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ON THE TIME-DEPENDENT PROPERTIES OF THE LATTICE MODEL OF THE LORENTZ GAS

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ABSTRACT

Far from equilibrium properties of a one dimensional lattice model of the Lorentz gas are studied by means of a correlated walk description. The exact time evolution of the distribution function of the non-Markovian stochastic process underlying the walk is obtained. The time relaxation of the system, the Boltzmann entropy and other time dependent thermodynamic potentials are given in exact and closed form. It is also shown that the local equilibrium condition is satisfied, even though the system is far from equilibrium. Finally in the limit of long times, the ideal gas thermodynamic properties are obtained.

RESUMEN

Se estudian las propiedades lejos del equilibrio de un modelo de red unidimensional del gas de Lorentz usando una descripción de camino correlacionado. Se obtiene la evolución temporal exacta de la función distribución del proceso estocástico no-Markoviano asociado al camino. La relajación temporal del sistema, la entropía de Boltzmann y otros potenciales termodinámicos dependientes del tiempo se dan en forma exacta y cerrada. Se demuestra además que se satisface la condición de equilibrio local, a pesar de que el sistema está lejos del equilibrio. Finalmente en el límite de tiempos largos, se obtienen las propiedades del gas termodinámico ideal.

1. INTRODUCTION

The study of nonequilibrium phenomena is beset with many difficulties of physical and mathematical nature. These difficulties have motivated theorists to devise and study the simplest models which exhibit any resemblance with the systems occurring in the real world, with the hope that the deeper insights offered by the exact treatment, or the mathematical trasparency of the models, will compensate for the unrealistic simplifications in the formulation.

One of these models is that of a system of independent particles moving among randomly distributed fixed scatteres. This system is commonly known in statical mechanics, at least when the scatteres are hard spheres, as the Lorentz gas[1] or Sinai's billiards[2]. Here we shall consider the particular case of a uniform distribution of scatteres to model the scattering of particles by the lattice points of a solid.

It has been shown by Fujita *et al.*[3] that the dynamics of a Lorentz gas molecule may be simulated in terms of a correlated walk[4] on a cubic lattice by assuming that when a particle hits a fixed scatterer, the particle will suffer forward or backward scattering with different probabilities. The fixed scatterer is not necesarily a hard sphere, it may be an anisotropic scatterer, for instance an electric dipole, or even an isotropic scatterer in the presence of an external field.

So far, the only analytic solution that has been found for this Lorentz lattice gas, corresponds to the particular case of initial conditions where all the particles are located at some point in the lattice[8,9,10].

Unfortunately this solution is cumbersome and difficult to handle. We will show in this paper that for spatially homogeneous initial conditions the corresponding solution is elementary and so the dynamics of the model can be analyzed at the light of straighforward calculations.

More specifically, we consider the one dimensional version of this model which corresponds to the X projection of the three dimensional motion of the particles. We will show that for periodic boundary conditions and far from equilibrium initial conditions, the exact and analytic time evolution of this Lorentz lattice gas can be derived.

For this purpose we first analize the non-Markovian process underlying a walker moving of a one dimensional periodic lattice with lattice constant $a_0 = 1$ and lenght L. The probability of finding the walker at the discrete position $X = xa_0$ at the discrete time $t = N\tau_0$, if the walker is moving form left to right (positive velocity), is described by $P_+(X,N)$. Similarly, when the walker moves from right to left (negative velocity), the corresponding probability is $P_-(X,N)$. Clearly, the knowledge of these distribution functions provides a complete description of the stochastic process associated with the motion of the walker, since the specification of P_+ and P_- is equivalent to the knowledge of a one particle distribution function, $f(x,v,t)$, of the Lorentz type. In fact,

$$P_+(X,N) \equiv f(x = Xa_0, v > 0, t = N\tau_0) \qquad , \qquad (1.1a)$$

$$P_-(X,N) \equiv f(x = Xa_0, v < 0, t = N\tau_0) \qquad , \qquad (1.1b)$$

where the magnitude of the velocity, v, is a constant given by $v = a_0/\tau_0$. Thus, P_+ and P_- describe the time evolution of a Lorentz lattice gas whose phase-space consists of ($\Omega = 2L$) points, as shown in Fig. 1.

