Since the total energy is fixed, there is less energy left over to distribute amongst the rest of the elements in the system. This is not the case for the rotators, since there is no energy cost for their location in the channel. Thus the kinetic temperature of the particles decreases with height whereas that of the rotators remains constant. Still, it is amusing to note that in spite of having different kinetic temperatures, or precisely because they have different kinetic temperatures, the scatterers and the particles are in equilibrium with each other. We present a sketch of the kinetic effects involved in this apparent failure of collisions to yield equipartition of kinetic energy in Appendix A.

For completeness, we also calculate the particle density, which can be expressed as:
\[
C(x_0) \propto \int_{-\infty}^{\infty} d^2 p_0 \Omega_{N-1,M} \left( E - q\mathcal{E}x_0 - \frac{p_0^2}{2m} \right).
\]
(33)

$C(x_0)$ must now be normalized to $N$, the number of particles in the system. Using Eq (33) we obtain:
\[
C(x_0) = \frac{N(q\mathcal{E}L)^{2N+M/2-2}}{N} \Phi_{N-1} \left( 2N + M/2 - 2 \left| \frac{E - q\mathcal{E}x_0}{q\mathcal{E}L} \right| \right)
\]
(34)

where the normalization constant $\mathcal{N}$ is
\[
\mathcal{N} = \frac{1}{q\mathcal{E}(2N + M/2 - 1)} \left( E^{2N+M/2-1} + S_1 + S_2 \right)
\]
(35a)
\[
S_1 = \sum_{n=1}^{n^*} \frac{(N - 2n)(N - 1)!}{n!(N - n)!} (E - nq\mathcal{E}L)^{2N+M/2-1}
\]
(35b)
\[
S_2 = \sum_{n=n^*}^{N-1} \frac{(N - 1)!}{n!(N - n - 1)!} (E - nq\mathcal{E}L)^{2N+M/2-1}
\]
(35c)
where \( n^* = \text{Int}[\frac{E}{q^2 T}] \). The convoluted expression for \( \mathcal{N} \) arises from the fact that the integral of some terms of the sum are cut by the step function in the expressions, whereas others are cut by the finite size \( L \) of the system. It is, of course \( C(x_0) \), the density profile of the particles, which becomes the familiar exponential in the thermodynamic limit.

V. GENERAL SYSTEMS

While the explicit calculations presented above apply directly to the SLG, we argue that the effects illustrated with this model are rather general. Our observations rest essentially on (13) and (25), in which we express the probability of finding a particle, respectively a disk, with a given kinetic energy in terms of the microcanonical partition function. The reasoning leading to these equations is, of course, entirely general.

If we take an arbitrary system, it is necessary to resort to approximations, but the result is quite similar to the ones obtained for the SLG. For the sake of simplicity, we limit ourselves here to a finite number \( N \) of particles only confined by the field, that is, we neglect the effect of a confining box altogether. One has in the general case, for the particles subjected to the field:

\[
\ln \rho(p_0|x_0) = \ln \Omega_{N-1,M}(E - qE x_0 - \frac{p_0^2}{2m}) - \ln \Omega_{N-1,M}(E) + K
\]

\[
\approx K - \left( qE x_0 + \frac{p_0^2}{2m} \right) \frac{\partial}{\partial E} \ln \Omega_{N,M}(E) + \frac{1}{2} \left( qE x_0 + \frac{p_0^2}{2m} \right)^2 \frac{\partial^2}{\partial E^2} \ln \Omega_{N,M}(E)
\]

\[
= K' - \frac{p_0^2}{2m k_B T_M} - \frac{1}{2} \left( qE x_0 + \frac{p_0^2}{2m} \right)^2
\]

\[
= K'' - \frac{p_0^2}{2m k_B T_M} \left( 1 + \frac{qE x_0}{C_V T_M} \right) - \frac{p_0^4}{8 m^2 C_V k_B T_M^2}
\]

where \( K \) and its primed variants denote additive constants independent of \( p_0 \), corresponding to the undetermined multiplicative constant in (13), and \( C_V \) is the heat capacity at constant volume. The second term clearly shows that the temperature has the kind of dependence stated in this paper. Indeed

\[
\frac{dT(x_0)}{dx_0} = -\frac{qE}{C_V}
\]

up to terms of higher order in \( 1/N \). The third term in (36), on the other hand, indicates a deviation from the Maxwellian in microcanonical systems at the \( 1/N \) level. It thus generates a correction to \( T \) of order \( 1/N \) but independent of \( x_0 \).

