

A Gas of Brownian Particles in Statistical Dynamics

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We consider a large number of particles on a one-dimensional lattice IZ in interaction with a heat particle; the latter is located on the bond linking the position of the particle to the point to which it jumps. The energy of a single particle is given by a potential $V(x)$, $x \in Z$. In the continuum limit, the classical version leads to Brownian motion with drift. A quantum version leads to a local drift velocity which is independent of the applied force. Both these models obey Einstein's relation between drift, diffusion, and applied force. The system obeys the first and second laws of thermodynamics, with the time evolution given by a pair of coupled non linear heat equations, one for the density of the Brownian particles and one for the heat occupation number; the equation for a tagged Brownian particle can be written as a stochastic differential equation.

KEY WORDS: Brownian motion; nonlinear; fluctuation-dissipation; entropy; stochastic differential equation.

1. INTRODUCTION

Einstein⁽¹⁾ introduced the mathematical theory of Brownian motion by means of the heat equation. Actually, for consistency he should have considered the heat equation with drift, which in one dimension takes the form

$$\frac{\partial f}{\partial t} = \kappa \frac{\partial^2 f}{\partial x^2} + v \frac{\partial f}{\partial x} \quad (1)$$

Here, $f(x, t)$ is the probability density that the particle is at x at time t . From this we deduce that v is the mean velocity. The equation was derived

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by considering a spherical particle, having reached its terminal speed, moving in a frictional medium under a constant force F . He showed that the parameters of the model are related by

$$v = \frac{\kappa F}{k_B T} \quad (2)$$

where k_B is Boltzmann's constant and T is the temperature of the medium; Eq. (2) was the world's first fluctuation-dissipation theorem. This theory does not describe the initial stages of the motion, before the particle has speeded up or slowed down to its terminal velocity; nor does it take into account the work done on the particle by the applied force. When the particle moves at a steady speed all this work ought to be converted into heat, but the presumed infinite size of the system and the presumed rapid dissipation of this heat tempts one to disregard local increases in temperature. To take these details into account needs a more microscopic description.

In this paper we apply the methods of statistical dynamics⁽²⁾ to these problems. Statistical dynamics is a generalization of Hamiltonian dynamics designed to obey the first and second laws of thermodynamics. In *isothermal dynamics* the system is maintained at a constant temperature, either by controlled heat flows at the boundary, or by postulating that the conductivity is infinite, and the volume infinite. Einstein's model, then, is an isothermal one. If we are to keep track of local heating the temperature will depend on space and time, and we need to set up a model of *isolated dynamics*, in which energy is conserved. In kinetic theory, heat is thermalised kinetic energy, but in statistical dynamics we lump the thermalised energy of photons and phonons in with the kinetic energy, and represent heat by one or more oscillators, called heat-particles. These we localise on the bonds, or edges, of the lattice (in a model with discrete space). We impose the *hypothesis of local thermodynamic equilibrium*, *LTE*, an idea due to Schwarzschild.⁽³⁾ *LTE* assumes that all the kinetic energy is thermalised, and that the oscillator on each bond is in a thermal state at some beta (where $\beta k_B T = 1$). This hypothesis is generally not true in Hamiltonian dynamics, in that if it is true of the initial state, it will not be true after a short time. The *LTE*-map, denoted by Q , implements the hypothesis by replacing the state of the oscillator on each bond by the thermal state with the same mean energy. This considerably simplifies the dynamics, but makes the reduced system nonlinear. The map Q is entropy non-decreasing, and by construction conserves mean energy, and so gives rise to one step in the dynamics which obeys both laws of thermodynamics, provided that energy-conservation is taken to refer to mean energy. Q replaces the state of the

combined system, Brownian particle and oscillator, by the product state, and so forces the correlation, set up by the interaction between them, to be zero. If only one Brownian particle is present, we can measure the correlation experimentally by finding the the position of the particle, and then measuring the temperature at the same point. The correlation thus measured will not be zero unless there is some physical effect that spoils the correlation. If there is a gas of Brownian particles, and we consider the dynamics of a tagged particle, this effect is due to the random presence of the other particles; they heat up the liquid in the same way, whether or not we measure the position of the tagged particle. For this reason, we consider that our models will describe a gas of particles rather than a single one. The map Q is the second step in the dynamics; the first step is given by an energy-conserving bistochastic map, which determines the nature of the model in question.

Heat-particles under the name of caloric, or phlogiston, have not got a good reputation in science, and were abandoned by the middle of the 19th Century. I think that the mistake was to insist that they be conserved in time; heat is not, by itself, conserved, but can be transformed into other forms of energy. For this reason, we model the heat-particles by neutral bosons, which are readily absorbed and emitted by matter. In this way they become the vehicles for the transfer and dissipation of energy.

Statistical dynamics can be formulated in classical as well as quantum probability. The former is a special case of the latter, in which all observables commute; thus there is a sample space, Ω , taken to be countable in ref. 2. The bounded random variables on Ω form the algebra \mathcal{A} of observables. \mathcal{A} is an abelian W^* -algebra. The set of probability measures on Ω is the state-space, Σ . In quantum probability, we start with a possibly non-abelian W^* -algebra \mathcal{A} , and Σ is taken to be the set of normal states on \mathcal{A} . The dynamics (for discrete time) in either case is given by a map $\tau: \Sigma \rightarrow \Sigma$ giving the change in the state in one time-step, say from time t to time $t + 1$. In the absence of time-varying external fields, τ is independent of time. We write the action of τ on the right, so that each initial state $p \in \Sigma$ defines an orbit

$$p, p\tau, p\tau^2, \dots$$

We require that this law of dynamics obeys the first and second laws of thermodynamics. This is achieved by constructing τ as the composition of two maps, each obeying both laws. The first stage is a bistochastic map $T: \mathcal{A} \rightarrow \mathcal{A}$, which certainly does not decrease the Shannon–von Neumann entropy of a state, and so obeys the second law. To express the first law we must specify the total energy of the system, including heat. In classical

probability, the energy is a random variable $\mathcal{E}: \Omega \rightarrow \mathbf{R}$; this divides Ω into energy shells

$$\Omega = \bigcup_E \Omega_E, \quad \text{where } \Omega_E = \{\omega \in \Omega: \mathcal{E}(\omega) = E\} \quad (3)$$

Then T is said to conserve energy if T maps the indicator function of Ω_E to itself, for each E . In the quantum case, \mathcal{E} is a self-adjoint operator and T is said to conserve energy if it maps each spectral resolution of T to itself. A simple example of such an operator is conjugation by the scattering operator of the theory. In either case we immediately have the conservation of mean energy

$$p \cdot T\mathcal{E} = p \cdot \mathcal{E} \quad (4)$$

Here, $p \cdot X$ denotes the expectation of the observable X in the state p .