In the next section 2 we give the finite difference equations that the above distributions satisfy and we discuss the physical interpretation of the parameters involved. A solution of these equations is obtained for spatially homogeneous initial conditions in section 3 and its evolution towards equilibrium is studied. Using this solution, in section 4 we explicitly evaluate some non-equilibrium thermodynamic potentials of the system and show that the local equilibrium hypothesis

holds for any degree of departure from equilibrium. Finally, in section 5 some thermal equilibrium properties, like the equation of state and the internal energy, are obtained.
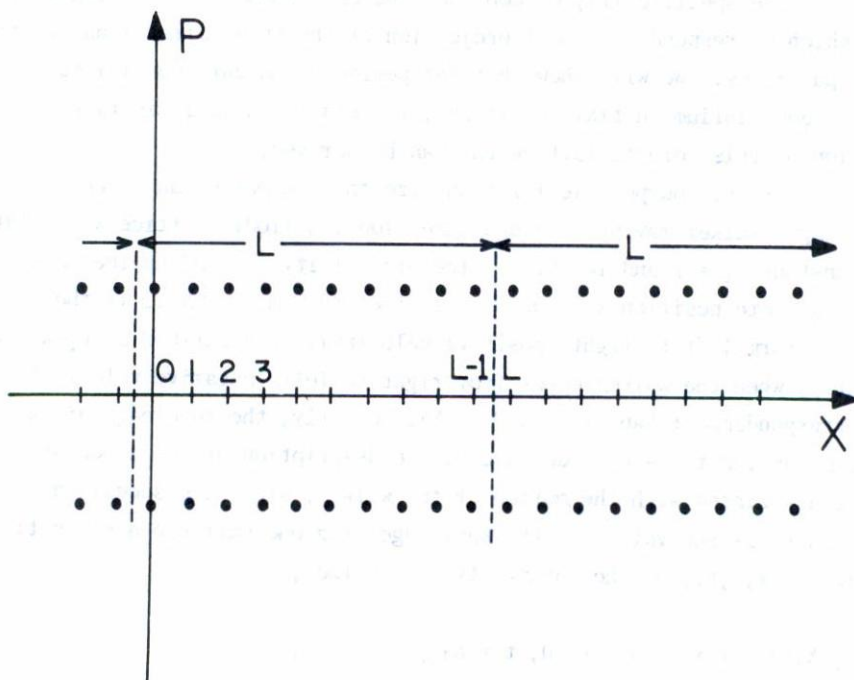
Fig. 1. Phase space for one dimensional periodic lattice of lattice constant $a_0 = 1$ and length L.

2. PROPERTIES OF THE MODEL

The probabilities for making succesive steps, P_+ and P_-, introduced in the previous section are described through transition probabilities that keep memory of the previous step and which are defined as

a: probability of stepping right if the previous step was to the right
b: probability of stepping right if the previous step was to the left
c: probability of stepping left if the previous step was to the right

d: probability of stepping left if the previous step was to the left

In terms of these quantities the equations of motion describing the correlated walk on the lattice are found to be

$$P_+(X, N+1) = aP_+(X-1,N) + bP_-(X-1,N) \quad , \tag{2.1a}$$

$$P_-(X, N+1) = cP_+(X+1,N) + dP_-(X+1,N) \quad . \tag{2.2b}$$

Notice that the normalization condition (CONSERVATION OF PARTICLES)

$$\sum_x \left\{ P_+(X,N) + P_-(X,N) \right\} = 1 \tag{2.2a}$$

implies that

$$a + c = 1 \quad , \qquad b + d = 1 \tag{2.2b}$$

and, therefore, there are only two independent transition probabilities. Actually, in order to describe more clearly the physical role of the transition probabilities, it is convenient to introduce two independent parameters, namely, the bias factor ϵ (also called the external field parameter), defined by

