CONTRIBUTION TO THE STATISTICAL MECHANICAL THEORY OF BROWNIAN MOTION

E. BRAUN GUITLER

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PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR IN DE WISKUNDE EN NATUURWETENSCHAPPEN AAN DE RIJKSUNIVERSITEIT TE LEIDEN, OP GEZAG VAN DE RECTOR MAGNIFICUS DR. W. DEN BOER, HOOGLERAAR IN DE FACULTEIT DER LETTEREN, TEN OVERSTAAN VAN EEN COMMISSIE UIT DE SENAAT TE VERDEDIGEN OP WOENSDAG 24 JUNI 1964 TE 16 UUR

DOOR

ELIEZER BRAUN GUITLER
GEBOREN TE MEXICO CITY IN 1940

DRUKKERIJ PASMANS - v. d. VENNESTRAAT 76 - DEN HAAG

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A mis padres

A Guítele

A mis hermanos

Op verzoek van de Faculteit der Wiskunde en Natuurwetenschappen volgen hier enkele gegevens over mijn studie.

In 1957 begon ik mijn studie aan de Universidad Nacional Autónoma de Mexico (UNAM) te Mexico City en behaalde in september 1961 de graad van Fisico.

Van juni 1959 tot september 1961 werkte ik onder leiding van Prof. J. de Oyarzabal op het gebied van de zwakke wisselwerking tussen elementaire deeltjes.

Gedurende de academische jaren 1959 en 1961 gaf ik aan de UNAM colleges in wiskunde en natuurkunde.

Van december 1959 tot januari 1962 maakte ik deel uit van een researchgroep op het Instituto Nacional de la Investigación Científica die onder leiding van Dr. R. Gall onderzoek verrichtte over kosmische straling.

Vanaf januari 1962 was ik werkzaam op het Instituut-Lorentz voor theoretische natuurkunde, waar ik onder leiding van Prof. Dr. P.Mazur onderzoek verrichtte op het gebied van de statistische mechanica, o.m. over de statistische mechanica van irreversibele processen.

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CONTENTS

INTRODUCTION

Recently some attention has been devoted to the problem of finding statistical mechanical models for Brownian motion.

Hemmer[1], Rubin[2], and Turner[3] have studied the motion of a heavy particle in an assembly of coupled harmonic oscillators with nearest neighbour interaction. They found that for a sufficiently large mass, the motion of the heavy particle in the one dimensional assembly is almost that of a free Brownian particle. As pointed out by Toda[4] and Hori[5] the heavy particle rigorously performs Brownian motion only in the limit as its mass M and the force constant α characterizing the nearest neighbour interaction, both tend to infinity in such a way that the ratio α/M^2 remains finite.

On the other hand, Kac, Mazur and Ford[6] have shown that for particles of equal mass, any particle will perform Brownian motion in the "heat bath" consisting of all other particles if the harmonic interactions are of a very special (long range) type. In fact, Brownian motion may then only be rigorously obtained in the limit as a "cut off frequency", limiting the spectrum of normal modes frequencies, tends to infinity. It was also shown that if in this type of assembly any particle is acted upon by an arbitrary external force, then its motion becomes that of a Brownian particle in this field of force.

All the above mentioned results refer to systems with an infinite number of particles.

In this thesis we study the general motion of a particle in an harmonic oscillator assembly. In particular we obtain the conditions under which this particle will perform Brownian motion.

In chapter I we solve formally the equations of motion of the particle of interest, in the presence of an arbitrary external force acting on it. With the aid of this solution we rewrite the equations of motion in a form which bears a structural resemblance to the Langevin equation.

We also study the statistics of the particle in an initially conditional canonical ensemble, which describes the randomness of the remaining particles of the assembly (heat bath).

In chapter II we first discuss the model of Kac, Mazur and Ford. We then proceed to study the general motion of the particle of interest in the case that its mass is infinitely large. We find the conditions under which it performs Brownian motion. The mass M of the particle of interest and the time t have to tend to infinity in such a way $\tau = t/M$ remains infinite. Then Brownian motion is obtained, provided that the interactions satisfy some very general requirement, independent of their precise form: the spectral density $G(\omega^2)$ of eigenvalues ω of the interaction matrix has to be proportional to ω^{-1} for $\omega \to 0$.

We also study the motion of a heavy particle when this condition is not satisfied.

A generalization of our results to system of D dimensions is presented.

In chapter III we analyze the quantum mechanical behaviour of an infinitely heavy particle.

As is shown in chapter II there are two classically equivalent procedures for taking the limit $M \to \infty$. Quantum mechanically they are not equivalent.

We obtain for both cases a "Langevin operator equation" for the heavy particle in the presence of an arbitrary external force. They differ in the quantum mechanical correlation function for the "random force operator". The solution of the Langevin operator equation is studied for the case that a linear external force is applied to the heavy particle.

Finally we obtain the form of the position distribution function of the heavy particle at an arbitrary time.

CHAPTER I.

DYNAMICS AND STATISTICS OF A PARTICLE IN HARMONIC OSCILLATOR ASSEMBLIES

1. Introduction.

In the present chapter we shall study the dynamical and statistical properties of a particle coupled to a system of 2N harmonic oscillators.

In section 2 we give a formal solution of the equations of motion for the particle of interest, in the presence of an arbitrary external force acting on that particle only. With the help of this solution, we then rewrite the equations of motion in a form which bears a structural resemblance to the Langevin equation describing Brownian motion of a particle in the presence of an external force.

In section 3 we introduce a statistical element by assuming the "medium", consisting of the 2N oscillators to be initially in "thermal equilibrium with respect to the particle of interest", i.e. we describe the medium initially with a conditional canonical distribution function. It should be stressed that this is the only assumption of a statistical nature that we shall make throughout our investigation. The previously derived Langevin-type equation is then interpreted as a stochastic equation containing a stochastic force. The covariance of this force is obtained from the momentum autocorrelation function of the particle of interest in the absence of an external force.

Finally, in section 4 we discuss some general properties of this momentum autocorrelation function.

2. Dynamics of a particle coupled to a harmonic system.

Let us consider a one dimensional system of 2N+1 particles interacting with harmonic forces. The Hamiltonian of the system is

$$H^{(0)} = \sum_{k=-N}^{N} \tfrac{1}{2} \frac{p_k^2}{M_k} + \tfrac{1}{2} \sum_{j,k=-N}^{N} x_j A_{jk} x_k \,, \tag{2.1}$$

where M_k, p_k and x_k denote the mass, momentum and displacement of the k-th particle, respectively. We take

$$\begin{aligned} M_k &= 1, \quad \text{for } k \neq 0 \\ M_0 &= M. \end{aligned} \tag{2.2}$$

The equations of motion corresponding to the Hamiltonian (2.1) are

$$\dot{x}_k = \frac{\partial H^{(0)}}{\partial p_k} = p_k / M_k \tag{2.3}$$

$$\dot{p}_k = -\frac{\partial H^{(0)}}{\partial x_k} = -\sum_j A_{kj} x_j . \tag{2.4}$$

In order to insure conservation of the total momentum of the system, we must have, according to (2.4)

$$0 = \sum_k \dot{p}_k = -\sum_j x_j \sum_k A_{kj}$$

for arbitrary displacements x_j. Therefore

$$\sum_j A_{kj} = 0 . \tag{2.5}$$

We now proceed to solve the equations of motion. To this end we make the following canonical transformation

$$p_k' = M_k^{-1/2}\, p_k , \qquad x_k' = M_k^{1/2}\, x_k . \tag{2.6}$$

In terms of these variables the Hamiltonian becomes

$$H^{(0)} = \sum_k \tfrac{1}{2} p_k'^2 + \tfrac{1}{2} \sum_{j,k} x_k' \, B_{kj} \, x_j' \tag{2.7}$$

where the symmetric matrix B_{jk} is defined by

$$B_{jk} = (M_j M_k)^{-\frac{1}{2}} \, A_{jk} \, . \tag{2.8}$$

From (2.5) we find that B has to satisfy the following condition

$$\sum_k M_k^{\frac{1}{2}} \, B_{jk} = 0. \tag{2.9}$$

The equations of motion corresponding to the Hamiltonian (2.7) are

$$\dot{x}_k' = p_k' \tag{2.10}$$

$$\dot{p}_k' = - \sum_j B_{kj} x_j' \tag{2.11}$$

The solutions of these equations are

$$x_k'(t) = \sum_j (\cos B^{\frac{1}{2}} t)_{kj} \, x_j'(0) + \sum_j (B^{-\frac{1}{2}} \cdot \sin B^{\frac{1}{2}} t)_{kj} \, p_j'(0) \tag{2.12}$$

and

$$\dot{x}_k'(t) = p_k'(t) = \sum_j (\cos B^{1/2} t)_{kj}\, p_j'(0) - \sum_j (B^{1/2}.\sin B^{1/2} t)_{kj}\, x_j'(0) \quad (2.13)$$

where (cos $B^{1/2}t$), etc. are defined by their series expansions.

Using (2.6) we find the solutions in terms of the original variables

$$x_k(t) = \sum_j M_k^{-1/2} (\cos B^{1/2} t)_{kj} M_j^{1/2} x_j(0) + \sum_j M_k^{-1/2} (B^{-1/2}.\sin B^{1/2} t)_{kj} M_j^{-1/2} p_j(0) \quad (2.14)$$

and

$$p_k(t) = \sum_j M_k^{1/2} (\cos B^{1/2} t)_{kj} M_j^{-1/2} p_j(0) - \sum_j M_k^{1/2} (B^{1/2}.\sin B^{1/2} t)_{kj} M_j^{1/2} x_j(0). \quad (2.15)$$

Now let us assume that the zeroeth particle is acted upon by an arbitrary external force $F(x_0)$ which may be derived from a potential,

$$F(x_0) = -\frac{\partial V(x_0)}{\partial x_0}. \quad (2.16)$$

Then the Hamiltonian of the system is

$$H = \sum_k \tfrac{1}{2} \frac{p_k^2}{M_k} + \tfrac{1}{2} \sum_{j,k} x_j A_{jk} x_k + V(x_0). \quad (2.17)$$

The formal solutions of the equations of motion corresponding to this Hamiltonian are

$$x_k(t) = \sum_j M_k^{-\frac{1}{2}} (\cos B^{\frac{1}{2}} t)_{kj} M_j^{\frac{1}{2}} x_j(0) + \sum_j M_k^{-\frac{1}{2}} (B^{-\frac{1}{2}}.\sin B^{\frac{1}{2}} t)_{kj} M_j^{-\frac{1}{2}} p_j(0) +$$

$$+ M_k^{-\frac{1}{2}} \int_0^t dt' \, [B^{-\frac{1}{2}}.\sin B^{\frac{1}{2}} (t-t')]_{k0} \, M^{-\frac{1}{2}} F(x_0(t')) \quad (2.18)$$

and

$$p_k(t) = M_k \dot{x}_k(t) = \sum_j M_k^{\frac{1}{2}} (\cos B^{\frac{1}{2}} t)_{kj} M_j^{-\frac{1}{2}} p_j(0) - \sum_j M_k^{\frac{1}{2}} (B^{\frac{1}{2}}.\sin B^{\frac{1}{2}} t)_{kj} M_j^{\frac{1}{2}} x_j(0) +$$

$$+ M_k^{\frac{1}{2}} \int_0^t dt' \, [\cos B^{\frac{1}{2}} (t-t')]_{k0} \, M^{-\frac{1}{2}} F(x_0(t')) \, . \quad (2.19)$$

In particular we have for the zeroeth particle, from (2.2) and (2.19)

$$p_0(t) = (\cos B^{\frac{1}{2}} t)_{00} p_0(0) + M^{\frac{1}{2}} \sum_{j \neq 0} (\cos B^{\frac{1}{2}} t)_{0j} \, p_j(0) -$$

$$- M^{\frac{1}{2}} \sum_j (B^{\frac{1}{2}}.\sin B^{\frac{1}{2}} t)_{0j} M_j^{\frac{1}{2}} x_j(0) + \int_0^t dt' \, [\cos B^{\frac{1}{2}} (t-t')]_{00} \, F(x_0(t')) \, . \quad (2.20)$$

Differentiating this equation with respect to time one finds

$$\dot{p}_0(t) = -(B^{1/2}.\sin B^{1/2}t)_{00}p_0(0) - M^{1/2} \sum_{j \neq 0} (B^{1/2}.\sin B^{1/2}t)_{0j}\, p_j(0) -$$

$$- M^{1/2} \sum_j (B.\cos B^{1/2}t)_{0j}\, M_j^{1/2} x_j(0) + F(x_0(t)) -$$

$$- \int_0^t dt' \, [B^{1/2}.\sin B^{1/2}(t-t')]_{00}\, F(x_0(t')) \,. \qquad (2.21)$$

Eliminating $p_0(0)$ from (2.20) and (2.21) we then obtain

$$\dot{p}_0(t) - F(x_0(t)) = -\gamma(t)\, p_0(t) + E(t) +$$

$$+ \int_0^t dt' \, [\gamma(t) - \gamma(t-t')]\, [\cos B^{1/2}(t-t')]_{00} F(x_0(t')) \qquad (2.22)$$

where the time dependent "friction coefficient", $\gamma(t)$ is given by

$$\gamma(t) = \frac{(B^{1/2}.\sin B^{1/2}t)_{00}}{(\cos B^{1/2}t)_{00}} = -\frac{d}{dt} \ln (\cos B^{1/2}t)_{00} \,, \qquad (2.23)$$

and the force $E(t)$ by

$$E(t) = M^{1/2} \sum_{k \neq 0} \{\gamma(t)\, (\cos B^{1/2}t)_{0k} - (B^{1/2}.\sin B^{1/2}t)_{0k}\} p_k(0) -$$

$$- M^{1/2} \sum_{k \neq 0} \{\gamma(t)\, (B^{1/2}.\sin B^{1/2}t)_{0k} + (B.\cos B^{1/2}t)_{0k}\} (x_k(0) - x_0(0)) \,. \qquad (2.24)$$

Here we have used (2.9). We note that E(t) is independent of the external force $F(x_0)$, and depends only on the initial state of the "medium" consisting of the 2N particles of unit mass. In fact, it depends only on the initial values of their momenta and their displacements relative to the zeroeth particle.

3. Stochastic motion of the zeroeth particle.

Let the initial momentum $p_0(0)$ and displacement $x_0(0)$ be specified. Furthermore we take the medium to be in "thermal equilibrium with respect to the zeroeth particle" at t = 0, i.e. we assume that it may be described by the non-stationary canonical distribution function

$$f' = e^{-\beta H'} \tag{3.1}$$

where $\beta = (k_B T)^{-1}$, and

$$H' = \sum_{k \neq 0} \tfrac{1}{2} p_k^2 + \tfrac{1}{2} \sum_{j,k \neq 0} (x_j - x_0) A_{jk} (x_k - x_0) \tag{3.2}$$

which in view of (2.2) and (2.8) may also be written as

$$H' = \sum_{k \neq 0} \tfrac{1}{2} p_k^2 + \tfrac{1}{2} \sum_{j,k \neq 0} (x_j - x_0) B_{jk} (x_k - x_0). \tag{3.3}$$

Then E(t) given by (2.24) is seen to be a sumvariable of Gaussian random variables, and thus a Gaussian random process.

