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► **To cite this version:**

M. Combescure, D. Robert. A semiclassical approach in the linear response theory. Conference Internationale on Quantum Results in Mathematical Physics, Dec 2001, Taxco, Mexico. pp.83-88. in2p3-00012232

HAL Id: in2p3-00012232

<https://hal.in2p3.fr/in2p3-00012232>

Submitted on 7 Apr 2003

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A semiclassical Approach in the Linear Response Theory

M. Combescure and D. Robert

ABSTRACT. We consider a quantum system of non-interacting fermions at temperature T , in the framework of linear response theory. We show that semiclassical theory is an appropriate framework to describe some of their thermodynamic properties, in particular through asymptotic expansions in \hbar (Planck constant) of the dynamical susceptibilities. We show how the orbits of the classical motion in phase space manifest themselves in these expansions, in the regime where T is of the order of \hbar .

Consider a system of non-interacting fermions confined by an external potential and in contact with an exterior reservoir at temperature T . Assume that a time-varying external perturbation drives the system out to, but near of, its equilibrium state. The response of this quantum system to an external time-dependent perturbation is a subject of high physical interest, which can be investigated experimentally, in particular the so-called “dynamical susceptibility”. A complete rigorous analysis of this problem is still lacking, although recent progress is being made in the understanding of non-equilibrium statistical mechanism, and of its link with the underlying chaotic dynamics [11, 12, 18].

A semi-empirical route which has been proposed (see classical textbooks [14, 15]) consists, for small perturbation, of investigating the response function “to first order of the perturbation”, i.e. the so-called “linear response theory”. This semi-empirical route has been given a firmer foundation (see the book by Bratelli and Robinson [4]) where a link with the KMS condition is established. (See also recent progress in [18]).

In this paper we rederive, formally, the first order response function for the quantum fermionic system under study, i.e. the so-called “generalized Kubo formula” (see also [2]) and investigate semiclassical expansions of it, assuming suitable “chaoticity assumptions” on the one-body underlying classical dynamics. These semiclassical expansions are developed in a similar spirit as previous studies on the “semiclassical magnetic response for non-interacting electrons” [1, 5, 7, 10, 13, 16, 17] i.e. we exhibit a low temperature regime where the closed classical orbits of one-particle motion manifest themselves as oscillating corrections to the response function.

We shall present here the physical objects under study, and give some assumptions under which a mathematical treatment can be applied.

Consider a system of non-interacting fermions living in \mathbb{R}^n , each fermion being

subject to a one-body Hamiltonian \widehat{H} which is the Weyl quantization of a classical Hamiltonian $H(q, p)$ of the form

$$(0.1) \quad H(q, p) = \frac{p^2}{2m} + V(q)$$

with $V \in C^\infty(\mathbb{R}^n)$ such that

$$(0.2) \quad V(q) \geq c_0(1 + q^2)^{s/2} \quad s, c_0 > 0 .$$

Under these assumptions, \widehat{H} is self-adjoint in $L^2(\mathbb{R}^n)$ and its spectrum is pure point, and contained in $[0, \infty)$. Assume our system is in contact with a reservoir at temperature T , and chemical potential μ , and define the Fermi-Dirac function, as usual:

$$(0.3) \quad f(x) = \left(1 + e^{\beta(x-\mu)}\right)^{-1}$$

where $\beta = 1/kT$ (k being the Boltzmann constant). Then the total number of fermions in the system is related to T and μ by:

$$(0.4) \quad N = f(\widehat{H})$$

where the trace is taken in the operator sense in $\mathcal{H} = L^2(\mathbb{R}^n)$, and the trace-one operator:

$$(0.5) \quad \widehat{\rho}_{eq} = N^{-1} f(\widehat{H})$$

is the "equilibrium state" for the fermionic system under consideration.

