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A semiclassical Approach in the Linear Response Theory

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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 $\hat{H}$ 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, $\hat{H}$ 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:

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

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

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

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

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

where $\hat{A}$ 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:

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

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

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

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 $\hat{H}(t)$ (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:

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

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

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

with $\tilde{\eta} \in C_0^\infty(\mathbb{R})$ 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:

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

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

$$\begin{aligned} |\partial_q^\alpha \partial_p^\beta B(q, p)| &\leq C_{\alpha\beta} & |\alpha| + |\beta| &\geq 2 \\ |\partial_q^\alpha V| &\leq C_\alpha & |\alpha| &\geq 2 \end{aligned}$$

Our result is as follows:

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

$$\begin{aligned} \chi_{A,B}(s, \omega) &\asymp -i\hbar^{-n} \delta_0(s) \otimes \widetilde{C'_{A,B}}(\omega) + \sum_{j \geq 1} \hbar^{j-n} \mu_j(s, \omega) \\ &+ \sum_{\gamma: T_\gamma \neq 0} \frac{\pi e^{i(S_\gamma/\hbar + \nu_\gamma \pi/2)}}{\hbar \sigma \sinh(\pi T_\gamma/\sigma) |\det(1 - P_\gamma)|^{1/2}} \left(\delta_{T_\gamma}(s) \otimes \sum_k c_{\gamma*,k} \delta(\omega - \frac{2k\pi}{T_{\gamma*}}) + \sum_{j \geq 1} \hbar^j \nu_{j,\gamma}(s, \omega) \right) \end{aligned}$$

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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