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The Master Equation for the Interference Term and the Approach to Equilibrium in Quantum Many-Body Systems

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Synopsis. The techniques developed by VAN HOVE for deriving a master equation to general order in the perturbation for the transition probability are now applied to the interference term. A master equation to general order for the partial interference term is obtained, which, in the limit of small perturbation, leads to a Pauli master equation for the interference term itself. The long-time behaviour of the interference term is discussed. By means of these results, one can write down a complete master equation without any random phase assumption. The ergodic behaviour of a quantum many-body system is demonstrated for a large class of physical quantities, and the approach to micro-canonical equilibrium is discussed.

1. Introduction

PAULI derived his well-known master equation in the limit of small perturbation, making use of the so-called repeated random phases assumption[1]). VAN HOVE, using special properties of the perturbing potential valid for a great number of large quantum-systems having physical interest, derived a master equation to general order in λ and discussed the approach to equilibrium of a quantum many-body system in a series of papers[2])*). Underlying was the assumption of random phases for the initial state only**), corresponding to rapidly varying phases as a function of the state variables α, which are quantum numbers for the eigenfunctions of the unperturbed hamiltonian. Following this assumption, the contribution of the phase-dependent interference term to the occupation probability density $p_t(\alpha)$ was neglected for every time of interest, and $p_t(\alpha)$ was expressed by means of phase-independent terms

*) Here quoted as S_1, S_2 and S_3.
**) Other assumptions on the initial states have also been considered by VAN HOVE in the weak-coupling case (S_1).

only. It was then possible to derive the PAULI master equation from the general one, in the limiting case of small perturbation without the repeated random phase assumption. The approach to equilibrium has been discussed to general order in λ by considering the singularities of corresponding Fourier-transformed expressions. By assuming some additional conditions, VAN HOVE was able to show that for a diagonal operator A with an eigenvalue $A(\alpha)$ which is a smooth function of α, the statistical equilibrium reached corresponds to the micro-canonical one. In this connexion, FIERZ[3]) pointed out the importance (a) of considering a broader class of macroscopic operators than the diagonal ones, and (b) of an appropriate discussion of the interference term, so far neglected. As regards (a), the ergodic behaviour for quantum many-body systems was extended in S_3 to a larger class of non-diagonal operators B, and its implications for the classical case were discussed.

Concerning (b), a first step was made by PROSPERI[4]). In his paper, this author shows, under some restrictive assumptions, that the class of hamiltonians considered by VAN HOVE also satisfy abstract ergodicity conditions: for this, Prosperi also considers the non-diagonal contributions, i.e. the interference term I_t. What we discuss in the present paper is the time evolution and the asymptotic behaviour of this interference term. Our results are consistent with those derived by PROSPERI. However, our work has been inspired by VAN HOVE's papers, and only represents a straightforward application to the non-diagonal part of his own way of dealing with the problem. Starting from an expression for the interference term, which expression is equivalent to that given by PROSPERI[4]), a general equation is derived for the interference term, it being of the same type as that obtained for the transition probability, i. e. an inhomogeneous integro-differential equation of non-markoffian character. To lowest order in λ we get the same PAULI master equation as for the transition probability, however with another initial condition. Within this limit, it was also possible to derive an explicit solution. The discussion, to general order in λ, of the asymptotic behaviour of the interference term is based on an analysis of the singularities of the Fourier-transformed non-diagonal term. We have considered only the case in which all states α are dissipative, characterized as they are by some regularity properties of the diagonal part of the resolvent $R_l(\alpha)$. Approach to statistical equilibrium is observed without any random phase assumption, even for the initial state. Under the same supplementary hypothesis as made by VAN HOVE for the diagonal part alone (validity of a generalized microscopic reversibility or detailed balance and interconnexion of states having the same unperturbed energy), the equilibrium is a microcanonical one. The probability distribution of the total energy in the initial state now contains contributions from the phase-dependent terms. The calculation is first made for a class of diagonal operators A; the generalization to the non-diagonal operators B considered by VAN HOVE [2]) is straightforward.

2. Van Hove's Derivation of the Master Equation for the Transition Probability

In this section we summarize the assumptions and the results of VAN HOVE's master equation derivation. We refer to his papers [2]) for further details. We assume that the hamiltonian of the system may be written as:

$$H = H_0 + \lambda V \tag{2.1}$$

The eigenstates $| \alpha \rangle$ of H_0 are supposed to be known and to form a complete set.

$$H_0 \, | \alpha \rangle = \varepsilon(\alpha) \, | \alpha \rangle \tag{2.2}$$

where α represents a collection of quantum numbers characterizing the state, and $\varepsilon(\alpha)$ is the unperturbed energy of the system in the state $| \alpha \rangle$. In the limit of an infinite system, the eigenstates are normalized to:

$$\langle \alpha \, | \, \alpha' \rangle = \delta(\alpha - \alpha') \, . \tag{2.3}$$

Any operator O can be split into a 'diagonal part' O^{d} and a 'non-diagonal part' O^{nd} defined by:

$$\begin{aligned} \langle \alpha \, | \, O \, | \, \alpha' \rangle &= \langle \alpha \, | \, O^{\mathrm{d}} \, | \, \alpha' \rangle + \langle \alpha \, | \, O^{\mathrm{nd}} \, | \, \alpha' \rangle = \\ &= O^{\mathrm{d}}(\alpha) \, \delta(\alpha - \alpha') + O^{\mathrm{nd}}(\alpha \, \alpha') \end{aligned} \tag{2.4}$$

where: $O^{\mathrm{d}} \, | \, \alpha \rangle = | \, \alpha \rangle \, O^{\mathrm{d}}(\alpha)$, and $O^{\mathrm{nd}}(\alpha \, \alpha')$ has only singularities of smaller order than $\delta(\alpha - \alpha')$. The perturbation λV has special properties in the representation $| \, \alpha \rangle$. In particular, it is supposed that V has a vanishing diagonal part, but that operators of the type $V A_1 V \dots A_n V$ have a non-vanishing diagonal part for A_j-diagonal operators.

We define as 'irreducible diagonal part':

$$(V A_1 V \, \dots \, A_n V)_{\mathrm{id}}$$

the diagonal operator, the matrix elements of which are obtained by keeping all intermediate states different from one another and from the initial and final states. In the same way, an 'irreducible non-diagonal part':

$$(V A_1 V \, \dots \, A_n V)_{\mathrm{ind}}$$

is defined for a non-diagonal operator.

We now consider a diagonal operator A and assume that its eigenvalue $A(\alpha)$ is a smooth function of the α's. Let us introduce the time evolution operator U_t:

$$U_t = \exp[-i\,(H_0 + \lambda V)\,t] \quad (\hbar = 1)\,. \tag{2.5}$$

We may write:

$$\begin{aligned} \langle\alpha\,|\{U_{-t}\,A\,U_t\}_{\mathrm{d}}\,|\,\alpha'\rangle &= \int d\alpha_0\,A(\alpha_0)\,P_t(\alpha_0\,\alpha)\,\delta(\alpha-\alpha')\,, \\ \langle\alpha\,|\{U_{-t}\,A\,U_t\}_{\mathrm{nd}}\,|\,\alpha'\rangle &= \int d\alpha_0\,A(\alpha_0)\,I_t(\alpha_0\,\alpha\,\alpha')\,. \end{aligned} \tag{2.6}$$

In order to interpret the physical significance of the two functions P_t and I_t defined in (2.6), let us consider the wave function of the system at time $t = 0$ expanded in the α-eigenfunctions:

$$|\,\varphi_0\rangle = \int d\alpha\,|\,\alpha\rangle\,c(\alpha)\,, \tag{2.7}$$

with $|\,\varphi_0\rangle$ normalized to one:

$$\langle\varphi_0\,|\,\varphi_0\rangle = \int d\alpha\,|\,c(\alpha)\,|^2 = 1\,. \tag{2.7a}$$

We introduce a coarse-grained probability density $p_t(\alpha)$ at the time t:

$$\langle\varphi_t\,|\,A\,|\,\varphi_t\rangle = \int d\alpha_0\,A(\alpha_0)\,p_t(\alpha_0) \tag{2.8}$$

where $|\,\varphi_t\rangle = U_t\,|\,\varphi_0\rangle$.
One obtains:

$$p_t(\alpha_0) = \int d\alpha\,P_t(\alpha_0\,\alpha)\,|\,c(\alpha)\,|^2 + \int d\alpha\,d\alpha'\,I_t(\alpha_0\,\alpha\,\alpha')\,c^*(\alpha)\,c(\alpha')\,. \tag{2.8a}$$

Therefore, the quantity $P_t(\alpha_0\,\alpha)$ can be interpreted as coarse-grained transition probability from α to α_0 during the time interval t, and $I_t(\alpha_0\alpha\alpha')$ as a function describing the time evolution of the interference effects between the initial states.