The second stage of the map τ is where the *LTE*-map enters; it is a projection, or reduction, Q , which increases entropy, while conserving mean energy. Generally, Q can be identified as the map which, given the state p , replaces it by the reduced state pQ , the state of maximum entropy subject to the condition that the means of all "slow variables" are the same in the state p as in the state pQ . This is described in refs. 2, 4, and 5. Our slow variables are the same as the "gross variables" of ref. 6. The energy must be chosen to be one of the slow variables; in this paper, any function of the position operator of the Brownian particle will be taken to be slow, as well as the energy of each heat-particle. Other variables, such as the correlations of the particle with the heat, are not slow variables. With this choice, the map Q coincides with the *LTE*-map. We replace the *hypothesis* of local thermodynamic equilibrium by the *LTE*-map: just do it.

In the next section we give the classical version of the Brownian particle on a lattice in a potential $V(x)$, in which the work done by the potential reappears as heat. We get a generalisation of the heat equation with drift when we take a scaled continuum limit. The model obeys Einstein's relation Eq. (1) when the temperature is constant. In Section 3 we give a quantum model, in which the dynamics is derived from a plausible scattering operator. In Section 4 we compute the local changes to the betas caused by the thermalisation of the work done by the potential. We arrive at a coupled system of non-linear equations for which the energy is conserved and the entropy increases. The equation for the Brownian particle generates a stochastic process which obeys a non-linear stochastic differential equation driven by a Gaussian process. We claim that this is the equation obeyed by the tagged Brownian particle.

2. THE CLASSICAL BROWNIAN PARTICLE

We consider a tagged particle (one taken from the cloud of particles) moving at its terminal velocity on a lattice $\mathcal{A} = l\mathbb{Z}$ in a potential $V(x)$, $x \in \mathcal{A}$. Here l is the distance between the points of \mathcal{A} . The probability that the particle is at $x \in \mathcal{A}$ is interpreted as being proportional to the density of particles at the site. There is no kinetic energy attached to the particle; we describe this as saying that the particle is already moving at its terminal velocity, and that its kinetic energy, other than this constant amount, is fully thermalised; this thermal energy is shared with the medium and the electromagnetic field, and is accounted for by the heat-particle. Following ref. 2 we shall denote objects associated with the particle by the subscript c , denoting chemical, and those associated with heat will get the subscript γ , for photon. We aim to arrange things so that the energy gained by the particle from the potential is all converted into heat which is deposited locally.

The sample space of the tagged particle is $\Omega_c = \mathbb{Z}$, so a configuration $\omega_c \in \Omega_c$ is given by specifying the position x of the particle. Its energy when at x is $\mathcal{E}_c(x) = V(x)$. The heat-particles are harmonic oscillators, one sitting on each bond or link, $b_x = (x, x + l)$, with sample space

$$\Omega_{\gamma x} = \{0, 1, 2, \dots\}$$

where $n_x \in \Omega_{\gamma x}$ specifies the number of quanta present. The energy at the bond b_x is that of an oscillator of frequency ν_x :

$$\mathcal{E}_{\gamma x} = 2\pi\hbar\nu_x n_x \tag{5}$$

The total configuration of the thermal energy is described by the double sequence $\{n\} = \{\dots, n_{-1}, n_0, n_1, \dots, n_x, \dots\}$ in the sample space

$$\Omega_\gamma = \prod_x \Omega_{\gamma x} \tag{6}$$

and the total energy of the system, particle plus heat, is the random variable

$$\mathcal{E}(\omega_c, \omega_\gamma) = \mathcal{E}(x; \{n\}) = \mathcal{E}_c(x) + \mathcal{E}_\gamma(\{n\}) = V(x) + \sum_{x \in \mathcal{A}} 2\pi\hbar\nu_x n_x \tag{7}$$

We see that this might be unbounded, and may not be finite for some configurations with an infinite total number of heat-particles. Nevertheless we shall be able to define an energy-conserving dynamical law on the space of

regular measures (those for which the measure of any open set is the limit of the measures of any increasing family of finite sets inside it).

To construct an energy-conserving bistochastic map T , we allow that the Brownian particle, when at $x + l$, can move to x , gaining energy $V(x + l) - V(x)$; we take it that this is positive. This energy is converted into heat rather than kinetic energy. The simplest model is to assume that that this occurs by the creation of one quantum on the link b_x . For this process to conserve energy, we need

$$V(x + l) - V(x) = 2\pi\hbar\nu_x \tag{8}$$

If the particle is at x this transition can be reversed, provided that $n_x > 0$; the particle jumps from x to $x + l$, absorbing one quantum from the link b_x . Suppose that in one time-step dt the jump $x \rightarrow x + l$ occurs with probability $\lambda(n_x) = \lambda_1(n_x) dt$, independent of the state of the system outside the bond b_x . Since the jump cannot occur without absorbing a quantum, we see that $\lambda(0) = 0$. Microscopic reversibility is achieved by the requirement that the transitions $x + l \rightarrow x$ and $x \rightarrow x + l$ have equal probability. The state with the particle at x , and with given occupation $\{n_y\}_{y \in A}$ is then linked to only two states, and the transition is given by the infinite symmetric stochastic matrix T :

$$\begin{matrix} & \omega_1 & \omega_2 & \omega_3 \\ \omega_1 & \left(1 - \lambda(n_{x-l} + 1) - \lambda(n_{x-2l} + 1) \right. & \lambda(n_{x-l} + 1) & 0 \\ \omega_2 & \left. \lambda(n_{x-l} + 1) \right) & 1 - \lambda(n_{x-l} + 1) - \lambda(n_x) & \lambda(n_x) \\ \omega_3 & 0 & \lambda(n_x) & 1 - \lambda(n_x) - \lambda(n_{x+l}) \end{matrix} \tag{9}$$

The notation is to mean that when the matrix indicates a transition to a state with occupation number -1 then the entry in the matrix is taken to be zero. This can be achieved if $\lambda(0) = 0$. The rows and columns are labelled by states $\omega_i, i = 1, 2, 3$; here, ω_1 is the point of Ω with the Brownian particle at $x - l$, the occupation of the bond b_{x-l} equal to $n_{x-l} + 1$, and all the other bonds b_y occupied by n_y heat-particles; ω_2 is the point with the particle at x and all the bonds b_y occupied by n_y heat-particles; ω_3 is the point with the Brownian particle at $x + l$, the bond b_x occupied by $n_x - 1$ heat-particles and all the other bonds b_y occupied by n_y heat-particles, thus:

$$\begin{aligned} \omega_1 &= (x - l; n_{x-l} + 1, n_x, n_{x+l}, \dots) \\ \omega_2 &= (x; n_{x-l}, n_x, n_{x+l}, \dots) \\ \omega_3 &= (x + l; n_{x-l}, n_x - 1, n_{x+l}, \dots) \end{aligned}$$