$$\epsilon = a - d = b - c \tag{2.3}$$

and the correlation factor, δ defined as

$$\delta = a - b = d - c \quad . \tag{2.4}$$

ϵ is a measure of any bias in one direction, it may depend on an external field (which does not perform any work on the system) or on anisotropies of the lattice or any other perturbing effect. Its range is $-1 \leq \epsilon \leq +1$. On the other hand, δ measures the amount of correlation between two succesive steps, in such a way that for maximum correlation the walker eventually will keep full motion in the same direction of the external

field. Clearly, for vanishing correlation two succesive steps will be statistically independent and the whole problem is reduced to the usual random walk. For bias toward the right ($\epsilon > 0$) the range of δ is $0 \le \delta \le 1 - \epsilon$.

Hence the stochastic process may be described in terms of either of the two sets $(a,b,c,d,)$ or (ϵ,δ) with the following connection between them

$$2a = 1 + \epsilon + \delta ,$$
$$2b = 1 + \epsilon - \delta ,$$
$$2c = 1 - \epsilon - \delta ,$$
$$2d = 1 - \epsilon + \delta .$$

(2.5)

3. SOLUTION FOR HOMOGENEOUS INITIAL CONDITIONS

In order to solve the set of equations (2.1) we have to choose a boundary condition at $X = 0$ and $X = L-1$. Since for a large volume we expect that the effect of the boundary condition will not be so important on the bulk properties of the gas, we choose periodic boundary conditions for mathematical simplicity. This periodic character of the solution, suggests the use of finite Fourier series, so we define the transformation

$$\vec{P}(r,N) = \sum_{X=0}^{L-1} P(X,N)\exp(i2\pi rX/L) .$$

(3.1)

Under this transformation the coupled set of equations (2.1) may be written as

$$\vec{P}(r,N) = \underset{\sim}{M} \cdot \vec{P}(r,N-1)$$

(3.2)

where the probability vector $\vec{P}$ is defined as

$$\vec{P}(r,N) \equiv \begin{bmatrix} P_+(r,N) \\ P_-(r,N) \end{bmatrix}$$

(3.3)

and the transition matrix $\underset{\sim}{M}$ is given by

$$\underset{\sim}{M} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \tag{3.4}$$

with $A = ae^{ik}$, $B = be^{ik}$, $C = ce^{-ik}$, $D = de^{-ik}$ and where

$$k \equiv 2\pi r/L \; . \tag{3.5}$$

Clearly the solution of Eq. (3.2) is given by

$$\vec{P}(r,N) = \underset{\sim}{M}^N \cdot \vec{P}(r,N=0) \tag{3.6}$$

with

$$\underset{\sim}{M}^N = \alpha(N)\underset{\sim}{M} - \delta\alpha(N-1) \; \mathbf{1} \tag{3.7}$$

where $\alpha(N)$ depends on the eigenvalues λ_+, λ_- of the matrix $\underset{\sim}{M}$,

$$2\lambda_{\pm} = A + D \pm \left[(A+D)^2 - 4\delta \right]^{\frac{1}{2}}$$

through the expression

$$\alpha(N) \equiv \frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-} \; . \tag{3.8}$$

Therefore, the final solution $P(X,N)$ is given by the inverse
Fourier transform of (3.6), namely

$$\vec{P}(X,N) = \frac{1}{L} \sum_{r=0}^{L-1} \vec{P}(r,N)\exp(-i2\pi rX/L) \tag{3.9}$$

The most important initial condition $P(X,N=0) = \begin{pmatrix} \delta x_0 \\ 0 \end{pmatrix}$

which generates the Green's function, has been discussed elsewhere[5,8,9,10].
Unfortunately this analytic solution is rather involved and will not be
considered here. However, there is one initial condition which generates
the easiest analytic solution, namely, any homogeneous (position independent)
initial condition, $P(X, N = 0) = P(N = 0)$. For this case we have

$$\vec{P}(r, N = 0) = \vec{P}(N = 0) L \delta_{r, mL} \quad , \quad m = 0, \pm 1, \pm 2, \ldots \quad (3.10)$$

We have choosen this particular initial condition, hoping to show
how the irreversible behavior of the system develops, having at the same
time a very transparent and elementary mathematics.