The 'random phase assumption' for initial time, corresponding to the assumption of rapidly varying phases for the $c(\alpha)$ as a function of α, allows the description of the time evolution of the system towards equilibrium, in terms of $P_t(\alpha_0\,\alpha)$ alone. The interference term is considered negligible during this time period.

$P_t(\alpha_0\,\alpha)$ itself, in the weak coupling limit ($\lambda \to 0$, $t \to \infty$, $\lambda^2 t$ finite) obeys the Pauli master equation with the initial condition:

$$P_0(\alpha_0\,\alpha) = \delta(\alpha_0 - \alpha)\,. \tag{2.9}$$

The general order behaviour is best discussed on the basis of the resolvent defined by:

$$R_l = (H_0 + \lambda V - l)^{-1}, \quad l \text{ complex number} \tag{2.10}$$

which is related to U_t by means of the relation:

$$U_t = \frac{-1}{2\pi i} \int_\gamma dl\, e^{-ilt} R_l \tag{2.11}$$

γ is a counter-clockwise integration contour in the complexe plane, encircling a sufficiently large portion of the real axis.

Let us define:

$$\begin{aligned} \langle \alpha \,|\{R_l A R_{l'}\}_d\,|\, \alpha' \rangle &= \delta(\alpha - \alpha') \int d\alpha_0\, A(\alpha_0)\, X_{l\,l'}(\alpha_0\, \alpha)\,, \\ \langle \alpha \,|\{R_l A R_{l'}\}_{nd}\,|\, \alpha' \rangle &= \int d\alpha_0\, A(\alpha_0)\, Y_{l\,l'}(\alpha_0\, \alpha\, \alpha')\,. \end{aligned} \tag{2.12}$$

The functions $X_{l\,l'}(\alpha_0\,\alpha)$ and $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ are related to $P_t(\alpha_0\,\alpha)$ and $I_t(\alpha_0\,\alpha\,\alpha')$ respectively through the relations:

$$\begin{aligned} P_t(\alpha_0\,\alpha) &= \frac{-1}{(2\pi)^2} \int_\gamma dl \int_\gamma dl'\, e^{i(l-l')t}\, X_{l\,l'}(\alpha_0\,\alpha)\,, \\ I_t(\alpha_0\,\alpha\,\alpha') &= \frac{-1}{(2\pi)^2} \int_\gamma dl \int_\gamma dl'\, e^{i(l-l')t}\, Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')\,. \end{aligned} \tag{2.13}$$

The reduction of $\{R_l A R_{l'}\}_d$ to its irreducible diagonal part leads to the following expression for $X_{l\,l'}(\alpha_0\,\alpha)$:

$$\begin{aligned} X_{l\,l'}(\alpha_0\,\alpha) &= D_l(\alpha_0)\, D_{l'}(\alpha_0)\, \delta(\alpha_0 - \alpha) + \lambda^2 D_l(\alpha_0)\, D_{l'}(\alpha_0) \Big[W_{l\,l'}(\alpha_0\,\alpha) + \\ &+ \lambda^2 \int d\alpha_1\, W_{l\,l'}(\alpha_0\,\alpha_1)\, D_l(\alpha_1)\, D_{l'}(\alpha_1)\, W_{l\,l'}(\alpha_1\,\alpha) + \ldots \Big] D_l(\alpha)\, D_{l'}(\alpha) \end{aligned} \tag{2.14}$$

where D_l is the diagonal part of R_l and $W_{l\,l'}(\alpha_0\,\alpha)$ is defined by:

$$\begin{aligned} &\{(V - \lambda V D_l V + \ldots)\, A\, (V - \lambda V D_{l'} V + \ldots)\}_{id}\, |\alpha\rangle = \\ &= |\alpha\rangle \int d\alpha_0\, A(\alpha_0)\, W_{l\,l'}(\alpha_0\,\alpha)\,. \end{aligned} \tag{2.15}$$

In the next section we shall derive a corresponding expression for $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$, which was first explicitly given by PROSPERI[4]).

We now consider the spectral component $P_{E,t}(\alpha_0\,\alpha)$ of $P_t(\alpha_0\,\alpha)$:

$$P_t(\alpha_0\,\alpha) = \int_{-\infty}^{+\infty} dE\; P_{E,t}(\alpha_0\,\alpha)\;;$$

$$P_{E,t}(\alpha_0\,\alpha) = \frac{s(t)}{2\,\pi^2}\int_\gamma dl\; e^{2ilt}\, X_{E+l,\,E-l}(\alpha_0\,\alpha) \tag{2.16}$$

which represents the partial transition probability at energy E and $s(t) = t/|t|$.

For $P_{E,t}(\alpha_0\alpha)$, a general master equation of non-markoffian character can be derived from the following equation for $X_{l\,l'}(\alpha_0\,\alpha)$:

$$(l - l')\; X_{l\,l'}(\alpha_0\,\alpha) = \big(D_l(\alpha_0) - D_{l'}(\alpha_0)\big)\,\delta\,(\alpha_0 - \alpha) +$$

$$-\, i\,\lambda^2 \int \tilde{W}_{l\,l'}(\alpha_0\,\alpha_1)\; d\alpha_1\; X_{l\,l'}(\alpha_1\alpha) + i\,\lambda^2 \int d\alpha_1\; \tilde{W}_{l\,l'}(\alpha_1\,\alpha_0)\; X_{l\,l'}(\alpha_0\,\alpha) \tag{2.17}$$

where $$\tilde{W}_{l\,l'}(\alpha_0\,\alpha) = i\,\big(D_l(\alpha_0) - D_{l'}(\alpha_0)\big)\; W_{l\,l'}(\alpha_0\,\alpha)\,. \tag{2.18}$$

3. General Properties of the Interference Term

Our first aim is to derive an expression for $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ in terms of irreducible non-diagonal parts.

From the definition of $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$, and expressing the resolvent in its irreducible contributions, we have:

$$\int d\alpha_0\; A(\alpha_0)\; Y_{l\,l'}(\alpha_0\,\alpha\,\alpha') = \langle\alpha\,|\,\{[D_l + (-\lambda\,D_l\,V\,D_l + \ldots)_{\text{ind}}]\; A\;\big[(D_{l'} + $$
$$+ (-\lambda\,D_{l'}\,V\,D_{l'} + \;\ldots)_{\text{ind}}]\}_{\text{nd}}\;|\alpha'\rangle\,.$$

We note first that reducible contributions can only arise from identities between intermediate states to the right and to the left of the state $|\,\alpha_0\rangle$ as schematically shown in Fig. 1.

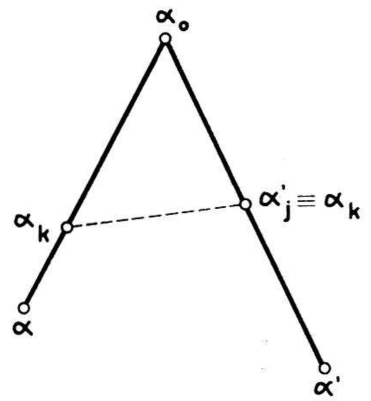

Fig. 1

Reducible contribution to $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$

The corresponding subdiagonal contribution is simply $X_{l\,l'}(\alpha_0\,\alpha_k)$. We also note that interlocked pairs of identical intermediate states are excluded (Property (iii) of S_2, p. 445) – Fig. 2:

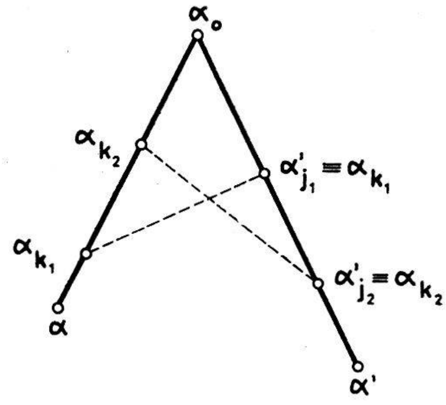

Fig. 2
Excluded reducible contribution to $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$

In the same approximation as for $X_{l\,l'}(\alpha_0\,\alpha)$ (this means, in the limit of a very large system[5]), we therefore obtain for $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$:

$$Y_{l\,l'}(\alpha_0\,\alpha\,\alpha') = \int d\alpha_1\, X_{l\,l'}(\alpha_0\,\alpha_1)\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha') \tag{3.1}$$

where $V_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ is a non-diagonal operator defined by:

$$\langle\alpha\,|\,\{(1 - \lambda\, D_l\, V + \lambda^2\, D_l\, V\, D_l\, V + \ldots)\, A\, (1 - \lambda\, V\, D_{l'} + \lambda^2\, V\, D_{l'}\, V\, D_{l'} + \\ + \ldots)\}_{\text{ind}}\,|\,\alpha'\rangle = \int d\alpha_0\, A(\alpha_0)\, V_{l\,l'}(\alpha_0\,\alpha\,\alpha')\,. \tag{3.2}$$

(3.1) can also be put into another form:

$$\{R_l\, A\, R_{l'}\}_{\text{nd}} = \{(1 - \lambda\, D_l\, V + \ldots)\, (R_l\, A\, R_{l'})_{\text{d}}\, (1 - \lambda\, V\, D_{l'} + \ldots)\}_{\text{ind}} \tag{3.1a}$$

from which the expression indicated by PROSPERI[4]) is immediately derived.