Thus in one time-step the dynamics of the probability measures is given by:

$$p'(\omega_2) = \lambda(n_{x-l} + 1) p(\omega_1) + (1 - \lambda(n_{x-l} + 1) - \lambda(n_x)) p(\omega_2) + \lambda(n_x) p(\omega_3) \tag{10}$$

or in more detail,

$$p'(x; \{n_y\}) = \lambda(n_{x-l} + 1) p(x-l; n_{x-l} + 1, n_x, \dots) + (1 - \lambda(n_{x-l} + 1) - \lambda(n_x)) p(x; \{n_y\}) + \lambda(n_x) p(x+l; n_{x-l}, n_x - 1, \dots) \tag{11}$$

The choice of this form for the operator T is not forced on us; in the first place, we could allow x to jump by more than a distance l , or for the number of heat quanta to change by more than one at a time; secondly, λ could depend on x or on $V(x)$.

In statistical dynamics, one time-step is implemented by applying the transpose matrix $T^d = T$, followed by the thermalising map Q . To find Q in our case, we must identify the slow variables; then Q replaces p' by the state of maximum entropy, subject to having the same mean for all the slow variables. The slow variables are chosen to be the vector space spanned by any function of x , and the energies \mathcal{E}_{yx} of all the bonds. Let \mathcal{M}_c be the marginal map onto the states of the algebra \mathcal{A}_c generated by the bounded random variables on Ω_c , and let \mathcal{M}_{yx} be the marginal map for the algebra \mathcal{A}_{yx} . The action of Q is then to replace p' by

$$p'Q = \mathcal{M}_c p' \otimes \bigotimes_y s_{y, \beta_y} \tag{12}$$

here, s_{y, β_y} is the canonical state

$$s_{y, \beta_y} = Z_{\beta_y}^{-1} e^{-\beta_y \mathcal{E}_{yy}} \tag{13}$$

with the same mean for the bond-energy (=heat) at b_y as the state p' and therefore also as the marginal state $\mathcal{M}_{yx} p'$. Since Q has just been applied at time $t-1$ the state p at time t is a product state of the form

$$p(x; \{n_y\}) = p(x) \otimes_y s_{y, \beta_y} \tag{14}$$

This is called the hypothesis of *LTE*, combined with the Boltzmann's stosszahlansatz. In our model it is not a hypothesis, but part of the construction. The usual hypothesis is that the state $p'Q$ is close to p' , which is not true in our model, because the needed thermalising forces have been left out, to be replaced by the map Q . In statistical dynamics the hypothesis really takes the form that the resulting dynamics is a good model for

describing a tagged particle moving in a dense liquid containing many such particles; this is ultimately an experimental question.

The marginal distribution, $p(x)$, describing the position of the Brownian particle, is given by

$$p(x) = \sum p(x; \{n_y\}) \quad (15)$$

where the sum is over all configurations $\{n_y\}$ of all the heat-particles. So after one time-step the distribution is

$$\begin{aligned} p'(x) &= \sum p'(x; \{n_y\}) \\ &= \sum p(x-l; n_{x-l}+1, n_x, \dots) \lambda(n_{x-l}+1) + \sum p(x; \{n_y\}) \\ &\quad - \sum \lambda(n_{x-l}+1) p(x; n_{x-l}, n_x, \dots) - \sum \lambda(n_x) p(x; \{n_y\}) \\ &\quad + \sum \lambda(n_x) p(x+l, n_{x-l}, n_x-1, \dots) \end{aligned} \quad (16)$$

Let

$$\begin{aligned} \bar{\lambda}(y) &= \sum_{n_y \geq 0} s_{y, \beta_y}(n_y) \lambda(n_y) \\ &= \sum_{n_y \geq 1} s_{y, \beta_y}(n_y) \lambda(n_y) \end{aligned} \quad (17)$$

since $\lambda(0) = 0$. Then doing the sums in Eq. (10) gives

$$\begin{aligned} p'(x) &= \bar{\lambda}(x-l) p(x-l) + p(x) \\ &\quad - \bar{\lambda}(x-l) \exp \beta_{x-l}(V(x) - V(x-l)) p(x) \\ &\quad - \bar{\lambda}(x) p(x) + p(x+l) \bar{\lambda}(x) \exp \beta_x(V(x+l) - V(x)) \end{aligned} \quad (18)$$

This map gives one step of a Markov process; the coefficients $\bar{\lambda}$ depend on space and time through their dependence on $s_x(n_x)$ which, in isolated dynamics, themselves depend on time. In the thermal state of an oscillator at beta β , the quantum of energy is related to the mean occupation number $\bar{n}(x)$ by

$$\bar{n}^{-1}(x) = (e^{2\pi\beta_x h\nu_x} - 1) \quad (19)$$

We may use this to eliminate the Boltzmann factors from Eq. (18) to get

$$\begin{aligned} \frac{p(x, t + dt) - p(x, t)}{dt} &= \bar{\lambda}_1(x, t)(p(x + l, t) - p(x, t)) \\ &\quad - \bar{\lambda}_1(x - l, t)(p(x, t) - p(x - l, t)) \\ &\quad + \bar{n}^{-1}(x) \bar{\lambda}_1(x) p(x + l, t) \\ &\quad - \bar{n}^{-1}(x - l) \bar{\lambda}_1(x - l) p(x, t) \end{aligned} \tag{20}$$

Here, $\bar{\lambda}_1 dt = \bar{\lambda}$. Let us take the simple case when

$$\lambda_1(0) = 0, \quad \lambda_1(n) = \lambda_0, \quad \text{if } n \geq 1 \tag{21}$$

then

$$\bar{\lambda}(x) = \sum_{n \geq 1} s_{x, \beta_x}(n) = \lambda_0 e^{-\beta_x l V'(x)} = \lambda_0 \bar{n}(x) (1 + \bar{n}(x))^{-1}$$

Then the equation becomes

$$\frac{dp}{dt} = \lambda_0 \left\{ (p(x + l) - p(x)) - (p(x) - p(x - l)) + \frac{p(x)}{1 + \bar{n}(x)} - \frac{p(x - l)}{1 + \bar{n}(x - l)} \right\} \tag{22}$$

The occupation number \bar{n} is time-dependent, and obeys a non-linear heat equation with a source provided by the work done by the Brownian particle's potential. The resulting coupled equations obey both laws of thermodynamics. This is derived in Section 4. The microscopic dynamics of the classical particle, in which we choose $\lambda_1(n)$ as in Eq. (21) is similar to the choice made in ref. 7, which leads to activity-led equations. If we choose another natural function for λ , namely $\lambda_1(n) = n\lambda_0$ then we get a result similar to that in quantum field theory, including Einstein's stimulated emission. To have an interpretation as a discrete stochastic process, however, requires an ultraviolet cut-off, since $n\lambda_0 dt$ becomes greater than 1 for large n . We shall treat this case in quantum mechanics in Section 3, where we shall find that the discrete-time theory is well defined. The interesting non-linearity of the dynamics, described in Section 4, comes from the response of the medium to the presence of the gas of particles, when we treat the total system as isolated. In the usual theory (of Smoluchowski), under isothermal conditions, there is no dynamics for $\bar{n}(x)$, and therefore none for beta, as it is supposed to be fixed from outside.

