# DIFFUSION, MOBILITY AND THE EINSTEIN RELATION

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Abstract. We investigate the Einstein relation $\sigma = \beta D$ between the diffusion constant $D$ and the "mobility" , of a "test particle" interacting with its environment : $\beta^{-1}$ is the temperature of the system where $D$ is measured and $\sigma E$ is the drift in a constant external field $E$ . The relation is found to be satisfied for all model systems in which we can find a unique stationary non-equilibrium state of the environment, as seen from the test particle in the presence of the field. For some systems, e.g. infinite systems of hard rods in one dimension, we find non unique stationary states which do not satisfy the Einstein relation. For some models in a periodic box the Einstein relation is the most direct way of obtaining $D$ . A precise macroscopic formulation of the Einstein relation which makes it mathematically very plausible is given.

## I. Introduction.

We investigate stationary states of various classical model systems in which a charged "test particle" (tp) is subject to a constant external field $E$ in the x-direction . The suitably defined drift or mean velocity of this tp , $u(E)$ , is generally expected, for small fields to be proportional to the diffusion constant $D$ of the tp at $E = 0$ , when the system is in equilibrium. More precisely,

$$\sigma \equiv \lim_{E \to 0} \frac{u(E)}{E} = \beta D \tag{1.1}$$

where $\beta$ the reciprocal of the temperature characterizing the equilibrium state of the system at $E = 0$ . (We set Boltzmann's constant and the charge of the tp equal to unity. We use the usual physicist's normalization for $D$ : for standard Brownian motion, $(dW)^2 = dt$ , $D = 1/2$ , and for the general one dimensional Brownian motion $\langle W_D(t)^2 \rangle = 2Dt)$ .

Equation (1.1) is the first example of a class of general relations between linear transport coefficients and equilibrium fluctuations e.g. $\sigma$ and $D$ . It was derived by Einstein for Brownian particles in a fluid using physically intuitive quasi-equilibrium arguments [1]. Their most general formulation, as Einstein-Green-Kubo (EGK) relations, is usually derived via formal perburbation arguments around the equilibrium state, see below and refs.[2].

The validity of the EGK relations, or at least of some of their experimental consequences appear well established in many cases. A convincing mathematical derivation, and in some cases even a precise formulation, is however lacking at present [3] . The purpose of this presentation is to discuss the meaning and status of equation (1.1) for various model systems

Formulation of Problem.

We shall call a system for which the tp has differentiable spatial trajectories, i.e. in which the microscopic velocity $\underline{v}$ , $\underline{v} \in \mathbb{R}^d$ of the tp is well defined a mechanical system. For such a system

$$u(E) = \langle v_x \rangle_E \, , \quad \beta^{-1} = M \langle v_x^2 \rangle_o \tag{1.2}$$

where $M$ is the mass and $v_x$ the x-component of $\underline{v}$ . The subscripts $E$ and $0$ refer to expectation values in the appropriate stationary measures with and without the field. The microscopic action of the field in such a mechanical system is an acceleration $M^{-1}E$ of the test particle in the x-direction - while leaving all other interactions unchanged. We shall later discuss different models of such mechanical systems. Note that according to our terminology a particle whose velocity undergoes an Ornstein-Uhlenbeck process is a mechanical system. A system which evolves in a deterministic manner according to Newton's equations of motion will be called Newtonian.

In addition to mechanical models we shall also consider systems where the microscopic dynamics is modeled by Brownian motion, a continuous spatial process whose velocity is not well defined. In these models the



electric field acts by adding a drift term proportional to $Edt$ to the displacement of the tp . The definition of $\beta$ appearing in (1.1) is now related to the behavior of the tp in equilibrium with an external "confining potential" . A similar situation occurs for models in which the position of the tp takes values on a lattice, $X \in \mathbb{Z}^d$ . Here the electric field acts to "suitably" bias jumps in the x-direction .

In general, for mechanical and non-mechanical systems in which the tp is free to move in all of $\mathbb{R}^d$ or $\mathbb{Z}^d$ , there will be no stationary probability measure completely describing the entire systems, environment plus tp , since the position of the latter will not be localized in the "steady state". However, if we ignore the position of the tp and consider only the remaining coordinates, describing the environment relative to the tp (including the velocity of the tp in the case of mechanical systems), this problem disappears. It is to stationary probability measures for this relative description - the environment seen from the test particle - to which $\langle \; \rangle_o$ and $\langle \; \rangle_E$ refer.

For mechanical systems it is natural to define $u(E)$ as $\langle v_x \rangle_E$ , but this makes no sense for non-mechanical systems. However, in all cases $X(t)$ , (the x-coordinate of) the position of the tp at time $t$ $(X(0)=0)$ can be naturally defined as a random variable on the path space for the evolution of the environment seen from the tp , equipped with the invariant path measure $P_E$ arising from $\langle \; \rangle_E$ . We then have that $\langle X(t) \rangle_E/t$ is independent of $t$ and we define $u(E)$ by (we abuse notation and write $\langle \; \rangle_E$ for the expectation with respect to $P_E$) ,

$$u(E) \equiv \langle X(1) \rangle_E \tag{1.3}$$

This definition agrees with the previous one in the case of mechanical systems, since in this case $X(t) = \int_0^t v(s)ds$ . We also note that if the process describing the evolution of the environment seen by the tp starting from the state $\langle \; \rangle_E$ is ergodic, then

$$\lim_{t\to\infty} \frac{X(t)}{t} = u(E) \tag{1.4}$$

a.s. with respect to $P_E$ .

Observe also that while for mechanical systems the diffusion constant $D$ is given by $\int_0^\infty \langle v_x(0)\, v_x(t) \rangle_o \, dt$, an expression which makes no sense for non-mechanical systems, in all cases (under consideration) we have

$$D = \lim_{t\to\infty} (2t)^{-1} \langle X(t)^2 \rangle_o \tag{1.5}$$

Note that equation (1.1) implies in particular that $\sigma$ is zero whenever $D$ vanishes. This is trivial in the case where the tp is confined to a compact spatial region by an external potential, e.g. by walls. It is more interesting in the one dimensional system of Brownian particles with hard cores or lattice gases with jumps restricted to nearest neighbor empty sites. In these cases it is known [4] that $\langle X^2(t) \rangle \sim t^{1/2}$ so that $D$ is zero. We show indeed that in these cases $u(E) = 0$ : In fact the infinite volume stationary measures $\langle \ \rangle_E$ for $E \neq 0$ turn out to be limits of finite volume $E \neq 0$, stationary states containing $N$ particles with either periodic or rigid wall boundary conditions. In the latter case the finite volume states are generalized Gibbsian for which of course $u(E) = 0$, while in the periodic case we verify (1.1) for finite $N$, with $u_N(E)$, $D_N \sim N^{-1}$.

The situation is less clear for interacting Newtonian particles with hard cores. The diffusion constant for a tp, having the same mass $M$ as the other "fluid" particles, is non-zero [5]. However, just as for Brownian particles, we explicitly find stationary measures as limits of finite volume (generalized) Gibbs states. These states, which are spatially identical to those found for Brownian particles, have Maxwellian velocities, so that $u(E) = 0$. (They are however no longer limits of stationary states with periodic boundary conditions). Moreover, by Galilean invariance, these states are imbedded in a family, members of which can be found assigning $u(E)$ any value whatsoever. Presumably, none of these states have anything to do with the Einstein relation, not even the one(s) for which it is satisfied. We expect, but do not prove, that there are also other stationary states, arising in the limit $t \to \infty$ (under the evolution with $E \neq 0$) from the initial state $\langle \ \rangle_o$, for which we expect that the Einstein relation is satisfied. Indeed, in cases where there is more than one stationary state $\langle \ \rangle_E$ (for given $\beta$ and density), it is only for those arising in the above way that we expect the Einstein relation to be satisfied and hence we believe that $u(E)$



**should be defined in these states. In fact this is essentially what the usual derivation of the Kubo formulas (EGK relations), via perturbation of the equilibrium state in effect does [2]. We present it here as heuristics.**

Perturbation Argument.