If we additionally have another species which is not affected by the external field, its kinetic temperature will be unaffected by the field and thus independent of \( x \). This kinetic temperature
of this species will differ in general from the kinetic temperature of the other species. We thus see that quite generally the kinetic temperature neither equilibrates between different heights, nor between different species. On the other hand, the microcanonical temperature is a characteristic of the whole system, but, contrary to the kinetic temperature, there is no clear way of attributing it to any part of the system, such as a species, or a position.

VI. NUMERICAL SIMULATIONS

To check the validity of our results, we have performed extensive molecular dynamics simulations of the system as well as Monte Carlo simulations, since with the latter no problems arise with the sampling of the $N$-particle phase space. For all the simulations, particle and disk masses were set to one, $m = M = 1$, as well as the interaction parameter $\eta = 1$, which controls the energy exchange between particles and scatterers. To calculate local averages, the channel of Fig. 1 is divided in $S$ “strips” of width $\Delta x = L/S$, where $L$ is the total channel length.

The density $C(x)$, and kinetic temperature $T_K(x)$ were obtained as the time average of particle number per area and the time average of the kinetic energy per particle in each strip.

In Fig. 2 we show that $T_K(x)$ is indeed not constant for our closed, many-particle system, as expected from our results. However, the kinetic temperature measured in the molecular dynamics simulations appears to display a very slight, but possibly systematic, deviation from the value obtained analytically. We believe that such discrepancies may arise from the fact that the presence of the field affects the ergodicity properties of the system. In particular, some configurations are hard to reach from generic initial conditions; for example in those for which the disks have a large share of the energy, particles become confined to the region near the bottom of the channel. To check whether this was the case, we performed microcanonical Monte Carlo simulations, in which particles were allowed to fly under the influence of the field, and after a certain amount of time, they would either exchange energy with a random scatterer or randomly rotate their velocity vector. The kinetic temperatures for this simulation agree quite well with the theoretical prediction (see Fig. 3).

The density of particles $C(x)$ is also shown in Fig. 2 (inset); it was measured for both the SLG and the normal Lorentz gas for similar simulations with an applied field $E = -0.5$, where all particles are initially at height $x = 15$ while discs and particles have zero kinetic energy. We observe that in the SLG the density profile is indeed barometric; in contrast, in the normal Lorentz gas particles cannot go beyond their maximum initial energy: it is therefore impossible to obtain
such a barometric profile without some kind of interaction, as provided for example by the SLG model.

Spinning Lorentz gas. $N = 90, E = 720, L = 30, \mathcal{E} = -0.5$

FIG. 2: Kinetic temperature profile in the SLG for $N = 90$ particles inside the closed slab with length $L = 30$ (see Fig. 1), with an external applied field $\mathcal{E} = -0.5$ and system energy of $E = 720$. These results were obtained by Molecular Dynamics simulation (segmented lines). The continuous line (red) is the theoretical prediction (21). We observe a slight discrepancy for $T_k(x)$ along the slab; the reason is presumably related to issues of non-ergodicity of the simulation. The short-segmented line (stars) indicates the temperature of the discs. These data are also significantly more noisy than in the Monte-Carlo simulations. In the inset, we show a semi-log plot of the density of particles $C(x)$ in the slab, compared to a similar simulation in the usual Lorentz gas (in crosses).

VII. CONCLUSION

Summarising: in isolated systems described by the microcanonical ensemble, the presence of an applied field gives rise to intrinsic equilibrium inhomogeneities: a spatially varying local kinetic temperature which differs from the thermodynamic temperature of the system. We argue that this result is general, and we illustrate the effect both analytically and numerically for the SLG model, subject to a constant external field, for which all calculations can be carried out explicitly. The
FIG. 3: This figure shows results from a Monte-Carlo simulation of the SLG model to obtain the kinetic temperature profile for $N = 90$ particles inside a closed slab of length $L = 30$ with an external applied field $E = -0.5$ and an initial energy of $E = 720$. The continuous line shows the simulation data while the discontinuous line (stars) is the theoretical prediction [21]. There are thus no approximations involved. The discontinuous line with crosses (green) indicates the temperature of the discs.