We define the momentum aurocorrelation function $\rho(t)$ of the zeroeth particle in a system for which $F(x_0) \equiv 0$, as

$$\rho(t) = \overline{p_0(t) p_0(0)}\ , \tag{3.4}$$

where $p_0(t)$ is given by equation (2.15), and where the bar denotes an average taken over the stationary canonical ensemble with distribution function

$$f^{(0)} = e^{-\beta H^{(0)}} . \tag{3.5}$$

Here $H^{(0)}$ is given by (2.1). Combining (2.15) and (3.4) we find that

$$\rho(t) = \beta^{-1} M (\cos B^{\frac{1}{2}} t)_{00} \tag{3.6}$$

which relates $\rho(t)$ to the (0,0) matrix element of $(\cos B^{\frac{1}{2}} t)$.

Recalling the fact that $E(t)$ is independent of $F(x_0)$ (cf. the discussion after equation (2.24)), we have according to the equation of motion (2.22) with $F(x_0) \equiv 0$

$$E(t) = \dot{p}_0(t) + \gamma(t)\, p_0(t) . \tag{3.7}$$

From this equation we obtain

$$E(t_0)\, E(t_0+t) = \frac{\partial}{\partial t_0} \{p_0(t_0)\, \dot{p}_0(t_0+t)\} + \gamma(t_0+t) \frac{\partial}{\partial t_0} \{p_0(t_0)\, p_0(t_0+t)\}$$

$$- \frac{\partial^2}{\partial t^2} \{p_0(t_0)\, p_0(t_0+t)\} + \gamma(t_0)\, \gamma(t_0+t)\, p_0(t_0)\, p_0(t_0+t) +$$

$$\{\gamma(t_0) - \gamma(t_0+t)\} \frac{\partial}{\partial t} \{p_0(t_0)\, p_0(t_0+t)\} . \tag{3.8}$$

By averaging the left hand side of this equation over the initial distribution function (3.1) we obtain the autocorrelation function of $E(t)$.

However, as is seen from (2.24), E(t) does not depend on $p_0(0)$, and we can replace the average over the initial distribution (3.1) by an average over the stationary distribution (3.5). We then obtain using (3.4) and the stationarity of (3.5)

$$< E(t_0)\,E(t_0+t) > = \overline{E(t_0)E(t_0+t)} = -\frac{\partial^2}{\partial t^2}\,\rho(t) + \gamma(t_0)\gamma(t_0+t)\,\rho(t) +$$

$$+ \{\,\gamma(t_0) - \gamma(t_0+t)\}\frac{\partial}{\partial t}\;\rho(t)\;. \qquad (3.9)$$

Thus, in an initial ensemble described by (3.1), the statistical behaviour of the zeroeth particle can in principle be determined from equation (2.22). This equation must be interpreted as a stochastic equation. The stochastic force E(t) is a Gaussian process with covariance given by (3.9).

We note that equation (2.22) bears at structural resemblance to the Langevin equation for Brownian motion of a particle in the presence of an external force

$$\dot{p}(t) - F(x(t)) = -\gamma p(t) + E_L(t)\;. \qquad (3.10)$$

Here γ is the friction constant, and $E_L(t)$ the Gaussian random force with covariance

$$\overline{E_L(t_0)\,E_L(t_0+t)} = 2\beta^{-1}M\gamma\,\delta(t)\;, \qquad (3.11)$$

where M is the mass of the Brownian particle and $\delta(t)$ is the Dirac delta function.

However (2.22) with the covariance (3.9) will reduce to (3.10) with the covariance (3.11), if and only if the following equality holds

$$(\cos B^{1/2}t)_{00} = e^{-\gamma\,|t|}\;. \qquad (3.12)$$

Indeed, $\gamma(t)$ is then no longer time dependent, but has the constant value γ, as follows immediately from (2.23), and as a consequence the last term on the right hand side in (2.22) would then vanish, whereas the covariance (3.9) reduces to (3.11).

In the following chapter we shall establish the conditions under which the equality (3.12) holds. At the same time we shall then obtain an explicit expression for the friction constant γ in terms of the interaction matrix **A**. But first we shall discuss in the next section some general properties of the quantity $(\cos B^{1/2}t)_{00}$, which is according to (3.4) and (3.6) essentially the momentum autocorrelation function.

4. Properties of the momentum autocorrelation function.

Let **U** be the matrix that diagonalizes the symmetric matrix **B**, with eigenvalues ω_k^2 ($k = -N,\ldots,N$). Then

$$B = U^{-1} \cdot \omega^2 \cdot U \tag{4.1}$$

where ω^2 is the diagonal matrix with elements ω_k^2. From equation (3.6) we can therefore write

$$\beta M^{-1} \rho(t) = (\cos B^{1/2}t)_{00} = \sum_k |U_{k0}|^2 \cos \omega_k t \,. \tag{4.2}$$

For a system with a finite number of particles this function, a finite sum of periodic functions, is an almost periodic function. This means that any value which is once achieved, will be achieved an infinite number of times.

Let us, for the sake of simplicity, consider the case that $M = 1$ and $|U_{k0}|^2 = n^{-1}$, with $n = 2N + 1$. Then we have

$$\beta\rho(t) = \frac{1}{n} \sum_k \cos \omega_k t \equiv \frac{1}{n}\, h(t) \,. \tag{4.3}$$

Let L(q) be the average frequency with which a value q is achieved by h(t). For large N, Kac[9] has shown that

$$L(bn^{1/2}) \simeq \frac{2\omega_0}{\pi}\ e^{-\frac{1}{2}b^2} \tag{4.4}$$

where

$$\omega_0^2 = \frac{1}{n}\sum_k \omega_k^2 \tag{4.5}$$

and where it is assumed that

$$\lim_{n\to\infty} \frac{1}{n^2} \sum_k \omega_k^4 = 0\ , \tag{4.6}$$

and that the frequencies ω_k are rationally independent.

On the other hand, starting from a formula given by Slater[10], Mazur and Montroll[11] have shown that in the case that (n−q) is small and n large

$$L(q) \simeq \frac{\omega_0}{2\pi^{3/2}}\ \left(\frac{1-\alpha}{\pi e}\right)^{\frac{1}{2}(n-1)} \simeq L(\alpha n) \tag{4.7}$$

where

$$\alpha = \frac{q-1}{n-1} \simeq \frac{q}{n}\ . \tag{4.8}$$

Consider a value of $\beta\rho(t) = n^{-1}h(t)$ in the range $(-bn^{-\frac{1}{2}}, bn^{-\frac{1}{2}})$, $(b\sim 0\,(1))$. The average frequency of recurrence for this value of $\beta\rho(t)$

is given by (4.4), whereas the average frequency corresponding to values of $\beta\rho(t) = \alpha$ $(0 < \alpha < 1)$ is given by (4.7). Thus, for the limit as N tends to infinity, the recurrence frequency for values in a range outside $(-bn^{-1/2}, bn^{-1/2})$, i.e. for values of $\alpha \sim O(1)$, becomes very small, while the frequency for values inside the range is of the order of ω_0.

In other words, when N is very large, the mean recurrence time (which is inversely proportional to the mean recurrence frequency) for values outside the range $(-bn^{-1/2}, bn^{-1/2})$ is very large compared with the available observation times, and there occurs an apparently irreversible trend towards "equilibrium". In this case the system will remain near "equilibrium" most of the time. Only when N is infinite, will the system rigorously tend to equilibrium and remain there. In this case the range $(-bn^{-1/2}, bn^{-1/2})$ shrinks to zero, and $\rho(t)$ vanishes as t tends to infinity; $p_0(t)$ and $p_0(0)$ then become independent of each other.

The case of what we shall call a perfect system (M = 1) has explicitly been studied for two different types of harmonic interactions between the particles. The first one is a system with nearest neighbours interactions, in which one has[12]

$$\omega_k = \omega_L \left|\sin \frac{\pi k}{n}\right|, \qquad |U_{0k}|^2 = \frac{1}{n}, \tag{4.9}$$

where ω_L is the maximum frequency of the system. The momentum autocorrelation function in this case takes the form

$$\beta\rho(t) = \frac{1}{n} \sum_k \cos(\omega_L t \sin \frac{\pi k}{k}) . \tag{4.10}$$

In the limit as N tends to infinity let $\varphi = \pi k n^{-1}$ and $d\varphi = \pi n^{-1}$. Then

$$\beta\rho(t) = \frac{1}{\pi} \int_0^\pi \cos(\omega_L t \sin \varphi)\, d\varphi = J_0(\omega_L t) , \tag{4.11}$$

where J_r is the Bessel function of order r.

Secondly, Kac, Mazur and Ford[6] obtained for a system with special long range forces between the particles that (cf. Ch. II, section 2)

$$\rho(t) = \beta^{-1} e^{-\gamma |t|} . \tag{4.12}$$

Since we have shown in the preceding section that the zeroeth particle will perform Brownian motion if and only if $\rho(t)$ is of an exponential form, it follows from (4.11) and (4.12) that the first system does not give rise to Brownian motion for the zeroeth particle, wheras the second one does.

As for the case of a non perfect system ($M \neq 1$), Rubin[2] found taking $M = 2$ and nearest neighbours interactions that

$$\rho(t) = 2\beta^{-1} (\omega_L t)^{-1} J_1(\omega_L t) , \tag{4.13}$$

so that for this system one does not obtain Brownian motion for the zeroeth particle.

For very large M with nearest neighbours interactions, however, the behaviour of $\rho(t)$ becomes approximately exponential, as was shown by Hemmer[1] and Rubin[2] :

$$\rho(t) \sim e^{-\omega_L |t| / M} + R(|t|, M) . \tag{4.14}$$

The rest term R can be made to vanish by taking the limit $M \to \infty$. But then $\rho(t)$ reduces to a constant according to (4.14).

Takeno and Hori[5], following a suggestion given by Toda[4] have shown, however that the exponential form of $\rho(t)$ may be rigorously obtained from (4.14) by a double limiting procedure: $M \to \infty$, $\omega_L \to \infty$, $\omega_L / M = \gamma$ finite.

In the next chapter we shall present an alternative limiting procedure which yields the desired exponential behaviour. Moreover, our analysis will not be confined to the case of nearest neighbours interactions.

CHAPTER II.

BROWNIAN MOTION

1. Introduction.

In this chapter we study the conditions under which the particle of interest labeled by the number 0 will perform Brownian motion.

In section 2 we consider the case that the zeroeth particle is of unit mass, i.e. all the particles in the system are equal. As has been shown the particle then behaves as a Brownian particle for a very special interaction[6].

In section 3 we analyze the case that the mass M of the particle of interest is infinitely large. We show that as the time t and the mass M both tend to infinity in such a way that their ratio remains finite, the heavy particle performs Brownian motion provided that the interactions satisfy some very general requirement, independent of their precise form: Brownian motion is obtained only if the spectral density $G(\omega^2)$ of eigenvalues ω^2 of the interaction matrix is proportional to ω^{-1} for $\omega \to 0$. (This is the case, for instance, for nearest neighbours interactions in one dimension). We also study the motion of a heavy particle when this condition is not satisfied.

In section 4 we generalize our results to systems of higher dimensionality. In particular we study the case of a simple cubic lattice.

In section 5 we give an explicit example of an interaction matrix A such that a heavy particle will perform Brownian motion for any dimension.

Finally it is shown that the limit in which Browñian motion is obtained, corresponds to the "weak coupling" limit taken in the derivation of the master equation by perturbation techniques[7,8].

2. Brownian motion of a particle of unit mass.

In this section we consider the case that M=1, i.e. all the particles of the system are equal. In this case, we have according to (I.2.8)

$$B_{jk} = A_{jk} . \tag{2.1}$$

Consider

$$(\cos A^{1/2}t)_{00} = \int_{-\infty}^{\infty} d\omega \cos\omega t \, \{\delta(A^{1/2} - \omega)\}_{00} = \int_{-\infty}^{\infty} d\omega \cos\omega t \, S_1(\omega) \qquad (2.2)$$

where the spectrum $S_1(\omega)$ is given by

$$S_1(\omega) = \tfrac{1}{2} \{ \delta(A^{1/2} - \omega) + \delta(A^{1/2} + \omega)\}_{00} \, . \qquad (2.3)$$

Using the following representations of the δ-functions

$$\delta(A^{1/2} - \omega) = \frac{1}{\pi} \lim_{\epsilon \to 0+} \operatorname{Im} [A^{1/2} - (\omega + i\epsilon) I]^{-1} \qquad (2.4)$$

$$\delta(A^{1/2} + \omega) = -\frac{1}{\pi} \lim_{\epsilon \to 0+} \operatorname{Im} [A^{1/2} + (\omega + i\epsilon) I]^{-1} \, , \qquad (2.5)$$

where I is the unit matrix, equation (2.3) may be written as

$$S_1(\omega) = \lim_{\epsilon \to 0+} \frac{1}{\pi} \operatorname{Im} (\omega + i\epsilon) \, Q_{00}((\omega + i\epsilon)^2) \qquad (2.6)$$

with

$$Q(z^2) = (A - z^2 I)^{-1} \qquad (2.7)$$

the resolvent of the matrix A.

So far we have not made any specific assumption concerning the interaction matrix A. Let us suppose that A_{jk} is defined as follows

$$A_{jk} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta f(\theta) \, e^{i(j-k)\theta} \, . \qquad (2.8)$$

In order to insure that A is a symmetric, positive semi-definite matrix with the property (I.2.5), we take $f(\theta)$ to be a positive, even function with $f(0)=0$. The matrix A then has the property that

$$A_{jk} = A_{|j-k|} \, . \qquad (2.9)$$

We shall also take $f(\theta)$ to be bounded and piecewise monotonic.

As we discussed in section 4 of chapter I, in order that $(\cos A^{1/2}t)_{00}$ tends to zero as t tends to infinity, or equivalently, in order that the spectrum $S_1(\omega)$ be continuous, the number of particle in the system must be infinite. We shall therefore at this point take the limit of an infinite number of particles.

From (2.8) it may be shown that as N tends to infinity, Q_{00} may be written as

$$Q_{00}(z^2) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; \frac{1}{f(\theta) - z^2} \, . \tag{2.10}$$

Assume now that $f(\theta)$ is defined as follows:

$$f(\theta) = \begin{cases} \gamma^2 \mathrm{tg}^2\theta \, , & \text{for } 0 \le |\theta| \le \theta_L \, , \; \pi - \theta_L \le |\theta| \le \pi \\ \gamma^2 \mathrm{tg}^2 \theta_L \equiv \omega_L^2 \, , & \text{for } \theta_L \le |\theta| \le \pi - \theta_L \end{cases} \tag{2.11}$$

with $|\theta| < \pi/2$.