Using the well-known identity:

$$R_l - R_{l'} = (l - l')\, R_l\, R_{l'} \tag{3.3}$$

and taking the non-diagonal part, we get the relation

$$R_l^{\text{nd}}(\alpha\,\alpha') - R_{l'}^{\text{nd}}(\alpha\,\alpha') = (l - l') \int d\alpha_0\, Y_{l\,l'}(\alpha_0\,\alpha\,\alpha') = \\ = (l - l') \int d\alpha_0\, X_{l\,l'}(\alpha_0\,\alpha_1)\, d\alpha_1\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha')\,. \tag{3.4}$$

By means of the corresponding diagonal-part relation

$$D_l(\alpha) - D_{l'}(\alpha) = (l - l') \int d\alpha_0 \, X_{l\,l'}(\alpha_0\,\alpha) \tag{3.5}$$

we obtain

$$R_l^{\mathrm{nd}}(\alpha\,\alpha') - R_{l'}^{\mathrm{nd}}(\alpha\,\alpha') = \int d\alpha_0 \left(D_l(\alpha_0) - D_{l'}(\alpha_0)\right) V_{l\,l'}(\alpha_0\,\alpha\,\alpha') \,. \tag{3.6}$$

This last expression can easily be derived directly from the definition of $V_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ for $A = D_l - D_{l'}$, and from the irreducible expression of R_l^{nd}.

To the lowest order in λ, $V_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ is given by:

$$V_{l\,l'}^{(1)}(\alpha_0\,\alpha\,\alpha') = -\lambda\, V(\alpha\,\alpha') \left(\delta(\alpha_0 - \alpha)\, D_{l'}^{(0)}(\alpha') + D_l^{(0)}(\alpha)\, \delta(\alpha_0 - \alpha')\right) \tag{3.7}$$

where

$$D_l^{(0)} = (H_0 - l)^{-1} \,.$$

For $l \to \infty$, $V_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ has a non-vanishing limit. The same is true for l'. For large l and l', $V_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ approaches to zero as $|\,l\,|^{-1} \sim |\,l'\,|^{-1}$. From the asymptotic behaviour of $X_{l\,l'}(\alpha_0\,\alpha)$ for large l and l' respectively, one sees that $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ approaches to zero as $|\,l\,|^{-1}$ for $l \to \infty$, as $|\,l'\,|^{-1}$ for $l' \to \infty$, and as $|\,l^2\, l'\,|^{-1} \sim |\,l\, l'^2\,|^{-1}$ when l and $l' \to \infty$.

4. Master Equation to General Order for the Interference Term

We consider the relation (2.17) for $X_{l\,l'}(\alpha_0\,\alpha_1)$, and we multiply this equation by $V_{l\,l'}(\alpha_1\,\alpha\,\alpha')$. Integration over α_1 yields:

$$\begin{aligned}(l - l') \int d\alpha_1\, X_{l\,l'}(\alpha_0\,\alpha_1)\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha') &= \int d\alpha_1\, \delta(\alpha_0 - \alpha_1) \left(D_l(\alpha_1) - D_{l'}(\alpha_1)\right) \times \\ \times\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha') - i\,\lambda^2 \int d\alpha_1\, d\alpha_2\, &\tilde{W}_{l\,l'}(\alpha_0\,\alpha_2)\, X_{l\,l'}(\alpha_2\,\alpha_1)\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha') + \\ + i\,\lambda^2 \int d\alpha_1\, d\alpha_2\, &\tilde{W}_{l\,l'}(\alpha_2\,\alpha_0)\, X_{l\,l'}(\alpha_0\,\alpha_1)\, V_{l\,l'}(\alpha_1\,\alpha\,\alpha') \,.\end{aligned}$$

From it, we immediately obtain a basic equation for $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$:

$$\begin{aligned}(l - l')\, Y_{l\,l'}(\alpha_0\,\alpha\,\alpha') &= \left(D_l(\alpha_0) - D_{l'}(\alpha_0)\right) V_{l\,l'}(\alpha_0\,\alpha\,\alpha') + \\ - i\,\lambda^2 \int d\alpha_1\, \tilde{W}_{l\,l'}(\alpha_0\,\alpha_1)\, &Y_{l\,l'}(\alpha_1\,\alpha\,\alpha') + i\,\lambda^2 \int d\alpha_1\, \tilde{W}_{l\,l'}(\alpha_1\,\alpha_0) \times \\ &\times Y_{l\,l'}(\alpha_0\,\alpha\,\alpha') \,.\end{aligned} \tag{4.1}$$

From this basic equation, the derivation of a master equation for the interference term follows closely that given by Van Hove in S_2 for the transition probability P_t. Here too we obtain an equation to general order in λ not for I_t itself, but only for its spectral component $I_{E,t}$ defined by:

$$I_{E,t}(\alpha_0\,\alpha\,\alpha') = \frac{s(t)}{2\pi^2}\int_\gamma dl\, e^{2ilt}\, Y_{E+l,\,E-l}(\alpha_0\,\alpha\,\alpha') \quad \text{with} \tag{4.2}$$

$$I_t(\alpha_0\,\alpha\,\alpha') = \int_{-\infty}^{+\infty} dE\; I_{E,t}(\alpha_0\,\alpha\,\alpha')\,.$$

Following VAN HOVE, we introduce:

$$w_{E,t}(\alpha_0\,\alpha) = \frac{1}{2\pi^2}\int_\gamma dl\, e^{2ilt}\, \tilde{W}_{E+l,\,E-l}(\alpha_0\,\alpha)\,. \tag{4.3}$$

In the same way as for the diagonal part, and owing to the asymptotic behaviour of $\tilde{W}_{E+l,\,E-l}$ and of $Y_{E+l,\,E-l}$ for $l\to\infty$, we obtain the relation:

$$s(t)\int_\gamma dl\, e^{2ilt}\, \tilde{W}_{E+l,\,E-l}(\alpha_3\,\alpha_2)\; Y_{E+l,\,E-l}(\alpha_1\,\alpha\,\alpha') =$$

$$= 4\pi^3\int_0^t dt'\, w_{E,\,t-t'}(\alpha_3\,\alpha_2)\; I_{E,t'}(\alpha_1\,\alpha\,\alpha')\,.$$

Multiplying equation (4.1) for $Y_{E+l,\,E-l}(\alpha_0\,\alpha\,\alpha')$ by $\frac{1}{2\pi^2}\, s(t)\, i\int_\gamma dl\, e^{2ilt}$,

one finally gets:

$$\frac{dI_{E,t}(\alpha_0\,\alpha\,\alpha')}{dt} = g_{E,t}(\alpha_0\,\alpha\,\alpha') + 2\pi\lambda^2\int_0^t dt'\int d\alpha_1\, w_{E,\,t-t'}(\alpha_0\,\alpha_1)\; I_{E,t'}(\alpha_1\,\alpha\,\alpha') +$$

$$- 2\pi\lambda^2\int_0^t dt'\int d\alpha_1\, w_{E,\,t-t'}(\alpha_1\,\alpha_0)\; I_{E,t'}(\alpha_0\,\alpha\,\alpha') \tag{4.4}$$

where:

$$g_{E,t}(\alpha_0\,\alpha\,\alpha') =$$

$$= \frac{i\,s(t)}{2\pi^2}\int_\gamma dl\, e^{2ilt}\,\big(D_{E+l}(\alpha_0) - D_{E-l}(\alpha_0)\big)\, V_{E+l,\,E-l}(\alpha_0\,\alpha\,\alpha')\,. \tag{4.5}$$

The partial interference term $I_{E,t}(\alpha_0\alpha\alpha')$ obeys an integro-differential equation of general order in λ, which equation has the same structure as the general master equation derived by VAN HOVE for $P_{E,t}(\alpha_0\,\alpha)$. The present equation only differs from the other in its inhomogeneous term. It is therefore indicated to call it a general master equation for the (partial) interference term $I_{E,t}$. The lowest order equation that we shall derive from it will confirm this standpoint.

