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THE ERGODIC BEHAVIOUR OF QUANTUM MANY-BODY SYSTEMS

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Synopsis

By a pertubation technique adapted to the actual properties of gases and solids (and possibly also of liquids) we have established in previous papers that under suitable conditions a quantum many-body system approaches statistical equilibrium as far as those physical quantities are concerned which are diagonal in the unperturbed representation. This result is now extended to non-diagonal quantities of a type broad enough to include all observables of actual interest. A general discussion of the resulting ergodic theorem is given, and its implications for classical statistics are briefly analyzed. The paper ends with a discussion of a recent article by Ingraham on the application of our methods to the case of a very small perturbation. The main arguments of Ingraham are shown to be in error, and the inconsistencies he derives from them are thereby disproved.

1. *Introduction.* The approach of a quantum many-body system to statistical equilibrium has been studied in two previous papers [1]), to be referred to hereafter as S and S', on the basis of a separation of the hamiltonian H' into a main term H describing non-interacting plane wave excitations (like phonons or Bloch electrons in solids, free particles in gases) and a perturbation λV representing their mutual interaction. Using as basic representation the eigenstates $|\alpha>$ of H, each of which describes a set of plane wave excitations, we founded our treatment on the recognition that the matrix elements to be calculated according to perturbation theory exhibit remarkable diagonal singularities, *i.e.* singularities of the form $\delta(\alpha - \alpha')$. A systematic analysis of these singularities made it possible to study the time evolution of certain physical quantities A under the assumption of incoherent phases for the amplitudes $c(\alpha)$ of the initial state φ_0 of the system *)

$$\varphi_0 = \int |\alpha> d\alpha c(\alpha). \tag{1.1}$$

Under proper conditions it could be established that in the course of time the expectation value of A, which is (we put $\hbar = 1$)

$$\langle A \rangle_t = \langle \varphi_0 | U_{-t} A U_t | \varphi_0 \rangle, \quad U_t = \exp[-i(H + \lambda V)t], \tag{1.2}$$

*) A detailed definition of our notation is found in S'.

tends to the equilibrium value $\langle A\rangle_{eq}$ calculated on the basis of microcanonical ensemble theory. This was established for operators A diagonal in the $|\alpha\rangle$-representation, in the case of very small perturbation in S and for finite λV, *i.e.* to general order in the dimensionless parameter λ, in S'.

Our present aim is to extend the general order treatment of S' to a wide class of non-diagonal operators B **). This class is composed of the non-diagonal operators B given by a convergent series, each term of which is a product of creation and destruction operators for individual plane wave excitations. We assume the number of creation and destruction operators in each term of the series to be finite and independent of the large number N of particles in the system. In contrast to the diagonal operators A, the class of operators B just defined is broad enough to contain all quantities of practical interest. Since we will again be able to establish that the expectation value

$$\langle B\rangle_t = \langle\varphi_0|U_{-t}BU_t|\varphi_0\rangle \tag{1.3}$$

tends to the microcanonical equilibrium value $\langle B\rangle_{eq}$ we will have established, for all practical purposes, the ergodic behaviour of our system, using only the properties of the hamiltonian postulated in S' (sections 2 and 7) and the incoherent phase assumption for the initial state (1.1).

The rather broad scope of this result makes it desirable to discuss its significance, also in relation to classical statistics. Whereas the derivation of our main result

$$\langle B\rangle_t \to \langle B\rangle_{eq} \text{ for } t \to \pm\infty \tag{1.4}$$

is presented in the next section, section 3 will be devoted to this general discussion. Section 2 will make free use of the formal technique developed and applied in S'. Although the author is fully aware of the complication of this technique, he believes that the scope of the results may justify at least partially the involved nature of the mathematical methods. Section 3 gives a nontechnical discussion which can be largely followed without knowledge of the detailed formalism of section 2 and S'. Section 4 presents a refutation of a critical discussion of S recently published by Ingraham.