3. THE QUANTUM BROWNIAN PARTICLE

In this model the physical space is the same as in the classical case, $\Lambda = l\mathbf{Z}$. The tagged particle moves on the lattice Λ , and so a pure state is described by a wave-function $\psi \in l^2(\mathbf{Z})$. The energy H_c of the Brownian particle is purely potential, and so is described by the multiplication operator M_V :

$$(H_c\psi)(x) = (M_V\psi)(x) = V(x)\psi(x), \quad x = lz, \quad z \in \mathbf{Z}, \quad \psi \in l^2 \quad (23)$$

We place an oscillator on the bond $b_x = (x, x + l)$ of energy

$$2\pi\hbar\nu_x = V(x + l) - V(x) \quad (24)$$

This is designed so that one quantum is enough to supply the energy needed to send the particle up one step of the ladder, if $V(x + l) > V(x)$, which we assume from now on. The Hilbert space of the bond b_x is thus the Fock space $\mathcal{F}_x = l^2(\mathbf{N})$. The energy is

$$H_y(x) = 2\pi\hbar\nu_x a_x^* a_x \quad (25)$$

where a_x^* and a_x are the creation and annihilation operators on \mathcal{F}_x . The total heat energy is then

$$H_y = \sum_{x=-\infty}^{\infty} 2\pi\hbar\nu_x a_x^* a_x \quad (26)$$

At first, this makes sense only on the incomplete infinite tensor product space

$$\bigotimes_{x=-\infty}^{\infty} \Omega \otimes \mathcal{F}_x$$

where Ω is the product of vacuum states. However, H_y generates a well-defined automorphism of the C^* -algebra defined by infinitely many oscillators; for example we could take Segal's C^* -algebra,⁽⁸⁾ or the quasiloocal version.⁽⁹⁾ Then the definition of the time-evolution is purely algebraic, the same in all states. We shall need a relatively tractable class of states, such as occur when Ω is the product of thermal states at various betas.

The oscillator on the bond $b_x = (x, x + l)$ represents the thermalised phonons, the photons in the black-body radiation, as well as the thermalised kinetic energy of the Brownian particle. This confluence of roles expresses the adage that "there is only one kind of heat." We could imagine

that the falling particle could excite more than one mode of the electromagnetic field, but for simplicity we shall assume that only one oscillator is coupled to the Brownian particle on each bond. We cannot localise very soft photons in the interval $(x, x + l)$, and on the other hand a very hard photon cannot be produced by the limited energy $V(x + l) - V(x)$. The mean kinetic energy of the Brownian particle is also constrained by Heisenberg's uncertainty relation. So in the quantum model we cannot take the limit $l \rightarrow 0$ in the literal sense and still get a realistic model; indeed the time interval is supposed to be large compared with the microscopic interaction time. Nevertheless, it is mathematically convenient to consider the limit, since l is very small; we shall then arrive at the quantum analogue of Brownian motion with drift.

We take the algebra of the Brownian particle and the heat to be

$$\mathcal{A} = \mathcal{A}_c \otimes \mathcal{A}_y \tag{27}$$

here, \mathcal{A}_c is the set of all bounded operators on $l^2(\mathbb{Z})$. The ambiguity of the C^* -tensor product is resolved by choosing it to be the inductive limit of the spatial products of \mathcal{A}_c with \mathcal{A}_{γ_n} , the W^* closed algebra of the Schrödinger representation of n oscillators, localised in a finite subset of \mathcal{A} ; it is thus a quasilocal algebra in the sense of Haag.⁽⁹⁾ Our next task is to choose a Hermitian operator T commuting with the total energy which causes the desired transition. We want a state on \mathcal{A} of the form

$$\psi_c \otimes \phi_y = \delta_x \otimes \phi_{n+1, x} \tag{28}$$

to make a transition to

$$\delta_{x+l} \otimes \phi_{n, x} \tag{29}$$

and *vice versa*; here, δ_x is the wavefunction which is 1 at x and zero elsewhere, and $\phi_{n, x}$ is a state on \mathcal{A}_y with n quanta present on the bond b_x . Let

$$X = \sum_{x \in \mathbb{Z}} x P_x \tag{30}$$

be the spectral resolution of the position operator X of the Brownian particle, and let U be the translation operator by one step on \mathcal{A} ; then

$$(U\psi_c)(x) = \psi_c(x - l), \quad \psi_c \in l^2(\mathcal{A}) \quad \text{which means} \quad U\delta_x = \delta_{x+l} \tag{31}$$

Let λ , the transition rate, be real, and define

$$T_x = \lambda \{ U P_x \otimes a_x + U^* P_{x+l} \otimes a_x^* \} \tag{32}$$

This is Hermitian, since

$$(UP_x)^* = P_x^* U^* = U^* P_{x+l} \tag{33}$$

Since UP_x is bounded, T_x has a dense set of analytic vectors in the space $l^2(A) \otimes \mathcal{F}_x$, and T_x is essentially self-adjoint on this set. The heat-energy at bond b_y , with $y \neq x$, commutes with T_x ; the remaining energy near x ,

$$H_x = H_c \otimes 1 + 1 \otimes H_y(x) = M_V \otimes 1 + 1 \otimes 2\pi\hbar v_x a_x^* a_x \tag{34}$$

is also self-adjoint on its domain. We now show that it commutes with T_x .

Theorem 35. $[T_x, H_x] = 0$.

