The density matrix of a dissipative system
R. Omnès

To cite this version:
10.1051/jphys:019850046010100 . jpa-00209942
The density matrix of a dissipative system

R. Omnès
Laboratoire de Physique Théorique et Hautes Energies, Université Paris-Sud, 91405 Orsay, France
(Reçu le 1er juin 1984, accepté le 25 septembre 1984)

Résumé. — Partant de la théorie de la réponse linéaire et d'une expression phénoménologique du type du chaos quantique pour les éléments de matrice du courant électrique, nous établissons au premier ordre en calcul de perturbation la forme de la matrice densité d'un conducteur porteur de courant en contact avec un thermostat. Cette forme est remarquablement simple et suggère une généralisation naturelle dans laquelle un hamiltonien brisant l'invariance de sens du temps décirait le système à tous les ordres du calcul de perturbation.

Abstract. — Using linear response theory and a phenomenological quantum-chaos expression for the matrix elements of current in a conductor carrying current and in contact with a thermostat, we have obtained to first order in perturbation theory the statistical density matrix of the system. It turns out to have a very simple form which suggests a generalization in which a time-oriented Hamiltonian would describe the system to all orders of perturbation theory.

1. Introduction.

The present work is concerned with the rather elementary question of finding the statistical density matrix of a dissipative system in contact with a thermostat. More precisely, we consider the case of a current-carrying conductor.

Our starting point is a simple property for the matrix elements of the current which is typical of quantum chaos (Eq. (3)). Although some properties of chaos are used, our approach does not rely on fundamental principles but on simple phenomenology.

We find that, to first order in perturbation, the density matrix of the conductor is of the form $\exp(-\beta H)$ where $H$ turns out not to depend on $\beta$ (which is not obvious a priori for a system out of thermal equilibrium). More precisely, one has

$$H = H_0 - E_0 \int_{-\infty}^{0} \dot{X}(t) \, dt$$

(0)

where $H_0$ is the Hamiltonian of the unperturbed conductor, $E_0$ the applied electric field, $X$ the dipole moment along the field and $\dot{X} = dX/dt$. Because of the chaotic behaviour of matrix elements, the integral in equation (0) has nothing to do with its naive value $X(0)$.

If $H$ is interpreted as a Hamiltonian, it is found to break time-reversal invariance and to have memory of past fluctuations.

We propose to generalize equation (0) to define intrinsically the Hamiltonian $H(t)$ of a dissipative system, when $X(t)$ is supposed to evolve with $H(t)$. Some cancellations of divergences in the calculation of noise to higher order in perturbation theory may suggest a deeper meaning for equation (0).

2. The matrix elements of current.

Let us consider a cylindrical conductor with axis along the $x$-direction and length $L$. The $x$-component of the total dipole moment is denoted by $X$ and its time derivative $\dot{X}$ is related to the current intensity $I$ by $\dot{X} = IL$.

Some information about the matrix elements of the operator $I$ can be obtained through a comparison of the Nyquist formula with the quantum expression of the noise intensity. When no external potential is applied to the conductor, the noise in $I$ is given by the quantum formula [1-4]
where \( S_f(\omega) \) is the spectral density of noise for \( I \), the states \( |i\rangle, |j\rangle \) are eigenstates of the conductor Hamiltonian \( H_0 \) with energies \( E_i, E_j \); \( I_{ij} \) is the matrix element \( \langle i | I | j \rangle \), \( \omega_{ij} \) is an energy difference \( \omega_{ij} = E_j - E_i \) or a frequency (using \( \hbar = 1 \)) and \( F \) is the free energy.

According to the fluctuation-dissipation theorem (Nyquist formula), \( S_f(\omega) \) is related to the resistance \( R(\omega) \) by

\[
S_f(\omega) = \frac{1}{2} kT R^{-1}(\omega) .
\]

Now, it is known that \( R^{-1}(\omega) \) is essentially a constant for a large range of values and behaves as \( (\omega^2 \tau^2 + 1)^{-1} \) for large \( \omega, \tau \) being the mean free time for electrons.