Let the time evolution of the appropriate probability measure be given by the forward generator of the process $L_o + EL_1$

$$\frac{\partial \mu}{\partial t} = (L_o + EL_1)\mu \tag{1.6}$$

where $L_o$ and $L_1$ are independent of $E$. We consider now the state at time $t > 0$ when $\mu(0) = \mu_o$, the equilibrium state, when $E = 0$ ; $L_o \mu_o = 0$. Then by the standard Dyson formula

$$\mu(t) = \mu_o + E \int_0^t \exp[(t-t')L_o] L_1 \mu(t') dt' \tag{1.7}$$

Let now $U = U_o + U_1 E$ be the function whose expectation value in the correct stationary state is $u(E)$. (For a mechanical system $U_o = v_x$, $U_1 = 0$ ; for a diffusion system $U_1$ is a constant). We then write formally, assuming that the average of $U$ converges as $t \to \infty$ to the correct $u(E)$ and that the limit (1.1) exists and is given by letting $t \to \infty$ after expanding $\langle U \rangle$ in $E$,

$$\sigma = \langle U_1 \rangle_o + \int_0^\infty \langle U_o^{(0)}(t') A \rangle_o \, dt' \tag{1.8}$$

where

$$A = \mu_o^{-1} L_1 \mu_o = L_1 \log \mu_o \quad . \tag{1.9}$$

The subscript $\langle \ \rangle_o$ means that the average is with respect to $\mu_o$ and the superscript $U_o^{(o)}(t')$ indicates that the time evolution is taken with the generator $L_o$. For a mechanical system (1.8) is simply

$$\sigma = \beta \int_0^\infty \langle v_x(t') v_x \rangle_o \, dt' = \beta D \tag{1.10}$$

A similar formula [6] is obtained for a diffusive system with the appropriate choice of $U_o$.

We have avoided making precise statement about the limits $t \to \infty, E \to 0$ leading to (1.8). This is deliberate; we have no rigorous (or even very convincing) arguments about the validity of (1.8) for general systems [3]. It is precisely this lack of knowledge which led us to the present work. We believe that in addition to the specific models considered explicitly here the formulation in the last section has some promise of leading to rigorous results for general systems. In particular that formulation makes Einstein's original argument precise and very convincing.

We proceed to give some examples of models with "static" environments for which the Einstein relation holds. In later sections we will investigate models with "dynamic" environments in which the tp is one of the particles in an interacting system and give a new formulation of the Einstein relation.

## II. Static Environments.

### a) Markovian Mechanical Models.

In this widely used class of models the velocity of the tp undergoes either i) a Markov jump process specified by a transition rate $K(v,v')dv$ or ii) an Ornstein-Uhlenbeck process. (We take here $v \in \mathbb{R}$ since extra dimensions do not introduce any essential new elements.) Setting $x(0) = 0$ the position at time $t$ is given by $x(t) = \int_0^t v(t')dt'$. The position and the velocity distribution of the tp satisfies a "linear Boltzman equation"

$$\frac{\partial f(x,v,t)}{\partial t} + v\frac{\partial f}{\partial x} + \frac{1}{M}\left[-\frac{\partial U(x)}{\partial x} + E\right]\frac{\partial f}{\partial v} = (Kf)(x,v,t) \quad (2.1)$$



We have included here also a force term coming from an external potential $U(x)$ (which we generally take to be zero) in order to clarify the role of $E$. The operator $K$ on the right side of (2.1) represents the effect of the environment : it is the forward generator of the Markov velocity process and is independent of $U, E$ and $x$. $K$ is assumed to have a non-degenerate eigenvalue zero, corresponding to the Maxwellian velocity distribution $h_\beta(v)$

$$K h_\beta = 0 \quad (2.2)$$

$$h_\beta(v) = (2\pi/\beta M)^{-1/2} \exp[-(1/2)\beta M v^2] \quad . \quad (2.3)$$

The stationary solution of (2.1) for $E = 0$ is the equilibrium distribution

$$f_o(x,v) = C \exp[-\beta U(x)] h_\beta(v) \; . \quad (2.4)$$

$C$ is a normalization constant whose meaning is clear when $\exp[-\beta U(x)]$ is integrable - or the particle is in a rigid box. When $U(x) = 0$ or is bounded periodic with period $L$ it is simplest to interpret (2.4) as holding for $x$ in $\mathbb{R}/L$, i.e. we can think of the tp defined in the periodic box of length $L$. Alternatively $f_o$ is the stationary Poisson density of independent particles in the $x,v$ plane.

The diffusion constant $D$ for the tp undergoing the process defined by (2.1) with $U$ zero or bounded periodic can be shown to exist under mild assumptions on $K$, and to be given, as usual, by the integral of the velocity autocorellation function as in Equation (1.10) with $\langle\;\rangle_o$ referring to the normalized equilibrium distribution (2.4). It might appear that, in this case at least, very few additional assumptions are required to jusfity (1.8) and thus prove (1.1) (see however eq. (2.9) and the subsequent discussion). We do not attempt to investigate this here - instead we limit ourselves to two examples where $h(v;E)$ can be computed explicitly and (1.1) can thus be shown to hold.

For the OU process [9]

$$Kh = M^{-1}\gamma\frac{d}{dv}\,[vh + (\beta M)^{-1}\,\frac{d}{dv}\,h] \tag{2.5}$$

and $D = (\gamma\beta)^{-1}$. It is easy to check explicitely (or by performing a Galilean transformation) that for $U = 0$ the stationary velocity distribution is given by

$$h(v;E) = h_\beta(v - E/\gamma) \tag{2.6}$$

and so $\sigma = \gamma^{-1} = \beta D$.

A problem may arise, however, when $K$ is an integral operator (case i).

$$(Kh)(v) = \int K(v,v')h(v')dv' - \int K(v',v)h(v)dv' \tag{2.7}$$

so that $EL_1$ becomes a singular perturbation : $E$ multiplying the highest derivative. To see this let us consider the simplest jump process, one without memory,

$$K(v,v') = \tau^{-1}h_\beta(v) \tag{2.8}$$

with $\tau$ a constant.

The stationary solution of (2.1) can now be easily obtained for the case $U = 0$ ;

$$h(v;E) = \int_{-\infty}^{v} \alpha \exp -\alpha(v-v')\ h_\beta(v')dv'\,,\quad \alpha = M/\tau E \tag{2.9}$$

Clearly $h(v;E)$ is not differentiable at $E = 0$. The Einstein relation is nevertheless satisfied,

$$\langle v \rangle_E = \tau E/M = \beta DE\ . \tag{2.10}$$

The first part of (2.10) is obtained most easily by multiplying (2.1) by v and integrating over v , while the second equality follows readily from (1.10) (In fact the same method can be applied to the case $K(v,v') = W(v-\lambda v')$ , $W(n)$ even and integrable, $\lambda < 1$ . It gives $\sigma = \tau/(1-\lambda)M = \beta D$ , $\tau^{-1} = \int W(v)dv$).. Thus the existence of an expansion of



$h(v;E)$ about $E = 0$ , is certainly not necessary for (1.1) to hold, what is then ? Our formulation in section 5 suggests that (1.1) is valid in essentially all cases where the motion of the tp , for $E = 0$ , converges (in the limit of macroscopic length and time scales) to Brownian motion. The problem however remains open.

b. Diffusion in a Random Environment.

We continue the investigation of static environments by considering the motion of a test particle diffusing in a potential $U$ with a "conductivity" $a(x)$. The distribution function $\rho(x,t)$ for this model (there is no velocity variable) satisfies the equation

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\,(\gamma^{-1}[-\,\frac{\partial U}{\partial x} + E]\rho) = \frac{\partial}{\partial x}\,a\,\frac{\partial}{\partial x}\,\rho \tag{2.11}$$

with $a\gamma \equiv \beta^{-1}$ , independent of $x$ , required to make the stationary measure, for $E = 0$ , assume its equilibrium value, c.f. (2.4). For $U = 0$ and $a$ constant, the Einstein relation is then satisfied by assumption. The question about (1.1) now occurs when U and/or a is periodic or more generally themselves form a spatially stationary random process. We shall consider this case in one dimension where one can obtain explicit expressions for $\sigma$ and $D$ and show that they satisfy (1.1).

Consider ergodic, translation invariant random fields $U(x)$ and/or $a(x)$ , $x \in \mathbb{R}$ , defined on some probability space $\langle \Omega, A, P \rangle$.(We assume that $w$ may be identified with $U_w, a_w$ , or $(U_w, a_w)$ .)We write $\langle . \rangle$ for the expectation w.r.t. P . For each $w \in \Omega$ the forward generator of the corresponding process $X(w,t)$ is

$$L_w\rho = -\frac{\partial}{\partial x}\,[\gamma_w^{-1}(-\,\frac{\partial U_w}{\partial x} + E)\,\rho\,] + \frac{\partial}{\partial x}[a_w\,\frac{\partial}{\partial x}\,\rho] = L_o\rho - E\frac{\partial}{\partial x}(\beta a\rho) \tag{2.12}$$

and the stationary solutions to (2.11) satisfy

$$L_w\rho_w(x) = 0\ . \tag{2.13}$$

According to (2.12) $L_w\rho = \mathrm{div}\,J_w(\rho)$ , where $J_w$ is the current (operator).