The resolvent $Q_{00}(z^2)$ then becomes

$$Q_{00}(z^2) = \frac{1}{\pi} \int_{|\theta| \le \theta_L} d\theta \; \frac{1}{\gamma^2 \mathrm{tg}^2\theta - z^2} \; + \frac{1}{\pi} \, \frac{\pi - 2\theta_L}{\omega_L^2 - z^2} \quad . \tag{2.12}$$

Making the transformation of variables

$$x = \gamma \mathrm{tg}\theta \tag{2.13}$$

and taking the limit $\theta_L \to \pi/2$ $(\omega_L \to \infty)$, we find that

$$Q_{00}(z^2) = \frac{\gamma}{\pi} \int_{-\infty}^{\infty} dx \, \frac{1}{(\gamma^2 + x^2)(x^2 - z^2)}$$

$$= - \frac{1}{z(z + i\gamma)} \, . \tag{2.14}$$

Combining (2.6) and (2.14) we obtain

$$S_1(\omega) = \frac{\gamma}{\pi}\,\frac{1}{\omega^2+\gamma^2} \tag{2.15}$$

which yields when introduced into (2.2)

$$(\cos A^{1/2}t)_{00} = e^{-\gamma|t|}\,. \tag{2.16}$$

From (2.16) it then follows, as has been showed in the preceding chapter that the zeroeth particle performs Brownian motion (cf. the discussion after (I.3.11)).

We note the resemblance between the limit $\theta_L \to \pi/2$, or $\omega_L \to \infty$ as taken above, and the limit $M \to \infty$, $\omega_L \to \infty$, $\omega_L/M = \gamma$ finite, proposed by Toda for a heavy particle in a system with nearest neighbours interactions (cf. the end of ch. I). In both cases a "cut of" frequency tends to infinity and the forces between the particles therefore also tend to infinity.

If first order corrections in ω_L^{-1} to the above results are taken into account, the Brownian motion is only obtained inasmuch as time intervals of the order ω_L^{-1} are neglected and inasmuch as $\omega_L \gg \gamma$.

3. Brownian motion of a heavy particle.

We now turn to the case that the mass M of the zeroeth particle is larger than the mass of all other particles. From now on we shall call the zeroeth particle the heavy particle.

We proceed to investigate under what conditions the momentum autocorrelation function of a heavy particle will fall off exponentially in time.

To this end we write

$$(\cos B^{1/2}t)_{00} = (\cos M B^{1/2}\tau)_{00} = \int_{-\infty}^{\infty} d\omega \cos\omega\tau \,\{\, \delta(MB^{1/2} - \omega)\}_{00}$$

$$= \int_{-\infty}^{\infty} d\omega \cos\omega\tau \, S_M(\omega) \tag{3.1}$$

where

$$\tau = \frac{t}{M} \tag{3.2}$$

and where the spectrum $S_M(\omega)$ is given by

$$S_M(\omega) = \tfrac{1}{2} \{ \delta(MB^{1/2} - \omega) + \delta(MB^{1/2} + \omega)\}_{00} . \tag{3.3}$$

The new time scale τ defined by equation (3.2) has been introduced to enable us to study the motion of a particle in the limit as M tends to infinity. (In the original time scale an infinitely heavy particle will not react at all to the interaction with the medium).

Using the representations of the δ-functions as given by equations (2.4) and (2.5), equation (3.3) may be written as

$$S_M(\omega) = \lim_{\epsilon \to 0+} \mathrm{Im}\, \frac{1}{\pi} \frac{1}{M^2} (\omega + i\epsilon) R_{00}((\frac{\omega + i\epsilon}{M})^2) , \tag{3.4}$$

with

$$R(z^2) = (B - z^2 I)^{-1} \tag{3.5}$$

the resolvent of the matrix B.

We now proceed to establish a connection between the (0,0) matrix elements of the resolvent B and the resolvent A (as defined by (2.7)). Equation (I.2.8) may be written in matrix form as

$$B = M^{-1/2} . A . M^{-1/2} , \tag{3,6}$$

or equivalently,

$$M^{1/2} . B = A . M^{-1/2} . \tag{3.7}$$

Here the matrix M is diagonal and has elements $M_k \ \delta_{kj}$, with M_k given by (I.2.2). Solving equations (2.7) and (3.5) for A and B, respectively, and inserting the obtained expressions into equation (3.7) we find that

$$M^{1/2} . (R^{-1} + z^2 I) = (Q^{-1} + z^2 I) . M^{-1/2} . \tag{3.8}$$

Multiplying equation (3.8) from the right by **R** and from the left by **Q**, and taking the (0,0) matrix element, we then obtain, using (I.2.2)

$$R_{00}(z^2) = \frac{M\, Q_{00}(z^2)}{1 + z^2\,(1-M)\, Q_{00}(z^2)} \; . \tag{3.9}$$

We therefore have the relation

$$\lim_{M\to\infty} \frac{1}{M^2}\, z\, R_{00}\left(\frac{z^2}{M^2}\right) = \frac{\lim\limits_{M\to\infty} zM^{-1} Q_{00}\left(\frac{z^2}{M^2}\right)}{1 - z \lim\limits_{M\to\infty} z\, M^{-1} Q_{00}\left(\frac{z^2}{M^2}\right)} \; . \tag{3.10}$$

This result is completely general, valid for any matrix **A**. We now assume that A_{jk} is of the form (2.8). In the limit as N tends to infinity, $Q_{00}(z^2)$ is then given by equation (2.10)

$$Q_{00}(z^2) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; \frac{1}{f(\theta) - z^2} \; . \tag{3.11}$$

Making the change of variables

$$u^2 = f(\theta) \, , \tag{3.12}$$

equation (3.11) becomes

$$Q_{00}(z^2) = \frac{1}{2\pi} \int_{-u_0}^{u_0} du \; \frac{g(u)}{u^2 - u^2} \; . \tag{3.13}$$

Here g(u) is the positive frequency spectrum of normal modes for the case that all masses, including the mass of particle 0, are equal. We may also say that $(2u)^{-1}\, g(u) = G(u^2)$ is the spectrum of eigenvalues $\lambda = u^2$ of the matrix **A**. u_0 is the frequency corresponding to the maximum eigenvalue $\lambda_0 = u_0^2$. We have defined g(u) in such a way that

$$g(-u) = g(u) \,. \tag{3.14}$$

From equation (3.13) we have

$$z M^{-1} Q_{00}\left(\frac{z^2}{M^2}\right) = \frac{1}{2\pi}\int_{-u_0}^{u_0} du\, g(u)\, \tfrac{1}{2} \left\{ \frac{1}{u - z/M} - \frac{1}{u + z/M} \right\}. \tag{3.15}$$

In conformity with the physical ideas underlying the phenomenological theory of Brownian motion, we shall study the expressions obtained in the limit as M tends to infinity.

Using the fact that if $\mathrm{Im}\, z > 0$,

$$\lim_{M\to\infty} \frac{1}{u \mp z/M} = P\left(\frac{1}{u}\right) \pm i\pi\delta(u) \,, \tag{3.16}$$

where P denotes the principal value, we find from equation (3.15)

$$\lim_{M\to\infty} zM^{-1} Q_{00}\left(\frac{z^2}{M^2}\right) = \frac{1}{2\pi}\int_{-u_0}^{u_0} du\, g(u)\, i\pi\delta(u) = i\,\tfrac{1}{2}\, g(0). \tag{3.17}$$

Combination of (3.10) and (3.17) yields

$$\lim_{M\to\infty} \frac{1}{M^2}\, z\, R_{00}\left(\frac{z^2}{M^2}\right) = \frac{i\tfrac{1}{2}g(0)}{1 - i\tfrac{1}{2}g(0) z} \,. \tag{3.18}$$

Therefore, $S_M(\omega)$ as given by equation (3.4) becomes in this limit

$$\lim_{M\to\infty} S_M(\omega) \equiv S(\omega) = \frac{1}{\pi}\, \frac{\gamma}{\gamma^2 + \omega^2} \tag{3.19}$$

with

$$\gamma \equiv \tfrac{1}{2} g(0)\ . \tag{3.20}$$

From equation (3.1) we obtain

$$\lim_{\substack{M\to\infty\ t\to\infty \\ t/M = \tau}} (\cos B^{1/2} t)_{00} = \lim_{M\to\infty} (\cos M\, B^{1/2} \tau)_{00} = e^{-\gamma |\tau|}\ . \tag{3.21}$$

Therefore in this limit the heavy particle performs indeed Brownian motion (cf. Ch. I, section 3).

It should be stressed that we have assumed $g(0) = (2uG(u^2))_{u\,=\,0}$, where $G(u^2)$ is the spectrum of eigenvalues of the matrix $\mathbf{A}$ to be a non vanishing finite quantity. The matrix $\mathbf{A}$ may be otherwise completely arbitrary. Thus as should be expected, the detailed specification of the "medium" is not essential for the limiting Brownian motion type behaviour of a heavy particle. In fact, the one dimensional system with nearest neighbours interactions discussed by Hemmer, Rubin, Takeno and Hori is just a special case satisfying the above requirements. We shall come back in the final section to the discussion of the various limits taken in the derivation of the Langevin equation.

We now consider in more detail the case that $g(u)$ vanishes at the origin. In that case the average motion of the infinitely heavy particle is singular on the time scale (3.2). Let us therefore instead of (3.2) introduce the time variable

$$\tau = t/M^{1/2}\ . \tag{3.22}$$

We then have

$$(\cos B^{1/2} t)_{00} = (\cos M^{1/2} B^{1/2} \tau)_{00} = \int_{-\infty}^{\infty} d\omega \cos \omega\tau\, S'_M(\omega) \tag{3.23}$$

where

$$S'_M(\omega) = \lim_{\epsilon\to 0+} \operatorname{Im} \frac{1}{\pi M} (\omega + i\epsilon)\, R_{00}\left(\frac{(\omega + i\epsilon)^2}{M}\right)\ . \tag{3.24}$$

The matrix $R(z^2)$ is given by (3.5). In view of (3.9) we then have instead of (3.10)

$$\lim_{M\to\infty} \frac{1}{M}\, z\, R_{00}\left(\frac{z^2}{M}\right) = \frac{\lim\limits_{M\to\infty} z\, Q_{00}\left(\frac{z^2}{M}\right)}{1 - z \lim\limits_{M\to\infty} z\, Q_{00}\left(\frac{z^2}{M}\right)} \,. \tag{3.25}$$

On the other hand, we have from (3.13)

$$Q_{00}\left(\frac{z^2}{M}\right) = \frac{1}{2\pi} \int_{-u_0}^{u_0} du\, g(u) \frac{1}{2u} \left\{ \frac{1}{u - z/M^{1/2}} + \frac{1}{u + z/M^{1/2}} \right\} \tag{3.26}$$

which in the limit $M \to \infty$ ($\mathrm{Im}\, z > 0$) becomes

$$\lim_{M\to\infty} z\, Q_{00}\left(\frac{z^2}{M}\right) = \frac{z}{2\pi}\, P \int_{-u_0}^{u_0} du\, \frac{g(u)}{u^2} \,. \tag{3.27}$$

The quantity ω_0^{-2}, defined by

$$\omega_0^{-2} = \frac{1}{2\pi}\, P \int_{-u_0}^{u_0} du\, \frac{g(u)}{u^2} \tag{3.28}$$

is finite for spectra behaving in the neighbourhood of the origin as $c|u|^n$, $n \geq 1 + \epsilon$, ($\epsilon > 0$).

Combining (3.24), (3.25), (3.27) and (3.28) we now find the following result for $S'_M(\omega)$:

$$\lim_{M\to\infty} S'_M(\omega) = \tfrac{1}{2}\delta(\omega - \omega_0) + \tfrac{1}{2}\delta(\omega + \omega_0) \,, \tag{3.29}$$

and with (3.23) for the limiting behaviour of $(\cos M^{1/2} B^{1/2} \tau)_{00}$

$$\lim_{\substack{M\to\infty\ t\to\infty \\ t/M^{1/2}=\tau}} (\cos B^{1/2}t)_{00} = \lim_{M\to\infty} (\cos M^{1/2}B^{1/2}\tau)_{00} = \cos \omega_0\tau. \quad (3.30)$$

We thus note that for the case $\lim_{u\to 0+} u^{-n}g(u) = c > 0,\ (n \geq 1+\epsilon)$,
the average motion of the heavy particle **appears** to be periodic with frequency ω_0. This result should not be interpreted to imply that the motion of the heavy particle in the infinite "heat bath" is then purely reversible. In fact, we found that on the more compressed time scale (3.2), the momentum autocorrelation function $\rho(\tau)$ has already relaxed to zero, for all $\tau \neq 0$. Therefore our result implies that on the time scale $\tau = t/M^{1/2}$ the motion of a very heavy particle will appear to be reversible, and that the characteristic times for the decay of the momentum autocorrelation function are very much larger than the characteristic time of an oscillation ω_0^{-1}. This corresponds, as it were to highly underdamped oscillation of the heavy particle. We shall discuss, in this connection in section 6 Rubin's result for the motion of a heavy particle in a 3-dimensional cubic lattice with nearest neighbours interactions. For such a system the relevant quantity g(u) behaves as cu^2 near the origin. We shall first, however, generalize our results to systems of higher dimensionality.

We also note that the formulae given were not sufficient to establish the limiting behaviour of the heavy particle for the case that $\lim_{u\to 0+} u^{-n}g(u) = b > 0,\ (0 < n \leq 1)$.

4. Motion of a heavy particle in a D-dimensional system.

In this section we generalize the foregoing results to the case of a D-dimensional system (D= 1,2, ...). Each particle has D degrees of freedom and is labeled with a D-dimensional vector $\vec{k}$, whose components k_α are integers such that $-N \ll k_\alpha \ll N$, with $\alpha = 1,2 \ldots, D$. We therefore have $(2N+1)^D$ particles in the system. The Hamiltonian of the system is

$$H^{(0)} = \sum_{\vec{k}} \tfrac{1}{2} \frac{(\vec{p}_{\vec{k}})^2}{M_{\vec{k}}} + \tfrac{1}{2} \sum_{\vec{j},\vec{k}} \vec{x}_{\vec{j}} \cdot A_{\vec{j}\vec{k}} \cdot \vec{x}_{\vec{k}} \quad (4.1)$$

where $\mathbf{A}_{\vec{j}\vec{k}}$ is a D-dimensional tensor. We denote by $\mathbf{A}$ the $D(2N+1)^D$ x$D(2N+1)^D$ matrix with elements $A^{\alpha\beta}_{\vec{j}\vec{k}}$, where $\alpha,\beta = 1,2,\ldots,D$. We take

$$
\begin{aligned}
M_{\vec{k}} &= 1, \text{ for } \vec{k} \neq \vec{0} \\
M_{\vec{0}} &= M
\end{aligned}
\tag{4.2}
$$

Proceeding in the same way used to derive (I.2.22) we now obtain

$$
\begin{aligned}
&\dot{\vec{p}}_{\vec{0}}(t) - \vec{F}(\vec{x}_{\vec{0}}(t)) = -\gamma(t) \cdot \vec{p}_{\vec{0}}(t) + \vec{E}(t) + \\
&+ \int_0^t dt' \; \{\gamma(t) - \gamma(t-t')\} \cdot [\cos B^{1/2}(t-t')]_{\vec{0}\vec{0}} \cdot \vec{F}(\vec{x}_{\vec{0}}(t'))
\end{aligned}
\tag{4.3}
$$

with

$$
\vec{F}(\vec{x}_{\vec{0}}) = -\frac{\partial V(\vec{x}_{\vec{0}})}{\partial \vec{x}_{\vec{0}}} \quad , \tag{4.4}
$$

the external force applied on the heavy particle, and

$$
\gamma(t) = (\frac{d}{dt} \cos B^{1/2} t)_{\vec{0}\vec{0}} \cdot (\cos B^{1/2} t)^{-1}_{\vec{0}\vec{0}} \quad . \tag{4.5}
$$

The expression for the force $\vec{E}(t)$ is analogous to (I.2.24). Here

$$
B_{\vec{j}\vec{k}} = (M_{\vec{j}} M_{\vec{k}})^{-1/2} \, \mathbf{A}_{\vec{j}\vec{k}} \; . \tag{4.6}
$$

Note that the matrix element $(\cos B^{1/2}t)_{\vec{0}\vec{0}}$ and therefore γ (t) are D-dimensional tensors.