Already at the classical level, the behaviour of electron scattering in the conductor is expected to be chaotic in the Kolmogorov-Arnold-Moser sense. At the quantum level, this means that the matrix elements of \( I \) have random phases but depend very little, in their modulus, upon the eigenstates so that, when inserted into a sum, one can write phenomenologically an expression for the matrix elements such as \([5-13]\)

\[
I_{ij} I_{kl} = \delta_{ik} \delta_{jl} F^2(\omega^2 \tau^2 + 1)^{-1}
\]

where the number \( F^2 \) is essentially a constant.

It follows from equation (3) that the dipole operator \( X \), contrary to \( I \) is a badly behaved operator since

\[
X_{ij} X_{kl} = -(\omega_{ij} \omega_{kl})^{-1} \delta_{ik} \delta_{jl} F^2(\omega^2 \tau^2 + 1)^{-1} .
\]

Because of the \( \omega \)-factors in the denominator, calculations of the noise to higher than second order in perturbation theory meets with bad divergences so that, to our knowledge, there is no complete consistent theory.

3. Density matrix of a conductor.

We shall use these remarks concerning the character of operators to clarify the description of the statistical state for this dissipative system and more precisely, the density matrix of a conductor carrying current. Despite the fact that it is not in thermodynamic equilibrium because of dissipation, such a conductor should have a stationary density matrix when in contact with a thermostat.

Let us start from the theory of linear response, assuming that an adiabatically varying electric field

\[
E = \frac{1}{2} [E_0 \exp(-i\omega_0 t) + \text{c.c.}]
\]

is applied to the conductor. The average value of an arbitrary physical quantity \( Y \), after subtracting its average value at equilibrium, will behave as

\[
\langle Y \rangle = \frac{1}{2} [Y_0 \exp(-i\omega_0 t) + \text{c.c.}]
\]

and, to first order in \( E_0 \), one should have a generalized susceptibility \( \chi_{xy}(\omega) \) such that

\[
Y_0 = \chi_{xy}(\omega_0) E_0 .
\]

Taking for the Hamiltonian \( H = H_0 - XE \), one has formally, using perturbation theory [1]

\[
\chi_{xx}(\omega) = \frac{1}{2} \sum_{ij} \exp \beta(F-E) \{ X_{ij} Y_{kj}(\omega - \omega_{ij} + i0)^{-1} - Y_{ij} X_{kj}(\omega_{ij} + i0)^{-1} \} .
\]

Let us assume the existence of an adiabatically varying matrix density \( \rho(t) \) such that

\[
\langle Y(t) \rangle = \text{Tr}(\rho(t) Y) .
\]

Taking \( \rho(t) \) in the form

\[
\rho(t) = \rho_1 e^{-i\omega_0 t} + \rho_1^* e^{i\omega_0 t} .
\]

One sees that \( \rho_1 \) should satisfy the relation

\[
\text{Tr}(\rho_1 Y) = Y_0 = \chi_{xy}(\omega_0) E_0 .
\]

This relation should be true for any operator \( Y \) and any adiabatic value of \( \omega_0 \). It therefore defines uniquely in principle \( \rho_1(\omega) \) and, in the limit \( \omega_0 \to 0 \), it defines the density matrix \( \rho = \rho_1 + \rho_1^* \) for the stationary dissipative system.

Let us look for a matrix \( \rho(t) \) in the form

\[
\rho(t) = \exp[-\beta(H_0 + U(t))] Z^{-1}
\]

where \( Z \) is a number and we try to find an operator

\[
U(t) = \frac{1}{2} (\hat{U} \exp(-i\omega_0 t) + \hat{U}^* \exp(i\omega_0 t))
\]

such that (12) be satisfied to first order in perturbation. Here again the calculation is straightforward and gives

\[
\rho_{ij} = \exp \beta(F-E_j) \delta_{ij} \left[ 1 + \beta \sum_k \exp \beta(F-e_k) \hat{U}_{kk} \right] - \omega_{ij}^{-1} U_{ij} \exp \beta(F-E_j) \exp \beta(F-E_i)
\]

wherefrom, using (13)
\[ Y_0 = -\frac{1}{2} \sum_{ij} \omega_{ij}^{-1} \bar{U}_{ij} Y_\mu \left[ \exp \beta (F - E_j) - \exp \beta (F - E_i) \right] + \]
\[ + \frac{1}{2} \beta \left[ \sum_i \exp \beta (F - E_i) Y_{\mu} \right] \left[ \sum_i \exp \beta (F - E_i) \bar{U}_{\mu} \right]. \quad (14) \]