Thus the first integration constant of (2.13) is the current $J = J(\rho_w)$ , which can be interpreted as

$$J(\rho_w) = \lim_{t\to\infty} \frac{N_0(t)}{t}$$

where $N_0(t)$ is the (expected) signed number of crossings of the origin (total flux) up to time $t$ of independent particles, each performing $X(w,t)$ and distributed initially according to a non homogeneous Poisson process of density $\rho_w(x)$ .

If $P$ is ergodic one can prove (using ergodicity of the process induced in the space of the environments) that the $\lim_{t\to\infty} \frac{X(w,t)}{t}$ exists and is independent of $w$ . Thus the effective velocity of the system is given by

$$u(E) = \lim_{t\to\infty} \frac{X(w,t)}{t} \quad , P \text{ a.s.} \tag{2.14}$$

and we have also that $< \rho_w(0) > u(E) = J(\rho_w)$ , so

$$u(E) = \frac{J(\rho_w)}{<\rho_w(0)>} \tag{2.15}$$

Now we compute $u(E)$ in two cases :

a) random potential ($a$ is constant $[=1]$ in eq. (2.11)) and

b) random conductivities ($U$ is zero in eq. 2.11).

For the case of a random potential the stationary density $\rho_w$ is the solution of the equation

$$\frac{\partial}{\partial x}(\gamma^{-1} [\frac{\partial U_w}{\partial x} - E] \rho) + \frac{\partial^2}{\partial x^2} \rho = 0 . \tag{2.16}$$

Putting the first integration constant $J(\rho_w) = 1$ we obtain

$$\rho_w(x) = \int_x^\infty e^{-\beta E(x'-x)} e^{\beta[U(x')-U(x)]} dx' \tag{2.17}$$

Taking $x = 0$ and using eq. (2.15) we get



$$u(E) = \frac{1}{<\rho_w(0)>} = \beta E \left( \int_0^\infty dx\, \beta E\, e^{-\beta E x} < e^{-\beta U(0)} e^{\beta U(x)} > \right)^{-1} \tag{2.18}$$

Thus

$$\sigma \equiv \lim_{E\to 0} \frac{u(E)}{E} = \beta(< e^{-\beta U(0)} > < e^{\beta U(0)} >)^{-1} \tag{2.19}$$

The rightmost factor is the diffusion constant $D$ of the tp moving in the random potential (provided e.g. $e^{-\alpha U(0)} \in L^2(p)$ and $P$ is mixing under translations) , so we have that $\sigma = \beta D$ .

For the case of random conductivities, stationary densities $\rho_w$ satisfy the equation

$$\frac{\partial}{\partial x} [a_w \frac{\partial}{\partial x} \rho] - \beta E \frac{\partial}{\partial x}(a_w \rho) = 0 .$$

Taking again the first integration constant $J(\rho_w) = 1$ we obtain, for $x = 0$ , $\rho_w(0) = \int_0^\infty \frac{e^{-\beta E x}}{a(x)} dx$ .

Thus $\sigma \equiv u(E) = \frac{1}{<\rho_w(0)>} = \beta E < 1/a >^{-1}$ which implies that

$$\lim_{E\to 0} \frac{u(E)}{E} = \beta < 1/a >^{-1}$$

It is known [7,6] that $< 1/a >^{-1}$ equals the diffusion coefficient in this case, so relation (1.1) has been verified for the cases of random potentials and random conductivities: see also Appendix B.

## III. Dynamic Environments.

### 1. Non-crossing Particles in one dimension.

#### a. Ornstein-Uhlenbeck Dynamics.

We consider first the case of mechanical particles on the line which interact via a finite range even pair potential $\phi(r)$ , smooth for $r > 0$ . In addition there is a hard core, i.e. they cannot cross. This is irrelevant when $\phi(r) \nearrow \infty$ as $r \searrow 0$ but we shall keep it anyway. When two particles meet, or collide, they exchange velocities. All particles have the same mass and between collisions they undergo independent Ornstein-Uhlenbeck (O.U.) processes with friction constants $\gamma/M$ and reciprocal temperature $\beta$, i.e.

$$dv_i = -(\gamma/M)[v_i\, dt - \sqrt{2/\beta\gamma}\, dW_i] - (1/M) \sum_{j \neq i} \frac{\partial}{\partial x_i} \phi(x_i - x_j) dt \qquad (3.1)$$

where the $W_i$ are independent standard Wiener processes. For a given density, the, presumably unique, stationary state of this system is a Gibbs state at temperature $\beta^{-1}$ for the Hamiltonian $H = (1/2)M v_i^2 + \Sigma_{j \leq i} \phi(x_i - x_j)$.

It is known rigorously for the case when $\phi(r) = 0$ but presumably true also for the general non-crossing case that the mean square displacement of a particle in an infinite system in equilibrium with particle density $\rho$ behaves asymptotically like $t^{1/2}$ [8] rather than $t$, and so $D = 0$.

The Einstein relation then predicts for this system (and other one dimensional non-crossing systems we discuss later) that $\sigma$ should be zero. As we shall see later this is true in a very strong sense with $u(E) = 0$ for all values of $E$ acting on a test particle.

We shall, however, first consider a system consisting of $N$ O.U. particles on a circle of length $L$. We show that the diffusion constant $D_N$ and mobility $\sigma_N$ are of $O(N^{-1})$ and satisfy the Einstein relation. The displacement $x(t)$ of the tp is now of course to be interpreted as $\int_0^t v(t')dt'$, i.e. like an angular variable.

To investigate the diffusion of a tp in such a system, we simply note two facts : a) since there is no crossing $D_N$ must equal $\overline{D}_N$, the diffusion constant of the "center-of-mass" $\overline{x}$ of the system. b) The motion of $\overline{x}$ is entirely independent of the forces between the particles (as long as they satisfy Newton's law of action and reaction). Thus, setting



$$\overline{x} = N^{-1} \sum_{i=1}^{N} x_i \;, \; x_1 \leq x_i \leq x_1 + L$$
$$\overline{v} = N^{-1} \sum_{i=1}^{N} v_i \;. \qquad (3.2)$$

We have from (3.1)

$$d\overline{v} = \frac{-\gamma}{M} [\overline{v}\, dt - \sqrt{2/\beta\gamma}\, N^{-1} \sum_{i=1}^{N} dW_i] \;. \qquad (3.3)$$

This gives immediately

$$D_N = \overline{D}_N = (\beta\gamma N)^{-1} \qquad (3.4)$$

When there is a field $E$ acting on a tp, say the first particle, then (3.1) is modified for $i = 1$ by the addition of a term $(E/M)dt$ on the right side. The center of mass velocity now satisfies the equation

$$d\overline{v} = \frac{-\gamma}{M} [\overline{v}\, dt - \sqrt{2/\beta\gamma}\, N^{-1} \sum_{i=1}^{N} dW_i] + \frac{E}{MN}\, dt \qquad (3.5)$$

It follows that in the stationary state, which we shall discuss next

$$u(E) = \langle \overline{v} \rangle_E = \frac{1}{N\gamma} E = \beta^{-1} D_N E \qquad (3.6)$$

Stationary States.

The stationary non-equilibrium state in the presence of a field on the tp is most easily obtained by considering the problem in the frame of reference moving with the average velocity of the system $E/\gamma N$. In this frame the stationary distribution of the fluid particles relative to the test particle is just the equilibrium measure in the presence of an electrostatic potential $E(x_i - x_1)/N$. More precisely, setting

$$y_i = (x_i - x_1) \in (0,L) \;, \; i = 2,\ldots,N \qquad (3.7)$$

the stationary ensemble density will have the form

$$\mu(x_1;\underline{y},\underline{v}) = L^{-1}[\exp[-\beta\hat{U}(\underline{y})] \prod_{i=1}^{N} h_\beta(\hat{v}_i)]/\hat{Z} \qquad (3.8)$$

$$= P(\underline{y},\underline{v})/\ L$$

where

$$(\underline{y},\underline{v}) = (y_2,\ldots y_N, v_1, v_2,\ldots,v_N) ,$$

$$\hat{v}_i = v_i - E/\gamma N \quad ,$$

$$\hat{U}(y) = \sum_{i=2}^{N} \{ \sum_{j>i}^{N} \phi(y_i - y_j) + \phi(y_i) + Ey_i/N\} , \qquad (3.9)$$

$P$ is the density for the environment measure and $\hat{Z}$ is a normalization constant. The stationarity of $\mu$ follows easily from the fact that $\mu$ is a canonical Gibbs state periodic in $x_1$, of period $L$ (in fact, independent of $x_1$).