To insure conservation of total momentum, A has to satisfy

$$\sum_{\vec{k}} A_{\vec{j}\vec{k}} = M_{\vec{j}}^{1/2} \sum_{\vec{k}} M_{\vec{k}}^{1/2} B_{\vec{j}\vec{k}} = 0. \tag{4.7}$$

Equation (I.3.9) for the covariance of the stochastic force $\vec{E}$ (t) becomes

$$< \vec{E}(t_0) \vec{E}(t_0 + t) > = -\frac{\partial^2}{\partial t^2} \rho(t) + \gamma(t_0) \cdot \rho(t) \cdot \tilde{\gamma}(t_0 + t) +$$

$$+ \gamma(t_0) \cdot \frac{\partial}{\partial t} \rho(t) - (\frac{\partial}{\partial t} \rho(t)). \tilde{\gamma}(t_0 + t) \tag{4.8}$$

with

$$\rho(t) = \beta^{-1} M (\cos B^{1/2}t)_{\vec{0}\vec{0}} , \tag{4.9}$$

and $\tilde{\gamma}$, the transpose of γ.

Equation (3.I) now becomes

$$(\cos B^{1/2}t)^{\alpha\beta}_{\vec{0}\vec{0}} = (\cos M B^{1/2}\tau)^{\alpha\beta}_{\underline{\vec{0}\vec{0}}} = \int_{-\infty}^{\infty} d\omega \cos \omega\tau S^{\alpha\beta}_{M}(\omega) . \tag{4.10}$$

Here $\tau = t/M$, and the spectrum $S^{\alpha\beta}_{M}(\omega)$ is given by

$$S^{\alpha\beta}_{M}(\omega) = \lim_{\epsilon \to 0+} \text{Im} \frac{1}{\pi M^2} (\omega + i\epsilon) R^{\alpha\beta}_{\underline{\vec{0}\vec{0}}} ((\frac{\omega + i\epsilon}{M^2})^2) \tag{4.11}$$

with

$$R(z^2) = (B - z^2 I)^{-1} . \qquad (4.12)$$

Defining

$$Q(z^2) = (A - z^2 I)^{-1}. \qquad (4.13)$$

equation (3.10) becomes

$$\lim_{M\to\infty} \frac{z}{M^2} R_{\vec{0}\vec{0}}\left(\frac{z^2}{M^2}\right) = \lim_{M\to\infty} z M^{-1} Q_{\vec{0}\vec{0}}\left(\frac{z^2}{M^2}\right) \cdot \{I - z \lim_{M\to\infty} z M^{-1} Q_{\vec{0}\vec{0}}\left(\frac{z^2}{M^2}\right)\}^{-1}$$

$$(4.14)$$

Generalizing (2.8) to D-dimensions, we now define the interaction matrix as follows

$$A^{\alpha\beta}_{\vec{j}\vec{k}} = \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi}\!\!\dots\int f_{\alpha\beta}(\vec{\theta})\, e^{i(\vec{j}-\vec{k})\cdot\vec{\theta}}\, d\vec{\theta} \qquad (4.15)$$

where $\vec{\theta}$ denotes the vector $(\theta_1,\dots,\theta_D)$. In order to insure the symmetry and reality of $A^{\alpha\beta}_{\vec{j}\vec{k}}$, $f(\vec{\theta})$ has to satisfy

$$f_{\alpha\beta}(\vec{\theta}) = f^*_{\beta\alpha}(\vec{\theta}) = f_{\beta\alpha}(-\vec{\theta}) \qquad (4.16)$$

where f^* denotes the complex conjugate of f. In other words, $f(\vec{\theta})$ is an hermitian matrix; its real part is an even function of $\vec{\theta}$, and its imaginary part is odd. Furthermore we take $f(\vec{\theta})$ to be a bounded, positive semi-definite matrix with $f(\vec{0}) = 0$.

From (4.13) and (4.15) we find, in the limit as N tends to infinity

$$Q^{\alpha\beta}_{\vec{0}\vec{0}}(z^2) = \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi}\!\!\dots\!\int d\vec{\theta}\, \{f(\vec{\theta}) - z^2 I\}^{-1}_{\alpha\beta} \quad (4.17)$$

Let $U(\vec{\theta})$ be the unitary which diagnolizes the hermitian positive definite matrix $f(\vec{\theta})$, and let $\Omega_\nu(\vec{\theta})$ be the positive eigenvalues. Then

$$f(\vec{\theta}) = U(\vec{\theta}) \cdot \Omega(\vec{\theta}) \cdot U^{-1}(\vec{\theta}) \quad (4.18)$$

where $\Omega(\vec{\theta})$ is the diagonal matrix with elements $\Omega_\nu(\vec{\theta})$. Inserting equation (4.18) into (4.17) we get

$$Q^{\alpha\beta}_{\vec{0}\vec{0}}(z^2) = \frac{1}{(2\pi)^D} \sum_{\nu=1}^{D} \int_{-\pi}^{\pi}\!\!\dots\!\int d\vec{\theta}\, U_{\alpha\nu}(\vec{\theta}) \{\Omega_\nu(\vec{\theta}) - z^2\}^{-1} U^{*}_{\beta\nu}(\vec{\theta}). \quad (4.19)$$

Now let us change variables according to

$$\begin{aligned} u_1^2 &= \Omega_\nu(\vec{\theta}) \\ u_2 &= \theta_2 \\ &\cdot \\ &\cdot \\ &\cdot \\ u_D &= \theta_D\,, \end{aligned} \quad (4.20)$$

and call $J_\nu(\vec{u})$ the Jacobian of the transformation. Equation (4.19) becomes

$$Q^{\alpha\beta}_{\vec{0}\vec{0}}(z^2) = \frac{1}{2\pi} \int_{-u_0}^{u_0} du_1\, g^{\alpha\beta}(u_1) \frac{1}{u_1^2 - z^2}\,, \quad (4.21)$$

where the spectral density matrix $g^{\alpha\beta}(u_1)$ is given by

$$g^{\alpha\beta}(u_1) = \frac{1}{(2\pi)^{D-1}} \sum_{\nu=1}^{D} \int_{-\pi}^{\pi} \ldots \int d^{D-1}u \, U'_{\alpha\nu}(\vec{u}) \, J_\nu(\vec{u}) \, U'^{*}_{\beta\nu}(\vec{u}) \, . \quad (4.22)$$

We have defined $g^{\alpha\beta}(u_1)$ to be an even function of u_1. In equation (4.21) $u_0 = \max\,(\max\, \Omega_1^{1/2}(\vec{\theta}),\ \max\, \Omega_2^{1/2}(\vec{\theta}),\ \ldots,\ \max\, \Omega_D^{1/2}(\vec{\theta})\,)$. Proceeding as we did in deriving equation (3.17), we find that

$$\lim_{M\to\infty} z\, M^{-1} Q^{\alpha\beta}_{\vec{0}\vec{0}} \left(\frac{z^2}{M^2}\right) = i\,(\gamma^{-1})^{\alpha\beta} \quad (4.23)$$

with

$$(\gamma^{-1})^{\alpha\beta} = \tfrac{1}{2}\, g^{\alpha\beta}(0). \quad (4.24)$$

From (4.14) and (4.23), we then find

$$\lim_{M\to\infty} \frac{z}{M^2} R_{\vec{0}\vec{0}} \left(\frac{z^2}{M^2}\right) = i\, \gamma^{-1} \cdot [I - iz\, \gamma^{-1}]^{-1} \, , \quad (4.25)$$

and from equations (4.10), (4.11) and (4.25),

$$\lim_{\substack{M\to\infty\ t\to\infty \\ t/M = \tau}} (\cos B^{1/2} t)_{\vec{0}\vec{0}} = \lim_{M\to\infty} (\cos M B^{1/2} \tau)_{\vec{0}\vec{0}} = e^{-\gamma|\tau|}. \quad (4.26)$$

From the properties of **A** it may be shown that $g^{\alpha\beta}(u)$ is a symmetric, positive matrix. It follows therefore from equation (4.24) that γ^{-1} is also a symmetric positive matrix and has D positive eigenvalues.

From equation (4.5) and (4.26) we find

$$\lim_{M \to \infty} M\, \gamma(\tau) = \gamma, \qquad \tau > 0, \tag{4.27}$$

so that equation (4.3) becomes asympotically the Langevin equation in D dimensions

$$\dot{\vec{p}}_{\vec{0}}(\tau) - M\vec{F}(\vec{x}_{\vec{0}}(\tau)) = -\gamma \cdot \vec{p}_{\vec{0}}(\tau) + M\vec{E}(\tau), \quad \tau > 0. \tag{4.28}$$

The covariance of the Gaussian random force $\vec{E}(\tau)$ is found by combining (4.8), (4.9), (4.26) and (4.27)

$$\lim_{M \to \infty} M < \vec{E}(\tau_0)\, \vec{E}(\tau_0 + \tau) > = 2\beta^{-1}\gamma\, \delta(\tau). \tag{4.29}$$

Thus, in this limit the heavy particle will indeed perform Brownian motion in D dimensions.

The D positive eigenvalues of γ represent the characteristic friction constants of the system. Note that we must impose the condition that these eigenvalues are finite, non vanishing quantities. Or in other words, that the matrix $\mathbf{g}(0)$ with elements $g^{\alpha\beta}(0)$ is positive definite. This last condition generalizes the condition stated in section 3 for the Brownian motion in a one-dimensional system.

For the case that the particles are placed in a simple cubic lattice we use the symmetry property that

$$T \cdot A_{T.(\vec{j}-\vec{k})} \cdot T^{-1} = A_{\vec{j}\vec{k}}, \tag{4.30}$$

where T is the matrix corresponding to a rotation of $\pi/2$ around any lattice direction, taking the equilibrium position of the heavy particle as origin. From equation (4.13) we find that the resolvent Q has to satisfy

$$T \cdot Q_{T\cdot\vec{j},\, T\cdot\vec{k}} \cdot T^{-1} = Q_{\vec{j}\vec{k}}\,, \tag{4.31}$$

and in particular the $(\vec{0},\vec{0})$ matrix element

$$T \cdot Q_{\vec{0}\vec{0}} \cdot T^{-1} = Q_{\vec{0}\vec{0}}\,, \tag{4.32}$$

which implies that $Q_{\vec{0}\vec{0}}$ is of the form

$$Q^{\alpha\beta}_{\vec{0}\vec{0}} = Q_{\vec{0}\vec{0}}\, \delta_{\alpha\beta}\,. \tag{4.33}$$

(The matrix A is also of the form $A^{\alpha\beta}_{\vec{0}\vec{0}} = A_{\vec{j}\vec{k}}\, \delta_{\alpha\beta}$, so that the Hamiltonian of the system is then the sum of D independent and equal "one degree of freedom per lattice point" Hamiltonians.)

Using equations (4.23) and (4.33) we now find that

$$(\gamma^{-1})^{\alpha\beta} = \gamma^{-1}\, \delta_{\alpha\beta}\,. \tag{4.34}$$

On the other hand we have (cf. equation (4.21))

$$g^{\alpha\beta}(u) = g(u)\, \delta_{\alpha\beta} \tag{4.35}$$

where $g(u) = 2u\, G(u^2)$; $G(u^2)$ is the spectrum of eigenvalues $\lambda = u^2$ of the matrix with elements $A_{\vec{j}\vec{k}}$.

From equations (4.24), (4.34), and (4.35) it follows that

$$\gamma = 2/g(0)\,, \tag{4.36}$$

which is equivalent to the result in the one dimensional case: the heavy particle will now perform Brownian motion in a D dimensional isotropic system (there is only one characteristic friction constant) if g(0) is a non vanishing, finite quantity. In a cubic lattice with nearest neighbours interactions this is only true for D = 1. It is however possible to find classes of matrices **A** for which $0 < g(0) < \infty$; the corresponding systems therefore exhibit the Brownian motion type behaviour for a heavy particle. In the next section we give an example of such a matrix **A**.

If on the other hand g(0) vanishes and if $\lim_{u \to 0+} u^{-n}\, g(u) = c > 0$. $(n \geq 1 + \epsilon)$, the result obtained in this case for the one dimensional system will hold (cf. the end of section 3).

5. Example of an interaction giving rise to Brownian motion in D dimensions.

As an example, consider a simple cubic lattice with

$$f(\vec{\theta}) = (1 - e^{-\nu\theta_1^2}) \prod_{\alpha=2}^{D} (1 - e^{-\nu|\theta_\alpha|})\,,\ 0 < \nu < \infty \tag{5.1}$$

In this case the Jacobian of the transformation (4.20) is given by

$$J(\vec{u}) = \frac{u_1}{\nu^{1/2}} \{ [-\ln (1-u_1^2 \prod_{\alpha=2}^{D} (1-e^{-\nu|u_\alpha|})^{-1})]^{1/2} [1-u_1^2 \prod_{\alpha=2}^{D} (1-e^{-\nu|u_\alpha|})^{-1}]$$

$$\times \prod_{\alpha=2}^{D} (1-e^{-\nu|u_\alpha|}) \}^{-1}\,, \tag{5.2}$$

and the friction constant by

$$\gamma = 2/g(0) = 2\nu^{1/2} \{\tfrac{\nu}{2}(\text{arc tg } (1-e^{-\nu\pi})^{1/2} - \pi/4)^{-1}\}^{D-1}, \qquad (5.3)$$

which is finite for any D.