Thus, using Eqs. (3.9), (3.10) and after some elementary algebra
we find that

$$P_+(X, N) = \left[a(1 - \delta^N) - \delta(1 - \delta^{N-1}) \right] \frac{P_+(N = 0)}{1 - \delta} + b(1 - \delta^N) \frac{P_-(N = 0)}{1 - \delta} \quad (3.11)$$

and

$$P_-(X, N) = c(1 - \delta^N) \frac{P_+(N = 0)}{1 - \delta} + \left[d(1 - \delta^N) - \delta(1 - \delta^{N-1}) \right] \frac{P_-(N = 0)}{1 - \delta} \cdot (3.12)$$

It should be stressed that these solutions are valid only for
arbitrary homogeneous initial conditions that satisfy the normalization
condition, Eq. (2.2a). We now consider two particular initial conditions.
First a far from equilibrium case where initially all the walkers in the
lattice are moving to the right. Then

$$P_+(N = 0) = \frac{2}{\Omega} \quad , \quad P_-(N = 0) = 0 \quad , \quad (3.13)$$

where Ω is the number of points in phase space ($\Omega = 2L$).

Substituting Eq. (3.13) into Eqs. (3.11) and (3.12) we obtain

$$P_\pm(N) = \frac{1}{\Omega} \left[1 \pm \delta \pm \epsilon \frac{1 - \delta^N}{1 - \delta} \right] \quad . \quad (3.14)$$

These solutions imply that as a result of the collisions between walkers and lattice scatteres the initial condition Eq. (3.13) can not persist, instead it evolves in time according to Eq. (3.14) toward a stationary state given by

$$P_\pm (N \to \infty) = \frac{1}{\Omega} \left[1 \pm \frac{\varepsilon}{1 - \delta} \right] \quad . \tag{3.15}$$

Notice that for zero bias factor ($\varepsilon = 0$) the stationary distribution is Ω^{-1} for both directions of motion, which is just the micro canonical distribution. Of course, for non-vanishing bias factor the stationary distribution is different according to the direction of the velocity with respect to the external field. As for the dependence on the correlation factor δ, note that for vanishing correlation there are two different stationary distributions

$$\lim_{\delta \to 0} P_\pm (N \to \infty) = \frac{1}{\Omega} (1 \pm \varepsilon) \tag{3.16}$$

and for maximum correlation, $\delta = 1 - \varepsilon$ one of the initial distributions persists, namely

$$\lim_{\delta \to 1 - \varepsilon} P_+ (N \to \infty) = \frac{2}{\Omega} \quad , \tag{3.17a}$$

$$\lim_{\delta \to 1 - \varepsilon} P_- (N \to \infty) = 0 \quad . \tag{3.17b}$$

Hence for maximum correlation the walkers move unconstrained in the direction of the bias factor and never have the chance of reversing its motion.

As a second initial condition let us now examine the case where the system is in thermal equilibrium,

$$P_+ (N = 0) = P_- (N = 0) = \frac{1}{\Omega} \quad . \tag{3.18}$$

This equation corresponds to a microcanonical distribution without an external field. Substitution of Eq. (3.18) into Eqs. (3.11) and (3.12) leads to

$$P_\pm(N) = \frac{1}{\Omega}\left[1 \pm \epsilon\ \frac{1 - \delta}{1 - \delta}^N\right] \qquad , \tag{3.19}$$

which describes how the thermal equilibrium distribution evolves in time after the bias factor is turned on. Notice that for this case the stationary distribution is precisely the same as the previous initial condition, Eq. (3.15). That this is true for the general case of arbitrary homogeneous initial conditions can be proved from Eqs. (3.11) and (3.12). Taking the long-time limit of these equations we find

$$P_\pm(N \to \infty) = \frac{1}{\Omega}\left[1 \pm \frac{\epsilon}{1 - \delta}\right] \tag{3.20}$$

which proves that the stationary state is indeed independent of the particular form of the homogeneous initial conditions and so, after some time, the system forgets any initial distribution.