N.B. In choosing the domain of the $y_i$ in (3.7) we have used strongly the fact that there is a hard core between the tp and the fluid particles. This permits the discontinuity in the electrostatic potential and in $P(\underline{y},\underline{v})$ between $y_i = 0$ and $y_i = L$ which correspond simply to the right and left side of the tp.

To see more clearly what is happening, let us consider the case $\phi(r) = 0$, i.e. hard point particles. In this case $P$ is a product measure

$$P(\underline{y},\underline{v}) = h_\beta(\hat{v}_1) \prod_{i=2}^{N} [\lambda(y_i)h_\beta(\hat{v}_i)] \qquad (3.10)$$

where (changing the domain of $y_i$ to $(-1/2\,L, 1/2\,L)$ for future convenience) $\lambda(y)$ has the form

$$\lambda(y) = \begin{cases} C\exp\left[-\beta Ey/N\right], & 0 < y \le (1/2)L \\ C\exp\left[-\beta E(y+L)/N\right], & (-1/2)L \le y < 0 \end{cases} \qquad (3.11)$$

$$C = \beta E[1-\exp(-\beta E/\rho)]^{-1}/N , \quad \rho = N/L$$



Put differently, the distribution of the fluid particles relative to the position of the tp is Poisson with a density $\rho(y)h_\beta(v_i - E/\gamma N)$, $\rho(y) \equiv (N-1)\lambda(y)$.

Note that there is a discontinuity in $\rho(y)$ at the position of the tp. Putting $\rho(0+) = \rho_R$ and $\rho(0-) = \rho_L$, the densities to the right and left of the tp, we immediately find

$$\beta^{-1}[\rho_R - \rho_L] = (\tfrac{N-1}{N})E \qquad (3.12)$$

$$\rho_L/\rho_R = \exp[-\beta E/\rho] \qquad (3.13)$$

The left side of (3.12) represents the difference in pressure $\Delta p$, exerted on the tp by the fluid particles – the net remaining force on it

$$E - \Delta p = E/N = \gamma\, u(E) \qquad (3.14)$$

is just enough to produce the average motion.

Infinite Volume Stationary States.

Taking now the thermodynamic limit $N \to \infty$, $L \to \infty$, $N/L \to \rho$ of this stationary state, we obtain a Poisson field (for the environment measure) with constant densities $\rho_R$ $(\rho_L)$ for $y > 0 (< 0)$ with $\rho_R = \rho_L + \beta E$ and on either side of the tp a Maxwellian velocity distributions $h_\beta(v)$. In this "blocked" state the electric force on the tp is entirely balanced by the difference in pressure exerted by the fluid on its opposite sides and $u(E) = 0$ as it should be.

It is useful to note here, and this will be important later when we deal with other non-crossing systems, that this stationary measure can also be obtained directly as a limit of constrained equilibrium states in a box with rigid walls situated at $\pm L$. Suppose we want to obtain the infinite volume state with some specified density $\rho_L$ to the left of the tp . We then put $N_L = \rho_L L$ particles to the left of the tp and $N_R = [\rho_L + \beta E]L$ particles to the right of it. Because of the hard core interaction between the tp and the other particles $N_L$ and $N_R$ are conserved quantities. The corresponding equilibrium canonical ensemble density will therefore be given by (with now the particles labelled so that the o-th particle is the tp)

$$\mu(x_{-N_L}, v_{-N_L}, \dots, x_1, v_1, \dots, x_{N_R}, v_{N_R}) = Z^{-1} \prod_{i=-N_L}^{N_R} h_\beta(v_i) \cdot \exp[\beta E x_o] \chi(\underline{x}; N_L, N_R) \tag{3.15}$$

where $\chi$ is the characteristic function specifying that there be exactly $N_L$, $N_R$ particles on the left, right of $x_o$. It is now an easy exercise to show that this state leads to the blocked state when $L \to \infty$. (See section 4 for the lattice version). The above construction will work also when $\phi(r) \neq 0$. We will always end up with two semi-infinite Gibbs states which, except near the boundary, will be uniform with densities $\rho_L$ and $\rho_R$ determined by $p(\rho_R, \beta) - p(\rho_L, \beta) = E$ where $p(\rho, \beta)$ is the pressure in the (infinite one dimensional) Gibbs state with density $\rho$ at temperature $\beta$.

Remark. Going back to the stationary non-equilibrium state in the periodic box we can also take there the limit $L \to \infty$ with $N$ fixed. We obtain then a stationary environment measure in which there are no particles on the left and $N$ independent particles with exponentially decaying density on the right. The whole entity is moving to the right with a velocity $E/N\gamma$. Such a stationary state cannot be produced by starting with a rigid box and does not exist when $E = 0$; the particles would then disperse to infinity. To the extent that one can define a diffusion constant here it would correspond presumably to the center-of-mass of the block and would satisfy the Einstein relation.

b. Brownian and Jump Dynamics.

The above analysis can be carried out almost verbatim for the (positional part of) the distribution of interacting Brownian particles.



**The results are also essentially identical. The problem is a bit more complicated for particles on the 1-dimensional lattice which can only jump to unoccupied nearest neighbor sites . The absence of complete translational symmetry makes the computations awkward, particularly for the periodic case. They are given in section 4.**

c. Hamiltonian Dynamics.

When $\gamma$ is set equal to zero in (3.1), we are dealing with a conservative system whose evolution is governed by classical mechanics. It is clear that for such a system the velocity of the center of mass is a constant of the motion and thus $D_N$ is infinite. Similarly, under the action of a uniform (non-potential) field on the circle the finite systems center of mass keeps on accelerating, no stationary state is possible and $\sigma_N$ is also infinite.

The situation is different for the infinite system. Here it was shown by many authors [ 5 ] for the case $\phi = 0$, i.e. for hard point particles that $D = \langle|v|\rangle/\rho > 0$, where $\rho$ is the uniform density and $\langle|v|\rangle$ the expectation of the speed of the tp, which has the same mass as the other particles, is given in equilibrium by $(2/\pi M\beta)^{1/2}$. Einstein's relation would now appear to say that when the field is put on the tp there should result a non-equilibrium stationary state in which $u(E)/E \to \beta D$ as $E \to 0$. On the other hand the constrained Gibbs state constructed in (3.15) is stationary also for this system and as before, gives rise in the limit $L \to \infty$ to the "blocked" state in which $u(E) = 0$.

We believe but cannot prove that the resolution of this problem lies in the fact that the blocked state is not the appropriate stationary state for this system. Unlike the case of OU or Brownian particles, the blocked state is not unique here. In particular we expect that there exists an entirely different stationary state, one which would be obtained, as $t \to \infty$, if we turned on the field at $t = 0$ when the system is in equilibrium. Such a state should have quite a different velocity distribution for "out going" particles to the right and the left of the tp . If such a state exists it is presumably given by the construction (1.8) and satisfies the Einstein relation as is expected from the considerations in section 5.

2. Higher dimensions, Crossing particles.

The existence of a diffusion constant $D$, $0 < D < \infty$, for a tp in a general interacting system of particles has been proven so far only for : a) B-particles interacting via sufficiently soft superstable potentials [6,9]. b) Particles on a lattice at infinite temperatures in dimension greater than one (also in one dimension when the jumps extend beyond nearest neighbor sites [10]) and for OU particles - with bounded potentials [11].

In none of these systems is there any rigorous information about the existence of a stationary state in the presence of an electric field $E$ acting on the tp. In fact, for a mechanical system with "soft" interactions, the resistance of the fluid to the motion of the tp might be expected to decrease at large speeds of the latter, as the cross section does, and there will presumably not be any stationary state for $E > 0$. The Einstein relation might still hold however for some kind of "metastable" state in such a system or when $E$ is sealed properly : c.f. section 5. We shall therefore confine our discussion here to the case where the tp is OU or Brownian while the fluid particles are Newtonian. It will be seen that for these "mixed dynamics" the Einstein relation provides some interesting insights.