Proof.

$$\begin{aligned} [T_x, M_V \otimes 1] &= \lambda [UP_x \otimes a_x + U^* P_{x+l} \otimes a_x^*, M_V \otimes 1] \\ &= \lambda [U, M_V] P_x \otimes a_x + \lambda [U^*, M_V] P_{x+l} \otimes a_x^* \end{aligned}$$

Now

$$\begin{aligned} [T_x, H_x] &= [T_x, H_y(x)] \\ &= 2\pi\hbar\lambda \{UP_x v_x [a_x, a_x^* a_x] + U^* P_{x+l} v_x [a_x^*, a_x^* a_x]\} \\ &= 2\pi\hbar\lambda \{UP_x v_x a_x - U^* P_{x+l} v_x a_x^*\} \end{aligned}$$

Thus the theorem is proved if, on $l^2(A)$, we have

$$[U, M_V] P_x = -2\pi\hbar v_x UP_x \quad \text{and} \quad [U^*, M_V] P_{x+l} = 2\pi\hbar v_x U^* P_{x+l}$$

For the first, it is enough to apply it to δ_x :

$$(UM_V - M_V U) P_x \delta_x = (V(x) - V(x+l)) \delta_{x+l} = -2\pi\hbar v_x UP_x \delta_x$$

For the second it is enough to check it on δ_{x+l} :

$$\begin{aligned} U^* M_V P_{x+l} \delta_{x+l} &= M_V U^* P_{x+l} \delta_{x+l} = V(x+l) \delta_x - V(x) \delta_x \\ &= 2\pi\hbar v_x (U^* P_{x+l} \delta_{x+l}) \quad \blacksquare \end{aligned}$$

It is clear that T_x causes the desired transitions, and that $Ad \exp\{itT_x\}$ is an automorphism of \mathcal{A} that leaves the spectral projections of H pointwise fixed; the same can be said of the formal infinite sum, $T = \sum_x T_x$, whose multiple commutators with any creation operator vanishes; $Ad T$ therefore defines an automorphism of \mathcal{A} by inductive limit, which is therefore the desired completely positive bistochastic map giving the linear part of the dynamics.

We shall be interested in the time evolution of $X \in \mathcal{A}_c$ under τ :

$$X \mapsto e^{itT} X e^{-itT} = X + it[T, X] + (it)^2/2! [T, [T, X]] + \dots = \tau X \quad (36)$$

The map τ is linear; its dual action on the states will be denoted by τ^d , acting on the right. This is well defined for discrete time. In the continuum limit, we shall keep only the term of second order; this needs justification, since the individual terms in the expansion in Eq. (36) are unbounded. We call this the *anti-van-Hove limit*⁽²⁾: we measure time on the scale of the slow variables, say seconds, and one time-step, t , becomes very small as it is the time needed for the small region of space, of size l , to relax to equilibrium in the fast variables. The rate, λ , of reactions per second, becomes large, in such a way that $\lambda^2 t \rightarrow \lambda_0$ which is neither zero nor infinity. Put $T_0 = \lambda^{-1} T$. The terms of higher order formally vanish in this limit; we shall see that, if we take the expectation in the thermal state, the (otherwise dominant) term of first order vanishes. Then the finite difference quotient becomes a double commutator:

$$t^{-1}(\tau X - X) \sim -\lambda_0 [T_0, [T_0, X]] \quad (37)$$

The double commutator has many of the properties of the Laplacian acting on functions of x ; it is the square of a derivation, and generates a one-parameter semigroup of positive maps, which are contractions in various norms.

So far we have constructed the linear part of the time-step; in statistical dynamics we follow it by the randomizing map Q . Thus if we start with a state $\rho \in \Sigma(\mathcal{A})$, after one time-step we replace $\rho \tau^d$ by the product of the partial traces

$$\rho \mapsto \rho \tau^d \mapsto Tr_\gamma(\rho \tau^d) \otimes Tr_c(\rho \tau^d)$$

Then we replace the state of the heat-particle by the thermal state $\otimes_x \omega_{\gamma x}$ with the same mean energy on each bond b_x ; this is the LTE map, denoted Q_γ . Suppose that at time $t=0$, $\rho = \rho_c \otimes \rho_\gamma$. Then one time-step in the dynamics of the state of the Brownian particle is the map

$$\rho_c \mapsto \rho_c \otimes \rho_\gamma \mapsto (\rho_c \otimes \rho_\gamma) \tau^d Q \mapsto \rho'_c = Tr_\gamma((\rho_c \otimes \rho_\gamma) \tau^d) \quad (38)$$

This is linear in ρ_c and so has a dual acting on \mathcal{A}_c ; this gives one time-step of an observable, and is a stochastic map obeying detailed balance. It depends on time through ρ_γ , whose time-evolution is given by the map

$$\rho_\gamma \mapsto \rho_c \otimes \rho_\gamma \mapsto Tr_c((\rho_c \otimes \rho_\gamma) \tau^d) Q_\gamma \quad (39)$$

We see that the map given in Eq. (39) depends on the current state ρ_c of the Brownian particle, so that the combined action on the state of \mathcal{A} is not linear. This equation of motion will be studied in more detail in Section 4.

It is shown in ref. 2, Theorem 11.8, that one time-step of $X_c \in \mathcal{A}_c$ is

$$X_c \mapsto \omega_y(\tau(X_c \otimes 1)); \quad \text{here } \omega_y = \bigotimes_x \omega_{yx} \quad (40)$$

We now apply this to the time-evolution of the spectral projection P_x ; the term of zeroth order is P_x and the term of first order, due to T_x , is

$$\begin{aligned} P_x^{(1)} &= it\omega_y([T_x, P_x]) \\ &= it\lambda[UP_x a_x + U^*P_{x+l} a_x^*, P_x] \\ &= \lambda(UP_x a_x - U^*P_{x+l} a_x^*) \end{aligned}$$

Similarly,

$$[T_{x-l}, P_x] = -\lambda(P_x U a_{x-l} - U^*P_x a_{x-l}^*)$$

In the thermal state $\omega_y = \bigotimes_x \omega_{yx}$, the means of a_y and a_y^* are zero for any y , so $P_x^{(1)} = 0$ as promised. To compute the term of second order, note that the expectations of

$$[T_{x-l}, [T_x, P_x]] \quad \text{and} \quad [T_x, [T_{x-l}, P_x]]$$

vanish in the state $\bigotimes_x \omega_{yx}$; this leaves

$$\begin{aligned} [T_x, [T_x, P_x]] &= \lambda^2[UP_x a_x + U^*P_{x+l} a_x^*, UP_x a_x - U^*P_{x+l} a_x^*] \\ &= -2\lambda^2(P_{x+l}(N_x + 1) - P_x N_x) \end{aligned}$$

and similarly,

$$[T_{x-l}, [T_{x-l}, P_x]] = 2\lambda^2(P_x(N_{x-l} + 1) - P_{x-l}N_{x-l})$$

Note the factors N_x and $N_x + 1$; the latter includes Einstein's stimulated emission.⁽¹⁰⁾ The terms T_y , with $y \neq x$ or $x-l$, do not contribute; so

$$\begin{aligned} P_x^{(2)} &= -t^2/2\omega_y([T_x, [T_x, P_x]] + [T_{x-l}, [T_{x-l}, P_x]]) \\ &= t^2\lambda^2(\bar{n}_x(P_{x+l} - P_x) - \bar{n}_{x-l}(P_x - P_{x-l}) + P_{x+l} - P_x) \end{aligned}$$

where $\bar{n}_x = \omega_{yx}(N_x)$. In the anti-van Hove limit, we put $t\lambda^2 = \lambda_0$ and $t = dt$, to get the equation

$$\frac{\partial P_x}{\partial t} = \lambda_0(\bar{n}_x(P_{x+l} - P_x) - \bar{n}_{x-l}(P_x - P_{x-l}) + (P_{x+l} - P_x)) \quad (41)$$