With the initial condition

$$I_{E,0}(\alpha_0\, \alpha\, \alpha') = 0 \tag{4.6}$$

which is a result obtained from the definition of $I_{E,t}$ for $t = 0$ by deforming the integration path to infinity, the behaviour of $I_{E,t}$ is uniquely determined for all times.

We note that, here too, equation (4.4) only holds for $t \neq 0$. We were able to derive an equation for I_t itself only to the lowest order in λ, i.e. in the limiting case of small perturbation.

5. The Limiting Case of Small Perturbation

For the same reasons as for $P_{E,t}$, two time-scales exist in the evolution of $I_{E,t}$, which, in the limiting case of small perturbation, do not overlap. The initial stage for $I_{E,t}$ is determined by the behaviour of the rapidly varying functions $g_{E,t}$, and $w_{E,t}$, and is measured within the short-time scale, which is of the order of T_0, and is independent of λ. The approach of $I_{E,t}$ to its asymptotic value takes place during a much longer time, measured in a long-time scale of the order of T_1, where T_1 is proportional to λ^{-2}.

Neglecting terms of order λ^2, we have on the short time scale:

$$\frac{d I^{(1)}_{E,t}(\alpha_0\, \alpha\, \alpha')}{dt} = g^{(1)}_{E,t}(\alpha_0\, \alpha\, \alpha') \tag{5.1}$$

where

$$g^{(1)}_{E,t}(\alpha_0\, \alpha\, \alpha') = \frac{-i\,\lambda\, s(t)}{2\,\pi^2} \int_\gamma e^{2ilt} \left(D^{(0)}_{E+l}(\alpha_0) - D^{(0)}_{E-l}(\alpha_0)\right) \times$$
$$\times \{\delta(\alpha_0 - \alpha)\, D^{(0)}_{E-l}(\alpha') + \delta(\alpha_0 - \alpha')\, D^{(0)}_{E+l}(\alpha)\}\, V(\alpha\, \alpha')\, dl\,.$$

The integration over l can now easily be performed, and we obtain:

$$g^{(1)}_{E,t}(\alpha_0\, \alpha\, \alpha') = -\frac{\lambda\, s(t)\, V(\alpha\, \alpha')}{\pi} \Bigg\{\delta(\alpha_0 - \alpha') \left[\frac{e^{2i(\varepsilon' - E)t} - e^{2i(\varepsilon - E)t}}{\varepsilon - \varepsilon'} + \right.$$
$$\left. + \frac{e^{-2i(\varepsilon' - E)t} - e^{2i(\varepsilon - E)t}}{\varepsilon + \varepsilon' - 2E}\right] + \delta(\alpha_0 - \alpha) \left[\frac{e^{-2i(\varepsilon - E)t} - e^{-2i(\varepsilon' - E)t}}{\varepsilon' - \varepsilon} + \right.$$
$$\left. + \frac{e^{2i(\varepsilon - E)t} - e^{-2i(\varepsilon' - E)t}}{\varepsilon + \varepsilon' - 2E}\right]\Bigg\}\,. \tag{5.2}$$

In (5.2), and in the following formula and in others as well, we use the short notation ε_k for $\varepsilon(\alpha_k)$. Integration of (5.1) together with the initial condition (4.6) gives $I_{E,t}$, which in the upper limit of the short-time scale becomes:

$$I_E^{(1)}(\alpha_0\,\alpha\,\alpha') = \lim_{T\to\pm\infty} I_{E,T}^{(1)}(\alpha_0\,\alpha\,\alpha') = \frac{\lambda\,V(\alpha\,\alpha')}{\varepsilon-\varepsilon'}\,[\delta(\alpha-\alpha_0)-\delta(\alpha_0-\alpha')]\times$$
$$\times\,\delta(\varepsilon_0-E)\,. \tag{5.3}$$

In deriving this result, use was made of the asymptotic formula:

$$\int_0^T dt \int d\varepsilon\, e^{i\varepsilon t}\, F(\varepsilon) = \frac{T}{|T|}\, F(0) + i\int d\varepsilon\, F(\varepsilon)\left(\frac{1}{\varepsilon}\right)_P \tag{5.4}$$

the principal value part giving a vanishing contribution in (5.3).

We note that we obtain an expression independent of the direction of time only for $t \to \infty$. In general

$$I_{E,t}(\alpha_0\,\alpha\,\alpha') \neq I_{E,-t}(\alpha_0\,\alpha\,\alpha')\,.$$

$I_E^{(1)}(\alpha_0\,\alpha\,\alpha')$ now represents the initial condition for the long-time scale. In the mean for t large compared to T_0, the inhomogeneous term in (4.4) becomes negligible, and the homogeneous term alone determines the time variation of $I_{E,t}$, which variation is very slow, being of the order λ^2. We may therefore write:

$$\int_0^t dt'\, w_{E,t'}(\alpha_0\,\alpha_1)\, I_{E,t-t'}(\alpha_1\,\alpha\,\alpha') \cong I_{E,t}(\alpha_1\,\alpha\,\alpha') \int_0^\infty dt'\, w_{E,t'}(\alpha_0\,\alpha_1) =$$
$$= \frac{1}{2\pi}\,\tilde{W}_{E\mp i0,\,E\pm i0}(\alpha_0\,\alpha_1)\, I_{E,t}(\alpha_1\,\alpha\,\alpha') \tag{5.5}$$

where the upper signs are to be taken for positive, and the lower signes for negative time.

On the long-time scale, the master equation for $I_{E,t}$ is given by:

$$\frac{dI_{E,t}(\alpha_0\,\alpha\,\alpha')}{dt} = \lambda^2\int d\alpha_1\, \tilde{W}^{(1)}_{E\mp i0,\,E\pm i0}(\alpha_0\,\alpha_1)\, I_{E,t}(\alpha_1\,\alpha\,\alpha') +$$
$$-\,\lambda^2\int d\alpha_1\, \tilde{W}^{(1)}_{E\mp i0,\,E\pm i0}(\alpha_1\,\alpha_0)\, I_{E,t}(\alpha_0\,\alpha\,\alpha')\,, \quad \text{for} \quad t\sim T_1 \tag{5.6}$$

in which $\tilde{W}^{(1)}_{E\mp i0,E\pm i0}$ is taken to the first order in λ. Equation (5.6) must be integrated with $I_E^{(1)}(\alpha_0\,\alpha\,\alpha')$ as initial condition. In order to discuss the solution, we suppose $I_{E,t}$ to be developed in powers of λ and we obtain a system of differential equations of the form:

$$\frac{dI_{E,t}^{(2n+1)}(\alpha_0\,\alpha\,\alpha')}{dt} =$$
$$= 2\pi\lambda^2\int d\alpha_1\, W^{(1)}_{E\mp i0,E\pm i0}(\alpha_0\,\alpha_1)\, I_{E,t}^{(2n-1)}(\alpha_1\,\alpha\,\alpha')\,\delta(\varepsilon_0-E) +$$
$$-\,2\pi\lambda^2\int d\alpha_1\, W^{(1)}_{E\mp i0,E\pm i0}(\alpha_1\,\alpha_0)\, I_{E,t}^{(2n-1)}(\alpha_0\,\alpha\,\alpha')\,\delta(\varepsilon_1-E)\,.$$

Solving by recurrence, and noting that the initial condition for $I_{E,t}(\alpha_0\,\alpha\,\alpha')$ contains a factor $\delta(\varepsilon_0-E)$, one recognizes that the general solution is of the form:

$$I_{E,t}(\alpha_0\,\alpha\,\alpha') = J_t(\alpha_0\,\alpha\,\alpha')\,\delta(\varepsilon_0 - E)\,.$$

Integration over dE gives:

$$I_t(\alpha_0\,\alpha\,\alpha') = \int_{-\infty}^{+\infty} dE\; I_{E,t}(\alpha_0\,\alpha\,\alpha') = J_t(\alpha_0\,\alpha\,\alpha')\,.$$