2. *Approach to equilibrium for non-diagonal operators.* For any operator B of the type described above and for any set of diagonal operators $A_1, \ldots, A_n$ the matrix element

$$\langle\alpha|VA_1VA_2V\ldots A_\nu BA_{\nu+1}V\ldots A_nV|\alpha'\rangle \tag{2.1}$$

can have a $\delta(\alpha - \alpha')$-singularity for the same reasons and with the same properties as was the case for the matrix elements $\langle\alpha|VA_1V\ldots A_nV|\alpha'\rangle$

**) As in S and S' the adjectives diagonal and non-diagonal will always refer to the $|\alpha\rangle$-representation.

considered in S' (see S', section 2). The discussion of this singularity requires that (2.1) be written out as a sum over intermediate states α_j. In addition to having one V replaced by B this sum may differ from the sum (S'.2.6) *) by the fact that additional intermediate states may have to be introduced in between various factors of a single term of B. This would for example be the case if $B = V_1V_2$, V_1 and V_2 being individual terms in the expansion of V in products of creation and destruction operators. In this particular case one would obviously insert an additional intermediate state between V_1 and V_2. All considerations presented in S' (section 2) can be repeated for this slightly more general case, however, and we can define in addition the concept of *B-irreducible diagonal part*. It is the diagonal part, *i.e.* the $\delta(\alpha - \alpha')$-singular part, of (2.1) which is obtained when in the calculation of (2.1) one leaves out the diagonal part of each subproduct of the following type

$$\left.\begin{array}{l} VA_jV\ldots A_kV,\ (1 \leq j \leq k < \nu \text{ or } \nu + 1 < j \leq k \leq n), \\ VA_jV\ldots A_\nu BA_{\nu+1}V\ldots A_kV,\ (1 \leq j \leq \nu < k \leq n,\ k - j < n-1, \\ VA_jV\ldots A_\nu B,\ (1 \leq j \leq \nu),\quad BA_{\nu+1}V\ldots A_kV,\ (\nu + 1 \leq k \leq n). \end{array}\right\} \quad (2.2)$$

We denote by $\{VA_1V\ldots A_\nu BA_{\nu+1}V\ldots A_nV\}_{Bd}$ the diagonal operator defined by the B-irreducible diagonal part of (2.1). This concept may differ from the irreducible diagonal part defined in S' because of the possible occurrence of additional intermediate states inside B (these states are allowed to become equal to each other, to other intermediate states, to α or to α', and the corresponding subproducts, in contrast to the subproducts (2.2), may therefore contribute their diagonal part). The new concept can be extended in an obvious way to products of the type

$$BA_1V\ldots A_nV,\quad VA_1\ldots VA_nB. \quad (2.3)$$

Its importance will appear presently.

In analogy to our analysis in S', which made essential use of the quantity $X_{ll'}(\alpha\alpha')$ defined by (S'.4.14), we must consider the quantity $Y_{ll'}(\alpha)$ defined by

$$\{R_lBR_{l'}\}_d|\alpha> = |\alpha>Y_{ll'}(\alpha) \quad (2.4)$$

where R_l is the resolvent (S'.4.1). Reduction of diagonal parts, using (S'.4.4) and our definition of B-irreducible diagonal part, readily gives

$$\{R_lBR_{l'}\}_d = \{R_lB_{ll'}R_{l'}\}_d \quad (2.5)$$

with

$$B_{ll'} = \{(1 - \lambda VD_l + \lambda^2VD_lVD_l\ldots)B(1 - \lambda D_{l'}V + \lambda^2D_{l'}VD_{l'}V\ldots)\}_{Bd} \quad (2.6)$$

Hence, using (S'.4.14),

$$Y_{ll'}(\alpha) = \int B_{ll'}(\alpha')d\alpha'\dot{X}_{ll'}(\alpha'\alpha) \quad (2.7)$$

where $B_{ll'}(\alpha')$ is the eigenvalue of the diagonal operator $B_{ll'}$ for the state α'.

