Irreversibility of Systems Perturbed by Random Forces*

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The irreversibility of quantum mechanical systems perturbed by random forces is investigated by means of phenomonological equations derived from the Schrödinger equation. A semiquantitative discussion depending on an assumption of time reversal symmetry of the ensemble of random functions leads to a description of the irreversibility of a system with a finite number of states. A more general quantitative method utilizing "smoothed" density matrices produces a macroscopic description of systems tending to equilibrium states.

I. INTRODUCTION

ONE of the basic problems of statistical mechanics is to account for the irreversibility observed in physical systems. The investigation of this problem has proceeded by means of H theorems, ergodic theorems, and the derivation of differential equations describing the time change of the state probabilities.[1] From the assumption of such an equation Thomsen[2] has derived the relations between the ergodic hypothesis, the principle of detailed balance and the so-called λ hypothesis for systems with a finite number of states. More recently Jaynes[3] has generalized the work of Wangness and Bloch[4] to obtain a phenomenological description based on an assumption that the best criterion to use in statistical inference is that of maximum information.

These results may be obtained otherwise by an assumption that the quantum mechanical system in question is perturbed by small random forces, and certain additional assumptions characterizing the ensemble of random functions. In order to account for continuous measurements a smoothed density matrix is introduced. In Sec. II a semiquantitative approach yields a result of wide generality, while in Sec. III the assumption of "sliding averages" produces a result useful in describing continuous measurements.

II. RANDOM PERTURBATIONS

It is assumed: (i) That the system is acted on by a random external force which varies unpredictably to the extent that the probability of its being equal to any given function in the future is the same, no matter what function described it in the past. (ii) It is further assumed that the probability that the force is given by some particular function of time is equal to the probability that it is given by the function obtained from this one by reversal in respect to time.

The external force acting on the system will be assumed to act through a parameter of the system, designated by a. The system is described by a state function $\Psi=\sum_n c_n u_n(q,a)$ where the u_n are real energy eigenfunctions and the c_n are probability amplitudes, and q represents all the coordinates of the system. The c_n as functions of time are given by[5]

$$\dot{c}_m=-i\omega_m c_m+\dot{a}\sum_r \alpha_{mr}c_r, \tag{1}$$

where

$$\alpha_{ji}=\int u_i(q,a)\frac{\partial u_j(q,a)}{\partial a}dq, \tag{2}$$

and $\omega_m=E_m/\hbar$. It follows immediately that $\alpha_{ij}=-\alpha_{ji}$. If we assume a solution of the form

$$c_m(t)=\sum_s A_{ms}c_s(0), \tag{3}$$

it may be shown that the quantities A_{ms} obey a differential equation of the form Eq. (1) and that the matrix A is unitary.

If the random parameter a is not given as a particular function of time, but instead it is given only that a is equal to one of a number of given functions, each of which has a given probability of being a from the instant 0 to the instant t, then the prediction of a particular value of $c_p c_q^*$ at the instant t is impossible. The expectation value or ensemble average, however, is given by

$$\langle c_p(t)c_q^*(t)\rangle=\sum_m\sum_n\langle A_{pm}A_{qn}^*\rangle c_m(0)c_n^*(0). \tag{4}$$

Let it now be assumed that a varies unpredictably to the extent that the probability of its being equal to any given function in the future is the same, no matter what function described it in the past.

On this assumption, $\langle A_{pm}A_{qn}^*\rangle$ does not depend on the variation in a before the instant 0 or, consequently, on the amplitudes produced at that instant by the prior variation. Therefore, if only average initial values of $c_m c_n^*$ are given, $\langle A_{pm}A_{qn}^*\rangle$ will be the same for all

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the particular values of $c_m(0)c_n^*(0)$ included in the average $\langle c_m(0)c_n^*(0)\rangle$. Thus

$$\langle c_p(t)c_q^*(t)\rangle=\sum_m\sum_n\langle A_{pm}A_{qn}^*\rangle\langle c_m(0)c_n^*(0)\rangle. \quad (5)$$