Assume that this system, being in the far past prepared in the state (0.5) is submitted adiabatically to the one-body perturbed Hamiltonian

$$(0.6) \quad \widehat{H}(t) = \widehat{H} + \lambda \widehat{A}F(t)$$

where \widehat{A} is self-adjoint in $L^2(\mathbb{R}^n)$ (being the Weyl quantization of a symbol $A(q, p)$ that we shall make precise later), and F is any continuous function that equals one on the positive real axis, and is integrable on the negative real axis, for example:

$$(0.7) \quad F(t) = e^{nt} \quad t < 0 \quad F(t) = 1 \quad t \geq 0 .$$

In the "linear response theory" we try to solve the following problem : find a "density matrix" $\widehat{\rho}_{eq}(t)$ (i.e. a trace one operator in $L^2(\mathbb{R}^n)$) which, to the first order in the perturbation solves

$$(0.8) \quad i\hbar \frac{\partial \widehat{\rho}}{\partial t} = \left[\widehat{H}(t), \widehat{\rho} \right]$$

with "initial condition" at $t = -\infty$ being

$$(0.9) \quad \lim_{t \rightarrow -\infty} \widehat{\rho}_{eq}(t) = \widehat{\rho}_{eq} .$$

Let $V_\lambda(t, t_0)$ be the unitary evolution operator induced by $\widehat{H}(t)$ (namely solving

$$(0.10) \quad i\hbar \frac{dV_\lambda(t, t')}{dt} = \widehat{H}(t) V_\lambda(t, t')$$

with $V_\lambda(t_0, t_0) = 1$, and let

$$(0.11) \quad U(t) := e^{-it\widehat{H}/\hbar} .$$

We know using [19] that $V_\lambda(t, t')$ solution of (0.10) exists under the following :

Assumption 1: $A(q)$ is a multiplicative function dominated by $C(1 + q^2)$ in absolute value.

We can check that :

$$(0.12) \quad \widehat{\rho}(t, t_0; \lambda) = V(t, t_0) \widehat{\rho}_{eq} V(t_0, t)$$

solves (0.12) with $\widehat{\rho}(t_0) = \widehat{\rho}_{eq}$.

Moreover $\widehat{\rho}(t, t_0; \lambda)$ has a limit as $t_0 \rightarrow -\infty$, in the trace-class operator norm sense , which is called $\widehat{\rho}_{eq}(t; \lambda)$

Then using Duhamel's formula, we can write :

$$(0.13) \quad \widehat{\rho}_{eq}(t; \lambda) - \widehat{\rho}_{eq} = \frac{\lambda}{i\hbar} \int_{-\infty}^t dt' F(t') [\widehat{\rho}_{eq}, \widehat{A}_{t-t'}] + o(\lambda)$$

\widehat{A}_t being by definition the Heisenberg observable at time t (for the evolution governed by \widehat{H})

$$(0.14) \quad \widehat{A}_t = U(t) \widehat{A} U(t)^* .$$

Equation (0.13) is the linear response formula in this framework. It implies that if \widehat{B} is some self-adjoint operator that we want to measure in the “stationary” state $\widehat{\rho}_{eq}(t)$, the first order contribution in λ as $\lambda \rightarrow 0$ to the result :

$$(0.15) \quad J(t) = Tr \left\{ \widehat{B} (\widehat{\rho}_{eq}(t, \lambda) - \widehat{\rho}_{eq}) \right\}$$

is of the form :

$$(0.16) \quad J_L(t) = \lambda \int_{-\infty}^t dt' F(t') \Phi(t - t')$$

where

$$(0.17) \quad \Phi(t) = \frac{1}{i\hbar} Tr \left(\widehat{B} [\widehat{\rho}_{eq}, \widehat{A}_t] \right)$$

$$(0.18) \quad = \frac{1}{i\hbar} Tr \left(\widehat{\rho}_{eq} [\widehat{A}, \widehat{B}_{-t}] \right)$$

using the cyclicity of the trace.

We now take the Fourier transform, in the distributional sense of $\Phi(t)$, called the “generalized susceptibility” :

$$(0.19) \quad \chi_{A,B}(\omega) = \int_{-\infty}^{+\infty} \Phi(t) e^{i\omega t} dt$$

Our aim is to study the semiclassical behaviour of $\chi_{A,B}$ in distributional sense as $T \rightarrow 0$. Setting:

$$(0.20) \quad \sigma = \beta \hbar$$

and

$$(0.21) \quad f_\sigma(x) = (1 + e^{x\sigma})^{-1}$$

and given any real g in the Schwartz class we have formally:

$$(0.22) \quad \int \chi_{A,B}(\omega) g(\omega) d\omega = \frac{1}{i\hbar} \int_{-\infty}^{+\infty} Tr \left(f_\sigma \left(\frac{\widehat{H} - \mu}{\hbar} \right) [\widehat{A}, \widehat{B}_t] \right) \widetilde{g}(t) dt$$