This is the “reduced dynamics” of the abelian algebra generated by the position operator; this algebra is mapped to itself by the time-evolution, and can be regarded as the space of slow variables. The dynamics is linear at each time-step, for given field n_x ; it can thus be pushed onto the dual space, the states. Any normal state is linear sum of the point measures δ_x :

$$p = \sum_x p_x \delta_x$$

The induced action on the coefficients is the dual of the action on the δ_x , and therefore is the same as the action on P_x ; thus

$$\frac{\partial p_x}{\partial t} = \lambda_0(\bar{n}_x(p_{x+l} - p_x) - \bar{n}_{x-l}(p_x - p_{x-l}) + (p_{x+l} - p_x)) \quad (42)$$

In the further limit, $dx = l \rightarrow 0$, we see that

$$\bar{n}_x = \frac{e^{-\beta l V'}}{1 - e^{-\beta l V'}} \sim \frac{k_B T_x}{l V'_x} \quad (43)$$

we let $\lambda_0 \rightarrow \infty$ in such a way that $\lambda_0 l = \lambda_1$ remains fixed, to get the non-linear heat equation

$$\frac{\partial p_x}{\partial t} = \lambda_1 \left\{ k_B \frac{\partial}{\partial x} \left(\frac{T_x}{V'_x} \frac{\partial p_x}{\partial x} \right) + \frac{\partial p_x}{\partial x} \right\} \quad (44)$$

The drift velocity is λ_1 , and it obeys the Einstein relation Eq. (2), although here the terms’ dependence on temperature and applied force are not the same as in the classical model of Section 2. This difference is accounted for by the different form of the rate function $\lambda(n)$ in the two models, rather than the quantum nature of the present model.

4. THE TIME-EVOLUTION OF THE TEMPERATURE

4.1. The Temperature in the Classical Case

Let us find the dynamics of β_x according to the classical model of Sect. 2. By the first law of thermodynamics, which holds in our models, the

energy lost by the Brownian particle in moving from $x+l$ to x , namely $V(x+l) - V(x)$, assumed to be positive, must reappear as heat. The locality of the model ensures that this energy is deposited in the interval $(x, x+l)$. The *LTE*-map Q_γ ensures that this energy is thermalised during the time-step, and thus becomes heat. The state of the heat-particle after the map Q_γ is thus the product of local thermal states $\prod_x s_x(n_x)$, each determined by the local beta β_x by Planck's law:

$$s_x(n_x) = Z^{-1} \exp\{-2\pi\beta_x v_x n_x\} = Z^{-1} \exp\{-\beta_x (V(x+l) - V(x)) n_x\} \quad (45)$$

The thermal state s_x is determined by the current state $p(\omega) = p(x, \{n_y\})$ of the complete system by forming the marginal distribution

$$s_x(n_x) = \sum_{x \in \mathbf{Z}} \sum_{n_y, y \neq x} p(x, \{n_y\}) \quad (46)$$

Recall that $p(x)$ denotes the marginal distribution of the Brownian particle.

The beta on the bond b_x is altered in one time-step only by the occupation by the Brownian particle of the sites x or $x+l$. The probability of the configuration $\omega = (x, \dots, n_x, n_{x+l}, \dots)$ after one time-step of the linear part of the dynamics is according to Eq. (11),

$$\begin{aligned} p'(x, \dots, n_{x-l}, n_x, n_{x+l}, \dots) &= p(x) \cdots s_{x-l}(n_{x-l}) s_x(n_x) s_{x+l}(n_{x+l}) \cdots \\ &\quad - \lambda(n_x) p(x) \cdots s_{x-l}(n_{x-l}) s_x(n_x) s_{x+l}(n_{x+l}) \cdots \\ &\quad - \lambda(n_{x-l} + 1) p(x) \cdots s_{x-l}(n_{x-l}) s_x(n_x) \cdots \\ &\quad + \lambda(n_{x-l}) p(x-l) \cdots s_{x-l}(n_{x-l} + 1) s_x(n_x) \cdots \\ &\quad + \lambda(n_x) p(x+l) \cdots s_{x-l}(n_{x-l}) s_x(n_x - 1) \cdots \end{aligned} \quad (47)$$

with similar equations for $p'(x+l, \dots)$ and for $p'(y, \dots)$, $y \neq x, x+l$. After some tedious sums we get for the change in marginal distribution

$$\begin{aligned} s'_x(n_x) - s_x(n_x) &= \lambda(n_x)(p(x+l) s_x(n_x - 1) - p(x) s_x(n_x)) \\ &\quad - \lambda(n_x + 1)(p(x+l) s_x(n_x) - p(x) s_x(n_x + 1)) \end{aligned} \quad (48)$$

We can understand the four terms; the loss in probability of finding n_x quanta on the bond b_x is due to n_x being reduced to $n_x - 1$, and the Brownian particle moving from x to $x+l$ (the probability of this being $\lambda(n_x) p(x) s_x(n_x)$), or, if the Brownian particle had been at $x+l$, it moves down to x , changing

n_x to $n_x + 1$ (the probability for this is $\lambda(n_x + 1) p(x + l) s_x(n_x)$). Similarly for the two positive terms, which contribute to a gain in $s_x(n_x)$.