If $\langle c_m(0)c_n^*(0)\rangle=\delta_{mn}/W$, where W is the number of possible states of the system, it follows from Eq. (5) and the properties of A_{ij} that

$$\langle c_p(t)c_q^*(t)\rangle=\delta_{pq}/W, \quad (6)$$

and there is statistical equilibrium, with all possible states equally probable. If a is constant,

$$c_p(t)=c_p(0)e^{i\omega_p t}. \quad (7)$$

If a, though not constant, is changing slowly, the magnitudes of the probability amplitudes will change only slowly and, during any time in which the changes in magnitude are negligible, the approximation

$$c_p(t)=c_p(0)\exp(i\bar{\omega}_p t), \quad (8)$$

in which $\bar{\omega}_p$ denotes the time average of ω_p, will be valid. Thus, during any such time

$$c_p(t)c_q^*(t)=c_p(0)c_q^*(0)\exp[i(\bar{\omega}_p-\bar{\omega}_q)t]. \quad (9)$$

Corresponding to the different functions of the time to which a may be equal, there will be different values of $\bar{\omega}_p-\bar{\omega}_q$ for any unequal numbers p and q. However small may be the spread in the values of $(\bar{\omega}_p-\bar{\omega}_q)$, the values of $(\bar{\omega}_p-\bar{\omega}_q)t$ may be spread as widely as desired by decreasing da and thus increasing the time t in which any given variation in a takes place. If the spread of extreme values of $(\bar{\omega}_p-\bar{\omega}_q)t$ is made many times π, the distribution becomes practically uniform between 0 and 2π. With a uniform distribution in phase, $\langle\exp[i(\bar{\omega}_p-\bar{\omega}_q)t]\rangle$ and hence $\langle c_p(t)c_q^*(t)\rangle$ are zero for any two unequal numbers p and q.

Let it be supposed that this has taken place before the instant 0. Then $\langle c_m(0)c_n^*(0)\rangle$ is 0 for all unequal numbers m and n and

$$\langle c_p(t)c_p^*(t)\rangle=\sum_m\langle A_{pm}A_{pm}^*\rangle\langle c_m(0)c_m^*(0)\rangle. \quad (10)$$

Now $\langle c_pc_p^*\rangle$ is the probability of finding the system in the state p. Let it be denoted by f_p. $\langle A_{pm}A_{pm}^*\rangle$ is a function of t. Let it be denoted by $B_{pm}(t)$. Then

$$f_p(t)=\sum_m B_{pm}(t)f_m(0), \quad (11)$$

where since $\sum_r A_{mr}A_{nr}^*=\delta_{mn}=\sum_r A_{rm}A_{rn}^*$,

$$\sum_m B_{pm}(t)=\sum_m B_{mp}(t). \quad (12)$$

Differentiating these equations with respect to t and letting t be zero, we have

$$\dot{f}_p(0)=\sum_m \dot{B}_{pm}(0)f_m(0), \quad (13)$$

$$\sum_m \dot{B}_{pm}(0)=\sum_m \dot{B}_{mp}(0), \quad (14)$$

The first of these equations shows that $\dot{B}_{pm}(0)dt$ is the probability of the transition in the time dt from the state m to the state p, when it is given that the system is initially in the state m. To the extent that transitions are probable only between states of equal energy, the second equation is what Thomsen[2] has called the λ hypothesis, which, he has shown, implies the ergodic theorem and the second law of thermodynamics but not the principle of detailed balance or Onsager's reciprocities. Whether or not transitions are restricted to states of equal energy, these equations, derived from assumption (i) alone, are enough to show that random changes in an external coordinate can only increase the entropy of a system.

We may now show that under assumptions (i) and (ii) the system under consideration will exhibit microscopic reversibility.[2] Let us now make use of assumption (ii), that the probability that a is given by some particular function of the time is equal to the probability that it is given by the function obtained from this one by reversal in respect to the time. Thus, the graphs shown as I and II in Fig. 1 are equally probable as expressions for a.

To any point P' on Graph I, at the interval τ after the instant 0, there corresponds a point P'' on Graph II, at the same interval τ before the instant t, such that a has the same value at P'' as at P'. If Q' is a point on Graph I following the point P' at the interval $d\tau$, there is a corresponding point Q'' on Graph II, preceding the point P'' by the same interval $d\tau$, at which a has the same value as at Q'.

