

Semiclassical results in the linear response theory

Monique Combescure

*Laboratoire de Physique Théorique, CNRS - UMR 8627
Université de Paris XI, Bâtiment 210, F-91405 ORSAY Cedex, France
and*

*IPNL, Bâtiment Paul Dirac
4 rue Enrico Fermi, Université Lyon-1
F.69622 VILLEURBANNE Cedex, France
email monique.combescure@ipnl.in2p3.fr*

Didier Robert

*Département de Mathématiques
Laboratoire Jean Leray, CNRS-UMR 6629
Université de Nantes, 2 rue de la Houssinière,
F-44322 NANTES Cedex 03, France
email Didier.Robert@math.univ-nantes.fr*

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 closed orbits of the classical motion in phase space manifest themselves in these expansions, in the regime where T is of the order of \hbar .

1 Introduction

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 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 [5]) where a link with the KMS condition is established. (See also recent progress in [18]).

In this paper we rederive 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, 6, 8, 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.

Section 2 contains , for pedagogical purposes the basic framework of so-called “second quantization” in which the physical system under consideration can be studied and its thermodynamical properties mathematically investigated. Section 3 presents the so-called “linear-response theory”, and the dynamical susceptibility that will be studied in the semiclassical framework. Section 4 presents and derives the main results of this paper: a rigorous semiclassical expansion of the dynamical susceptibility under suitable assumptions on the physical system.

2 The physical model

Consider a system of non-interacting fermions, living in \mathbb{R}^n , subject to a one-body Hamiltonian \widehat{H} which is the Weyl quantization of a classical Hamiltonian $H(q, p)$ of the form

$$H(q, p) = \frac{p^2}{2m} + V(q) \quad (2.1)$$

with $V \in \mathcal{C}^\infty(\mathbb{R}^n)$ such that the following confining assumption holds:

Assumption 1:

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

Under these assumptions, \widehat{H} is self-adjoint in $L^2(\mathbb{R}^n) = \mathcal{H}$ and its spectrum is pure point, and contained in $]0, \infty)$.

Assume that the system of non-interacting fermions is infinite and in contact with a reservoir at temperature T . The study of thermodynamical properties of this system is performed within the framework of statistical mechanics which is well known, and that we recall here for completeness (see [6]). We introduce the so-called Fock space:

$$\mathcal{F}_a = \bigoplus_{n=0}^{\infty} (\otimes_a^n \mathcal{H}) \quad (2.2)$$

where $\otimes_a^n \mathcal{H}$ is the antisymmetric tensor product of \mathcal{H} , which physically represents the space of n-fermions states. The Hamiltonian of the infinite system is governed by the second quantization of \widehat{H} :

$$d\Gamma(\widehat{H}) = \widehat{\widehat{H}} \quad (2.3)$$

acting in \mathcal{F}_a . Similarly the number \widehat{N} of particles is a second quantized operator in \mathcal{F}_a :

$$\widehat{N} = d\Gamma(\mathbb{1}_{\mathcal{H}}) \quad (2.4)$$

Note that if $\{\psi_j\}_{j \geq 0}$ denotes an orthonormal basis of eigenfunctions of \widehat{H} , with eigenvalue E_j :

$$\widehat{H}\psi_j = E_j\psi_j \quad (2.5)$$

then:

$$\{\psi_{j_1} \wedge \psi_{j_2} \wedge \dots \wedge \psi_{j_n}\}_{j_1 < j_2 < \dots < j_n} \quad (2.6)$$

is an orthonormal basis of $\otimes_a^n \mathcal{H}$ consisting of eigenvectors of \widehat{H} with eigenvalue $E_{j_1} + \dots + E_{j_n}$.

According to the Pauli principle, the occupation number n_j of any state ψ_j in \mathcal{F}_a equals 0 or 1. Thus the spectrum of \widehat{H} can be rewritten as:

$$\sum_j n_j E_j$$

where n_j is the eigenvalue of $\widehat{N}_{j,n}$:

$$\widehat{N}_{j,n}(\psi_{j_1} \wedge \psi_{j_2} \wedge \dots \wedge \psi_{j_n}) = n_j(\psi_{j_1} \wedge \psi_{j_2} \wedge \dots \wedge \psi_{j_n}) \quad (2.7)$$

($\widehat{N}_{j,n}$ “tells” whether or not the state ψ_j is occupied in a given state of $\otimes_a^n \mathcal{H}$). We define:

$$\widehat{N}_j = \oplus_{n \geq 0} \widehat{N}_{j,n}$$

Obviously we have:

$$\begin{aligned} \widehat{N} &= \sum_{j \geq 1} \widehat{N}_j \\ \widehat{H} &= \sum_{j \geq 1} \widehat{N}_j E_j \end{aligned} \quad (2.8)$$

Note that: $[\widehat{H}, \widehat{N}] = 0$

In the grand-canonical formalism (see [6]), the Gibbs partition function is:

$$Z_G = \text{Tr} \left(e^{-\beta \widehat{H} + \kappa \widehat{N}} \right) \quad (2.9)$$

where κ and β are Lagrange multipliers:

$$\begin{aligned} \beta &= 1/kT \\ \kappa &= \beta\mu \end{aligned} \quad (2.10)$$