We begin with the O.U. mixed dynamics system, i.e. we set $\gamma = 0$ in (3.1) for all $i \neq 1$. It is quite easy to see that the stationary state of the system of $N$ particles in a periodic box with a field $E$ on the tp is simply the Galilean transform of the canonical Gibbs state : the positional part remains canonical Gibbs while the velocity part is transformed, $h_\beta(v_i) \to h_\beta(v_i - E/\gamma)$, independent of $N$. It follows furthermore from general arguments about spreading Markov processes, [12], that for non-degenerate interactions, i.e. when the phase space cannot be decomposed into separate components, this stationary state is unique.

The perturbation argument for the EGK relations given in section 1, which there seems no reason to doubt, then leads to the result that the diffusion constant for the tp in the equilibrium state, $E = 0$, of this periodic system is $(\beta\gamma)^{-1}$ ; the same as if there were no other particles present.



**This result, while a little surprising at first sight, seems not too unreasonable for the finite periodic system. After all the interactions between the particles conserve momentum and energy and the only dissipation occurs via the tp. In fact, we shall now prove this explicitely for the case where the tp is a B-particle.**

For the mixed dynamics in which the tp is Brownian, the tp has no velocity and in place of (3.1) for $i = 1$ we have

$$dx_1 = \gamma^{-1} E - \frac{\partial}{\partial x_1} \sum_{i=2}^{N} \phi(x_i - x_1)\, dt + 2/\beta\gamma\, dW$$

We can now compute the diffusion constant for $E = 0$. Let

$$V = \sum_{i=2}^{N} v_i .$$

Then
$$dx_1 + \gamma^{-1} M dV = \sqrt{2/\beta\gamma}\, dW .$$

and

$$\frac{x_1(t) - x_1(0)}{\sqrt{t}} = \sqrt{2/\beta\gamma}\,\frac{W(t)}{\sqrt{t}} - \gamma^{-1} M\, \frac{V(t) - V(0)}{\sqrt{t}}$$

Since $V(t)$ forms a stationary stochastic process (with $\langle V^2 \rangle_0 < \infty$) the last term on the right does not contribute in the limit $t \to \infty$. We therefore obtain that the diffusion constant of the tp is the same as if no other particles were present. (We also (more or less) immediately obtain the invariance principle for the motion of the tp).

Consider now the passage to the thermodynamic limit $N \to \infty$, $L \to \infty$, $N/L^d \to \rho$. We obtain then (for both the B and O.U tp) a uniform Gibbs state in the frame of reference moving with velocity $E/\gamma$.

It is clear however, that this stationary state is not the relevant one for the Einstein relation. For starting with an infinite system in equilibrium and putting the field on the tp will surely lead to a state in which the velocity of the fluid particles "far away" will remain essentially unaffected by the electric field in higher dimensions. Also in one dimension for crossing particles, the fluid far away will be moving relative to the tp . It is this state in which $u(E)$ should be computed. It will then presumably satisfy the Einstein relation, with the correct equilibrium $D$ for the infinite system.

We can say a little more about this model if we consider again the non-crossing case. For the finite system in a periodic box the fluid particles must have the same diffusion constant as the test particle, $D = (\beta\gamma)^{-1}$ . In the thermodynamic limit we will have the additional stationary states obtained as the Galilean transforms of the blocked states discussed earlier. This leads to the family of stationary states moving with the velocity $\alpha$ and having a pressure jump $\Delta p$ connected by the relation

$$\alpha = (E-\Delta p)/\gamma .$$

For $\gamma = 0$ , $E = \Delta p$ and $\alpha$ is arbitrary as we found for the purely mechanical system.

The question now arises as to what is the diffusion constant of the tp , again the same as that of the fluid particles because of non-crossing, in the infinite equilibrium system with $E = \Delta p = 0$ . For the O.U. tp, it is clearly not just $(\beta\gamma)^{-1}$ since when $\gamma \to 0$ it should go to $\langle |v| \rangle/\rho$ .

The origin of the problem with all these stationary states appears to be the interchange of limits $t \to \infty$ , necessary to obtain the stationary state for $E \neq 0$ and diffusion constant for $E = 0$ in the finite periodic system, with the thermodynamic limit $L \to \infty$ . We get the "wrong" stationary state and diffusion constant. What then is the right answer ?

## IV. Jump Processes on the Lattice.

### a) Infinite one dimensional lattice gas.

**We consider a one dimensional lattice gas in which all the particles but one have a symmetric rate of jump (i.e. the rate of jumping to**



**the right = the rate of jumping to the left = 1/2). The test particle is subjected to an external field : it jumps with the rate $p$ (resp. $q = 1-p$) to the right (left), $p \geq q$ . The relation between $p$ , $\beta$ and $E$ is given by $q/p = e^{-\beta E}$ . (For this choice the (formal) Gibbs state satisfies detailed balance). The interaction of the particles is merely simple exclusion, so when a particle attempts to jump to an occupied site the jump is suppressed.**

We describe the system directly as it is seen from the tagged particle ("environment process"). The generator acting on cylindric functions $f : \{0,1\}^{\mathbb{Z}} \cap \{\eta : \eta(0) = 1\}$ is given by

$$L_p f(\eta) = \sum_{\substack{x,y \neq 0 \\ x-y = 1}} (1/2)[f(\eta_{xy}) - f(\eta)] +$$

$$p[1-\eta(1)]\,[f(\tau_1 \eta_{01}) - f(\eta)] + q[1-\eta(-1)][f(\tau_{-1}\eta_{0-1}) - f(\eta)] \quad (4.1)$$

where $(\tau_x \eta)(z) = \eta(x+z)$ and

$$\eta_{xy}(z) = \begin{cases} \eta(z) & \text{if } z \neq x,y \\ \eta(x) & \text{if } z = y \\ \eta(y) & \text{if } z = x \end{cases}$$

The semigroup $S_p(t)$ corresponding to the generator $L_p$ determines a unique strong Markov process $\eta_t$ on $\{0,1\}^{\mathbb{Z}}$ , in such a way that $S_p(t)f(\eta) = E\, f(\eta_t)$ where $E$ denotes the expectation with respect to the process with initial configuration $\eta$ .

The set of extremal invariant measures $J_e$ is given by (see theorem A1 in the appendix)

$$J_e = \{\mu_\rho : 0 \leq \rho \leq 1\} \cup \{\tilde{\mu}_n : n \geq 0\} \quad (4.2)$$

where $\mu_\rho$ is a Bernoulli measure with parameters $\rho_\ell = \rho$ to the left of the origin and $\rho_r = (1-q/p) + \rho(q/p)$ to the right of the origin. Thus $q/p = \frac{1-\rho_r}{1-\rho_\ell}$ . $\mu_n$ is concentrated on configurations with no particles to the left of the origin and $n$ particles to its right (cf. eq. (A.11) below).

The position $X(t)$ of the tagged particle is given by the algebraic number of shifts of the system (corresponding to the last two terms in the generator (4.1)) in the interval $[0,t]$. Consider that the initial configuration $\eta(0)$ is distributed accordingly with $\mu_\rho\{X(t)\} \equiv 0$.

The Einstein relation in this case follows trivially : It is known (cf. [4] ) that when $E = 0$, $D = 0$ for all $\rho > 0$. On the other hand $U(E) = \frac{EX(t)}{t} = \lim_{t\to 0} \frac{EX(t)}{t} = p(1-\rho_r) - q(1-\rho_\ell) = 0$ for all $E$ and all $\rho > 0$.

The Einstein relation is, in fact, satisfied for this model in a somewhat stronger sense. In section c) below we show that for a sequence of periodic approximations the Einstein relation is satisfied with non-zero diffusion constant $D_N$ and mobility $\sigma_N$. Moreover, these quantities converge to their infinite volume values (0). Finally, we will see that the stationary states we have described in this section arise as limits of the stationary states for the periodic approximations.

In the next section, we show that the same thing is true for box approximations except that here, of course, the diffusion constant and drift are 0.

## b) Finite lattice gas.

We consider now finite approximations to the preceding model : the particles now move on a finite lattice of length $2L$ with reflecting walls at $-L$ and $L$. Note first that the Einstein relation is now trivial. Moreover, stationary states for this model are easy to find, even for $E \neq 0$, e.g. Gibbs states. The Gibbs states, however, don't have a good limit as $L \to \infty$. But if we condition the Gibbs states on the number of particles to the left and right of the tp, in the appropriate way as $L \to \infty$, we obtain a sequence of stationary states (stationary because particles cannot cross) converging to the measure $\mu_\rho$ of the infinite case. This is based on the fact that for these constrained Gibbs states, given the position $x$ of the tp, the particles on its left (right) are



uniformly independently distributed with density $\rho_\ell(\rho_r)$ - which depend upon $x$. What must do is show that $x$ is well localized as $L \to \infty$ at a position which gives the correct value for $\rho_\ell/\rho_r$. This we proceed to do.