Let Eq. (1) and its complex conjugate equation be written in the form

$$dc_m=-i\omega_m c_m dt+\sum_n \alpha_{mn}c_n da, \quad (15)$$

$$dc_m^*=i\omega_m c_m^* dt+\sum_n \alpha_{mn}c_n^* da. \quad (16)$$

At the point P'' on Graph II, ω_m and α_{mn}, which are functions only of a, have the same values as at P'. Also a increases by the same amount da between P'' and Q'' as between P' and Q'. But, from P' to Q', dt has the value $d\tau$, whereas, from P'' to Q'', it has the value $-d\tau$. Thus, if we write the preceding equations for these points on Graphs I and II, distinguishing by superscripts $(')$ and $('')$ the probability-amplitudes reckoned for the two graphs, we have:

$$\begin{aligned} dc_m'&=-i\omega_m c_m' d\tau+\sum_n \alpha_{mn}c_n' da,\\ dc_m''&=i\omega_m c_m'' d\tau+\sum_n \alpha_{mn}c_n'' da, \end{aligned} \quad (17)$$

$$\begin{aligned} dc_m'^*&=i\omega_m c_m'^* d\tau+\sum_n \alpha_{mn}c_n'^* da,\\ dc_m''^*&=-i\omega_m c_m''^* d\tau+\sum_n \alpha_{mn}c_n''^* da. \end{aligned} \quad (18)$$

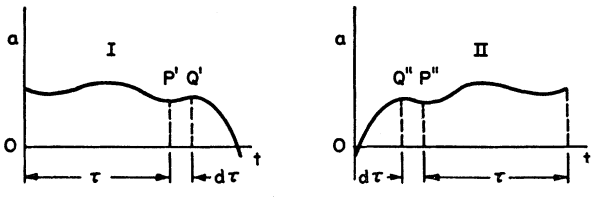

FIG. 1. $a=a(t)$ and its time-reversed graph.

Comparing these equations, we see that the probability-amplitudes reckoned for either graph vary with τ according to the equation which describes the complex conjugate amplitudes along the other graph. On Graph I, τ is 0 at the instant 0 and t at the instant t but, on Graph II, it is 0 at the instant t and t at the instant 0. Thus, if we write for Graph I,

$$c_m'(t)=\sum_n A_{mn}'c_n'(0), \tag{19}$$

we have for Graph II

$$c_m''(0)=\sum_n A_{mn}'^{*}c_n''(t). \tag{20}$$

But we have also for Graph II, from Eq. (17),

$$c_m''(0)=\sum_n c_n''(t)A_{nm}''^{*}. \tag{21}$$

Thus, we see that

$$A_{nm}''^{*}=A_{mn}'^{*}. \tag{22}$$

Similarly,

$$A_{nm}''=A_{mn}'. \tag{23}$$

Here let us choose the initial amplitudes the same on both graphs. We may write for Graph I

$$c_p'(t)c_q'^{*}(t)=\sum_m\sum_n A_{pm}'A_{qn}'^{*}c_m(0)c_n^{*}(0) \tag{24}$$

or

$$c_p'(t)c_q'^{*}(t)=\sum_m\sum_n A_{mp}''A_{nq}''^{*}c_m(0)c_n^{*}(0). \tag{25}$$

Adding the corresponding members of these two equations and dividing by 2, we obtain

$$c_p'(t)c_q'^{*}(t)=\tfrac{1}{2}\sum_m\sum_n(A_{pm}'A_{qn}'^{*}+A_{mp}''A_{nq}''^{*})c_m(0)c_n^{*}(0). \tag{26}$$

An exchange of superscripts gives

$$c_p''(t)c_q''^{*}(t)=\tfrac{1}{2}\sum_m\sum_n(A_{pm}''A_{qn}''^{*}+A_{mp}'A_{nq}'^{*})c_m(0)c_n^{*}(0). \tag{27}$$

Again adding corresponding members and dividing by 2, we obtain

$$\tfrac{1}{2}[c_p'(t)c_q'^{*}(t)+c_p''(t)c_q''^{*}(t)]=\tfrac{1}{2}\sum_m\sum_n[\tfrac{1}{2}(A_{pm}''A_{qn}'^{*}+A_{pm}''A_{qn}''^{*})+\tfrac{1}{2}(A_{mp}'A_{nq}'^{*}+A_{mp}''A_{nq}''^{*})]c_m(0)c_n^{*}(0). \tag{28}$$