Therefore:

$$I_{E,t}(\alpha_0\,\alpha\,\alpha') = I_t(\alpha_0\,\alpha\,\alpha')\,\delta(\varepsilon_0 - E) \tag{5.7}$$

within our approximation. In this way we obtain a differential master equation for I_t itself:

$$\frac{dI_t(\alpha_0\,\alpha\,\alpha')}{dt} = 2\pi\lambda^2\int d\alpha_1\,\delta(\varepsilon_0-\varepsilon_1)\,W^{(1)}_{\varepsilon_1\mp i0,\,\varepsilon_1\mp i0}(\alpha_0\,\alpha_1)\,I_t(\alpha_1\,\alpha\,\alpha') + \\ - 2\pi\lambda^2\int d\alpha_1\,\delta(\varepsilon_0-\varepsilon_1)\,W^{(1)}_{\varepsilon_0\mp i0,\,\varepsilon_0\pm i0}(\alpha_1\,\alpha_0)\,I_t(\alpha_0\,\alpha\,\alpha') \tag{5.8}$$

with the initial condition:

$$I_0(\alpha_0\,\alpha\,\alpha') = \frac{\lambda\,V(\alpha\,\alpha')}{\varepsilon-\varepsilon'}\,[\delta(\alpha_0-\alpha) - \delta(\alpha_0-\alpha')]\,. \tag{5.9}$$

The equation obtained is the same master equation as that derived by PAULI for $P_t(\alpha_0\,\alpha)$ in the weak field case, and whose solution is known. It is therefore possible to give an explicit solution of I_t in terms of P_t in the limiting case of small perturbation:

$$I_t(\alpha_0\,\alpha\,\alpha') = \frac{\lambda\,V(\alpha\,\alpha')}{\varepsilon-\varepsilon'}\,[P_t(\alpha_0\,\alpha) - P_t(\alpha_0\,\alpha')] \tag{5.10}$$

with $P_0(\alpha_0\,\alpha) = \delta(\alpha_0-\alpha)$.
Under the usual assumptions of detailed balance:

$$W^{(0)}(\alpha_0\,\alpha) = W^{(0)}(\alpha\,\alpha_0) \tag{5.11}$$

and of interconnexion of all states having equal unperturbed energy, the long-time limit for $P_t(\alpha_0\,\alpha)$ is given by:

$$\lim_{t\to\pm\infty} P_t(\alpha_0\,\alpha) = \frac{\delta(\varepsilon_0-\varepsilon)}{\int d\alpha_1\,\delta(\varepsilon_1-\varepsilon)}\,. \tag{5.12}$$

In the same limit, we have for $I_t(\alpha_0\,\alpha\,\alpha')$:

$$\lim_{t\to\pm\infty} I_t(\alpha_0\,\alpha\,\alpha') = \frac{\lambda\,V(\alpha\,\alpha')}{\int d\alpha_1\,\delta(\varepsilon_1-\varepsilon_0)}\left[\frac{\delta(\varepsilon_0-\varepsilon)-\delta(\varepsilon_0-\varepsilon')}{\varepsilon-\varepsilon'}\right]. \tag{5.13}$$

For $t \sim T_1 \to \infty$ the interference term tends towards an equilibrium value. This result does not follow from any assumption relative to the initial state, and it depends only on the properties of the hamiltonian. As we shall show later on, this remains true for I_t to general order in λ the only difference being that in the general case we cannot give any estimation for the time needed by the system for it to reach statistical equilibrium.

6. The Long-Time Behaviour of the Interference Term

In this section we investigate the asymptotic behaviour of the functions $I_{E,t}(\alpha_0\,\alpha\,\alpha')$ and $I_t(\alpha_0\,\alpha\,\alpha')$ for very large times, $t \to \pm\infty$, to general order in the perturbation. For this purpose, we have to determine the singularities of $Y_{E+l,\,E-l}$ as a function of the complex variable l. We limit our discussion to the case of a dissipative system. Analytically speaking, this restriction corresponds to the assumption that the function $D_l(\alpha_k)$ has no pole for an l in the domain of integration and for each state occurring as initial, final or intermediate state in the development of $Y_{l\,l'}(\alpha_0\,\alpha\,\alpha')$. In this case, the state $|\,\alpha_k\rangle$ is said to be dissipative. To be clearer, let us consider D_l written as:

$$D_l(\alpha) = (\varepsilon(\alpha) - l - \lambda^2\, G_l(\alpha))^{-1}\,. \tag{6.1}$$

$G_l(\alpha)$ has the property that for l approaching to the real axis, it approaches a finite limit:

$$\lim_{0<\eta\to 0} G_{E\pm i\eta}(\alpha) = K_E(\alpha) \pm i\, J_E(\alpha)\,. \tag{6.2}$$

The dissipative behaviour for the state $|\,\alpha\rangle$ implies that:

$$J_E(\alpha) \neq 0 \quad \text{for } E \text{ solution of the equation}$$

$$\varepsilon(\alpha) - E - \lambda^2\, K_E(\alpha) = 0\,. \tag{6.3}$$

Keeping this result in mind, and considering the equation:

$$\int d\alpha_0 (D_{E_0+l}(\alpha_0) - D_{E_0-l}(\alpha_0))\; V_{E_0+l,\,E_0-l}(\alpha_0\,\alpha\,\alpha') =$$
$$= 2\,l \int d\alpha_0\; Y_{E_0+l,\,E_0-l}(\alpha_0\,\alpha\,\alpha') \tag{6.4}$$

one realizes that $Y_{E_0+l,\,E_0-l}$ has a pseudo-pole of degree one for $l = 0$. The factor responsible for this singularity is $X_{E_0+l,\,E_0-l}$, as discussed in S_2.

In fact, for a dissipative system, $V_{E+l,\,E-l}$ is holomorphic in the whole complex plane except on a portion of the real axis; $X_{E+l,\,E-l}$ has no other singularities apart from $l = 0$, so that the pseudo-pole for $l = 0$ is the only singularity for $Y_{E+l,\,E-l}$. This pseudo-pole determines the long-time behaviour of $I_{E,t}$ according to the equation:

$$I_E^{\pm}(\alpha_0\,\alpha\,\alpha') = \lim_{t\to\pm\infty} I_{E,t}(\alpha_0\,\alpha\,\alpha') = \frac{1}{\pi}\lim_{0<\eta\to 0}\eta\, Y_{E\mp i\eta,\,E\pm i\eta}(\alpha_0\,\alpha\,\alpha') =$$

$$= \frac{1}{\pi}\lim_{0<\eta\to 0}\int d\alpha_1\,\eta\, X_{E\mp i\eta,\,E\pm i\eta}(\alpha_0\,\alpha_1)\; V_{E\mp i\eta,\,E\pm i\eta}(\alpha_1\,\alpha\,\alpha') =$$

$$= \int d\alpha_1\, q_E^{\pm}(\alpha_0\,\alpha_1)\; V_{E\mp i0,\,E\pm i0}(\alpha_1\,\alpha\,\alpha') \qquad (6.5)$$

where

$$q_E^{\pm}(\alpha_0\,\alpha) = \frac{1}{\pi}\lim_{0<\eta\to 0}\eta\, X_{E\mp i\eta,\,E\pm i\eta}(\alpha_0\,\alpha)\,. \qquad (6.5\,\mathrm{a})$$

An explicit evaluation of $q_E^{\pm}(\alpha_0\,\alpha)$ is only possible provided further assumptions are made. These assumptions are:

(i) Generalized microscopic reversibility*):

$$W_{l\,l'}(\alpha\,\alpha') = W_{l'\,l}(\alpha'\,\alpha) \quad \text{which implies} \qquad (6.6)$$

$$X_{l\,l'}(\alpha\,\alpha') = X_{l'\,l}(\alpha'\,\alpha)\,.$$

(ii) Interconnexion of states with equal unperturbed energy:

For two states $|\alpha\rangle$ and $|\alpha'\rangle$ with $\varepsilon(\alpha) = \varepsilon(\alpha')$, a succession of states $|\alpha_k\rangle$, $k = 1,2,\ldots,n$ of same energy $\varepsilon(\alpha_k) = \varepsilon(\alpha)$ exists, such that:

$$W^{(0)}(\alpha\,\alpha_1) \neq 0 \quad W^{(0)}(\alpha_1\,\alpha_2) \neq 0 \ldots \quad W^{(0)}(\alpha_n\,\alpha') \neq 0 \qquad (6.7)$$

where $W^{(0)}(\alpha_j\,\alpha_k)$ is the λ^0 term of $W_{l\,l'}(\alpha_j\,\alpha_k)$. This assumption also implies that the states $|\alpha\rangle$ are dissipative.