The interaction matrix $A_{\vec{h}}$ ($\vec{h} \equiv \vec{j}-\vec{k}$) corresponding to (5.1) is

$$A_{\vec{h}} = \frac{1}{(2\pi)^D} \{2\pi\delta_{h_1 0} - \tfrac{1}{2}(\tfrac{\pi}{\nu})^{1/2} e^{-h_1^2/4\nu} [\phi(\nu^{1/2}(\pi - \frac{ih_1}{2\nu})) +$$

$$+ \phi(\nu^{1/2}(\pi + \frac{ih_1}{2\nu})) - \phi(-\frac{ih_1}{2\nu^{1/2}}) - \phi(\frac{ih_1}{2\nu^{1/2}})]\} \prod_{\alpha=2}^{D} \{2\pi\delta_{h_\alpha,0} -$$

$$- \frac{2\nu}{h_\alpha^2 + \nu^2} [1 - (-)^{h_\alpha} e^{-\nu\pi}]\}. \qquad (5.4)$$

Here ϕ (x) is the error integral defined by

$$\phi(x) = \frac{2}{\pi^{1/2}} \int_0^x e^{-x^2} dx \qquad (5.5)$$

$\rightarrow$ In this case the range of the "central part" of the interaction ($h=(h_1,0,\dots,0)$) is different from the range of the non central part $(0,0,\dots,h_\alpha,\dots,0)$. Examples in which these ranges do no differ, but which do nevertheless lead to Brownian motion in D dimensions may also be constructed.

6. Conclusions.

To conclude this chapter we wish to make the following remarks. It has been shown that Brownian motion may occur in an infinite assembly if the mass M of the heavy particle tends to infinity, together with the time t, in such a way that t/M remains finite. This limit is equivalent, at least for a "free" particle (i.e. if $V(x_0)\equiv 0$) to the limit proposed by Toda for the case of an assembly with nearest neighbours interactions .Indeed, Toda's limit implies that the normal mode frequencies tend to infinity as M, so that therefore the characteristic times T_k for the assembly behave as M^{-1}. Thus the ratio t/T_k tends also to infinity as M. We have achieved the same result by taking T_k constant and letting t tend to infinity as M.

We also wish to remark that the limit $t\to\infty$, $M\to\infty$, t/M finite is equivalent to the weak coupling limit taken in the derivation of e.g. the master equation by perturbation techniques[7,8]. To demonstrate this consider the Hamiltonian (I.2.7.)

$$H^{(0)} = \sum_k \tfrac{1}{2} p_k'^2 + \tfrac{1}{2} \sum_{j,k} x_k' B_{kj} x_j' . \tag{6.1}$$

Using (I.2.8.) and (I.2.2.) we may also write

$$H^{(0)} = H_0 + \lambda V , \tag{6.2}$$

with the "unperturbed Hamiltonian"

$$H_0 = \sum_k \tfrac{1}{2} p_k'^2 + \sum_{j,k\neq 0} \tfrac{1}{2} x_j' A_{jk} x_K' \tag{6.3}$$

and with the "perturbation", the interaction between the heavy particle and the heat bath, given by

$$V = x_0' \{ \sum_{j\neq 0} A_{0j} x_j' + \tfrac{1}{2} M^{-\frac{1}{2}} A_{00} x_0' \} . \tag{6.4}$$

The "coupling constant" λ in (6.2) is

$$\lambda = M^{-1/2} . \qquad (6.5)$$

Now, to compute from a Hamiltonian of the general form (6.2) any macroscopic quantity or equation in the weak coupling limit, means[7,8] to take the limit $\lambda \to 0$, $t \to \infty$, in such a way that $\lambda^2 t$ remains finite. As we see from (6.5) this is precisely the limit in which we have obtained Brownian motion of the heavy particle. Thus as, e.g. in the derivation of the master equation, the weak coupling limit corresponds to a Markoffian behaviour.

Finally we note that Rubin's result[2] for a 3-dimensional cubic lattice with nearest neighbours interactions is in agreement, if properly interpreted, with our results. In fact, in a 3-dimensional cubic lattice with nearest neighbours one has $\lim_{u \to 0+} u^{-2} g(u) = c > 0$. Thus according to our results (cf. the end of section 4 and the end of section 3, no Brownian motion is obtained for the heavy particle, which performs strongly underdamped oscillations. According to Rubin, the motion of the particle is **almost** that of a Brownian harmonic oscillator. However, inspection of his formula (see reference 2, formula (75)) shows that the apparent friction constant β is very much smaller than the frequency of oscillation of the damped oscillator ω, and their ratio β/ω tends to zero as $M^{-1/2}$. Thus in a rigorous limit, Rubin's result is in agreement with ours.

ized coupling constant" g, is (5.7)

Now, to compute from a Hamiltonian of the general form (5.1) any macroscopic quantity or equation in the weak coupling limit means to take the limit $\lambda \to 0$, $t \to \infty$, in such a way that $\lambda^2 t$ remains finite. As we saw from (5.4) this is precisely the limit in which we have obtained Brownian motion of the heavy particle. Thus as, e.g. in the derivation of the master equation, the weak coupling limit corresponds to a dissipative behavior.

Finally we note that Rubin's result[2] for a 3-dimensional cubic lattice with nearest neighbours interactions is in agreement, if properly interpreted, with our results. In fact, for a 3-dimensional cubic lattice with nearest neighbours one has $\lim_{\mu \to 0+} a^2 \varphi(0) \neq 0$, $c > 0$. Thus according to our results (cf. the end of section 4 and the end of section 2), no Brownian motion is obtained for the heavy particle, which performs strongly underdamped oscillations. According to Rubin, the motion of the particle is almost that of a Brownian harmonic oscillator. However, inspection of his formula (see reference 2, formula (25)) shows that the frictional constant β is very much smaller than the frequency of oscillation of the damped oscillator ω, and their ratio β/ω tends to zero as $M^{-1/2}$. Thus in a dynamical limit Rubin's result is in agreement with ours.

CHAPTER III.

QUANTUM MECHANICAL MOTION OF A HEAVY PARTICLE IN HARMONIC OSCILLATOR ASSEMBLIES.

1. Introduction.

In this chapter we study the quantum mechanical behaviour of an infinitely heavy particle coupled to a harmonic system.

In section 2 we obtain the "Langevin operator equation" for the heavy particle, in the presence of an arbitrary external force acting on it.

Whereas classically there were two equivalent procedures for taking the limit $M \to \infty$, quantum mechanically they are not equivalent. The difference lies in the expressions for the covariance of the stochastic operator $E(t)$.

For the initial state of the system ,we now prescribe the initial average values of the position and momentum operators of the heavy particle. The rest of the system is, as in the classical case, assumed to be initially in "thermal equilibrium with respect of the heavy particle".

In section 3 we solve explicitly the Langevin operator equation in the case that the heavy particle is acted upon by a linear force. Furthermore we discuss the dispersion of the position operator as a function of time.

In section 4 we find that the position distribution function for the heavy particle is Gaussian at any time.

2. Derivation of the Langevin operator equation.

In chapter I we found that the classical motion of the heavy particle coupled to a system of harmonic oscillators is described by the Langevin-type equation (I.2.22). In the quantum mechanical case we get an identical equation with the difference that it should be interpreted as an operator equation. Indeed, the Heisenberg form of the quantum mechanical equations of motion for the operators x_k and p_k are

$$\dot{x}_k \equiv \frac{dx_k}{dt} = \frac{1}{i\hbar} [x_k , H] \qquad (2.1)$$

and

$$\dot{p}_k \equiv \frac{dp_k}{dt} = \frac{1}{i\hbar}\,[p_k\,,\,H]\,, \tag{2.2}$$

where $[a, b]$ denotes the commutator of a and b. Here the Hamiltonian H is given by

$$H = \tfrac{1}{2}\sum_k \frac{p_k^2}{M_k} + \tfrac{1}{2}\sum_{j,k} x_j A_{jk} x_k + V(x_0)\,, \tag{2.3}$$

where $V(x_0)$ is the external potential applied to the heavy particle.
Using the fact that

$$[x_k, p_n^2] = 2i\hbar\,\delta_{kn} p_n \tag{2.4}$$

and

$$[x_j x_n\,,\,p_k] = i\hbar(x_j\,\delta_{kn} + x_n\,\delta_{kj})\,, \tag{2.5}$$

we find from (2.1), (2.2) and (2.3) that

$$\dot{x}_k = p_k/M_k \tag{2.6}$$

$$\dot{p}_k = -\sum_j A_{kj} x_j + \delta_{k0}\,F(x_0), \tag{2.7}$$

where the force operator $F(x_0)$ is defined as

$$F(x_0) \equiv \frac{1}{i\hbar}\,[p_0\,,\,V(x_0)]\,. \tag{2.8}$$

From equations (2.6) and (2.7) we can now proceed as we did in chapter I, and obtain the operator equation.

$$p_0(t) = M^{1/2} \sum_k (\cos B^{1/2}t)_{0k} M_k^{-1/2} p_k(0) - M^{1/2} \sum_k (B^{1/2}.\sin B^{1/2}t)_{0k} M_k^{1/2} x_k(0) +$$

$$+ \int_0^t dt' \, [\cos B^{1/2}(t-t')]_{00} \, F(x_0(t')) \,. \qquad (2.9)$$

From this equation we find, with the aid of (2.6)

$$\ddot{x}_0(t) + \frac{1}{M} F(x_0) = - \gamma(t) \dot{x}_0(t) + \frac{1}{M} E(t) +$$

$$+ \int_0^t dt' \{\gamma(t) - \gamma(t-t')\} \, [\cos B^{1/2}(t-t')]_{00} \, F(x_0(t')), \qquad (2.10)$$

where $\gamma(t)$ and B_{jk} are given by (I.2.23) and (I.2.8), respectively. The operator E(t) is given by

$$E(t) = M^{1/2} \sum_{k \neq 0} \{\gamma(t)(\cos B^{1/2}t)_{0k} - (B^{1/2}.\sin B^{1/2}t)_{0k}\} \, p_k(0) -$$

$$- M^{1/2} \sum_{k \neq 0} \{\gamma(t)(B^{1/2}.\sin B^{1/2}t)_{0k} + (B.\cos B^{1/2}t)_{0k}\} \, (x_k(0) - x_0(0)) \,. \qquad (2.11)$$

For the initial state of the heavy particle we cannot assign definite values to both displacement and momentum, because of the uncertainty principle. We may, however, choose a wave packet such that the initial expectation values of the displacement and momentum operators are prescribed:

$$< x_0(0) > = R \qquad (2.12)$$

$$< p_0(0) > = \lambda = MV \qquad (2.13)$$

It may be verified that the wave functi on

$$\psi(x_0) = (2\pi\sigma')^{-1/4} \exp\{ \frac{i\lambda x_0}{\hbar} - \frac{(x_0 - R)^2}{4\sigma'} \} \quad (2.14)$$

will secure the correct initial expectation values. The initial dispersions then are

$$< x_0^2(0) - < x_0(0) >^2 > = \sigma' \quad (2.15)$$

$$< p_0^2(0) - < p_0(0) >^2 > = \frac{\hbar^2}{4\sigma'} , \quad (2.16)$$

so that the wave packet has a minimum spread

$$< x_0^2(0) - < x_0(0)>^2 > < p_0^2(0) - < p_0(0)>^2 > = \frac{\hbar^2}{4} . \quad (2.17)$$

The rest of the system is assumed, as in the classical case, to be initially in "thermal equilibrium with respect to the heavy particle", i.e. we assume that at $t = 0$, the (non-stationary) density matrix, in position representation, of the whole system is given by

$$f'(x'^n, x^n) = \psi^*(x_0') \psi(x_0) c' e^{-\beta H'} \prod_{j \neq 0} \delta(x_j' - x_0' - x_j + x_0) \quad (2.18)$$

with $n = 2N + 1$,

$$H' = \sum_{k \neq 0} \tfrac{1}{2} p_k^2 + \tfrac{1}{2} \sum_{j,k \neq 0} (x_j - x_0) A_{jk} (x_k - x_0) , \quad (2.19)$$

and where c' is a normalization constant.

The brackets in (2.12), (2.13) and (2.15)-(2.17) may now also be interpreted as averages over the initial ensemble (2.18).

Let us now define, for the purpose of calculating the covariance of the operator E(t) in the initial non-stationary ensemble (2.18) (cf. also chapter I, section 3), the quantum mechanical autocorrelation function $\rho(t)$ of the heavy particle in the absence of an external force as

$$\rho(t) = \overline{\{p_0(t_0)\, ,\, p_0(t_0+t)\}}\, , \qquad (2.20)$$

where $p_0(t)$ is given by (2.9) with $F(x_0) \equiv 0$, and $\{a,b\} \equiv \frac{1}{2}(ab+ba)$. The bar denotes an average taken over the stationary ensemble described by the density matrix

$$f^{(0)}(x'^n, x^n) = c\, e^{-\beta H^{(0)}} \prod_j \delta(x'_j - x_0)\, , \qquad (2.21)$$

where

$$H^{(0)} = \frac{1}{2}\sum_k \frac{p_k^2}{M_k} + \frac{1}{2}\sum_{j,k} x_j A_{jk} x_k\, . \qquad (2.22)$$

In Appendix C we show that the covariance of the operator E(t) may be written as

$$<\{E(t_0), E(t_0+t)\}> = \overline{\{E(t_0), E(t_0+t)\}} = \frac{\partial^2}{\partial t^2}\rho(t) +$$

$$+\gamma(t_0)\,\gamma(t_0+t)\,\rho(t) + (\gamma(t_0) - \gamma(t_0+t))\frac{\partial}{\partial t}\rho(t)\, . \qquad (2.23)$$

In the classical case there are two equivalent alternatives for taking the limit $M\to\infty$. The first one is to change to a new time scale $\tau = t/M$, and the other one is to change the interaction matrix **A** to M^2**A**. However, these two approaches are not equivalent in the quantum mechanical case, as we now proceed to show.

i) Consider the first case. We change to the new time scale

$$\tau = t/M . \tag{2.24}$$

Then, as was shown in chapter II, section 3

$$(\cos B^{1/2}t)_{00} = \int_{-\infty}^{\infty} d\omega \cos \omega t \, S_1(\omega) = \int_{-\infty}^{\infty} d\omega \cos \omega \tau S_M(\omega) , \tag{2.25}$$

where $S_M(\omega)$ is given by (II.3.4).

In the limit as the number of particles tends to infinity, and as $M\to\infty$ (see formula (II.3.19)) we have

$$\lim_{M\to\infty} S_M(\omega) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + \omega^2} , \tag{2.26}$$

and therefore

$$\lim_{\substack{M\to\infty, t\to\infty \\ \tau = t/M}} (\cos B^{1/2}t)_{00} = e^{-\gamma|\tau|} . \tag{2.27}$$

Here γ is given by (II.3.20).

In Appendix B we show that the quantum mechanical momentum autocorrelation function is given by

$$\frac{1}{M} \rho(t) = \frac{\hbar}{2} \left[B^{1/2} . \coth \frac{\beta\hbar B^{1/2}}{2} . \cos B^{1/2}t\right]_{00} . \tag{2.28}$$

This may also be written as

$$\frac{1}{M} \rho(t) = \frac{\hbar}{2} \int_{-\infty}^{\infty} d\omega \, \omega \coth \frac{\beta\hbar\omega}{2} \cos \omega t \, S_1(\omega)$$

$$= \frac{\hbar}{2} \int_{-\infty}^{\infty} d\omega \, \frac{\omega}{M} \coth \frac{\beta\hbar\omega}{2M} \, \cos \omega\tau S_M(\omega)$$

$$\xrightarrow[M\to\infty]{} \frac{\gamma\beta^{-1}}{\pi} \int_{-\infty}^{\infty} d\omega \, \frac{\cos \omega\tau}{\gamma^2 + \omega^2} = \beta^{-1} e^{-\gamma|\tau|}, \tag{2.29}$$

where use has been made of (2.26). We note that (2.29) is just the classical momentum autocorrelation function.