The left-hand member of this equation is simply the average of the two values of $c_p(t)c_q^{*}(t)$ characteristic of Graphs I and II. Similarly, $\frac{1}{2}(A_{pm}'A_{qn}'^{*}+A_{pm}''A_{qn}''^{*})$ is the average of the two values of $A_{pm}A_{qn}^{*}$, and $\frac{1}{2}(A_{mp}'A_{nq}'^{*}+A_{mp}''A_{nq}''^{*})$ is the average of the two values of $A_{mp}A_{nq}^{*}$. The average may be extended over all pairs of equally probable graphs of a to give

$$\langle c_p(t)c_q^{*}(t)\rangle=\tfrac{1}{2}\sum_m\sum_n\langle A_{pm}A_{qn}^{*}+A_{mp}A_{nq}^{*}\rangle c_m(0)c_n^{*}(0). \tag{29}$$

If zero time is any instant after the amplitudes have become uniformly distributed in phase, this equation gives, in analogy with Eq. (11)

$$f_p(t)=\tfrac{1}{2}\sum_m[B_{pm}(t)+B_{mp}(t)]f_m(0). \tag{30}$$

where, as before,

$$B_{pm}=\langle A_{pm}A_{pm}^{*}\rangle. \tag{31}$$

Therefore, the probability of transition in the time dt from a state initially given as m to the state p is $[\dot{B}_{pm}(0)+\dot{B}_{mp}(0)]dt$. Microscopic reversibility follows from the symmetry of this expression with respect to p and m, and Onsager's reciprocities and the principle of detailed balance follow from microscopic reversibility.

III. RANDOM PARAMETERS AND SLIDING AVERAGES

In this section we discuss the irreversibility of quantum systems in so far as they may be described by the assumption that they are acted on by a random perturbation which affects some parameter or several parameters of the system. For instance, we might think of a harmonic oscillator whose spring constant is affected by random perturbations. A macroscopic example would be a weight hanging on a spring which is not at absolute zero temperature and hence has small heat fluctuations affecting its stiffness. Another example would be an atom affected by a small radiation field, random in character, incoherent in nature; another example is a particle enclosed in a potential well whose "walls" undergo small random changes in height or location. We wish to examine the effect of such perturbations on the density matrix describing ensembles of such systems and hence to deduce the average behavior of systems as a function of time.

It is necessary to consider the ensemble of systems which will be considered in this section as the appropriate one to describe a system undergoing random perturbations. The density matrix is defined in terms of an average over an ensemble of systems in order to represent the incomplete knowledge usually obtained in determining the initial state of a large system. The ensemble must contain every possible system consistent with our measurements of the initial state of a system. It is necessary to enlarge the ensemble when additional uncertainties are added, as in the situation considered here where the systems are under the influence of random perturbations. We assume that each system with a set of initial conditions can be acted on by each member of the set of possible random functions. Thus, our ensemble consists of all possible sets of initial conditions paired with all possible random perturbing functions. We will be concerned with averages over initial conditions, averages over the ensemble of random functions and time averages over both density matrices and unitary transformations.

It is clear that the equations of motion for the density matrix, whose solution can be written $\rho(t)=U\rho(0)U^{-1}$, cannot exhibit irreversibility, as a consequence of group property of the transformation on $\rho(0)$. The instantaneous value of the density matrix depends on the instantaneous value of $U(t)$ and cannot in general exhibit a trend toward equilibrium.

However, since we find in general that systems tend toward equilibrium, we must employ reasoning outside quantum mechanics to explain this situation. The methods of doing this are many and various.[1] The aim of many of these methods is to produce a differential equation for the state probabilities which can yield solutions which are asymptotic to constants, or which show a tendency for the ensemble to "relax" to an equilibrium situation. Such treatments have been more successful in predicting the outcome of experiments, for example, nuclear induction experiments, than would seem warranted by the results achieved under some very far-reaching assumptions. We will show in this section that the results can be obtained on the basis of some simpler assumptions.