As a first consequence of our dynamical description notice that we can easily find the relaxation time of the system. For this purpose note that in Eqs. (3.11) and (3.12) the time dependence occurs only through the factor δ^N. But since $0 \leq \delta \leq 1$, this is a monotonically decreasing function, so we may write the identity

$$\delta^N = \exp(-N \ln \delta^{-1}) \tag{3.21}$$

and clearly the relaxation time is given by

$$N_0 = (\ln \delta^{-1})^{-1} \ . \tag{3.22}$$

Notice that for a vanishing correlation, $\delta \to 0$, the relaxation time is zero. This is to be expected since for a non-correlate walk, the homogeneous probability distribution does not even change in time, it remains in a stationary state. On the other hand, for maximum, correlation the relaxation time depends on the external field as $N_0 \approx \epsilon^{-1}$, if $|\epsilon| \ll 1$. So, the external field induces the particles to reach their stationary state at a faster rate. Finally, for maximum correlation without external field, $\delta \to 1$, the relaxation time is infinite and the particles never reach equilibrium.

4. NON-EQUILIBRIUM POTENTIALS

Let us first consider the Boltzmann entropy defined by

$$S(t) = -k \int f(x,p,t) \log f(x,p,t) \, dxdp \equiv -k \, H(t) \quad , \tag{4.1}$$

where k is Boltzmann's constant. For the correlated walk with homogeneous initial conditions Eq. (4.1) reduces to

$$S(N) = -\frac{k\Omega}{2} \left[P_+(N) \log P_+(N) + P_-(N) \log P_-(N) \right] \quad . \tag{4.2}$$

From this equation we can study our two particular cases, namely, thermal equilibrium initial conditions, Eq. (3.18), and far from equilibrium initial conditions, Eq. (3.13). For the first case we have

$$\frac{1}{k} S_1(N) = \log \Omega - \frac{1}{2} \left[1 + \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] \log \left[1 + \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] - $$
$$\tag{4.3a}$$
$$- \frac{1}{2} \left[1 - \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] \log \left[1 - \varepsilon \frac{1 - \delta^N}{1 - \delta} \right]$$

and for the second one

$$\frac{1}{k} S_2(N) = \log \Omega - \frac{1}{2} \left[1 + \delta^N + \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] \log \left[1 + \delta^N + \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] - $$
$$\tag{4.3b}$$
$$- \frac{1}{2} \left[1 - \delta^N - \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] \log \left[1 - \delta^N - \varepsilon \frac{1 - \delta^N}{1 - \delta} \right] \quad .$$

In these equations Ω represents the number of accesible points in phase-space for a system with constant energy. However, since in the next section we shall describe the equilibrium properties of our model, it is suggested by the usual treatment of the microcanonical enesemble[6] that the entropy should be calculated in the region of phase space between the surface E and $E + \Delta$. Under these assumptions we have

$$\Omega = 2L(2me)^{\frac{1}{2}} + O(\Delta) \tag{4.4}$$

In Fig. 2 the entropies given by Eqs. (4.3) are plotted as functions of time for specific values of ε and δ. For equilibrium initial conditions, which correspond to maximum disorder, the entropy, S_1 (N = 0) has a maximum value (log Ω) and the effect of applying a bias factor ($\varepsilon \neq 0$) is to increase the order in the system, *decreasing* the entropy in the course of time toward a final value compatible with the applied field. As for the second case where initially all the particles move toward the right, and which corresponds to maximum order in the system and minimum entropy, the collisions with the lattice are the mechanism by which the order is reduced. Therefore, due to such collisions the entropy, S_2, increases in the course of time. If there were no bias factor, the system would evolve toward a state of maximum disorder and maximum entropy (log Ω). However, the presence of the bias factor imposes an upper boundary to the disorder, and so the system reaches a final equilibrium state compatible with the value of the bias factor, which is the same as in the previous case.