Under these supplementary conditions, one can prove that q_E^{+} and q_E^{-} are equal, and that for λ smaller than a critical value λ_c they are given by:

$$q_E^{\pm}(\alpha_0\,\alpha) = q_E(\alpha_0\,\alpha) = \frac{\Delta_E(\alpha_0)\,\Delta_E(\alpha)}{\int d\,\alpha_1\,\Delta_E(\alpha_1)} \qquad (6.8)$$

with

$$\Delta_E(\alpha) = \frac{1}{2\pi i}\left(D_{E+i0}(\alpha) - D_{E-i0}(\alpha)\right)\,. \qquad (6.9)$$

For $I_E^{\pm}(\alpha_0\,\alpha\,\alpha')$, it follows that:

$$I_E^{\pm}(\alpha_0\,\alpha\,\alpha') = \int d\alpha_1\, q_E(\alpha_0\,\alpha_1)\; V_{E\mp i0,\,E\pm i0}(\alpha_1\,\alpha\,\alpha')\,. \qquad (6.10)$$

---

*) This relation, already assumed by VAN HOVE in S_2, corresponds to a very strong assumption. We hope to be able to show in a further paper how it can be avoided.

This equation is completely equivalent to the expression indicated by PROSPERI[4]) for the value of:

$$\frac{1}{\pi} \lim_{0<\eta\to 0} \eta \langle \alpha \,|\, (R_{E\mp i\eta} A\, R_{E\pm i\eta})_{\mathrm{nd}} \,|\, \alpha' \rangle = \int d\alpha_0\, A(\alpha_0)\, I_E^{\pm}(\alpha_0\, \alpha\, \alpha') \,. \qquad (6.11)$$

Using the explicit expression of $q_E(\alpha_0\, \alpha)$, and equation (3.6), we obtain:

$$I_E^{\pm}(\alpha_0\, \alpha\, \alpha') =$$

$$= \frac{1}{2\pi i} \frac{\Delta_E(\alpha_0)}{\int d\alpha_1\, \Delta_E(\alpha_1)} \int d\alpha_1 (D_{E+i0}(\alpha_1) - D_{E-i0}(\alpha_1))\, V_{E\mp i0,\, E\pm i0}(\alpha_1\, \alpha\, \alpha') =$$

$$= \frac{1}{2\pi i} \frac{\Delta_E(\alpha_0)}{\int d\alpha_1\, \Delta_E(\alpha_1)} \left(R^{\mathrm{nd}}_{E+i0}(\alpha\, \alpha') - R^{\mathrm{nd}}_{E-i0}(\alpha\, \alpha')\right). \qquad (6.12)$$

We note that under the same conditions as previously for $q_E^{\pm}$, the limit is independent of the direction of time:

$$I_E^{\pm}(\alpha_0\, \alpha\, \alpha') = I_E(\alpha_0\, \alpha\, \alpha') \,. \qquad (6.13)$$

Let us define the operator Q_E by the relation:

$$Q_E = \frac{1}{2\pi i} \lim_{0<\eta\to 0} (R_{E+i\eta} - R_{E-i\eta}) \,. \qquad (6.14)$$

For $I_E(\alpha_0\, \alpha\, \alpha')$, we get:

$$I_E(\alpha_0\, \alpha\, \alpha') = \frac{\Delta_E(\alpha_0)\, Q_E^{\mathrm{nd}}(\alpha\, \alpha')}{\int d\alpha_1\, \Delta_E(\alpha_1)} \,. \qquad (6.15)$$

After integration over dE, the final result is given by:

$$\lim_{t\to\pm\infty} I_t(\alpha_0\, \alpha\, \alpha') = I_{\pm\infty}(\alpha_0\, \alpha\, \alpha') = \int_{-\infty}^{+\infty} dE\, \frac{\Delta_E(\alpha_0)\, Q_E^{\mathrm{nd}}(\alpha\, \alpha')}{\int d\alpha_1\, \Delta_E(\alpha_1)} \,. \qquad (6.16)$$

Developing this last equation on both sides in powers of λ, and making use of the relations:

$$R^{(1)}_{E\pm i0}(\alpha\, \alpha') = \frac{-\lambda\, V(\alpha\, \alpha')}{(\varepsilon - E \mp i\,0)\, (\varepsilon' - E \mp i\,0)}\,; \qquad \Delta_E^{(0)}(\alpha) = \delta(E - \varepsilon) \qquad (6.17)$$

we obtain to the lowest order in λ:

$$I^{(1)}_{\pm\infty}(\alpha_0\, \alpha\, \alpha') = -\lambda\, \frac{V(\alpha\, \alpha')}{2\pi i} \int_{-\infty}^{+\infty} \frac{dE\, \delta(\varepsilon_0 - E)}{\int d\alpha_1\, \delta(\varepsilon_1 - E)} \left[\frac{1}{(\varepsilon - \varepsilon_0 - i\,0)\, (\varepsilon' - \varepsilon_0 - i\,0)} + \right.$$

$$\left. - \frac{1}{(\varepsilon - \varepsilon_0 + i\,0)\, (\varepsilon' - \varepsilon_0 + i\,0)}\right] = \frac{\lambda\, V(\alpha\, \alpha')}{\int d\alpha_1\, \delta(\varepsilon_1 - \varepsilon_0)} \left[\delta(\varepsilon - \varepsilon_0) - \delta(\varepsilon' - \varepsilon_0)\right] \left(\frac{1}{\varepsilon - \varepsilon'}\right)_P \,. \qquad (6.18)$$

This corresponds to the result (5.13) obtained in the weak field case, it being noted that the P can be dropped, for there is no singularity for $\varepsilon' \to \varepsilon$.

7. The Complete Master Equation and the Approach to Statistical Equilibrium

For a better understanding of the dynamic behaviour of the whole system under the influence of the perturbation, let us summarize the principal results so far obtained by considering together the diagonal and the non-diagonal part of the various expressions.

We define:

$$\langle \alpha \,|U_{-t}\, A\, U_t|\, \alpha' \rangle = \int d\alpha_0\, A(\alpha_0)\, Z_t(\alpha_0\, \alpha\, \alpha') \tag{7.1}$$

respectively:

$$\langle \alpha \,|R_l\, A\, R_{l'}|\, \alpha' \rangle = \int d\alpha_0\, A(\alpha_0)\, Z_{l\,l'}(\alpha_0\, \alpha\, \alpha') \tag{7.2}$$

where

$$Z_t(\alpha_0\, \alpha\, \alpha') = \frac{-1}{2\,\pi^2} \int_\gamma dl \int_\gamma dl'\, e^{i(l-l')t}\, Z_{l\,l'}(\alpha_0\, \alpha\, \alpha')\,. \tag{7.3}$$

We obtain:

$$\begin{aligned} Z_t(\alpha_0\, \alpha\, \alpha') &= P_t(\alpha_0\, \alpha)\, \delta(\alpha - \alpha') + I_t(\alpha_0\, \alpha\, \alpha')\,, \\ Z_{l\,l'}(\alpha_0\, \alpha\, \alpha') &= X_{l\,l'}(\alpha_0\, \alpha)\, \delta(\alpha - \alpha') + Y_{l\,l'}(\alpha_0\, \alpha\, \alpha')\,. \end{aligned} \tag{7.4}$$

Using relation (3.3), we get:

$$\begin{aligned} R_l(\alpha\, \alpha') - R_{l'}(\alpha\, \alpha') &= (l - l') \int d\alpha_0\, Z_{l\,l'}(\alpha_0\, \alpha\, \alpha') = \\ = \int d\alpha_0\, \big(D_l(\alpha_0) - D_{l'}(\alpha_0)\big)\, &\big(\delta(\alpha_0 - \alpha)\, \delta(\alpha - \alpha') + V_{l\,l'}(\alpha_0\, \alpha\, \alpha')\big)\,. \end{aligned} \tag{7.5}$$