Combining (I.2.23), (2.10), (2.27) and (2.29) we find that

$$\ddot{x}_0(\tau) + \frac{1}{M} F(x_0(\tau)) = -\gamma \dot{x}_0(\tau) + \frac{1}{M} E(\tau), \ \tau > 0 . \tag{2.30}$$

with the covariance of the operator $E(\tau)$ given by

$$\lim_{M\to\infty} \frac{1}{M} < \{E(\tau_0), E(\tau_0 + \tau)\} > = 2\beta^{-1} \gamma \, \delta(\tau), \tag{2.31}$$

as follows from (2.23), (2.27) and (2.29).

ii) If we now keep the original time scale and change the interaction matrix **A** to M^2**A**, we then find that

$$(\cos MB^{1/2} t)_{00} \xrightarrow[M\to\infty]{} e^{-\gamma|\tau|} \tag{2.32}$$

and from (2.28)

$$\frac{1}{M} \rho(t) = \frac{\hbar}{2} \, [MB^{1/2} \cdot \coth \frac{\beta\hbar MB^{1/2}}{2} \cdot \cos MB^{1/2} t]_{00}$$

$$= \frac{\hbar}{2} \int_{-\infty}^{\infty} d\omega \, \omega \coth \frac{\beta\hbar\omega}{2} \, \cos \omega t \, S_M(\omega)$$

$$\xrightarrow[M\to\omega]{} \frac{\hbar\gamma}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{\omega \coth \frac{\beta\hbar\omega}{2}}{\gamma^2+\omega^2} \cos\omega t \equiv \rho'(t). \tag{2.33}$$

Here we have used (2.26). The explicit value of $\rho'(t)$ is[13]

$$\rho'(t) = \frac{\hbar\gamma}{2}\left\{ e^{-\gamma|\tau|} \cot\pi\gamma\tau_q + \frac{2}{\pi}\sum_{n=1}^{\infty} \frac{n\, e^{-n|\tau|/\tau_q}}{n^2-(\gamma\tau_q)^2} \right\} \tag{2.34}$$

where

$$\tau_q = \frac{\beta\hbar}{2\pi} . \tag{2.35}$$

Therefore, in this case we find from (2.10), (2.23), (2.32) and (2.33) that

$$\ddot{x}_0(t) + \frac{1}{M} F(x_0(t)) = -\gamma\dot{x}_0(t) + \frac{1}{M} E(t) , \tag{2.36}$$

with the covariance of $E(t)$

$$\lim_{M\to\infty} \frac{1}{M} < \{E(t_0), E(t_0+t)\} > = -\frac{\partial^2}{\partial t^2}\rho'(t) + \gamma^2\rho'(t) . \tag{2.37}$$

We note that in the classical case we were furthermore able to show that in the initial conditional canonical ensemble, $E(t)$ is a Gaussian random process. We did not succeed, in general, in obtaining a quantum analog of this statement. We shall therefore instead first study in the next section the Langevin operator equation for the case of a linear external force, and then in section 4 discuss for this particular case the full time dependent distribution for the displacement x_0.

3. Solution of the Langevin operator equation in the case of a linear external force.

The Langevin equations (2.30) and (2.36) obtained in the preceding section, may in principle be solved for any external force $F(x_0)$. However, in practice, this is only possible, as in the classical case for linear forces:

$$\frac{1}{M} F(x_0) = \kappa x_0 \,. \tag{3.1}$$

We shall now study the two cases considered in section 2.

i) In this case equation (2.30) becomes

$$\ddot{x}_0(\tau) + \kappa x_0(\tau) = -\gamma \dot{x}_0(\tau) + \frac{1}{M} E(\tau),\ \tau > 0 \,. \tag{3.2}$$

The formal solution to this equation is

$$x_0(\tau) = e^{-\frac{1}{2}\gamma\tau} [x_0(0) \cos \nu\gamma\tau + (\frac{\dot{x}_0(0)}{\gamma} + \frac{x_0(0)}{2}) \frac{\sin \nu\gamma\tau}{\nu}] +$$

$$+ \frac{1}{\nu\gamma} \int_0^\tau d\tau' \, e^{-\frac{1}{2}\gamma(\tau-\tau')} \sin \nu\gamma(\tau-\tau') \frac{1}{M} E(\tau') \,, \tag{3.3}$$

where we have taken

$$\kappa = k\gamma^2 \tag{3.4}$$

and

$$\nu = (k - \tfrac{1}{4})^{\frac{1}{2}} \,. \tag{3.5}$$

Using (2.12) and (2.13) and the fact that the average value of $E(\tau)$ vanishes, we find that

$$\lim_{M\to\infty} \langle x_0(\tau)\rangle = e^{-\frac{1}{2}\gamma\tau}\left[R\cos\nu\gamma\tau + \left(\frac{V}{\gamma} + \tfrac{1}{2}R\right)\frac{\sin\nu\gamma\tau}{\nu}\right], \tag{3.6}$$

which is the classical value.

Using (2.15), (2.16), (3.3) and (3.6) we obtain for the dispersion

$$\langle x_0^2(\tau) - \langle x_0(\tau)\rangle^2\rangle = e^{-\gamma\tau}\left\{\sigma'\left(\cos\nu\gamma\tau + \tfrac{1}{2}\frac{\sin\nu\gamma\tau}{\nu}\right)^2 + \frac{\hbar^2}{4M^2\sigma'\gamma^2\nu^2}\sin^2\nu\gamma\tau\right\} +$$
$$+ \frac{1}{M^2\nu^2\gamma^2}\int_0^\tau d\tau'\int_0^\tau d\tau'' e^{-\frac{1}{2}\gamma(\tau'+\tau'')}\sin\nu\gamma\tau'\sin\nu\gamma\tau''\langle\{E(\tau'),E(\tau'')\}\rangle \tag{3.7}$$

Taking

$$\sigma' = M^{-1}\sigma \tag{3.8}$$

and using (2.31) we find that

$$\lim_{M\to\infty} M\langle x_0^2(\tau) - \langle x_0(\tau)\rangle^2\rangle = e^{-\gamma\tau}\left\{\sigma\left(\cos\nu\gamma\tau + \frac{\sin\nu\gamma\tau}{2\nu}\right)^2 + \frac{\hbar^2}{4\sigma\gamma^2\nu^2}\sin^2\nu\gamma\tau\right\} + \frac{\beta^{-1}}{\kappa}\left\{1 - e^{-\gamma\tau}\left(1 + \frac{1}{2\nu^2}\sin^2\nu\gamma\tau + \frac{1}{\nu}\sin\nu\gamma\tau\cos\nu\gamma\tau\right)\right\}. \tag{3.9}$$

We note that except for the first bracket in the right hand side, this result is the classical one. The first bracket is due to the fact that there is an initial uncertainty in the position and momentum of the heavy particle. For times $\tau >> 1/\gamma$, we have

$$\lim_{M\to\infty} M < x_0^2(\tau) - < x_0(\tau) >^2> = \frac{\beta^{-1}}{\kappa} , \tag{3.10}$$

which is the classical equipartition value.

ii) In this case the dispersion of $x_0(t)$ is given by

$$\lim_{M\to\infty} M< x_0^2(t) - < x_0(t)> ^2> = e^{-\gamma t} \{\sigma(\cos \nu\gamma\tau + \frac{\sin \nu\gamma t}{2\nu})^2 +$$

$$+ \frac{\hbar^2}{4\sigma \gamma^2 \nu^2} \sin^2 \nu\gamma t\} + I(t) , \tag{3.11}$$

where σ' is given by (3.8), and where

$$I(t) = \frac{1}{\nu^2 \gamma^2} \int_0^t dt' \int_0^t dt'' \, e^{-\frac{1}{2}\gamma(t'+t'')} \sin \nu\gamma t' \sin \nu\gamma t''$$

$$\times \frac{1}{M} <\{E(t') , E(t'')\} > . \tag{3.12}$$

Changing to the variables

$$\zeta = t' + t'' , \qquad \eta = t' - t'' , \tag{3.13}$$

I(t) becomes with the aid of (2.37)

$$I(t) = \frac{1}{2\nu^2\gamma^2} \left(\int_0^t d\zeta \int_0^\zeta d\eta + \int_t^{2t} d\zeta \int_0^{-\zeta+2t} d\eta \right) \sin\tfrac{1}{2}\nu\gamma(\zeta+\eta)$$

$$x \sin\tfrac{1}{2}\nu\gamma(\zeta-\eta)\, e^{-\frac{1}{2}\gamma\zeta} \left\{ -\frac{\partial^2}{\partial\eta^2}\rho'(\eta) + \gamma^2\rho'(\eta) \right\} . \qquad (3.14)$$

Performing the integrations and using (2.33) and (2.34) we find that

$$\lim_{M\to\infty} M\langle x_0^2(t) - \langle x_0(t)\rangle^2\rangle = \frac{\hbar\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega \coth\frac{\beta\hbar\omega}{2}}{(\kappa-\omega^2)^2 + \gamma^2\omega^2} -$$

$$- \frac{\hbar}{2k\gamma^2} (\cot\pi\tau_q)\, e^{-\gamma t} \left(1 + \frac{1}{2\gamma^2}\sin^2\nu\gamma t + \frac{1}{\nu}\sin\nu\gamma t\cos\nu\gamma t\right) +$$

$$+ e^{-\gamma t} \left\{ \sigma\left(\cos\nu\gamma t + \frac{\sin\nu\gamma t}{2\nu}\right)^2 + \frac{\hbar^2}{4\sigma\gamma^2\nu^2}\sin^2\nu\gamma t \right\} +$$

$$+ 0\left(e^{-t/\tau_q}\right), \quad t \geq 0 . \qquad (3.15)$$

Here τ_q, given by (2.35), is a new characteristic time which represents a quantum mechanical effect.

In the derivation of (3.15) we have taken $k = 0(1)$ and $\tau_q \ll 1/\gamma$. This situation still may correspond to very low temperatures.

We see that for $t \gg \tau_q$ the time dependence in (3.15) is essentially classical.

For times $t \gg 1/\gamma$ the dispersion (3.15) becomes

$$\sigma_{eq} = \frac{\hbar\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega \coth\frac{\beta\hbar\omega}{2}}{(k\gamma^2 - \omega^2)^2 + \gamma^2\omega^2}$$

$$= \frac{\hbar}{2\nu\gamma} \frac{\sinh(\nu\gamma\beta\hbar)}{\cosh(\nu\gamma\beta\hbar) - \cos(\tfrac{1}{2}\gamma\beta\hbar)} - \frac{\hbar\gamma}{\pi}\tau_q^2\,\zeta(3) , \qquad (3.17)$$

where ζ (z) is the Riemann function. The second equality holds if $k = 0$ (1) and $\tau_q \ll 1/\gamma$. (The exact value of the integral is computed in Appendix D).

The expression (3.17) is the quantum mechanical equipartition value for the displacement x_0.

In the classical limit ($\hbar \to 0$, or $\beta \to 0$)

$$\sigma_{eq} \to \frac{\gamma}{\beta\pi} \int_{-\infty}^{\infty} d\omega \, \frac{1}{(k\gamma^2 - \omega^2)^2 + \gamma^2\omega^2} = \frac{1}{\beta k \gamma^2} = \frac{1}{\beta\kappa} = \sigma_{eq}^{(cl)} \, . \tag{3.18}$$

Consider now the case that the heavy particle is weakly coupled to the harmonic assembly, in the sense that $\gamma \to 0$, $k \to \infty$ and $\kappa = k\gamma^2$ finite. Then $\nu\gamma \to k^{1/2}\gamma = \kappa^{1/2}$. From formula (D.11) of Appendix D we then find

$$\sigma_{eq} = \frac{\hbar}{2\kappa^{1/2}} \coth \frac{\beta\hbar\,\kappa^{1/2}}{2} \, . \tag{3.19}$$

Let us now discuss in more detail the two main results (3.17) an (3.19).

The fact that for $t \to \infty$ the quantum mechanical equipartition value (3.17) is reached (as it should be) at the same time indicates that one may not speak in this case of (a quantum mechanical) Brownian motion in the usual sense: indeed this equipartition value contains reference to the structure of the heath bath through its explicit dependence on γ. In the classical case this is not so (cf. equation (3.18)): it is in fact one of the characteristics of Brownian motion that the equipartition value is independent of the structure of the system. Of course in an extended sense one might still speak of a quantum mechanical Brownian motion even in that case, since this motion is described by a Langevin operator equation.

On the other hand the result (3.19) shows that for weak coupling ($\gamma \to 0$, $k \to \infty$, $\kappa = k\gamma^2$ finite) we may speak of a quantum mechanical Brownian motion in a customary sense: the equipartition value is now that of a single quantum oscillator and is independent of the structure of the system.

4. Quantum mechanical distribution function for the displacement of the heavy particle.

In this section we discuss the form of the quantum mechanical distribution function of $x_0(t)$ in the case that a linear force $M\kappa x_0$ is applied to the heavy particle. The Hamiltonian of the system may then be written as

$$H = \tfrac{1}{2} \sum_k \frac{p_k^2}{M_k} + \tfrac{1}{2} \sum_{j,k} x_j C_{jk} x_k , \qquad (4.1)$$

where

$$C_{jk} = A_{jk} + M\kappa\, \delta_{j0}\, \delta_{k0} . \qquad (4.2)$$

In an n-dimensional notation, the solutions corresponding to the Hamiltonian (4.1) are

$$p^n(t) = \mathbf{a} \cdot p^n(0) + \mathbf{b} \cdot x^n(0) \qquad (4.3)$$

$$x^n(t) = \mathbf{d} \cdot x^n(0) + \mathbf{c} \cdot p^n(0) , \qquad (4.4)$$

where $n \equiv 2N + 1$, p^n and x^n are n-dimensional vectors with components p_k and x_k, respectively; $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$ are nxn dimensional, time dependent matrices.

Let $f_w(x^n,p^n;t)$ be the Wigner distribution function of the system at time t. It is defined by[14]

$$f_W(x^n,p^n;t) = (\pi\hbar)^{-n} \int dy^n\, \rho(x^n + y^n, x^n - y^n;t) \exp\left(\frac{2ip^n.x^n}{\hbar}\right) \qquad (4.5)$$

where $\rho(x^n,x'^n;t)$ is the coordinate representation of the density matrix at time t, and

$$p^n \cdot x^n = \sum_k p_k x_k \, , \quad dy^n = \prod_k dy_k \, .$$

From (4.5) we obtain by inversion

$$\rho(x^n,x'^n;t) = \int dp^n f_W(\tfrac{1}{2}(x^n + x'^n),p^n;t) \exp\{-\frac{ip^n.(x^n - x'^n)}{\hbar}\}. \quad (4.6)$$

The position distribution function $\rho(x^n;t)$ is given by the diagonal part of the density matrix. From (4.6) we find that

$$\rho(x^n;t) \equiv \rho(x^n, x^n;t) = \int dp^n \, f_W(x^n,p^n;t) \, . \quad (4.7)$$

The position distribution function for the heavy particle is

$$\rho(x_0;t) = \int dx^{n-1} \rho(x^n;t) \, , \quad (4.8)$$

where the integration is performed over all the x's except x_0.