*) This symbol refers to Eq. (2.6) of S'

In analogy to (S'.4.13) we have

$$U_{-t}BU_t = -(2\pi)^{-2}\int_\gamma dl \int_\gamma dl' \exp[i(l-l')t]R_lBR_{l'} \tag{2.8}$$

where the contour γ in the complex plane encircles an interval of the real axis sufficiently large to include the whole energy spectrum of the system and is described counterclockwise. Calculating the expectation value of (2.8) for the initial state φ_0, and using the incoherent phase assumption for the amplitudes $c(\alpha)$ of φ_0 one obtains

$$\langle B\rangle_t = -(2\pi)^{-2}\int_\gamma dl \int_\gamma dl' \exp[i(l-l')t]Y_{ll'}(\alpha)d\alpha|c(\alpha)|^2. \tag{2.9}$$

The long time limit of this quantity is found by repeating for $Y_{ll'}$ the discussion carried our for $X_{ll'}$ in section 6 of S'. No new difficulty occurs in this discussion because the quantity $B_{ll'}(\alpha')$ by virtue of its definition remains finite and has only finite discontinuities for l and l' crossing the real axis. According to (2.7) the pseudopoles of $Y_{E+l,E-l}$ therefore coincide with those of $X_{E+l,E-l}$. In analogy with (S'.6.18) one finds for the limit of (2.9) as $t \to \pm\infty$

$$\langle B\rangle_{\pm\infty} = \pi^{-1}\int_{-\infty}^{\infty} dE \int \lim_{0<\eta\to 0}\{\eta Y_{E\mp i\eta,E\pm i\eta}(\alpha)\}d\alpha|c(\alpha)|^2. \tag{2.10}$$

We go back to (2.7) and remember that $B_{ll'}$ remains finite when l and l' approach the real axis. This gives

$$\lim \eta\ Y_{E\mp i\eta,E\pm i\eta}(\alpha) = \int B_{E\mp i0,E\pm i0}(\alpha')d\alpha' \lim \eta X_{E\mp i\eta,E\pm i\eta}(\alpha'\alpha). \tag{2.11}$$

The limit on the righthand side has been calculated in section 7 of S', with the result (see (S'.7.9) and (S'.7.17) and the third equation thereafter)

$$\pi^{-1}\lim \eta X_{E\pm i\eta,E\mp i\eta}(\alpha'\alpha) = \Delta_E(\alpha')\Delta_E(\alpha)[\int \Delta_E(\alpha'')d\alpha'']^{-1}. \tag{2.12}$$

We obtain by substitution

$$\langle B\rangle_{\pm\infty} = \int_{-\infty}^{\infty} \langle B\rangle_E p_E dE. \tag{2.13}$$

$p_E dE$, defined by (S'.7.22), is the probability that the total energy $H+\lambda V$ be included between E and $E+dE$ for the system in its initial state φ_0, under the incoherent phase assumption. The quantity $\langle B\rangle_E$ is defined by

$$\langle B\rangle_E = [\int \Delta_E(\alpha'')d\alpha'']^{-1}\int B_{E\mp i0,E\pm i0}(\alpha')d\alpha'\Delta_E(\alpha'). \tag{2.14}$$

As will now be shown, it is equal to the microcanonical average of B on the energy shell $H+\lambda V = E$ and its value is independent of the double sign appearing in the definition.

The microcanonical average of B is

$$Sp(BQ_E)/Sp(Q_E), \tag{2.15}$$

Q_E being the projection operator on the energy shell $H+\lambda V = E$. One has

$$Q_E = \delta(H+\lambda V - E) = (2\pi i)^{-1}\lim_{0<\eta\to 0}(R_{E+i\eta} - R_{E-i\eta}).$$

But the resolvent verifies

$$R_{E+i\eta} - R_{E-i\eta} = 2i\eta R_{E+i\eta} R_{E-i\eta},$$

a relation which enables us to write

$$Sp(BQ_E) = \pi^{-1} \lim \eta Sp(R_{E\mp i\eta} B R_{E\pm i\eta}) = \pi^{-1} \int d\alpha \lim \eta Y_{E\mp i\eta, E\pm i\eta}(\alpha).$$