In order to avoid the singularity in $x = 0$ of $f_\sigma(x)$, (\widetilde{f}_σ being the Fourier Transform of f_σ) we replace f_σ by:

$$(0.23) \quad f_{\sigma,\eta} = f_\sigma * \eta$$

with $\widetilde{\eta} \in C_0^\infty(\mathbb{R})$ and therefore study a corresponding "regularized susceptibility", or in other words a distribution $\chi_{A,B}(s, \omega)$ in two variables s and ω in $\mathcal{D}'(\mathbb{R}^2)$ such that (0.22) is replaced by:

$$(0.24) \quad \int \int \chi_{A,B}(s, \omega) \widetilde{\eta}(s) g(\omega) ds d\omega = \frac{1}{2i\pi\hbar} \int \int Tr \left(e^{is(\widehat{H} - \mu)/\hbar} [\widehat{A}, \widehat{B}_t] \right) \widetilde{f}_\sigma(s) \widetilde{\eta}(s) \widetilde{g}(t) ds dt$$

Let ϕ^t be the classical flow induced by Hamiltonian (0.1). Consider Σ_μ the energy surface conserved by the flow:

$$(0.25) \quad \Sigma_\mu = \{(q, p) \in \mathbb{R}^{2n} : H(q, p) = \mu\}$$

We call $d\Sigma_\mu$ the Liouville measure on Σ_μ , so that the correlation of classical observables A and B on Σ_μ is defined by:

$$(0.26) \quad C_{A,B}(t) = \int_{\Sigma_\mu} A \cdot B_t d\Sigma_\mu$$

where $B_t(z) = B[\phi^t(z)]$. Moreover if γ is any periodic orbit on Σ_μ , and γ^* the corresponding primitive orbit, with period T_{γ^*} , we introduce the correlation function

$$(0.27) \quad c_{\gamma^*}(t) = \int_0^{T_{\gamma^*}} A_s(q, p) B_{s+t}(q, p) ds \quad (q, p) \in \gamma^*$$

c_{γ^*} being T_{γ^*} -periodic it admits the Fourier-series expansion:

$$(0.28) \quad c_{\gamma^*}(t) = \sum_{k=-\infty}^{k=+\infty} c_{\gamma^*,k} e^{2ikt\pi/T_{\gamma^*}}$$

To each γ is associated a corresponding "linearized Poincaré map" called P_γ , a classical action along γ called S_γ , and a Maslov index ν_γ (see [6]).

Let us assume that ϕ^t on Σ_μ satisfies the:

Gutzwiller Assumption:

Assumption 2 The periodic orbits γ are non-degenerate, i.e the Poincaré maps do not have 1 as eigenvalue (which implies that they are isolated).

Moreover B has to obey:

Assumption 3

$$|\partial_q^\alpha \partial_p^\beta B(q, p)| \leq C_{\alpha\beta} \quad |\alpha| + |\beta| \geq 2$$

$$|\partial_q^\alpha V| \leq C_\alpha \quad |\alpha| \geq 2$$

Our result is as follows:

THEOREM 0.1. *Under Assumptions 1,2,3, we have, in distributional sense in $\mathcal{D}'(\mathbb{R}^2)$:*

$$\chi_{A,B}(s, \omega) \asymp -i\hbar^{-n} \delta_0(s) \otimes \widetilde{C'_{A,B}}(\omega) + \sum_{j \geq 1} \hbar^j \mu_j(s, \omega)$$

$$+ \sum_{\gamma: T_\gamma \neq 0} \frac{\pi e^{i(S_\gamma/\hbar + \nu_\gamma \pi/2)}}{\hbar \sigma \sinh(\pi T_\gamma/\sigma) |\det(1 - P_\gamma)|^{1/2}} \left(\delta_{T_\gamma}(s) \otimes \sum_k c_{\gamma^*,k} \delta(\omega - \frac{2k\pi}{T_{\gamma^*}}) + \sum_{j \geq 1} \hbar^j \nu_{j,\gamma}(s, \omega) \right)$$

where μ_j and $\nu_{j,\gamma}$ are distributions in $\mathcal{D}'(\mathbb{R}^2)$ such that $\text{Supp}(\mu_j) \subseteq \{0\} \times \mathbb{R}$, $\text{Supp}(\nu_{j,\gamma}) \subseteq \{T_\gamma\} \times \mathbb{R}$.

Proof: The complete proof is given in [8]. The idea is to develop the trace as an integral over coherent states in \mathcal{H} , and to obtain the asymptotic expansions in \hbar by stationary phase theorems as in [6].

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