On the other hand, the Wigner distribution function at time t may be written in terms of its initial value as follows

$$f_W(x^n,p^n;t) = \int dx'^n \, dp'^n \, f_W(x'^n,p'^n;0) \, P(x'^n,p'^n | x^n,p^n;t) \quad (4.9)$$

where $P(x'^n,p'^n|x^n,p^n;t)$ is the propagator of the Wigner distribution function. For a system of harmonic oscillators, this propagator is known to be equal to the classical conditional probability density in phase space (cf. Appendix A):

$$P(x'^n,p'^n \mid x^n,p^n;t) = \delta(x^n - \mathbf{d} \cdot x'^n - \mathbf{c} \cdot p'^n)\,\delta(p^n - \mathbf{a} \cdot p'^n - \mathbf{b} \cdot x'^n), \quad (4.10)$$

where each δ-function stands for a product of n δ-functions.

Using (2.14) and (2.18) we find that the initial Wigner distribution function is Gaussian, and therefore, according to (4.10) and (4.9), $f_W(x^n,p^n;t)$ also. Thus we see from (4.7) that $\rho(x^n;t)$ is Gaussian, and finally from (4.8) that the distribution function for the position of the heavy particle is normal.

APPENDIX A

Consider a harmonic oscillator with the Hamiltonian

$$H = \tfrac{1}{2}P^2 + \tfrac{1}{2}\omega^2 Q^2 , \tag{A.1}$$

and let $\psi_\mu(Q)$ and E_μ denote the eigenfunctions and eigenvalues of H, respectively:

$$H\psi_\mu(Q) = E_\mu \psi_\mu(Q) . \tag{A.2}$$

By definition the Wigner distribution function is[14]

$$f_W(Q,P) \equiv (\pi\hbar)^{-1} \int dy\, \rho(Q + y, Q - y) \exp\left(\frac{2iPy}{\hbar}\right) \tag{A.3}$$

with the density matrix $\rho(Q',Q)$ given by

$$\rho(Q',Q) = \frac{1}{Z} \sum_{\mu=0}^{\infty} e^{-\beta E_\mu} \psi_\mu^*(Q')\, \psi_\mu(Q) \tag{A.4}$$

and

$$Z = \sum_{\mu=0}^{\infty} e^{-\beta E_\mu} . \tag{A.5}$$

Inserting in (A.4) the explicit eigenfunctions and eigenvalues of the harmonic oscillator, we find

$$\rho(Q',Q) = (\frac{\alpha}{\pi})^{1/2} \frac{1}{Z} \sum_{\mu=0}^{\infty} e^{-\beta\hbar\omega(\mu+1/2)} (\mu!\,2^{\mu})^{-1} e^{-1/2\,\alpha(Q'^2+Q^2)}$$

$$\times H_{\mu}(\alpha^{1/2}Q')\,H_{\mu}(\alpha^{1/2}Q) \,, \qquad (A.6)$$

where H_{μ} are Hermite polinomials and

$$\alpha = \omega/\hbar \,. \qquad (A.7)$$

Using the abbreviations

$$\alpha^{1/2}Q = x \,, \quad \beta\hbar\omega = \beta' \,, \qquad (A.8)$$

equation (A.6) becomes[15]

$$\rho(Q',Q) = \frac{1}{Z}(\frac{\alpha}{\pi})^{1/2} e^{-(x'^2+x^2)/2} \sum_{\mu=0}^{\infty} (\mu!\,2^{\mu})^{-1} e^{-\beta'(\mu+1/2)} H_{\mu}(x)H_{\mu}(x')$$

$$= \frac{1}{Z}\,(\frac{\alpha}{2\pi\sinh\beta'})^{1/2}\ \exp\{-1/4(x+x')^2 \operatorname{tgh}\frac{\beta'}{2}\ -$$

$$-1/4\,(x-x')^2\ \coth\frac{\beta'}{2}\}\,, \qquad (A.9)$$

or

$$\rho(Q',Q) = \frac{1}{Z}\,(\frac{\omega}{2\pi\hbar\sinh\beta\hbar\omega})^{1/2}\ \exp\{-1/4\frac{\omega}{\hbar}\,(Q+Q')^2 \operatorname{tgh}\frac{\beta\hbar\omega}{2}\ -$$

$$-1/4\frac{\omega}{\hbar}\,(Q-Q')^2\ \coth\frac{\beta\hbar\omega}{2}\ \}\,. \qquad (A.10)$$

Inserting (A.10) into (A.3) and performing the integration, we obtain for the Wigner distribution function

$$f_W(Q,P) = (\pi\hbar \coth\frac{\beta\hbar\omega}{2})^{-1} \exp\{-\frac{1}{\hbar\omega} \,\mathrm{tgh}\, \frac{\beta\hbar\omega}{2} (P^2 + \omega^2 Q^2)\} \quad (A.11)$$

where we have used the fact that

$$Z = (2 \sinh \frac{\beta\hbar\omega}{2})^{-1} . \quad (A.12)$$

For the propagator of the Wigner distribution function $P(Q',P'|Q,P;t)$ we have the following expression (cf. ref. 16, eq. 2 – 35)

$$P(Q',P'|Q,P;t) = \frac{2}{\pi\hbar} \iint e^{-2iP'Y'/\hbar} K(Q'+Y'|Q+Y;t)$$

$$K(Q'-Y'|Q-Y;t)\, e^{+2iPY/\hbar} dY\, dY' \quad (A.13)$$

where $K(Q'|Q;t)$ is the propagator of the wave function, given by

$$K(Q'|Q;t) = \sum_{\mu=0}^{\infty} e^{-iE_\mu t/\hbar} \psi^*_\mu(Q')\, \psi_\mu(Q) . \quad (A.14)$$

Comparing (A.4) and (A.14) we find that

$$K(Q'|Q;t) = [Z(\beta)\, \rho(Q',Q;\beta)]_{\beta=it/\hbar} , \quad (A.15)$$

and therefore, from (A.9) and (A.12) we get

$$K(Q'|Q;t) = \left(\frac{\omega}{2i\pi\hbar \sin\omega t}\right)^{1/2} \exp\left\{-\frac{i}{4}\frac{\omega}{\hbar}(Q+Q')^2 \, \mathrm{tg}\,\frac{\omega t}{2} + \right.$$

$$\left. + \frac{i}{4}\frac{\omega}{\hbar}(Q-Q')^2 \cot\frac{\omega t}{2}\right\}. \qquad (A.16)$$

Inserting (A.16) into (A.13) we find that the propagator of the Wigner distribution function is

$$P(Q',P'|Q,P;t) = \delta(Q - Q'\cos\omega t - \frac{P'}{\omega}\sin\omega t)\,\delta(P - P'\cos\omega t + Q'\omega\sin\omega t).$$

$$(A.17)$$

We note that this is just the classical propagator in phase space.

For a system of n independent harmonic oscillators, and without symmetrization of the wave function, the Wigner distribution function and its propagator are just the product of the Wigner distribution function and its propagator of each harmonic oscillator, respectively.

APPENDIX B

We compute the quantum mechanical momentum autocorrelation function $\rho(t)$:

$$\rho(t) = \mathrm{Tr}\,\{p_0(t_0)\,,\,p_0(t_0+t)\}\,f^{(0)}\,, \tag{B.1}$$

where

$$f^{(0)} = \frac{1}{Z}\,e^{-\beta H^{(0)}} \tag{B.2}$$

with

$$H^{(0)} = \sum_j \tfrac{1}{2}\,\frac{p_j^2}{M_j} + \tfrac{1}{2}\sum_{j,k} x_j\,A_{jk}\,x_k \tag{B.3}$$

and

$$Z = \mathrm{Tr}\,f^{(0)}\,. \tag{B.4}$$

Let us perform the transformation

$$p_k' = M_k^{-\frac{1}{2}}\,p_k\,,\qquad x_k' = M_k^{\frac{1}{2}}\,x_k\,. \tag{B.5}$$

Then (B.1) and (B.3) become

$$\rho(t) = M\,\mathrm{Tr}\,\{p_0'(t_0)\,,\,p_0'(t_0+t)\}\,f^{(0)} \tag{B.6}$$

and

$$H^{(0)} = \tfrac{1}{2} \sum_j p_j'^2 + \tfrac{1}{2} \sum_{j,k} x_j' B_{jk} x_k' , \tag{B.7}$$

respectively. Here

$$B_{jk} = (M_j M_k)^{-\frac{1}{2}} A_{jk} . \tag{B.8}$$

Now, we change to normal coordinates,

$$p_k' = \sum_\alpha U_{k\alpha} P_\alpha , \qquad x_k' = \sum_\alpha U_{k\alpha} Q_\alpha . \tag{B.9}$$

Therefore we have,

$$\rho(t) = M \sum_{\alpha\nu} U_{0\nu} U_{0\alpha} \mathrm{Tr}\{P_\nu(t_0), P_\alpha(t_0+t)\} f^{(0)} \tag{B.10}$$

with

$$H^{(0)} = \tfrac{1}{2} \sum_\alpha P_\alpha^2 + \tfrac{1}{2} \sum_\alpha \omega_\alpha^2 Q_\alpha^2 \tag{B.11}$$

and

$$\omega_\alpha^2 \delta_{\alpha\nu} = \sum_{jk} U_{\alpha j} B_{jk} U_{k\nu} . \tag{B.12}$$

It may be shown[17] that the autocorrelation function can be written as

$$\mathrm{Tr}\{P_\nu(t_0), P_\alpha(t_0+t)\}f^{(0)} = \iint P'_\nu P''_\alpha f_W(Q'^n,P'^n;t_0;Q''^n,P''^n;t_0+t)$$

$$dQ'^n dP'^n dQ''^n dP''^n$$

$$= \iint P'_\nu P''_\alpha f_W(Q'^n,P'^n;t_0) \cos\{\frac{\hbar}{2}(\frac{6}{6Q'^n}\cdot\frac{\partial}{\partial P'^n} - \frac{6}{6P'^n}\cdot\frac{\partial}{\partial Q'^n})\}$$

$$P(Q'^n,P'^n|Q''^n,P''^n;t)\, dQ'^n dP'^n dQ''^n dP''^n \,. \qquad (B.13)$$

Here $f_W(Q'^n,P'^n;t_0;Q''^n,P''^n;t_0+t)$, $f_W(Q'^n,P'^n;t_0)$, $P(Q'^n,P'^n \mid Q''^n,P''^n;t)$ are the joint Wigner distribution function, the Wigner distribution function and its propagator, respectively. The 6-symbol denotes differentiation "to the left", We now integrate (B.13) by parts, and recall the fact (cf. the end of Appendix A) that for the Hamiltonian (B.11), the Wigner distribution function and its propagator are products of single Wigner distribution functions and its propagator, respectively. Using (A.11) and (A.17) we find that

$$\mathrm{Tr}\{P_\nu(t_0)\,,\,P_\alpha(t_0+t)\}f^{(0)} = \delta_{\nu\alpha}\frac{\hbar}{2}\,\omega_\nu \coth\frac{\beta\hbar\omega_\nu}{2}\cos\omega_\nu t\,. \qquad (B.14)$$

Inserting (B.14) into (B.10), and using (B.12) we obtain that

$$\rho(t) = M\sum_\nu U_{0\nu}\,\frac{\hbar}{2}\,\omega_\nu \coth\frac{\beta\hbar\omega_\nu}{2}\,\cos\omega_\nu t\, U_{0\nu}$$

$$= M\frac{\hbar}{2}\,[B^{1/2}\cdot\coth\frac{\beta\hbar B^{1/2}}{2}\cdot\cos B^{1/2}t]_{00}\,. \qquad (B.15)$$

APPENDIX C

Consider

$$H^{(0)} = \sum_{k=0} \frac{p_k^2}{2M_k} + \tfrac{1}{2} \sum_{j,k\neq 0} (x_j - x_0)\, A_{jk} (x_k - x_0)$$

$$= \frac{p_0^2}{2M} + \sum_{k\neq 0} \tfrac{1}{2}\, p_k^2 + \tfrac{1}{2} \sum_{j,k\neq 0} (x_j - x_0)\; A_{jk}\; (x_k - x_0)$$

$$\equiv \frac{p_0^2}{2M} + H' \; . \tag{C.1}$$

Transforming to coordinates

$$p_k = \sum_{\alpha\neq 0} U_{k\alpha} P_\alpha$$

$$k \neq 0 \tag{C.2}$$

$$x_k - x_0 = \sum_{\alpha\neq 0} U_{k\alpha} Q_\alpha$$

where $U_{k\alpha}$ is an element of the orthogonal matrix which diagnolizes the matrix with elements A_{jk} ($j,k \neq 0$). (The $U_{k\alpha}$ introduced here should not be confused with the $U_{k\alpha}$ of Appendix B, which diagonalizes the complete matrix A_{jk}). The Hamiltonian (C.1) then becomes

$$H^{(0)} = \frac{p_0^2}{2M} + \sum_{\alpha\neq 0} \tfrac{1}{2}(P_\alpha^2 + \omega_\alpha^2\, Q_\alpha^2)\;, \tag{C.3}$$

where

$$\omega_\alpha^2\, \delta_{\alpha\beta} = \sum_{j,k\neq 0} U_{\alpha j} A_{jk} U_{k\beta}\, . \tag{C.4}$$

It should be noted that these ω_α's are not the normal modes of the whole system. Indeed, the $Q_\alpha (\alpha \neq 0)$ are functions of x_0.

Calling

$$Q_0 \equiv x_0 \ , \ P_0^2 \equiv \frac{p_0^2}{M} \ , \ \omega_0 \equiv 0 \ , \tag{C.5}$$

we may write (C.3) as follows

$$H^{(0)} = \sum_{\alpha \neq 0} \tfrac{1}{2}(P_\alpha^2 + \omega_\alpha^2 Q_\alpha^2) \ , \tag{C.6}$$

The canonical Wigner distribution function corresponding to the Hamiltonian (C.6) is

$$f_W^{(H^{(0)})} = \frac{1}{Z} \prod_\alpha \exp\{-\frac{1}{\hbar\omega_\alpha} \operatorname{tgh} \frac{\beta\hbar\omega_\alpha}{2} (P_\alpha^2 + \omega_\alpha^2 Q_\alpha^2)\}$$

$$= \frac{1}{Z_0} e^{-\beta P_0^2/2} \frac{1}{Z'} \prod_{\alpha \neq 0} \exp\{-\frac{1}{\hbar\omega_\alpha} \operatorname{tgh} \frac{\beta\hbar\omega_\alpha}{2} (P_\alpha^2 + \omega_\alpha^2 Q_\alpha^2)\}$$

$$= \frac{1}{Z_0} e^{-\beta p_0^2/2M} f_W^{(H')} \ , \tag{C.7}$$

where $f_W^{(H')}$ is the canonical Wigner distribution function corresponding to the Hamiltonian H'. Here Z, Z_0 and Z' are normalization constants.