In particular, $Z_{l\,l'}(\alpha_0\, \alpha\, \alpha')$ obeys the equation:

$$\begin{aligned} (l - l')\, Z_{l\,l'}(\alpha_0\, \alpha\, \alpha') &= \big(D_l(\alpha_0) - D_{l'}(\alpha_0)\big)\, \big(\delta(\alpha_0 - \alpha)\, \delta(\alpha - \alpha') + \\ &+ V_{l\,l'}(\alpha_0\, \alpha\, \alpha')\big) - i\,\lambda^2 \int d\alpha_1\, \tilde{W}_{l l'}(\alpha_0\, \alpha_1)\, Z_{l\,l'}(\alpha_1\, \alpha\, \alpha') + \\ &+ i\,\lambda^2 \int d\alpha_1\, \tilde{W}_{l\,l'}(\alpha_1\, \alpha_0)\, Z_{l\,l'}(\alpha_0\, \alpha\, \alpha') \end{aligned} \tag{7.6}$$

from which a general master equation can be derived for a $Z_{E,\,t}(\alpha_0\, \alpha\, \alpha')$ defined mathematically for $t \neq 0$ as:

$$Z_{E,\,t}(\alpha_0\, \alpha\, \alpha') = \frac{1}{2\,\pi^2}\, s(t) \int_\gamma dl\, e^{2\,i\,l\,t}\, Z_{E+l,\,E-l}(\alpha_0\, \alpha\, \alpha') \tag{7.7}$$

where

$$Z_t(\alpha_0\,\alpha\,\alpha') = \int_{-\infty}^{+\infty} dE\; Z_{E,t}(\alpha_0\,\alpha\,\alpha')\,.$$

The general master equation valid for $t \neq 0$ is expressed by

$$\frac{dZ_{E,t}(\alpha_0\,\alpha\,\alpha')}{dt} = h_{E,t}(\alpha_0\,\alpha\,\alpha') + 2\pi\lambda^2 \int_0^t dt' \int d\alpha_1\, w_{E,t-t'}(\alpha_0\,\alpha_1)\, Z_{E,t'}(\alpha_1\,\alpha\,\alpha') +$$
$$- 2\pi\lambda^2 \int_0^t dt' \int d\alpha_1\, w_{E,t-t'}(\alpha_1\,\alpha_0)\, Z_{E,t'}(\alpha_0\,\alpha\,\alpha') \qquad (7.8)$$

where:

$$h_{E,t}(\alpha_0\,\alpha\,\alpha') =$$
$$= \frac{i}{2\pi^2}\, s(t) \int_\gamma dl\; e^{2ilt} \left(D_{E+l}(\alpha_0) - D_{E-l}(\alpha_0)\right) \left(\delta(\alpha_0-\alpha)\,\delta(\alpha-\alpha') +\right.$$
$$\left. + V_{E+l,E-l}(\alpha_0\,\alpha\,\alpha')\right) \qquad (7.9)$$

and $w_{E,t}(\alpha_0\,\alpha)$ is given by (4.3).
Equation (7.8) must be supplemented by the initial condition:

$$Z_{E,0}(\alpha_0\,\alpha\,\alpha') = 0\,. \qquad (7.10)$$

In the limiting case of small perturbation, $Z_t(\alpha_0\,\alpha\,\alpha')$ itself obeys a PAULI master equation:

$$\frac{dZ_t(\alpha_0\,\alpha\,\alpha')}{dt} = 2\pi\lambda^2 \int d\alpha_1\, \delta(\varepsilon_0-\varepsilon_1)\, W^{(1)}_{\varepsilon_0 \mp i0,\, \varepsilon_0 \pm i0}(\alpha_0\,\alpha_1)\, Z_t(\alpha_1\,\alpha\,\alpha') +$$
$$- 2\pi\lambda^2 \int d\alpha_1\, \delta(\varepsilon_0-\varepsilon_1)\, W^{(1)}_{\varepsilon_0 \mp i0,\, \varepsilon_0 \pm i0}(\alpha_1\,\alpha_0)\, Z_t(\alpha_0\,\alpha\,\alpha') \qquad (7.11)$$

with the initial condition:

$$Z_0(\alpha_0\,\alpha\,\alpha') = \delta(\alpha_0-\alpha)\,\delta(\alpha-\alpha') + \frac{\lambda V(\alpha\,\alpha')}{\varepsilon-\varepsilon'} \left(\delta(\alpha_0-\alpha) - \delta(\alpha_0-\alpha')\right). \qquad (7.12)$$

For a dissipative system, the singularity that determines the asymptotic behaviour of $Z_t(\alpha_0\,\alpha\,\alpha')$ is a pseudo-pole of degree one of the function $Z_{E+l,\,E-l}(\alpha_0\,\alpha\,\alpha')$ for $l = 0$ and E solution of the equation $\varepsilon(\alpha) - E - \lambda^2 \times K_E(\alpha) = 0$. [Where $K_E(\alpha)$ is defined by (6.1) and (6.2)]. For very long times:

$$Z_E^{\pm}(\alpha_0\,\alpha\,\alpha') = \lim_{t\to\pm\infty} Z_{E,t}(\alpha_0\,\alpha\,\alpha') = \frac{1}{\pi} \lim_{0>\eta\to 0} \eta\, Z_{E\mp i\eta,\, E\pm i\eta}(\alpha_0\,\alpha\,\alpha') =$$
$$= \int d\alpha_1\, q_E^{\pm}(\alpha_0\,\alpha_1)\, [\delta(\alpha_1-\alpha)\,\delta(\alpha-\alpha') + V_{E\mp i0\;E\pm i0}(\alpha_1\,\alpha\,\alpha')]\,. \qquad (7.13)$$

Under the assumptions of generalized detailed balance $[W_{l\,l'}(\alpha\,\alpha') = W_{l'\,l}(\alpha'\,\alpha)]$, and of interconnexion of states of same unperturbed energy, we obtain:

$$Z_E^{\pm}(\alpha_0\,\alpha\,\alpha') = Z_E(\alpha_0\,\alpha\,\alpha') = \frac{\Delta_E(\alpha_0)\,Q_E(\alpha\,\alpha')}{\int d\alpha_1\,\Delta_E(\alpha_1)} \tag{7.14}$$

where Q_E is defined by (6.14), and Δ_E by (6.9). From (7.14), one immediately derives

$$\lim_{t\to\pm\infty} Z_t(\alpha_0\,\alpha\,\alpha') = Z_{\pm\infty}(\alpha_0\,\alpha\,\alpha') = \int_{-\infty}^{+\infty} dE\,\frac{\Delta_E(\alpha_0)\,Q_E(\alpha\,\alpha')}{\int d\alpha_1\,\Delta_E(\alpha_1)}\,. \tag{7.15}$$

For a diagonal operator A, whose eigenvalue is a smooth function of the state variables α's, we therefore get:

$$\lim_{t\to\pm\infty} \langle\alpha\,|U_{-t}\,A\,U_t|\,\alpha'\rangle = \int_{-\infty}^{+\infty} dE\,\frac{\int d\alpha_0\,A(\alpha_0)\,\Delta_E(\alpha_0)}{\int d\alpha_1\,\Delta_E(\alpha_1)}\,Q_E(\alpha\,\alpha')\,. \tag{7.16}$$

Let us now consider our system to be at time $t = 0$ in the quantum state:

$$|\varphi_0\rangle = \int d\alpha\,|\alpha\rangle\,c(\alpha)$$

and a time T such that the limit value of (7.16) is practically attained for the diagonal operator A. The expectation value at time t for $|\,t\,| \lesssim T$ is given by:

$$\langle A\rangle_t = \langle\varphi_t\,|\,A\,|\,\varphi_t\rangle = \langle\varphi_0\,|U_{-t}\,A\,U_t|\,\varphi_0\rangle$$

so that

$$\langle A\rangle_t = \int d\alpha_0\,d\alpha\,d\alpha'\,A(\alpha_0)\,Z_t(\alpha_0\,\alpha\,\alpha')\,c^*(\alpha)\,c(\alpha')\,. \tag{7.17}$$

For $t \to \pm\,T$, this expression approaches the limit:

$$\lim_{t\to\pm T} \langle A\rangle_t \cong \int_{-\infty}^{+\infty} dE\,\langle A\rangle_E\,p_E \tag{7.18}$$

where

$$\langle A\rangle_E = \frac{\int d\alpha_0\,A(\alpha_0)\,\Delta_E(\alpha_0)}{\int d\alpha_1\,\Delta_E(\alpha_1)} \tag{7.19}$$

and

$$p_E = \int d\alpha\,d\alpha'\,Q_E(\alpha\,\alpha')\,c^*(\alpha)\,c(\alpha')\,. \tag{7.20}$$

Now, Q_E is the projection operator on the energy shell $H_0 + \lambda\,V = E$, and $\langle A\rangle_E$ is the micro-canonical average of a diagonal operator A on the energy shell E. On the other hand, when the system is in its initial state

$|\varphi_0\rangle$, the probability for the total energy $H_0 + \lambda V$ to have a value between E and $E + dE$ is:

$$\langle\varphi_0 | Q_E | \varphi_0\rangle \, dE = \int d\alpha \, d\alpha' \, Q_E(\alpha \, \alpha') \, c^*(\alpha) \, c(\alpha') \, dE \tag{7.21}$$

p_E therefore gives the probability distribution of the total energy in the initial state.