Equation (48) is the linear part of the dynamics; the *LTE* map replaces the detailed information about the state $s_x(n_x)$ of the bond by a description in terms of one parameter, which can be the temperature or its inverse, beta. This is the canonical coordinate in the language of information geometry.⁽¹³⁾ Alternatively we can describe the state by the mixture coordinate, the mean energy or mean occupation number, \bar{n}_x , related to β by Planck's law, Eq. (18) if s_x is a thermal state. Since we regard the local energy of the bond as a slow variable, the *LTE*-map does not change the expectation of this energy, and we may define the state after the *LTE*-map as the thermal state with the same values of \bar{n}_x . The change in \bar{n}_x in one time step is therefore

$$\begin{aligned} \bar{n}'_x - \bar{n}_x &= \sum_{n_x} (s'_x(n_x) - s_x(n_x)) n_x \\ &= p(x) \sum_{n_x} n_x \{s_x(n_x + 1) \lambda(n_x + 1) - s_x \lambda(n_x)\} \\ &\quad + p(x + l) \sum_{n_x} n_x \{s_x(n_x - 1) \lambda(n_x) - s_x(n_x) \lambda(n_x + 1)\} \end{aligned} \quad (49)$$

which reduces to

$$\frac{\partial \bar{n}_x}{\partial t} = \lambda_0 (p(x + l) - e^{-\beta(V(x+l) - V(x))} p(x)) \quad (50)$$

Notice that the ratio of the absorption rate to the emission rate of energy by the particle is the usual Boltzmann factor $\exp\{-\beta(V(x + l) - V(X))\}$, and not proportional to \bar{n}_x , as in the form of Kirchoff's law used by Chandrasekhar;⁽¹¹⁾ the discrepancy is due to hidden inclusion of the Einstein factor for induced emission in the emission coefficient j . This is clearer in ref. 12, where j_v includes a term proportional to the intensity I_v , which is proportional to \bar{n} . As a result, the coefficient j_v of Eq. (38) of ref. 11, p. 8, should depend on temperature, according to the factor $(1 - e^{-\beta h\nu})^{-1}$, which cancels out a similar factor in \bar{n} , leaving the Boltzmann factor as here. This is seen in Eq. (58) below. Our present model, with the choice of $\lambda(n)$ given in Eq. (21), has no induced emission, Chandrasekhar's form of what he calls the Kirchoff-Planck law is not correct in this case. It is fair to say that Kirchoff was not aware of the non-linear nature of the interaction of radiation with matter when he formulated his law, and that Chandrasekhar was too polite to say that it was wrong.

Combined with Eq. (22), Eq. (50) gives a system of coupled non-linear finite-difference equations for the fields $p(x, t)$ and $\bar{n}(x, t)$. There is no problem in showing the existence of solutions for any initial fields for which $n_x \geq 0$, and $p(x) \geq 0$, summable. By construction, probability is conserved, energy is conserved, and entropy is non-decreasing. We could add a diffusion term to the equation of motion of the occupation number by modifying the microscopic dynamics with the addition of a hopping term.

To take the continuum limit of Eq. (22), write $\lambda_0 l^2 = \kappa$, the scaled diffusion constant, and $k_B = 1$, for simplicity. Also note that $\bar{n}_x \sim T(x, t)/lV'(x)$ and $(1 + \bar{n}_x)^{-1} \sim lV'(x)/T(x, t)$ as $l \rightarrow 0$. Also, put $f(x, t) = p(x, t)/l$; this is the probability density. In the limit $l \rightarrow 0$ Eq. (22) becomes

$$\frac{\partial f}{\partial t} = \kappa \frac{\partial^2 f(x, t)}{\partial x^2} + \kappa \frac{\partial}{\partial x} \left(\frac{V'(x) f(x, t)}{T(x, t)} \right) \quad (51)$$

Let us parametrise the state of the heat-particle by the temperature. Then in the same limit as above, with $\lambda_0 l^2$ being replaced by κ , we get from Eq. (50) the rate equation

$$\frac{\partial T(x, t)}{\partial t} = \kappa V'(x) e^{-\beta V(x)} \frac{\partial}{\partial x} (e^{\beta V(x)} p(x)) \quad (52)$$

Now we see a difficulty; we want to get a coupled system of equations for f and T , but as $p(x) = lf(x)$, we see that the right-hand side of Eq. (52) goes to zero as $l \rightarrow 0$, and the temperature does not appear to change. This defeats the purpose of the model, which was to rectify the (finite) loss of energy by the gas of Brownian particles by a gain in the temperature. The reason for this is that as $l \rightarrow 0$ the number of oscillators per unit length, l^{-1} , becomes infinite and so does the specific heat $C = k_B/l$ of the system; since the energy-change is finite, the change in temperature must be infinitesimal in order to conserve energy. The way out is to replace $p(x)$ in Eq. (52), not by lf but by f/C , and to regard C as experimentally given; for simplicity, and to be consistent with the way we took the limit of Eq. (22) we take it to be independent of x and temperature. Thus our final equation for T is

$$\frac{\partial}{\partial t} T(x, t) = \kappa V'(x) C^{-1} \left(\frac{V'(x)}{T(x, t)} f(x, t) + \frac{\partial}{\partial x} f(x, t) \right) \quad (53)$$

We can add a term of second order to this if we like, to represent heat conduction.

We now get expressions for the energy and entropy of the total system in the limit as $l \rightarrow 0$. The energy is given by

$$\begin{aligned}
 E(t) &= \sum_x p(x, t) l^{-1} V(x) l + \sum_x l V' \bar{n}(x, t) \\
 &\sim \int f(x, t) V(x) dx + C \int T(x, t) dx \tag{54}
 \end{aligned}$$

and the entropy is given by

$$\begin{aligned}
 S(t) &= - \sum_x p(x, t) \log p(x, t) - \sum_x \sum_{n_x} s_{x, t}(n_x) \log(s_{x, t}(n_x)) \\
 &\sim - \int f(x, t) \log f(x, t) dx + C \int \log T(x, t) dx \tag{55}
 \end{aligned}$$

(omitting some infinite time-independent terms and terms of smaller order in l). Let us assume that at each time, f and f' vanish at infinity. One then checks easily that E is conserved in time and that

$$\frac{dS}{dt} = \kappa \int f(x, t) \left\{ \frac{\partial \log f(x, t)}{\partial x} + \frac{V'(x)}{T(x, t)} \right\}^2 dx \geq 0 \tag{56}$$

We have thus successfully modified the classical theory of Brownian motion to conform with the first and second laws of thermodynamics.