For both cases the stationary state, defined by $N \to \infty$, is given by

$$\frac{1}{k} S_{1,2} (N \to \infty) = \log \Omega - \frac{1}{2} \left(1 + \frac{\varepsilon}{1 - \delta}\right) \log \left(1 + \frac{\varepsilon}{1 - \delta}\right) -$$

$$\text{(4.5)}$$

$$- \frac{1}{2} \left(1 - \frac{\varepsilon}{1 - \delta}\right) \log \left(1 - \frac{\varepsilon}{1 - \delta}\right) .$$

Furthermore, if in addition the bias factor ε vanishes, the system reaches equilibrium and the entropy evolves toward its microcanonical value given by the logarithm of the number of microstates, that is,

$$\lim_{\varepsilon \to 0} \frac{1}{k} S_{1,2} (N \to \infty) = \log \Omega . \qquad \text{(4.6)}$$

This result gives the maximum value of the entropy of the system and is evident, as indicated by Eq. (4.5), that the presence of any bias factor $0 \leq \varepsilon \leq 1$ will decrease this value, yielding a stationary state of lower entropy. Also note that for the case of maximum correlation, $\delta = 1 - \varepsilon$, the entropy is given by
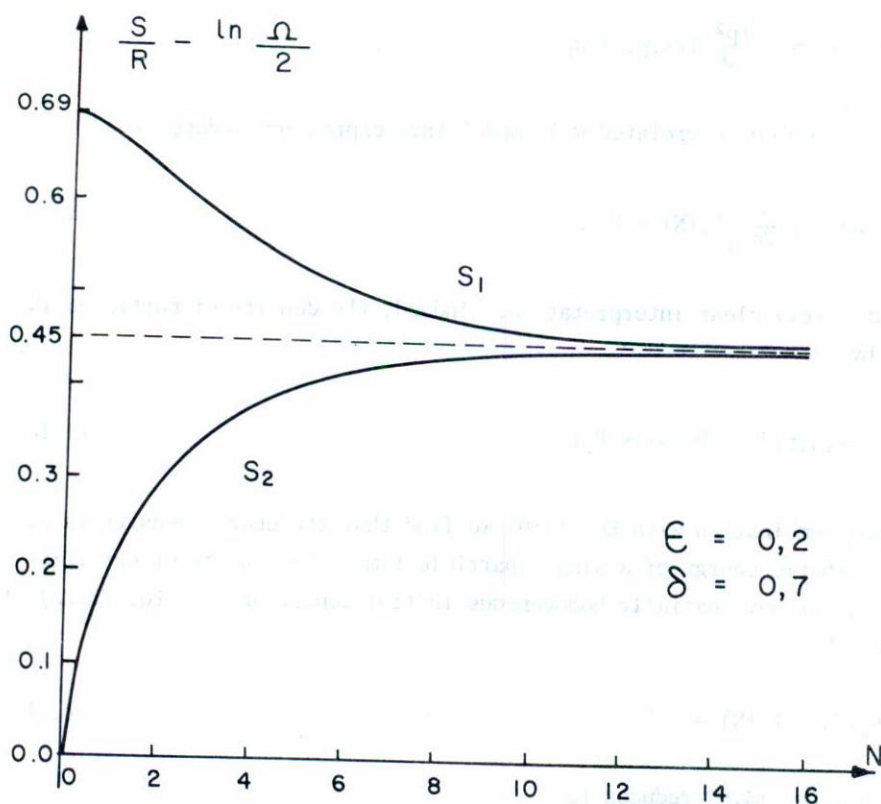
Fig. 2. Time evolution of entropy for equilibrium (——) and far form equilibrium initial conditions (-----) as given by Eqs. (4.3) and (4.4), respectively.