Let g be a function dependent on p^{n-1}, $x^{n-1}-x_0$, where the excluded coordinates are p_0 and x_0. Consider

$$\bar{g} = \int f_W{}^{(H^{(0)})} \, g \, dp^n \, dx^n$$

$$= \int dp^{n-1} \, d(x^{n-1}-x_0) \, g(p^{n-1}, x^{n-1}-x_0) \, f_W^{(H')} \frac{1}{Z_0} \int dp_0 \, dx_0 \, e^{-\beta p_0^2/2M}$$

$$= \int dp^{n-1} \, d(x^{n-1}-x_0) \, g(p^{n-1}, x^{n-1}-x_0) \, f_W^{(H')}$$

$$= \int dp^n \, d(x^{n-1}-x_0) \, dx_0 \, g(p^{n-1}, x^{n-1}-x_0) \, f_W^{(H')} \, f_W(x_0,p_0) \tag{C.8}$$

where

$$f_W(x_0,p_0) = (\pi\hbar)^{-1} \int dy \, \psi^*(x_0 + y)\psi(x_0 - y) \exp\left(\frac{2ip_0 y}{\hbar}\right) \tag{C.9}$$

with $\psi(x_0)$ given by (III.2.14).

Since $f_W^{(H')} \, f_W(x_0,p_0)$ is the Wigner distribution function corresponding to the initial ensemble (III.2.18), equation (C.8) implies that

$$\bar{g} = \langle g \rangle \, . \tag{C.10}$$

In computing the covariance of E(t), we may therefore calculate it as an average over the stationary canonical ensemble described by (III.2.21). We can proceed as in the classical case to derive equation (III.2.23) (cf. chapter I, section 3).

APPENDIX D

Consider the integral

$$I = \int_{-\infty}^{\infty} d\omega \, \frac{\omega \coth u\,\omega \cos\omega\, t}{\omega^4 + 2a^2\,\omega^2\cos 2\theta + a^4} = \tfrac{1}{2}\int_{-\infty}^{\infty} d\omega \, \frac{\omega \coth u\,\omega}{\omega^4 + 2a^2\omega^2\cos 2\theta + a^4}$$

$$x\,(e^{i\omega t} + e^{-i\omega t}) \equiv \tfrac{1}{2}(I_+ + I_-)\,, \qquad \text{(D.1)}$$

with $t \geq 0$, and $0 < \theta < \pi/2$.

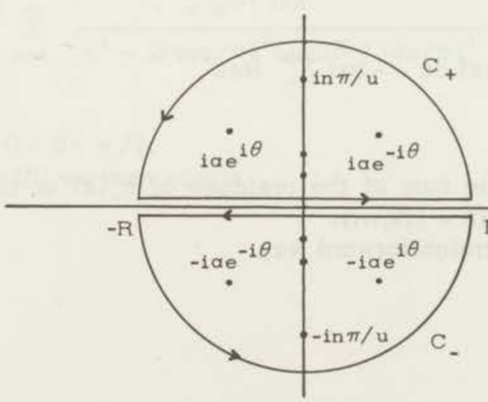
The integrals I_+ and I_- represent integrations along the entire length of the real axis, of the functions

$$h_{\pm}(z) = \frac{z \coth uz}{z^4 + 2a^2 z^2 \cos 2\theta + a^4}\, e^{\pm izt}\,, \qquad \text{(D.2)}$$

respectively.

The functions $h_{\pm}(z)$ have simple poles at the points

$$z = \pm\, iae^{\mp i\theta}\,,\; z = \pm\, in\pi/u,\; (n = 1,2,\ldots)$$



Let C_+ denote the upper half of the circle $|z| = R$, where $R > a$. Integrating the function $h_+(z)$ counterclockwise around the boundary of the semicircular region, we have

$$\int_{-R}^{R} h_+(z)\, dz + \int_{C_+} h_+(z)\, dz = 2\pi i \; \Sigma_+^R \,\text{Res}, \tag{D.3}$$

where Σ_+^R Res is the sum of the residues of $h_+(z)$ at the poles $z = iae^{\pm i\theta}$, $in\pi/u$ $(n = 1,2,\ldots, \frac{n\pi}{u} < R)$.

It may be shown that

$$\lim_{R\to\infty} \int_{C_+} h_+(z)\, dz = 0, \text{ for } t \geq 0. \tag{D.4}$$

Therefore

$$I_+ = \int_{-\infty}^{\infty} h_+(z)\, dz = 2\pi i \; \Sigma_+^\infty \,\text{Res} . \tag{D.5}$$

Analogously

$$I_- = \int_{-\infty}^{\infty} h_-(z)\, dz = -2\pi i \; \Sigma_-^\infty \,\text{Res} , \tag{D.6}$$

where Σ_-^∞ Res is the sum of the residues of $h_-(z)$ at the poles $z = -iae^{\pm i\theta}$, $z = -in\pi/u$ $(n = 1,2,\ldots)$.

We obtain in a straightforward way

$$\text{Res } h_+(z)\ (\text{at } z = i\alpha e^{-i\theta}) = -\text{Res } h_-(z)\ (\text{at } z = -i\alpha e^{-i\theta})$$

$$= (4i \sin 2\theta)^{-1} e^{-\alpha t e^{-i\theta}} \coth(i\alpha u e^{-i\theta}) \tag{D.7}$$

$$\text{Res } h_+(z)\ (\text{at } z = i\alpha e^{i\theta}) = -\text{Res } h_-(z)\ (\text{at } z = -i\alpha e^{i\theta})$$

$$= -(4i \sin 2\theta)^{-1} e^{-\alpha t e^{i\theta}} \coth(i\alpha u e^{i\theta}) \tag{D.8}$$

$$\text{Res } h_+(z)\ (\text{at } z = i|n|\pi/u) = -\text{Res } h_-(z)\ (\text{at } z = -i|n|\pi/u)$$

$$= \frac{i}{u^2} \frac{n\pi e^{-n\pi t/u}}{(n\pi)^4 - 2(\alpha u n\pi)^2 \cos 2\theta + (\alpha u)^4} \tag{D.9}$$

Combining (D.1), (D.5) - (D.9) we find that

$$I = \frac{\pi e^{-\alpha t\cos\theta}}{\alpha^2 \sin 2\theta} \frac{\sin(2\alpha u\cos\theta)\sin(\alpha t\sin\theta) + \sinh(2\alpha u\sin\theta)\cos(\alpha t\sin\theta)}{\cosh(2\alpha u\sin\theta) - \cos(2\alpha u\cos\theta)}$$

$$- 2\left(\frac{u}{\pi}\right)^2 \sum_{n=1}^{\infty} \frac{n e^{-n\pi t/u}}{n^4 - 2(\alpha u n/\pi)^2 \cos 2\theta + (\alpha u/\pi)^4}, \tag{D.10}$$

with $t \geq 0$, $0 < \theta < \pi/2$.

From (D.10) we then obtain

$$\int_{-\infty}^{\infty} d\omega \frac{\omega \coth \tfrac{1}{2}\beta\hbar\omega}{(k\gamma^2 - \omega^2)^2 + \gamma^2\omega^2} = \frac{\pi}{\gamma^2\nu} \frac{\sinh(\gamma\nu\beta\hbar)}{\cosh(\gamma\nu\beta\hbar) - \cos(\tfrac{1}{2}\gamma\beta\hbar)} -$$

$$-2\left(\frac{\beta\hbar}{2\pi}\right)^2 \sum_{m=1}^{\infty} \frac{m}{m^4 - m^2(\beta\hbar\gamma/2\pi)^2(1-2k) + k^2(\beta\hbar\gamma/2\pi)^4} \quad \text{(D.11)}$$

For the case that $\beta\hbar\,\gamma/2\pi \ll 1$ and $k = 0(1)$, the sum in (D.11) reduces to

$$\sum_{m=1}^{\infty} \frac{1}{m^3} = \zeta(3) = 1.202\ldots \quad \text{(D.12)}$$

where $\zeta(z)$ is the Riemann function.

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SAMENVATTING

Het ontwikkelen van een statistisch mechanisch model voor de Brownse beweging vormt het onderwerp van verschillende recente onderzoekingen.

Hemmer, Rubin en Turner hebben de beweging onderzocht van een zwaar deeltje in een systeem bestaande uit gekoppelde harmonische oscillatoren met naaste buren-wisselwerking. Zij hebben laten zien dat in een één-dimensionaal systeem een zwaar deeltje zich min of meer als een vrij Browns deeltje gedraagt als de massa van het zware deeltje maar groot genoeg is. Toda en Takeno en Hori merkten op dat zuivere Brownse beweging slechts verkregen wordt na een dubbele limietovergang waarbij zowel de massa M van het zware deeltje als de koppelingsconstante α, die de naaste buren-wisselwerking karakteriseert, oneindig groot worden, en wel op zodanige wijze dat de verhouding α/M^2 eindig blijft.

Anderzijds hebben Kac, Mazur en Ford laten zien dat in een systeem, geheel en al bestaande uit deeltjes van gelijke massa, een willekeurig deeltje zich al Browns deeltje zal gedragen in het "warmtebad" dat gevormd wordt door de overige deeltjes, als de harmonische wisselwerkingskrachten van een zeer speciale vorm zijn (lange dracht). Voor een systeem van gelijke deeltjes kan men zuivere Brownse beweging nl. alleen afleiden m.b.v. een limietovergang waarbij een "cut-off"frequentie", die het frequentiespectrum van de normaaltrillingen begrenst, oneindig groot wordt. Voorts bleek de beweging van een deeltje dat een uitwendige kracht ondergaat in deze limiet over te gaan in die van een Browns deeltje in hetzelfde uitwendige krachtveld.

Bovengenoemde resultaten hebben steeds betrekking op systemen bestaande uit oneindig veel deeltjes.

In dit proefschrift wordt de beweging onderzocht van een deeltje in een systeem bestaande uit harmonische oscillatoren, waarbij meer in het bijzonder de voorwaarden worden afgeleid waaronder dat deeltje zich als een Browns deeltje gedraagt.

In hoofdstuk I wordt een formele oplossing gegeven van de bewegingsvergelijkingen voor een bepaald deeltje dat een uitwendige kracht ondergaat. M.b.v. deze oplossing worden de bewegingsvergelijkingen zo geschreven dat zij een structurele analogie met de Langevin-vergelijking vertonen.

Tevens wordt, m.b.v. de statistische mechanica, het gedrag van het deeltje onderzocht in een initiëel conditioneel kanoniek ensemble dat de random-verdeling van de overige deeltjes beschrijft (warmtebad).

In hoofdstuk II wordt eerst het model van Kac, Mazur en Ford besproken, Vervolgens wcrdt de beweging van één bepaald deeltje onderzocht in het geval dat de massa M van dat deeltje oneindig groot wordt, waarbij de voorwaarden worden afgeleid waaronder het zich als een Browns deeltje gedraagt. Wanneer men de massa M en de tijd t oneindig groot laat worden, op zodanige wijze dat de verhouding $\tau = t/M$ eindig blijft, verkrijgt men Brownse beweging, mits de wisselwerking aan een zeer algemene voorwaarde voldoet, die geen speciale beperkingen oplegt aan de gedetailleerde vorm van de wisselwerking: de spectrale dichtheid $G(\omega^2)$ van eigenwaarden ω van de wisselwerkingsmatrix dient evenredig te zijn met ω^{-1} voor $\omega \to 0$.

Ook het geval dat de spectrale dichtheid niet aan bovengenoemde voorwaarde voldoet wordt nader onderzocht.

In hoofdstuk III wordt een quantum mechanische analyse van het gedrag van een oneindig zwaar deeltje gegeven.

Terwijl klassiek de limiet $M \to \infty$ op twee equivalente manieren genomen kan worden, zoals bewezen wordt in hoofdstuk II, leiden deze twee procedures quantum mechanisch tot verschillende resultaten. Wel vindt men in beide gevallen voor het zware deeltje (dat de invloed van een willekeurig uitwendig krachtveld ondergaat) een "Langevin operator-vergelijking", maar deze twee vergelijkingen verschillen onderling in de quantum mechanische autocorrelatiefunctie van de "random kracht-operator". De oplossing van de Langevin operator-vergelijking wordt onderzocht voor het geval dat de op het zware deeltje werkende uitwendige kracht lineair is.

Tenslotte wordt de vorm bepaald van de plaats-distributiefunctie van het zware deeltje op een willekeurige tijd.

E Braun/Cuitler

STELLINGEN

I

Rubin's statement that a heavy particle in a 3-dimensional cubic lattice with nearest neighbours harmonic forces performs harmonic Brownian motion is questionable.

R.R.Rubin, J.Math.Phys. *2* (1961)
Chapter II of this thesis.

II

A particle initially described by a Gaussian wave function and coupled to an assembly of oscillators initially in thermal equilibrium, will have a Gaussian position distribution function at any time.

Chapter III of this thesis.

III

In deriving classical Brownian motion of a particle mass $M \to \infty$, coupled to a harmonic assembly, there are two equivalent procedures for taking this limit: changing to a new time scale $\tau = t/M$ or enhancing the interaction matrix **A** to M^2**A**. These two alternatives are not equivalent in the quantum mechanical case.

Chapter III of this thesis.

IV

The quantum mechanical momentum autocorrelation function of an infinitely heavy particle, coupled to a harmonic assembly, becomes the classical function for the case $\tau_q \ll t \ll \tau_r$, where τ_q and τ_r are a quantum mechanical characteristic time and the relaxation time, respectively.

V

Contrary to their statement, Maradudin and Wallis do not compute the true dielectric susceptibility. However this quantity may be obtained from their result.

A.A. Maradudin and R.F.Wallis, Phys.Rev. *123*, (1961), 777

VI

The mean phonon lifetime in a one-dimensional anharmonic lattice with nearest neighbours interaction, to the lowest order approximation in the anharmonic force constant, is independent of the wave number.

A.A. Maradudin and A.E. Fein. Westinghouse Research Laboratories Scientific Paper 62-129-103 P.(1962) (Pittsburgh, Pensylvania)

VII

In order to verify the Onsager symmetry relations beyond reasonable doubt, both the Soret and Dufour effects in dense media should be measured.

VIII

For large values of Störmer's constant γ, Störmer's inner allowed zone shrinks into the corresponding characteristic line of force of the magnetic dipole.

C.Störmer, Polar Aurora (Oxford University Press, 1955)

IX

The latitudes of the mirror points in a dipole field for values of γ larger than 2.5, as obtained from the differential equations of motion agree with those obtained by the approximation of constant magnetic moment.

H.C. Alfvén and C. Fälthammer, Cosmical Electrodynamics (Oxford University Press, 1963).

X

The only geographic coordinates of two geomagnetic equivalent points in the dipole model which changed appreciably in the period 1845-1955, due to secular variation are the radius and the longitude.

XI

Messiah's derivation of the fact that the quantum number l, related to the eigenvalues of the orbital angular momentum operator $l(l+1)$ is an integer, is not satisfactory.

A. Messiah, Quantum Mechanics (North-Holland Publ. Co. Amsterdam, 1962)