4.2. The Temperature in the Quantum Case

The equation of motion of the number density in the quantum model of a Brownian particle given in Section 3 is easy to find. Since we are to find the expectation value in a thermal state, the term of first order in Eq. (36), $it[T, N_x]$, vanishes. Since the model is local, the double commutator $[T, [T, N_x]]$ uses only T_x , and we get

$$\begin{aligned}
 [T, [T, N_x]] &= \lambda [T_x, \{UP_x a_x - U^* P_{x+l} a_x^*\}] \\
 &= -2\lambda^2 [UP_x a_x, U^* P_{x+l} a_x^*] \\
 &= -2\lambda^2 \{UP_x U^* P_{x+l} a_x a_x^* - U^* P_{x+l} UP_x a_x^* a_x\} \\
 &= -2\lambda^2 \{P_{x+l} a_x a_x^* - P_x a_x^* a_x\}
 \end{aligned}$$

so that the second-order term of the equation for the number operator is

$$N'_x - N_x = -t^2 \lambda^2 / 2 [T, [T, N_x]] = t^2 \lambda^2 \{P_{x+l} a_x a_x^* - P_x a_x^* a_x\} \tag{57}$$

Taking the expectation value in the state $p \otimes \prod_x s_x$, in which the term of first order vanishes, gives

$$\frac{d\bar{n}_x}{dt} = \lambda_0 \{ p_{x+l}(\bar{n}_x + 1) - p_x \bar{n}_x \} \quad (58)$$

Combined with Eq. (42), this gives an infinite set of coupled non-linear differential equations for the time evolution of the fields $p(x, t)$ and $\bar{n}_{x, t}$; let us suppose that we have a solution. By construction this defines an orbit through the state space of density matrices of the total system, such that mean energy is conserved and entropy is non-decreasing.

Now let us take the continuum limit in the same way as we did to get Eq. (44), namely, put $\lambda_1 = l\lambda_0$, and use $\bar{n}_x l V' \sim T$; then we get

$$\frac{dT}{dt} = \lambda_1 V' \left(\frac{T}{lV'} (p_{x+l} - p_x) + p_{x+l} \right) \quad (59)$$

which in the limit $l \rightarrow 0$ gives

$$\frac{dT}{dt} = \lambda_1 (T p' + p V') \quad (60)$$

This suffers from the same problem as the classical model, namely, the specific heat becomes infinite as $l \rightarrow 0$; as there, we replace p by f/C . This leads to the equation for the temperature

$$C \frac{\partial T(x, t)}{\partial t} = \lambda_1 \left(T(x, t) \frac{\partial f(x, t)}{\partial x} + V'(x, t) f(x, t) \right) \quad (61)$$

Again, this equation of motion coupled with Eq. (44) written for f instead of p , leads to the conservation of energy, and the non-decrease of entropy; these are defined as for the classical model, by Eqs. (54) and (55). Indeed, we find

$$\dot{S} = \lambda_1 \int \frac{V' f}{T} \left(\frac{T f'}{f V'} + 1 \right)^2 dx \geq 0$$

It is natural to add a diffusion term, unrelated to the parameter λ_1 , due to direct hopping of quanta from bond to bond at rate κ_1 to the right-hand side, giving a heat equation with source:

$$C \frac{\partial T}{\partial t} = \kappa_1 \frac{\partial^2 T}{\partial x^2} + \lambda_1 \left(T \frac{\partial f}{\partial x} + V' f \right)$$

The diffusion term contributes a positive amount to \dot{S} , unless T is independent of x . From this, for a state to be stationary requires

$$Tf' = -fV'$$

where f and T are independent of time, and T is independent of x ; this can only occur if f is a Gibbs state at temperature T relative to the potential $V(x)$. This is not always possible, since we also require f to have finite L^1 -norm.

Similarly, the coupled equations where the heat capacity C is any positive function of x and T also lead to the first and second laws.

5. CONCLUSION AND OUTLOOK

In this paper we have succeeded in modifying the heat equation with drift so that the resulting non-linear system obeys the first and second laws of thermodynamics. Two models were studied, called the classical and the quantum model respectively, in which the gas of Brownian particles moves in one dimension in a potential $V(x)$. The state is described by a particle density f and a temperature field T , both varying in space and time. The equations of motion are given by

$$\frac{\partial f}{\partial t} = \kappa \frac{\partial^2 f}{\partial x^2} + \kappa \frac{\partial}{\partial x} \left(\frac{V'f}{T} \right) \tag{62}$$

$$C \frac{\partial T}{\partial t} = \kappa_1 \frac{\partial^2 T}{\partial x^2} + \kappa V' \left(\frac{V'f}{T} + \frac{\partial f}{\partial x} \right) \tag{63}$$

$$\frac{\partial f}{\partial t} = \lambda_1 \left\{ \frac{\partial}{\partial x} \left(\frac{T}{V'} \frac{\partial f}{\partial x} \right) + \frac{\partial f}{\partial x} \right\} \tag{64}$$

$$C \frac{\partial T}{\partial t} = \kappa_1 \frac{\partial^2 T}{\partial x^2} + \lambda_1 \left(T \frac{\partial f}{\partial x} + V'f \right) \tag{65}$$

In either case the energy and entropy are given by

$$E = \int f(x, t) V(x) dx + C \int T(x, t) dx \tag{66}$$

$$S(t) = - \int f(x, t) \log f(x, t) dx + C \int \log T(x, t) dx \tag{67}$$

These are obtained from the discrete microscopic theory by a suitable limit, dropping some infinite time-independent terms. The first and second laws

are expressed by the time-independence of E , and the increasing nature of $S(t)$.

It is not difficult to generalise these models to several dimensions, and to cases where the specific heat C and the diffusion constant κ depend on position and temperature; we just have to make different choices for the variation of the density of the oscillators with temperature, and for the transition probability $\lambda(n)$. The models thus obtained will also satisfy both laws.

It remains to prove the existence of global solutions in L^1 for given nonnegative initial conditions, and to show the expected positivity of the solutions. The classical version is quasilinear, and we have succeeded⁽¹⁴⁾ in showing that solutions exist for small times if the initial temperature is strictly positive, and the domain (in \mathbf{R}^n) has no boundaries. Some assumptions on the potential V , and on the initial state, are needed. The existence of solutions in other domains, with self adjoint boundary conditions on the Laplacian, is still an open problem. The quantum equation is fully non-linear, and the existence of evolutions, even for small times, is still open.

The slow variables of the microscopic models includes all the measurable functions of the Brownian particle; this enables us to set up, before the continuum limit is taken, a “non-linear stochastic process” in discrete time and space, which will describe the statistics of a tagged particle. We first give the initial distribution p and the beta fields at each site, and then solve for $p(x, t)$ and $n(b_x, t)$. We can then guide the stochastic process by the solution, and construct a process whose density at time t is $p(x, t)$. This is described in ref. 2, pp. 255 and 256, and in more detail in ref. 4 and 5. The point is that when the slow variables form an algebra, then the Heisenberg dynamics obtained as the dual to the flow through the states is a positive map, and so defines a process. A new problem then arises: once we have solutions $f(x, t)$ and $T(x, t)$ of our equations, (which we have, for small times, in the classical case) we can construct an associated stochastic process for the position of the tagged particle

$$dX_t = (2\kappa)^{1/2} dB_t + T^{-1}(x, t) V'(x) dt \quad (68)$$

The interpretation of such a process poses interesting further questions.

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