In the box $-L,L$ put the tp and $N$ additional particles, $M$ of them to the left of the tp. The position of the test particle we denote by $x$. The (average) density to the left is $\rho_\ell = M/(L+x)$ ; the density to the right of the tp is $\rho_r = 1-\rho_\ell = N-M/(L-x)$ Let $M/L \sim a$ and $N-M/L \sim b$ as $L \to \infty$. Then, writing $y = x/L$, $\rho_\ell \sim a/1+y \equiv \rho_\ell(y)$ and $\rho_r \sim b/1-y \equiv \rho_r(y)$.

The distribution of the tp corresponding to the constrained Gibbs state (i.e. conditioned on there being $M(N-M)$ particles to the left (right)) when the field acts as before $(q/p = e^{-\beta E})$ is given by

$$f(x) \sim e^{\beta Ex} \binom{L+x}{M} \binom{L-x}{N-M} .$$

Using the approximation $\ln n! \sim n \ln n$, we obtain

$$f(x) = e^{F(x)}$$

where

$$F(x) = \beta E x + (L+x) \ln(L+x) +$$

$$+ (L-x) \ln (L-x) - (L+x-M) \ln(L+x-M)$$

$$- M \ln M - (N-M)\ln(M-N) - (L-x-(N-M)) \ln(L-x-(N-M)) .$$

Under the change of variables $y = x/L$ we obtain $F(x) \sim L\phi(y)$

where $\phi(y) = \beta Ey + (1+y)\ln(1+y)+(1-y)\ln(1-y)-(1+y-a)\ln(1+y-a)$

$$-(1-y-b)\ln(1-y-b)+g(N,M)$$

where $g(N,M)$ arises from the terms of $F(x)$ which don't depend upon $x$.

We thus have that the distribution of $y \sim e^{L\phi(y)}$ so that for large $L$ $y$ is near the maximum $y_o$ of $\phi(y)$. Setting $\phi'(y_o) = 0$ we find that

$$e^{-\beta E} = \frac{(1+y_o)(1-b-y_o)}{(1-y_o)(1-a+y_o)}$$

i.e.,

$$q/p = \frac{1-\rho_r(y_o)}{1-\rho_\ell(y_o)} \quad .$$

Moreover $e^{L\phi(y)} \sim e^{-L/2\phi''(y_o)(y-y_o)^2}$, so that $|y-y_o| \sim 1/\sqrt{L}$. Thus in the thermodynamic limit $y$ is localized at $y_o$ and hence we obtain the state described in section 4a).

c) EGK <u>relation for a periodic lattice model.</u>

We here consider the symmetric lattice gas with the tp subjected to an electric field as in section 4a but now with the particles moving in a one dimensional periodic box of length $L+1$, $L > 1$. Let $X(t)$ be the position of the tp in $\mathbb{Z}$ induced by our process : $X(t)$ is the algebraic number of jumps performed by the tp up to time $t$ (jumps to the left make a negative contribution). Let $0 = X_o(t) < X_1(t) < \ldots < X_N(t) \leq L$ be the positions of the particles relative to the tp and let $Y_i(t) = X_i(t) + X(t)$, $i = 0,\ldots,N$, define the motion of the $i^{th}$ particle in $\mathbb{Z}$ ($Y_o(t) = X(t)$.) Then by considering the motion $\bar{Y}(t)$ of the center of mass

$$\bar{Y}(t) = (1/N+1) \sum_{i=0}^{N} Y_i(t) \qquad (4.3)$$

we easily compute the diffusion constant for $E = 0$, at least in the limit $L \to \infty$ : It is easy to check that $\bar{Y}(t)$ is a martingale (with respect to the $\sigma$-algebra generated by the motion of the entire system up to time $t$). Therefore, since $|Y_o(t) - \bar{Y}(t)| < L$ for all $t \geq 0$, we have that

$$D = \frac{E(\bar{Y}(t)^2)}{2t} = \lim_{t\to 0} \frac{E(\bar{Y}(t)^2)}{2t}$$



$$= \left\langle \frac{\sum_{i=0}^{n} 1(X_{i+1}-X_i>1)}{(N+1)^2} \right\rangle_0 \qquad (4.4)$$

Here $1(\ )$ is the indicator function and $X_{N+1} \equiv L+1$. The last equation follows easily from the fact that each particle jumps to each <u>unoccupied</u> neighboring site with rate 1/2 .

We are primarily interested in the situation in which $N$ and $L$ are fixed. In this case the RHS of (4.4) is not as easy to compute as it is when $\langle\ \rangle_o$ is Bernoulli with density $\rho$ (grand canonical ensemble). With this slight modification we find that

$$D = \left\langle \frac{\sum_{x=0}^{L} \eta(x)(1-\eta(x+1))}{[\Sigma\eta(x)]^2} \right\rangle_o$$

$$\sim \frac{\rho(1-\rho)L}{(L\rho)^2} = \frac{1-\rho}{\rho}\frac{1}{L}$$

since for large $L\rho$ we have that $\Sigma\eta(x) \sim L\rho$

We don't wish to make the approximation above more precise, since we will compute $D$ and $u$ explicitly after again slightly modifying the model. The real problem is with the computation of $u(E)$: in order to compute $u(E)$ we need detailed information on the stationary measure $\langle\ \rangle_E$ which is not so easy to obtain.

Nevertheless, if instead of fixing the length $L+1$ of the box and allowing $N$ to be random we fix $N$ and allow $L$ to be random in an appropriate way the computations become much easier. Consider the process $\xi_t^N(y) \in \mathbb{N}^{N+1}$, $y = 0,\ldots,N$ where $\xi_t(y)$ is the number of empty sites to the right of the $y$-th particle. Let $\nu = \nu_{\rho,E,N}$ be a probability measure on $\mathbb{N}^{N+1}$ satisfying

a) $\langle L \rangle = \langle \sum_{y=0}^{N} (\xi(y)+1) \rangle = \frac{(N+1)}{\rho}$ .

b) $\nu$ is a product measure (i.e. $\xi(y)$ are independent random variables) of geometric distributions with parameters $a_y$ (i.e

$$\nu(\xi(y) = k) = a_y^k \, (1-a_y))$$

c) $a_y$ satisfies the balance equations (4.5) below. One can prove by direct computation that $\nu$ is stationary for the process $\xi_t^N(y)$, and hence defines a stationary state $\langle\ \rangle_E$ for our periodic system (with random length).

We want to compute $\lim_{E\to 0} \frac{u(E)}{E}$. We find it convenient to consider the quantity

$$c \equiv c(\rho,E,N) = \frac{u(E)}{p-q}$$

since $\beta E \sim p-q$ as $E \to 0$,

$$\sigma = \lim_{(p-q)\to 0} \beta\cdot c \ .$$

Since $a_y = \nu\{\xi:\xi(y) > 0\}$ the average velocity of the $y$-th particle, $y \neq 0$, is given by $(1/2)a_y - (1/2)a_{y-1}$ while that of particle zero is $pa_o - qa_N$. (We are identifying $N$ with $-1$). We thus have that $a_y$, $0 \leq y \leq N$ must satisfy the following equations $(q/p = e^{-\beta E})$.

$$\begin{aligned} (1/2)a_y - (1/2)a_{y-1} &= c(p-q) \\ pa_o - qa_N &= c(p-q) \end{aligned} \qquad (4.5)$$

from which it follows that (for $E > 0$)

$$a_o = c(2Nq+1)$$

$$a_N = c(2Np+1)$$

$$a_y = (1-y/N)a_o + (y/N)a_N \ ; \ 0 < y < N$$

The relationship between $\rho$ and $c$ is then given by (cf. a) above)

$$1/\rho = \nu\left\{\frac{\sum_{y=0}^{N}(\xi(y)+1)}{N+1}\right\} = (1/N+1)\sum_{y=0}^{N}\frac{1}{1-a_y} =$$



$$\frac{1}{\rho} = \frac{N}{N+1}\sum_{y=0}^{N}\frac{1}{N-(N-y)c(2Nq+1)-yc(2Np+1)}$$

and taking the limit $(p-q)\to 0$ we obtain

$$\frac{1}{\rho} = \frac{N}{N+1}\sum_{y=0}^{N}(N-N(N+1)\lim_{(p-q)\to 0} c)^{-1} = (1-(N+1)\lim_{p-q\to 0} c)^{-1}$$

Thus

$$\sigma = \lim_{(p-q)\to 0} \beta c = \frac{\beta(1-\rho)}{N+1} \ .$$

On the other hand, (see eq. 4.4)

$$D = \frac{\sum_{y=0}^{N} \langle 1(x_{y+1}-x_y > 1)\rangle_o}{(N+1)^2}$$

$$= \sum_{y=0}^{N} \left\langle \frac{1(\xi(y)>0)}{(N+1)^2} \right\rangle_o = \frac{(N+1)(1-\rho)}{(N+1)^2} = \frac{1-\rho}{N+1}$$

This proves relation (1.1) for this model.