Here we have calculated the trace in the $|\alpha>$-representation. The limit under the integral sign has been found in (2.11) and (2.12). It gives

$$Sp(BQ_E) = \int B_{E\mp i0, E\pm i0}(\alpha') d\alpha' \Delta_E(\alpha'). \tag{2.16}$$

If one now remembers that $Sp(Q_E)$ is $\int \Delta_E(\alpha'') d\alpha''$ as remarked in S', one reaches the announced identity of (2.14) and (2.15) for either value of the double sign appearing in the former expression. Returning to (2.13) we see that the long time limit of $\langle B \rangle_t$ agrees with the equilibrium value

$$\langle B \rangle_{eq} = \int \langle B \rangle_E p_E dE \tag{2.17}$$

of the quantity B as deduced from microcanonical ensemble theory. The ergodic behaviour of our system is thereby established for all observable quantities B of the type described in section 1 and for initial states with incoherent phases. It may be noted that the main difference between the derivation just given and the treatment of diagonal quantities A in S and S' lies in the replacement of A by the diagonal operator $B_{ll'}$.

3. *Discussion.* We have been able to establish that under specified conditions an isolated many-body system approaches microcanonical equilibrium. This has been achieved in the quantum description and we have made essential use of very special properties of the system in this description. In the first place, our analysis is entirely based on the existence of a special orthonormal set of states α, composed of plane wave excitations. In this special representation the total hamiltonian is assumed to split into a diagonal part H and an off-diagonal part λV, and matrix elements of the form (2.1) are supposed to exhibit diagonal singularities with very definite properties. Secondly, we establish the approach to microcanonical equilibrium in a slightly unusual way. What we do is to study physical quantities represented by operators O with definite properties in the α-representation, and establish that their expectation value $\langle O \rangle_t$ tends in the course of time toward the equilibrium average value $\langle O \rangle_{eq}$ calculated from microcanonical theory. Finally our analysis follows the time evolution of the system for $t \to \pm \infty$ beginning with an initial state $\varphi_0 = \int |\alpha> d\alpha c(\alpha)$. We show that $\langle O \rangle_t$ splits into two terms, one depending on the $|c(\alpha)|^2$ only, and the second depending on the relative phases of $c(\alpha)$ for different α's. We simply leave out the phase-dependent term on the ground that it will vanish for all times of practical interest if the initial amplitudes $c(\alpha)$ have incoherent phases.

Our result $\langle O\rangle_t \to \langle O\rangle_{eq}$ is established for the phase-independent part of $\langle O\rangle_t$. This result, being truly non-trivial and involving quite subtle properties of the diagonal singularities mentioned above, seems to us in itself to give additional support to the soundness of the incoherent phase assumption.

Obviously the systems we study are quite special, we use a special representation in expressing their properties and we discuss the approach to equilibrium for special operators O. All these special features, however, are realized in the most common physical examples of ergodic systems, solids, gases and liquids (although for the latter the large size of λV may make our treatment more doubtful). We feel therefore confident that despite its apparent lack of generality our method is quite well adapted to the difficult problem of establishing ergodicity for realistic systems. In fact it is only by complete exploitation of the special conditions assumed that we have been able to study our system in so much greater detail than is the case in the conventional investigations of the ergodic problem *) and to actually carry out a true proof of ergodic behaviour.

Although quantum-mechanical in nature, our analysis applies also to the physical situations one usually calls classical, i.e. when the values of all observable quantities of interest depend on Planck's constant only through negligibly small corrections. For such situations it is important to translate our results into the language of classical theory. The main point in this translation is that the state of the system at any time, although a single quantum state $\varphi_t = U_t\varphi_0$, must be described classically by an ensemble of points in $6N$-dimensional phase space (N being the number of particles). This cannot be otherwise, because the quantum-mechanical wave function corresponding to a single point in classical phase space is a very special type of wave packet and cannot possess the incoherent phases we require φ_t to have for $t = 0$ in our analysis **). This correspondence between single quantum states and classical ensembles leads to certain consequences which we now want to describe.