The second term drops out since it is proportional to the equilibrium average value of \( Y \) which has been put equal to zero in the definition of the measured quantity \( Y \). Comparing Equation (15) for \( Y_0 \) with the equations (7) and (8), written in the form

\[ Y_0 = \frac{1}{2} \left\{ \exp \beta (F - E_i) \left( \omega - \omega_{ij} + it0 \right)^{-1} \right\} + \]
\[ \exp \beta (F - E_j) \left( \omega_{ij} - \omega - it0 \right)^{-1} \times E_o X_{ij} Y_{ji} \quad (15) \]

and identifying (14) and (15) one obtains an expression for \( U_{ij} \) which gives, in the limit \( \omega \to 0 \):

\[ \bar{U}_{ij} = -E_o \omega_{ij} X_{ij}(\omega_{ij} - it0)^{-1} \quad (16) \]
\[ \bar{U}_{ij} = iE_o \dot{X}_{ij}(\omega_{ij} - 0)^{-1}. \quad (17) \]

In the Heisenberg representation, equation (17) is equivalent to

\[ \bar{U}_{ij}(t) = -E_o \int_{-\infty}^{t} \dot{X}(t') dt' \quad (18) \]

or finally

\[ \rho(0) \sim \exp -\beta \left[ H_0 - E_0 \int_{-\infty}^{0} \dot{X}(t') dt' \right]. \quad (19) \]

This looks very much like a naive expression

\[ \exp -\beta(H_0 - E_0 X) \quad (20) \]

which however would give in place of equation (17) the expression

\[ \bar{U}_{ij} = iE_o \dot{X}_{ij} \omega_{ij}^{-1}. \quad (21) \]

The two expression (17) and (21) differ as \( \omega_{ij}^{-1} \) is replaced by \( (\omega_{ij} - it0)^{-1} \). This is a non-trivial difference since, according to equation (3), the matrix elements \( \dot{X}_{ij} \) do not vanish for \( \omega_{ij} \to 0 \). This property of a system exhibiting quantum chaos is to be contrasted with the free electron model where \( \dot{X}_{ij} \) vanishes for \( \omega_{ij} = 0 \).

4. Conclusion

Our main conclusion is therefore that one can find, to first order in perturbation theory, the density matrix of a dissipative conductor in contact with a thermostat. It happens to be of the form \( \exp(-\beta H) \), up to the usual normalization constant, with

\[ H = H_0 - E_0 \int_{-\infty}^{0} \dot{X}(t') dt' \quad (22) \]

or, more generally \( \rho(t) = \exp -\beta H(t) \) with

\[ H(t) = H_0 - E_0 \int_{-\infty}^{t} \dot{X}(t') dt' \quad (23) \]

This result suggests a generalization: assume that \( \dot{X}(t') \) is given in the integral by

\[ \dot{X}(t) = V^{-1}(t) \dot{X}(- \infty) V(t) \quad (24) \]

with

\[ i \frac{\partial V}{\partial t} = H(t) V(t) \quad (25) \]

Then \( H(t) \) is intrinsically defined by equation (23) and can be computed to any desired order of perturbation theory, although the calculations are somewhat involved.

Perhaps the most interesting property of such a Hamiltonian is the way by which it violates time-reversal invariance. Even at the level of equation (24), it is noticeable that, assuming nowhere time-reversal breaking, and using only a property of matrix elements characteristic of quantum chaos, we obtain an operator having memory in a well-defined and correct direction of time.

The mathematical origin of the choice in time direction can easily be traced back to equation (8). It comes at a certain stage in the calculation in defining the evolution operator as equal to identity at time \( t = -\infty \).

An obvious check in the significance of our last assumption (Eqs. (25) and (26)) is to consider what happens to the divergences of \( S_{ij}(\omega) \) when one goes further than first order perturbation. The calculations are however difficult and many perturbation graphs have to be computed. On a few typical ones, we have found a reduction of divergences and it is therefore quite interesting to find a systematic and convenient way for performing these calculations to check whether or not this expression for \( H(t) \) has a real physical meaning or is no more than an amusing and simple remark.
References