An essential element in our discussion will be the concept of the sliding average. In many treatments of this problem, an essential step is to average over high-frequency contributions to the derivative of the density matrix so as to obtain the slower "secular" variation. We will consider that our measuring apparatus is such that it performs an averaging of the form

$$\frac{1}{2T}\int_{t-T}^{t+T} f(t')dt'. \tag{32}$$

This is the time domain analog of the finite slit width of a spectroscope. This average is applicable to those cases where the measurement is a continuous process, and an unavoidable smoothing occurs.

Specifically we will consider the sliding average of the density matrix

$$[\rho(t)]_{Av}{}^{T}=\frac{1}{2T}\int_{t-T}^{t+T}\rho(t')dt'. \tag{33}$$

We see that

$$\frac{d[\rho(t)]_{Av}{}^{T}}{dt}=\frac{\rho(t+T)-\rho(t-T)}{2T}. \tag{34}$$

We will compute the right side of this equation and thus obtain an expression for the "smoothed" density matrix.

One further essential averaging must be performed, however. This is the averaging over all possible random perturbing forces. It is assumed that a maximal quantum mechanical observation has been made on the system at time $t=0$, and that at the time $t-\tau>0$, we wish to predict the results of a measurement. During the time $t-\tau$ the random perturbations have been acting on the system and we must average over their possible effects. Thus the quantity

$$\left\langle\frac{d[\rho(t)]_{Av}{}^{T}}{dt}\right\rangle=\frac{d\hat{\rho}}{dt} \tag{35}$$

will be computed. It will be the "effective" density matrix, to be used in the computation of the expected value of any observable Q according to the formula $E(Q)=\mathrm{tr}(Q\hat{\rho})$.

It will be necessary to approximate $\rho(t+T)$ by means of the Picard method. Briefly, if $\dot{\rho}=F[t,\rho(t)]$, the method is to obtain the successive approximations:

$$\begin{aligned}&\rho_1(t)=\rho(0)+\int_0^t F(t',\rho(0))dt'\\ &\cdot\\ &\cdot\\ &\rho_n(t)=\rho(0)+\int_0^t F(t',\rho_{n-1}(t'))dt'\\ &\cdot\\ &\cdot\end{aligned} \tag{36}$$

We will adapt this method to the solution of the equation

$$\dot{\rho}=-i[B(t),\rho(t)], \tag{37}$$

where the square brackets indicate the commutator of B and ρ and B is a Hermitian matrix. We use a lower limit of $t-T$ rather than zero, in order to obtain an expression for the derivative of our "smoothed" density matrix, $d\hat{\rho}/dt$. The quantity $\hbar$ has been incorporated into B.

Thus, using the approximation through second order we obtain

$$\begin{aligned}\frac{\rho(t+T)-\rho(t-T)}{2T}&=-\frac{i}{2T}\int_{t-T}^{t+T}[B(t'),\rho(t-T)]dt'\\ &+\frac{1}{2T}\int_{t-T}^{t+T}\int_{t-T}^{t'}[B(t'),[B(t''),\rho(t-T)]]dt'dt''.\end{aligned} \tag{38}$$

We assume that a measurement has been made at $t=0$, where $t-T>0$, and a density matrix $\rho(0)$ obtained. Our measuring apparatus is assumed to perform a continuous observation with a smoothing time of $2T$, and we wish to find the change with time of the smoothed density matrix. We may compute $\rho(t-T)$ in the form $U(t-T)\rho(0)U^{-1}(t-T)$, thus

$$\begin{aligned}&\frac{\rho(t+T)-\rho(t-T)}{2T}\\ &=\frac{-i}{2T}\int_{t-T}^{t+T}[B(t'),U(t-T)\rho(0)U^{-1}(t-T)]dt'\\ &+\frac{1}{2T}\int_{t-T}^{t+T}\int_{t-T}^{t'}[B(t'),[B(t''),\\ &\qquad U(t-T)\rho(0)U^{-1}(t-T)]]dt'dt''.\end{aligned} \tag{39}$$