According to our theory, for sufficiently large times t the expectation value $\langle O\rangle_t$ of a physical quantity O becomes equal to the equilibrium value $\langle O\rangle_{eq}$. This holds equally well for the quantity O^2,

$$\langle O^2\rangle_t = \langle O^2\rangle_{eq} \text{ for large } t.$$

In general, of course, $\langle O^2\rangle_{eq}$ and $\langle O\rangle_{eq}^2$ are different, so that for large t the quantities $\langle O^2\rangle_t$ and $\langle O\rangle_t^2$ will be both constant in time and have different values, a fact which makes it quite clear that the classical analogue to the

*) The unsatisfactory nature of Von Neumann's approach [2]) to the quantum ergodic problem has now been clearly revealed [3]). It stems from the fact that Von Neumann's form of ergodic property actually imposes no restriction at all on the dynamical system.

**) Starting from a different standpoint [4]) Van Kampen has been led some time ago to take the same view concerning the relation between classical and quantum statistics [5]).

single quantum state φ_t of our system has to be an ensemble. If now measurements of O are made on one and the same system at various times, the measured values q_t will show a time dependence even for large t and, in classical situations (as defined above), the time averages of q_t and $(q_t)^2$ must be equal to $\langle O\rangle_t$ and $\langle O^2\rangle_t$ respectively, because the measuring process then cannot affect the observable properties of the system.

In our theory, a measurement of O at time t must be described in the conventional quantum-mechanical fashion as giving rise to a reduction of the state vector φ_t to another vector φ_t'. This interpretation holds always, even in classical situations. For the latter case we can translate it by saying that the measurement gives rise to a reduction of the classical ensembe associated with φ_t to the smaller ensemble associated with φ_t'. Although there is nothing wrong with this description, it differs in a non-trivial way from the picture conventionally adopted for a classical many-body system, in which at every instant t the system is regarded as being in one single point of $6N$-dimensional phase space. If our theory is valid, *a gas, liquid or solid in thermal equilibrium can never be said to be in one single point of its classical phase space, even at high temperatures where all measurable quantum effects are numerically negligible. It is in a single quantum state, the classical analogue of which is an ensemble.*

It should be stressed that this unorthodox view cannot lead to any observable discrepancy with the conventional picture of a classical system. Let us verify for example in our quantum description that for a classical situation (as defined above) a measurement carried out at time t does not affect the result of observations at later times $t' = t + \tau$. Let the quantity O be measured at time t, and the quantity O' at time t'. Assuming for simplicity O to have discrete eigenvalue O_n, all we have to establish is the identity

$$\langle\varphi_t|U_{-\tau}O'U_\tau O|\varphi_t\rangle = \sum_n O_n\langle\varphi_t|P_nU_{-\tau}O'U_\tau P_n|\varphi_t\rangle \tag{3.1}$$

where the P_n's are the projection operators verifying $O = \sum_n O_nP_n$. The righthand side of (3.1) includes the reduction of the state vector due to the first measurement, the lefthand side neglects it. Since $P_n^2 = P_n$ the difference between the two is

$$\sum_n O_n\langle\varphi_t|[P_n, U_{-\tau}O'U_\tau]P_n|\varphi_t\rangle.$$

The commutator being proportional to $\hbar$, this difference is indeed negligible in a classical situation.

4. *Refutation of Ingraham's criticism.* In a recent paper [6]) Ingraham has presented a severely critical discussion of our derivation in S of the master equation describing the approach to equilibrium in the case of a very small perturbation (limiting case $\lambda \to 0$, $t \to \infty$, $\lambda^2 t$ finite). In fact, if

this discussion were correct, it would imply complete invalidity of the contents of S, S' and the present paper. Ingraham's analysis, however, is based on a few patently wrong assertions and arguments. If these assertions and arguments are replaced by their corrected versions, the whole criticism of Ingraham becomes groundless and his considerations reduce to those of S and lead to the same conclusions. We would like to devote the last section of the present paper to a refutation of Ingraham's criticism, to which end it will be sufficient to indicate which basic arguments of this author are incorrect. We can concentrate on section 3 of Ingraham's paper, which contains the actual discussion of our work.