8. Extension of the Results to Non-Diagonal Operators B

What follows represents the natural extension of the results so far obtained for a diagonal operator A to the case of the more general class of non-diagonal operators defined in S_3. The non-diagonal operators B, considered by VAN HOVE, are given by convergent series, each term of which is a product of creation and destruction operators for individual plane wave excitations. It is assumed that the number of creation and destruction operators in each term of the series is finite and independent of the large number N of particles in the system.

Let us consider

$$U_{-t} \, B \, U_t = \frac{-1}{(2\pi)^2} \int_\gamma dl \int_\gamma dl' \, e^{i(l-l')t} \, R_l \, B \, R_{l'} \, . \tag{8.1}$$

In analogy to (3.1a), we now have:

$$\{R_l \, B \, R_{l'}\}_{\mathrm{nd}} = \{(1 - \lambda D_l V + \lambda^2 D_l V D_l V + \ldots) \, (R_l \, B \, R_{l'})_{\mathrm{d}} \times \\ \times (1 - \lambda V D_{l'} + \lambda^2 V D_{l'} V D_{l'} + \ldots)\}_{\mathrm{ind}} \tag{8.2}$$

where, following VAN HOVE:

$$\{R_l \, B \, R_{l'}\}_d = \{R_l \, B_{l\,l'} \, R_{l'}\}_{\mathrm{d}} \tag{8.3}$$

with

$$B_{l\,l'} = \{(1 - \lambda V D_l + \lambda^2 V D_l V D_l + \ldots) \, B \, (1 - \lambda D_{l'} V + \\ + \lambda^2 D_{l'} V D_{l'} V + \ldots)\}_{Bd} \, . \tag{8.4}$$

As in S_3, we mean by the subscript Bd that the 'B-irreducible diagonal' part of the expression (8.4) should be taken, i.e. that diagonal part in which subdiagonal intermediate states outside B are excluded; however, subdiagonal contributions involving at least one intermediate state inside B are allowed.

Let us define:

$$\langle \alpha \mid R_l \, B \, R_{l'} \mid \alpha' \rangle = z_{l\,l'}(\alpha\,\alpha') \tag{8.5}$$

with

$$z_{l\,l'}(\alpha\,\alpha') = \int d\alpha_0 \, B_{l\,l'}(\alpha_0) \; Z_{l\,l'}(\alpha_0\,\alpha\,\alpha') \tag{8.6}$$

and where $B_{l\,l'}(\alpha_0)$ is the eigenvalue of the diagonal operator $B_{l\,l'}$ for the state $|\,\alpha_0\rangle$ and $Z_{l\,l'}(\alpha_0\,\alpha\,\alpha')$ is given by (7.2).

In analogy to (7.17), we consider the expectation value:

$$\langle B \rangle_t = \langle \varphi_0 \mid U_{-t} \, B \, U_t \mid \varphi_0 \rangle \tag{8.7}$$

where the initial state $|\,\varphi_0\rangle$ is expanded in the $|\,\alpha\rangle$ eigenfunctions as in (2.7). We get:

$$\langle B \rangle_t = \frac{-1}{(2\,\pi)^2} \int_\gamma dl \int_\gamma dl' \, e^{i(l-l')t} \int d\alpha \, d\alpha' \, z_{l\,l'}(\alpha\,\alpha') \, c^*(\alpha) \, c(\alpha') \, . \tag{8.8}$$

The asymptotic behaviour of $\langle B \rangle_t$ is determined by the singularities of $z_{l\,l'}(\alpha\,\alpha')$ as a function of the complex variables l and l'. According to S_3 and to the results obtained in our previous paragraph, the pseudo-poles of $z_{E+l,\,E-l}$ are the same as those of $X_{E+l,\,E-l}$, so that in the limit for $t \to \pm\infty$ we find:

$$\langle B \rangle_{\pm\infty} = \frac{1}{\pi} \int_{-\infty}^{+\infty} dE \int d\alpha \, d\alpha' \lim_{0<\eta\to 0} \{\eta \, z_{E\mp i\eta,\,E\pm i\eta}(\alpha\,\alpha')\} \, c^*(\alpha) \, c(\alpha') =$$

$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} dE \int d\alpha_0 \, d\alpha \, d\alpha' \, B_{E\mp i0,\,E\pm i0}(\alpha_0) \lim_{0<\eta\to 0} \eta \, Z_{E\mp i\eta,\,E\pm i\eta}(\alpha_0\,\alpha\,\alpha') \times$$

$$\times \, c^*(\alpha) \, c(\alpha') \, . \tag{8.9}$$

Using equations (7.13) and (7.14), we obtain

$$\langle B \rangle_{\pm\infty} = \int_{-\infty}^{+\infty} dE \, \frac{\int d\alpha_0 \, d\alpha \, d\alpha' \, B_{E\mp i0,\,E\pm i0}(\alpha_0) \, \Delta_E(\alpha_0) \, Q_E(\alpha\,\alpha') \, c^*(\alpha) \, c(\alpha')}{\int d\alpha_1 \, \Delta_E(\alpha_1)} \, . \tag{8.10}$$

Q_E being the projection operator on the energy shell considered in (6.14). We now define

$$\langle B \rangle_E = \left[\int d\alpha \, \Delta_E(\alpha)\right]^{-1} \int d\alpha_0 \, B_{E\mp i0,\,E\pm i0}(\alpha_0) \, \Delta_E(\alpha_0) \tag{8.11}$$

and we get:

$$\langle B \rangle_{\pm\infty} = \int_{-\infty}^{+\infty} dE \, \langle B \rangle_E \, p_E \tag{8.12}$$

where p_E is the same as in (7.20).

The microcanonical average of B is

$$\mathrm{Sp}(B\,Q_E)\,/\,\mathrm{Sp}(Q_E) \tag{8.13}$$

Using (3.3), (6.5a), (6.6) (6.8) and (6.14), we can evaluate $\mathrm{Sp}(B\,Q_E)$:

$$\begin{aligned}\mathrm{Sp}(B\,Q_E) &= \frac{1}{\pi} \lim_{0<\eta\to 0} \eta\,\mathrm{Sp}(R_{E\mp i\eta}\,B\,R_{E\pm i\eta}) = \\ &= \frac{1}{\pi} \lim_{0<\eta\to 0} \eta\,\mathrm{Sp}(R_{E\mp i\eta}\,B_{E\mp i\eta, E\pm i\eta}\,R_{E\pm i\eta}) = \\ &= \frac{1}{\pi}\int d\alpha_0\,B_{E\mp i0, E\pm i0}(\alpha_0)\int d\alpha \lim_{0<\eta\to 0} \eta\,X_{E\mp i\eta, E\pm i\eta}(\alpha_0\,\alpha) = \\ &= \int d\alpha_0\,B_{E\mp i0, E\pm i0}(\alpha_0)\,\Delta_E(\alpha_0)\,.\end{aligned}$$

Consequently:

$$\mathrm{Sp}(B\,Q_E) = \int d\alpha_0\,B_{E\mp i0, E\pm i0}(\alpha_0)\,\Delta_E(\alpha_0)\,. \tag{8.14}$$

By comparing (8.14) with (8.11) and remembering that $\mathrm{Sp}(Q_E)$ is $\int d\alpha\,\Delta_E(\alpha)$, one recognizes that $\langle B\rangle_E$ is in fact the microcanonical average over the energy shell. We have therefore established the ergodic behaviour of our system also for the non-diagonal operators B, without any random phase assumption for the initial state.

9. Concluding Remarks

The main conclusion of our work is that the special properties of the pertubation responsible for the dissipative behaviour of the system are sufficient to derive the quantum mechanical transport equation. No random phase assumption at all is needed. On the other hand, we have established the approach to microcanonical equilibrium values for a class of diagonal operators, and this for arbitrary initial states. The result has been generalized to a wider class of macroscopic operators[5]). The fact that a special choice of initial states may give rise to large deviations from the equilibrium value after a very long time does not invalidate our result, because nothing is said (to general order in λ) about the relaxation time for the system, which of course strongly depends on the proper choice of the initial phases, and may even become infinite. So the question of approach to equilibrium is shifted to another question, i.e. how fast does the system do it. Now very little is known about the solution of the general master equation. The fact that the complete master equation which we have derived here is of the same type as that analyzed by Van Hove and Verboven[6]) increases the interest of their results.

Finally, we may point out that the dissipative, or non-dissipative, behaviour of a state with respect to a given perturbation is of primary importance for a discussion of irreversibility, and needs further investigations.

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