## V. Macroscopic Formulation of Einstein Relation.

In our discussions so far the tp has been treated entirely on a microscopic level - asking for a description of the stationary states of the tp on the spatial and temporal scale on which the basic dynamics of the model is prescribed. While this level clearly gives the most detailed information the Einstein relation concerns quantities, $D$ and $\sigma$ which are measured on very long, i.e. macroscopic, spatial and time scales. Furthermore being a linear transport coefficient, $\sigma$ is calculated in the limit $E \to 0$ so the system is really very close to equilibrium - hence, of course, the EGK relations. It seems therefore sensible to formulate the Einstein relation in a more macroscopic way. In fact this turns out to be possible and has the (not so incidental) advantage that it is not necessary to first find $u(E)$ at finite $E$ and then take the limit $E \to 0$. Instead one goes to the appropriate macroscopic length and time scales by setting

$$x' = \varepsilon x \ , \ t' = \varepsilon^2 t$$

where $\varepsilon$ is a small parameter related to the electric field $E$ which is assumed to change as $E = \varepsilon E'$. A form of (1.1) is then the following : A). If for $E' = 0$, when the system is in equilibrium, the rescaled trajectory of the test particle converges (weakly) to Brownian motion with diffusion constant $D$, i.e.

$$x_\varepsilon(t) \equiv \varepsilon x(t/\varepsilon^2) \xrightarrow[\varepsilon\to 0]{} W_D(t) \qquad (5.1)$$

then in the presence of a field $\varepsilon E$

$$x_\varepsilon(t; E) \xrightarrow[\varepsilon\to 0]{} \sigma E\, t + W_D(t) \ , \ \sigma = \beta D \ . \qquad (5.2)$$

We believe that A can in fact be proven for all non-mechanical cases considered here and in particular for a B-particle in a random environment or interacting with other B-particles [13] . It also seems to hold in the case of an O.U. particle in a periodic potential, recently shown by Rodenhausen to satisfy (1.1) [14].

It should be noted that the scaling of the electric field is just such that it remains effective, neither zero nor infinite, on the macroscopic scale $\sigma$ is then the mobility, as in Stoke's law, for a dilute concentration of B-particles in a fluid. It is presumably this situation which Einstein had in mind. We are now in a position to present what we regard as the best argument for the Einstein relation, a rigorous reformulation of Einstein's original argument. We first observe that if we drop from equation (5.2) the relation $\sigma = \beta D$ and replace $\sigma E$ in (5.2) by a more or less arbitrary function $u(E)$ of the field, what we obtain is a sort of regularity condition for the macroscopic behavior of the tp. Moreover, if the field is allowed to vary with $x$ on a macroscopic scale

$$E_\varepsilon(x) = \varepsilon F(\varepsilon x) = \nabla_x U(\varepsilon x)$$



the regularity condition (5.2) should become

$$x_\varepsilon(t; F) \xrightarrow[\varepsilon\to 0]{} \int_0^t u(F(x(s)))ds + W_D(t) \qquad (5.3)$$

(where the function $u \to u(F)$ does not depend on the particular field $x \to F(x)$ under consideration, and the environment has the same initial distribution as for $F = 0$, i.e. equilibrium).

Now suppose we have macroscopic regularity (5.3). Consider a potential $U(x) \to \infty$, $|x| \to \infty$, sufficiently rapidly. If the system is at temperature $\beta^{-1}$, so that it has a stationary state for which the marginal distribution of $x_\varepsilon \equiv x' \sim e^{-\beta U(x')}$, then the distribution $\rho_\beta \sim e^{-\beta U(x)}$ must also be stationary for the limiting diffusion. Since the current in this state must be zero, we have that

$$0 = J(\rho_\beta) = u(F(x))\, \rho_\beta(x) - D\nabla_x \rho_\beta$$

$$= u(F(x))\rho_\beta(x) - D\beta\, F(x)\rho_\beta(x)$$

so that $u(F)/F \equiv \sigma$ does not in fact depend on $F$ and $\sigma = \beta D$. (It does not much matter here whether we regard $x$ as in $\mathbb{R}$ or $\mathbb{R}^d$. Moreover for $d > 1$, it is sufficient to assume that the drift is a vector valued function $\underline{u}(\underline{F})$ of the local field. It then follows from the (Einstein) argument that $\underline{u}(\underline{F}) = \sigma\underline{F} = \beta D\underline{F}$, where $\sigma$ and $D$ may be tensors).

Put somewhat differently, if $\rho_\beta \sim e^{-\beta U(x)}$ is to be stationary for the limiting diffusion, whose (forward) generator is

$$L\rho = -\nabla\cdot(u(F)\rho(x)) + D\Delta\rho$$

then $\sigma$ and $D$ must be related by $\sigma = \beta D$. Thus the Einstein relation is more or less an immediate consequence of macroscopic regularity (5.3) and the very meaning of a system's being at temperature $\beta^{-1}$, as Einstein originally argued. (Interestingly enough this appears to be the case in the Newtonian system of hard points when the initial state, before the field is turned on, is a Gibbs state but not when the initial state is one in which all the particles move with velocities ±1[17].)

## APPENDIX A.

In this appendix we sketch the proof of equation (4.2) for the process of section 4 in the infinite lattice. More precisely we prove the following :

**Theorem A.1.** Let $\eta_t$ be the simple exclusion process as seen from the test particle ("environment process"), for which the motion of all the particles but the test particle moves with rates p(resp. q) to the right (left), $p > q$ , i.e. the infinitesimal generator is given in equation (4.1). Then, the set $J_e$ of extremal invariant measures for the process is given by

$$J_e = \{\mu_\alpha : 0 \leq \alpha \leq 1\} \bigcup \{\tilde{\mu}_n : n \geq 0\} \tag{A.1}$$

where $\mu_\alpha$ is a Bernoulli measure with parameters $\alpha_- = \alpha$ to the left of the origin and $\alpha_+ = (1+q/p) + \alpha(q/p)$ to the right of the origin, and $\mu_n$ is concentrated on configurations with no particles to the left of the origin and n-particles to its right (see equation A.11) below for a formal description).

In order to prove theorem A.1 we consider the following partition of $x$ :

$$\begin{aligned} X_\infty &= \{\eta : \sum_{x>0} \eta(x) = \sum_{x<0} \eta(x) = \infty \\ X_\infty^+ &= \{\eta : \sum_{x>0} \eta(x) = \infty , \sum_{x<0} \eta(x) < \infty\} \\ X_\infty^- &= \{\eta : \sum_{x>0} \eta(x) < \infty , \sum_{x<0} \eta(x) = \infty\} \\ X_n^+ &= \{\eta : \sum_{x>0} \eta(x) = n , \sum_{x<0} \eta(x) < \infty\} \end{aligned} \tag{A.2}$$

Now one can prove [15] that

$$J_e = [J \cap M(X_\infty)]_e \cup [J \cap M(X_\infty^+)]_e \cup [J \cap M(X_\infty^-)] \cup \cup [J \cap \bigcup_{n \geq 0} M(X_n^+)] \tag{A.3}$$



where $M(y)$ is the set of probability measures concentrated on $y$ . We prove theorem A.1 by showing :

$$[J \cap M(X_\infty)]_e = \{\mu_\alpha . \ 0 < \alpha \leq 1\} \tag{A.4}$$

$$[J \cap M(X_\infty^+)]_e = \mu_o \tag{A.5}$$

$$[J \cap M(X^-)]_e = \phi \tag{A.6}$$

$$[J \cap M(X_n^+) ] = \tilde{\mu}_n \quad , n \geq 0 \tag{A.7}$$

Proof of (A.4). Let us introduce the zero range process naturally related to the lattice gas as seen from the test particle we are discussing. A given configuration $\eta \in X_\infty$ can be represented by a doubly infinite sequence $x_i : i \in \mathbb{Z}$ , $x_i < x_{i+1}$ , $x_o = 0$ where $x_i$ denotes the site occupied by the i-th particle ($i \in \mathbb{Z}$) . (In the same way configurations belonging to $X_\infty^+$ and $X_\infty^-$ can be represented by semi-infinite sequences and those belonging to $X_n$ by finite sets of sites).