The first argument of Ingraham is developed on pp. 107 to 111 of his paper. It tends to show that our method of calculation violates the unitarity of the operator of motion

$$U(t) = \exp[-i(H + \lambda V)t].$$

The essential step is that unitarity of $U(t)$ would imply In (3.20) *), which itself entails In (3.22), i.e. the vanishing of all transition rates. The central error is In (3.20). In deriving this equation, Ingraham tacitly assumes that for $\lambda \to 0$, $t \to \infty$, $\lambda^2 t$ finite, the limit of a product of operators (in the case at hand $U_2^* U_2$) is equal to the product of the limits. This assumption is incorrect. Explicit calculation of the limit of the product gives an additional term in the righthand side of In (3.20), removing the inconsistency. Incidentally, while "deriving" In (3.20), Ingraham states that our use of a well known asymptotic formula, In (3.16), would result from a choice. This is patently wrong, because In (3.16) is a *mathematical identity* for $f(\epsilon)$ continuously differentiable and vanishing at least as fast as $|\epsilon|^\nu$, $\nu < 0$ for $\epsilon \to \infty$. No other formula would be correct, and no choice can therefore be made.

The second criticism of Ingraham is that ambiguities exist in our calculations, because in products containing 3 or more factors V several prescriptions could be followed in replacing sub-products VAV by their diagonal parts: various choices could be made for these subproducts leading to different results for the total expression (see pp. 112 and 113 of Ingraham's paper). Ingraham has not understood that all choices *have* to be made, and that in the limit $\lambda \to 0$, $t \to \infty$, $\lambda^2 t$ finite, the total expression is the sum of the contributions of all possible choices. Among the latter only a few give non-vanishing contributions in the limiting case considered; all these have been calculated in S, ensuring the correctness of our results in the weak coupling limit.

Misled by the errors just mentioned, Ingraham concludes to the invalidity of the fundamental property on which our work is based, to know the occurrence of diagonal singularities, In (3.1) in his paper. His misunderstanding of this property becomes quite clear when he states it to be

*) By this abbreviation we mean Eq. (3.20) of Ingraham's paper.

equivalent to the property In (3.30), where no summation is carried out on the intermediate state q_1. The summation is absolutely essential for the occurrence of the diagonal singularity. Consequently the operator A in In (3.1) must have eigenvalues $A(E''\alpha'') = A''$ varying smoothly with the parameters E'', α'', and In (3.30) is incorrect. For the same reason, the master equation established in S concerns the *probability density* to find our large system in unperturbed states, i.e. the probability averaged over a very large number of neighboring states. This is a coarse-grained probability distribution. Therefore Ingraham's statement that we "want to obtain irreversible effects while retaining the maximum information permitted by statistical mechanics" (p. 101), according to his introduction the very motivation of his critical study, is incorrect. Concerning the alternative diagonal property In (3.33) proposed by Ingraham, it will be sufficient to say that it does not hold for actual systems, as is easily verified on the example of the electron-phonon system described in the appendix of S'.

Having thus concluded to the invalidity of Ingraham's criticism, we may finally remark that this author seems to be quite confused concerning the order in which the various limiting processes $N \to \infty$, $\lambda \to 0$, $t \to \infty$ must be considered for obtaining the region of validity of a master or transport equation. The number of particles N must go to infinity first, λ and t being finite. When this limiting process, which is necessary e.g. to eliminate surface and shape-dependent effects, is completed, one can consider the limiting case $\lambda \to 0$, $t \to \infty$, $\lambda^2 t$ finite. One then obtains the master equation as derived in S. One can treat also, however, the case of finite λ and t, as was done in S' and the present paper.

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