$$\lim_{\delta \to 1-\epsilon} \frac{1}{k} S_{1,2}(N \to \infty) = \log \frac{\Omega}{2} \quad , \qquad (4.7)$$

which corresponds to a situation where the only microstates accesible to the system are those with positive momentum, owing to the presence of the bias. Thus, for maximum correlation the number of microstates is reduced to a half of its value in equilibrium

Next consider the kinetic energy density defined as

$$E(x,t) = L \int \frac{p^2}{2m} f(x,p,t) \, dp \qquad . \qquad (4.8)$$

For our correlated walk model this expression reduces to

$$E(N) = L \frac{p^2}{2m} \left| P_+(N) + P_-(N) \right| \qquad (4.9)$$

and has a very clear interpretation. Indeed, the density of particles is given by

$$\int f(x,p,t) \, dp = P_+(N) + P_-(N) \qquad (4.10)$$

and upon combination with Eq. (4.9) we find that the energy density is equal to the kinetic energy of a single particle times the density of particles. However, for any spatially homogeneous initial condition form Eq. (2.2a) it follows that

$$P_+(N) + P_-(N) = L^{-1} \qquad (4.11)$$

and thus, Eq. (4.9) reduces to

$$E = p^2/2m \qquad (4.12)$$

which is independent of time. This results is consistent with the features of our model, where the magnitude of momentum is constant and so is the kinetic energy. (This is so because the external field, $\varepsilon \neq 0$ does not make any work on the system). Clearly, this allows us to use the equipartition theorem and relate the magnitude of momentum to the temperature in equilibrium. Thus

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{kT}{2} \qquad (4.13)$$

where the angular brackets stand for an equilibrium average, and therefore

$$|\vec{p}| = (m \, k \, T)^{\frac{1}{2}} \qquad . \tag{4.14}$$

Finally, we now consider the Helmholtz free energy density A defined by

$$A(x,t) = L \int \left[\frac{p^2}{2m} + k \, T \, \log \, f(x,p,t) \right] f(x,p,t) \, dp \quad . \tag{4.15}$$

After using Eqs. (4.2) and (4.8) this equation becomes

$$A(N) = \left(E(N) - TS(N) \right) \qquad . \tag{4.16}$$

Thus, being the energy a constant, the time dependence of the free energy occurs only through the entropy. This equation which is valid for all times and arbitrarily far from equilibrium, expresses the validity of the *local equilibrium assumption* for our model. It should be emphasized that this result appears naturally in our treatment and that it was not establi shed by using methods valid only near equilibrium, such a Chapman Enskog's[7].

5. EQUILIBRIUM PROPERTIES

From the thermal equilibrium expression for the entropy given by Eq. (4.5), which may be rewritten as

$$S(E,L) = k \, \log \, \left(L(2m \, E)^{\frac{1}{2}} \right) - S_0(\epsilon,\delta) \tag{5.1}$$

with

$$2S_0(\epsilon,\delta) = \left(1 + \frac{\epsilon}{1-\delta}\right) \log \left(1 + \frac{\epsilon}{1-\delta}\right) + \left(1 - \frac{\epsilon}{1-\delta}\right) \log \left(1 - \frac{\epsilon}{1-\delta}\right), \tag{5.2}$$

we can derive all the thermodynamic properties of our model. For instance, the temperature, T, is given by

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_L = \frac{k}{2E} \qquad . \tag{5.3}$$

Similary, the equation of state is defined through

$$p = T \left(\frac{\partial S}{\partial L}\right)_E = \frac{kT}{L} \tag{5.4}$$

and form Eqs. (5.3), (5.4) it follows that

$$p = \frac{2E}{L} \tag{5.5}$$

as could have been expected, since our model has the termodynamical properties of a one dimensional ideal gas.

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