The effect vanishes in the limit $N \to \infty$, but only as $1/N$, so that it may be observable in small systems.

If we have another species in the system which is not affected by the external field, its kinetic temperature will be unaffected by the field. The kinetic temperature of this species will be quite close to the microcanonical temperature of the whole system, at least if the particle numbers are not too small. On the other hand, the two species’ kinetic temperatures will not equilibrate, so that we cannot identify it as the (local) thermodynamic temperature of the species.

Further, an interesting possibility should be pointed out: when small systems are considered in the microcanonical ensemble, the possibility of negative specific heat cannot be ruled out [9–11], particularly if the system has long range interactions and is close to a tricritical point. We therefore cannot exclude the possibility that a temperature gradient arises in which high lying particles actually have higher temperatures than low lying ones.

These results must be all carefully considered in any applications of statistical thermodynamics to small many-particle systems such as e.g. atomic clusters, nanoparticles or molecular/biological ensembles, since these systems may not necessarily be described using the thermodynamic limit.
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Appendix A: Kinetic observations on the failure of disks to equilibrate with particles

The conundrum arising from the behaviour of the scatterers may be best understood in the light of the following remarks: First, a high lying scatterer can have a kinetic temperature which is significantly higher than that of the particles in the system. Second: most of the time such a scatterer has no particle in its vicinity. Finally, if we calculate the mean kinetic energy of the scatterer conditional on the presence of a particle in the same cell, it is the same as the particle temperature at this height. The presence of several particles, as an entirely similar calculation to the ones performed here shows that the temperature of the scatterer will be still lower.

This leads to the conclusion that the scatterer must be significantly hotter when it finds itself in the absence of any particle than in the presence of one or more particles. Since the mere absence of particles cannot of itself heat up the scatterer, we must find a mechanism whereby the scatterer is preferentially heated to an anomalous extent at the precise moment when the last particle leaves the scatterer’s vicinity.

To this end, let us use an exceedingly simplified model of what takes place in the system. Consider two cells, an upper and a lower one. Each cell contains a scatterer, which always remains in the cell and only has kinetic energy.

Additionally the whole system contains one particle, which can alternate between the two cells, and which has both kinetic and potential energy, the latter being always $V/2$ in the upper cell and $-V/2$ in the lower. Such a system in the microcanonical ensemble has all the features we look for. In particular, the particle in the upper cell is significantly colder than the corresponding scatterer. Indeed, in that case, all the components have the same energy, which leads to the kinetic energy of the particle being more than that of the scatterer in the lower and less in the upper cell.

In order to generate the microcanonical ensemble, we use the following Monte-Carlo dynamics: at each step, with probability $\epsilon$ a move of the particle from one cell to the other is attempted. If the particle is in the upper cell, the move is always accepted and the particle’s kinetic energy is increased by $V$. Otherwise, the move is only accepted if the total energy of the particle is larger than $V$, The kinetic energy is then decreased by $V$. With probability $1 - \epsilon$, on the other hand,
the particle and the scatterer in the particle’s cell add up their kinetic energies and then proceed to redivide the total energy randomly. As is readily seen, this Markov process satisfies detailed balance with respect to the microcanonical ensemble and thus tends to it, at least if ergodicity is satisfied.

This systems displays exactly the kind of “paradox” described in this paper: on average, the scatterer has a different kinetic energy than the particle, yet, when $\epsilon$ is small they pass a long time together and equilibrate their kinetic energies, thus it is not clear intuitively from what effect the discrepancy in temperatures could arise. Indeed, it is not difficult to show in this simplified model, that the kinetic energy of a scatterer conditional on the presence of the particle in the cell, is indeed close to the particle kinetic energy.

Thus the only way in which the discrepancy can arise is in the last exchange of energy just before the particle changes cell. Indeed, if the particle leaves the upper cell for the lower one with an exceptionally small amount of kinetic energy, then the scatterer in the upper cell keeps an anomalously large amount of kinetic energy. Further, the particle in these circumstances will take a longer than normal time to come back to the upper cell. Thus the upper scatterer will have remained for an anomalously long time in a state of anomalously high kinetic energy. The repetition of this pattern is, as can be checked, sufficient to cause a finite difference in the kinetic energies of the upper scatterer and the particle in the upper cell.

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