No special assumptions are made on the initial density matrix $\rho(0)$. It is not necessarily diagonal. We assume

however that $U(t)$ is a member of an ensemble of transformations consisting of the possible transformations occurring with a random parameter. We now average Eq. (39) over this ensemble, obtaining [see Eq. (36)]

$$\frac{d\hat{\rho}(t)}{dt}=-\frac{i}{2T}\int_{t-T}^{t+T}[B(t'),\langle\rho(t-T)\rangle]dt'$$
$$+\frac{1}{2T}\int_{t-T}^{t+T}\int_{t-T}^{t'}[B(t'),[B(t''),\langle\rho(t-T)\rangle]]dt'dt''. \quad (40)$$

The ensemble average is extended over the set of random perturbations up to the time $(t-T)$, hence it may be interchanged with the integration, and does not apply to the matrices B. We now assume that $\langle\rho(t-T)\rangle$ is diagonal, due to action of the random perturbations occurring in the time interval $(0, t-T)$, and write

$$\frac{d\hat{\rho}(t)}{dt}=-\frac{i}{2T}\int_{t-T}^{t+T}[B(t'),\rho_d]dt'$$
$$+\frac{1}{2T}\int_{t-T}^{t+T}\int_{t-T}^{t'}[B(t'),[B(t'')dt'dt'',\rho_d]]dt'dt''. \quad (41)$$

Assuming that the time average $(1/2T)\int_{t-T}^{t+T}B(t')dt'$ is negligible and writing ρ in place of $\hat{\rho}$ we have for the diagonal elements

$$\dot{\rho}_{kk}=\sum_\alpha \rho_{kk}(1/2T)\int\int B_{k\alpha}(t')B_{\alpha k}(t'')dt'dt''$$
$$-\sum_\alpha \rho_{\alpha\alpha}(1/2T)\int\int B_{k\alpha}(t')B_{\alpha k}(t'')dt'dt''$$
$$-\sum_\alpha \rho_{\alpha\alpha}(1/2T)\int\int B_{k\alpha}(t'')B_{\alpha k}(t')dt'dt''$$
$$+\sum_\alpha \rho_{kk}(1/2T)\int\int B_{k\alpha}(t'')B_{\alpha k}(t')dt'dt'', \quad (42)$$

where the omitted limits are the same as in Eq. (41). By defining

$$\Omega_{k\alpha}(t)=(1/2T)\int\int[B_{k\alpha}(t')B_{\alpha k}(t'')$$
$$+B_{k\alpha}(t'')B_{\alpha k}(t')]dt'dt'' \quad (43)$$

we may write Eq. (42) as

$$\dot{\rho}_{kk}=\sum_\alpha \Omega_{k\alpha}(t)(\rho_{kk}-\rho_{\alpha\alpha}), \quad (44)$$

where $\Omega(t)$ is only slowly varying, and may be considered constant if T is sufficiently long.

We must now investigate the characteristics of the coefficients Ω. Recalling that B is Hermitian, we see that $\Omega_{\alpha k}=\Omega_{k\alpha}$ and that $\Omega_{\alpha k}{}^*=\Omega_{\alpha k}$, i.e., Ω is a real symmetric matrix. Thus, also Thomsen's λ hypothesis[2]

$$\sum_\alpha \Omega_{\alpha k}=\sum_\alpha \Omega_{k\alpha}, \quad (45)$$

is always satisfied in this approximation. Furthermore, we may verify that $\sum_k \dot{\rho}_{kk}=0$, by observing that

$$\sum_k \rho_{kk}\sum_\beta \Omega_{k\beta}=\sum_\beta \rho_{\beta\beta}\sum_k \Omega_{k\beta}$$

which follows immediately upon changing $\Omega_{k\beta}$ to $\Omega_{\beta k}$ and reversing dummy indices on the right side.

IV. CONCLUSIONS

It has been shown that under the assumption that the system is affected by small random perturbing forces, it was possible to obtain, in Sec. II, the equations which are normally used as a description of irreversible phenomena. There two additional assumptions were introduced which characterized the ensemble of random perturbations.

In order to obtain a result of wider applicability, the assumption of sliding averages was introduced in Sec. III and there the differential equation describing the "smoothed" density matrix was obtained. It is concluded that a macroscopic description of irreversible systems may be based on the assumption of small random perturbing forces, and that continuous measurements are described by the "smoothed" density matrix.

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