Let $x_u(t)$ be the position of the particle initially at site $x_u$ . The process $\xi_t = \{\xi_t(u)\}_{u \in \mathbb{Z}}$ , $\xi_t(u)$ describing the evolution of the number of sucessive empty sites to the right of the u-th particle, is the so called zero range process :

$$\xi_t(u) = x_{u+1}(t) - x_u(t) \quad . \tag{A.8}$$

It is a process with state space $y = \mathbb{N}^{\mathbb{Z}}$ and infinitesimal generator $L_{zr}$ given by (on h-cylindric)

$$\begin{aligned} L_{zr} h(\xi) &= p[h(\xi_{0,-1}) - h(\xi)] + q[h(\xi_{-10}) - h(\xi)] \\ &+ (1/2) \sum_{x \neq 0} [h(\xi_{x,x-1}) - h(\xi)] + (1/2) \sum_{x \neq -1} [h(\xi_{x,x+1}) - h(\xi)] \end{aligned} \tag{A.9}$$

where

$$\xi_{x,y}(z) = \begin{cases} \xi(z)-1 & \text{if } z = x \text{ and } \xi(x) > 0 \\ \xi(z)+1 & \text{if } z = y \text{ and } \xi(x) > 0 \\ \xi(z) & \text{if either } z \neq y \text{ , } z \neq x \text{ or } \xi(x) = 0 \end{cases}$$

A set of invariant measures for this process is described in [16]:

$$J(L_{zr}) = \{\gamma_a\}_{0 \leq a < 1}$$

where $\nu_a$ is the geometric product measure defined by

$$\gamma_a\{\eta(x) = k\} = a_x^k(1-a_x) \qquad \text{(A.10)}$$

where $a_x = a$ if $x < 0$ and $a_x = (q/p)a$ if $x \geq 0$ . We find $\{a_x\}$ by solving the detailed balance equation :

$$a_o(p+(1/2)) = a_{-1}q + a_1(1/2)$$

$$a_{-1}(q+(1/2)) = a_o p + a_{-2}(1/2) \qquad \text{(A.10.b)}$$

$$a_k = (1/2)(a_{k-1}+a_{k+1}) \qquad k \neq 0,1$$

$a_x = \gamma_a\{\eta(x) > 0\}$ , so $0 \leq a_x < 1$ .

From equation (A.10) one proves, using coupling techniques as in [15,16], that the only extremal invariant measures for the $\eta_t$-process on $M(X_\infty)$ are those described in equation (4.4).

Proof of (A.5) (A.6) (A.7).

In the semi-infinite and finite case one has to look for solutions of equation (A.10b) allowing one (or two) of the $a_k$ to be one. The state space for the corresponding zero range model is semi-infinite (or finite). For $X_\infty^+$ for instance, we consider $a_k = 1$ for a fixed $k < 0$ . This implies that in the corresponding zero range model at site $k$ "there are infinitely many particles" so, from site $k$ to site $k+1$ particles enter with intensity 1/2 (respect q) if $k < -1$ (resp. $k = -1$). ] the simple



exclusion picture $a_k = 1$ must be read : "there are no particles to the left of the (k+1)-th particle", so the rate of jumping to the left for the (k+1)-th particle equals 1/2 if $k < -1$ and p if $k = -1$ .

In the semi infinite case we find solutions of the equations analogous to equation (A.10.b) when $k \neq -1$ and which imply that the density of the invariant the measures must be that described in equation (A.5) for the simple exclusion model. To prove that $\mu_o$ is the only invariant measure requires coupling technicalities which we omit.

Equation (A.6) is studied similarly and the counterpart of equation (A.10.b) gives us that there are no solutions with $a_n < 1$ for $n < k$ and $a_k = 1$ for a fixed $k \geq 0$ .

Equation (A.7) is proven following the standard methods of finite state markov chains, which imply that

$$\tilde{\mu}_\eta\{\eta : x_{i_\ell} - x_{i_\ell -1} = b_{i_\ell} \text{ , } \ell = 1,\ldots,j \leq n\} = \prod_{\ell=1}^{j} a_n(i_\ell)[1-a_n(i_\ell)b_i]$$

where $$a_n(k) = \frac{z(p-q)}{(n+1)zp+1}\,k + \frac{(n+1)zq+1}{(n+1)2p+1} \quad . \qquad \text{(A.11)}$$

APPENDIX B.

In this appendix, we indicate how from $\rho_w$, the invariant non normalizable measure of section IIb, we may easily obtain an invariant probability measure for the "environment process". This is the process induced by $X(w,t)$ in the space $\Omega$ of environments by the relation

$$U_w(t) = \tau_{X(w,t)}\, U_w$$

(or imply $w(t) = \tau_{X(w,t)}w$) where $U_w$ is the configuration of environments at time $t = 0$ , and $\tau_x$ denotes translation by $x$ .

In fact, the probability measure

$$d\tilde{P} = \frac{\rho_w(0)dP}{\langle\rho_w(0)\rangle}$$

is invariant for the environment process. The key to this is the fact that $\rho_w(x)$ depends on $x$ only through the environment seen from $x$, i.e. $\rho_w(x) = \rho_{\tau_x w}(0)$. To see this note first that $\rho_w(x)dx\ P(dw)$ is invariant for the process $(X(t,w),w)$, in which the environment does not change. The second component of this process, $w_t \equiv w$, is of course not the environment process. However, after the change of variables $(x,w) \rightarrow (x,\tau_x w)$ we obtain the process $(X(t,w),w(t))$, with invariant measure $d\mu = \rho_w(0)dx\ P(dw)$. The $w$ marginal for this measure should be an invariant (probability) measure for the environment process, but unfortunately this is not well defined, since $\mu$ is not normalizable. But we may regard $x$ as a variable defined modulo $L$ (for any $L > 0$) both for the measure $\mu$ and for the process $(X(t,w),w(t))$ since both $\mu$ and the process $(X(t,w))$ don't essentially depend upon $x$, $X(t,w) - X(0,w)$ depending only upon the autonomous process $w(t)$. In this way we obtain a normalizable measure $\mu_L$ which is stationary for the process $(X(t,w),w(t))$ so that the $w$ marginal $\rho_w(0)P(dw)$ is stationary for $w(t)$.

The stationarity of $\tilde{P}$ may also be seen directly : We may assume without loss of generality that $\langle \rho_w(0) \rangle = 1$. Then, denoting the transition probability for the environment process by $Q^t$, and the transition probability for the position $x$ of the tp by $P_w^t$, we have, for $f$ a "nice" function of the environment, that

$$P(Q^t f) = \iint dx\ P(dw)\ \rho_w(0)\ P_w^t(0,x)\ f(\tau_x w)$$

$$= \iint dx\ P(dw)\ \rho_{\tau_{-x} w}(0) P^t_{\tau_{-x} w}(0,x)\ f(w)$$

$$= \iint dx\ P(dw)\ \rho_w(-x)\ P_w^t(-x,0) f(w)$$

$$= \int P(dw)\ f(w) \int dx\ \rho_w(x)\ P_w^t(x,0)$$



$$= \int P(dw)\ f(w)\ \rho_w(0) = \tilde{P}(f)$$

where we have used the translation invariance of $P$, the fact that $\rho_w(x) = \rho_{\tau_x w}(0)$, the homogeneity of the x-process : $P^t_{\tau_y w}(0,x) = P_w^t(y,y+x)$, and the stationarity of $\rho_w(x)$ under $P_w^t$.

Note that we didn't need to explicitly refer to this invariant probability measure to obtain $u(E)$. In general, assuming ergodicity $u(E) = \lim_{t\to\infty} \frac{X(t,w)}{t}$ $\tilde{P}$ a.s. where $\tilde{P}$ is the stationary probability measure for the environment process. But here $\tilde{P}$ is equivalent to $P$.


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