μ being the chemical potential, and the Trace (which we denote with capital T) being taken in \mathcal{F}_a . Then it can easily be shown (see [6]) that Z_G factorizes as:

$$Z_G = \prod_{j \geq 1} \left(1 + e^{-\beta(E_j - \mu)}\right) \quad (2.11)$$

The mean value F_j of the occupation number of ψ_j is then:

$$\begin{aligned} F_j &= Z_G^{-1} \text{Tr} \left(\widehat{N}_j e^{-\beta(\widehat{H} - \widehat{N})} \right) \\ &= \left(1 + e^{\beta(E_j - \mu)}\right)^{-1} \end{aligned} \quad (2.12)$$

Denoting by f the Fermi-Dirac function:

$$f(x) = (1 + e^x)^{-1} \quad (2.13)$$

the mean value of the number of particles in the grand-canonical ensemble is then:

$$\langle N \rangle = \sum_{j \geq 1} F_j = \text{tr} \left\{ f \left(\beta(\widehat{H} - \mu) \right) \right\} \quad (2.14)$$

where now the trace (which we here denote with small t) is taken in \mathcal{H} . The operator in \mathcal{H} :

$$\widehat{\rho}_{eq} := f \left(\beta(\widehat{H} - \mu) \right) \quad (2.15)$$

is called the Fermi-Dirac equilibrium one-body operator.

We now assume that the one-body Hamiltonian is slightly perturbed in a time-dependent way:

$$\widehat{H}_\lambda(t) = \widehat{H} + \lambda \widehat{A} F(t) \quad (2.16)$$

where λ is a small real parameter, and F of the form, with $\alpha > 0$:

$$F(t) = \begin{cases} e^{\alpha t} & t < 0 \\ 1 & t \geq 0 \end{cases} . \quad (2.17)$$

Starting at time $t = -\infty$ from the Fermi-Dirac one-body equilibrium state $\widehat{\rho}_{eq}$, and switching on the perturbation, we get a time-dependent “density matrix” $\widehat{\rho}_\lambda(t)$ (namely a trace one operator) obeying:

$$i\hbar \frac{\partial \widehat{\rho}_\lambda}{\partial t} = [\widehat{H}_\lambda(t), \widehat{\rho}_\lambda] \quad (2.18)$$

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

The PROBLEM is the following: to which extend does $\widehat{\rho}_\lambda(t)$ wander from the equilibrium state $\widehat{\rho}_{eq}$ as the perturbation is switched on?

3 The linear response theory

Physically, we aim to answer the above PROBLEM “to the first order in λ ”, whence the name “linear response theory”. In this section we give a rigorous framework to this program. Thus our first step is to set a convenient set of assumptions on the Hamiltonians under which mathematical results can be obtained.

Assumption 2

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

Under this assumption we know ([19]) that the unitary evolution operator generated by $\widehat{H}_\lambda(t)$, namely solving:

$$i\hbar \frac{\partial V_\lambda(t, t')}{\partial t} = \widehat{H}_\lambda(t) V_\lambda(t, t') \quad (3.1)$$

$$V_\lambda(t_0, t_0) = \mathbb{1}$$

exists. Moreover it obeys the Duhamel’s formula:

$$V_\lambda(t, t_0) = U(t - t_0) + \frac{\lambda}{i\hbar} \int_{t_0}^t dt' V_\lambda(t, t') F(t') \widehat{A}U(t' - t_0) \quad (3.2)$$

where we have denoted:

$$U(t) := e^{-it\widehat{H}/\hbar}. \quad (3.3)$$

We define:

$$\widehat{\rho}_\lambda(t, t_0) = V(t, t_0) \widehat{\rho}_{eq} V(t_0, t) \quad (3.4)$$

It is clearly a solution of (2.18) with $\widehat{\rho}_\lambda(t_0) = \widehat{\rho}_{eq}$.

We shall now justify the “**linear response theory**” in this context.

Proposition 3.1 *The mapping $\lambda \mapsto \widehat{\rho}_\lambda(t, t_0)$ given by (3.4) is differentiable near $\lambda = 0$ in the trace-class operator norm sense and we have :*

$$\left. \frac{d}{d\lambda} \widehat{\rho}_\lambda(t, t_0) \right|_{\lambda=0} = \frac{1}{i\hbar} \int_{t_0}^t dt' F(t') U(t-t') [\widehat{\rho}_{eq}, \widehat{A}] U(t'-t) . \quad (3.5)$$

Moreover $\widehat{\rho}_\lambda(t, t_0)$ has a limit as $t_0 \rightarrow -\infty$, in the trace-class operator norm sense, called $\widehat{\rho}_{eq}(t, \lambda)$ and which is also differentiable in λ . Moreover we have:

$$\left. \frac{d}{d\lambda} \widehat{\rho}_\lambda(t) \right|_{\lambda=0} = \frac{1}{i\hbar} \int_{-\infty}^t ds F(s) [\widehat{\rho}_{eq}, \widehat{A}_{t-s}], \quad (3.6)$$

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

$$\widehat{A}_t = U(t) \widehat{A} U(t)^* . \quad (3.7)$$

Proof: Inserting $\mathbf{1} = U(t_0 - t)U(t - t_0)$ and commuting with $\widehat{\rho}_{eq}^{1/2}$ we obtain :

$$\widehat{\rho}_\lambda(t, t_0) = V_\lambda(t, t_0) U(t_0 - t) \widehat{\rho}_{eq}^{1/2} \cdot \widehat{\rho}_{eq}^{1/2} U(t - t_0) V_\lambda(t_0, t) \quad (3.8)$$

Each of these two factors admits a limit as $t_0 \rightarrow -\infty$ in the norm trace sense. Namely using Duhamel's formula, we have :

$$(V_\lambda(t, t_0) U(t_0 - t) - \mathbf{1}) \widehat{\rho}_{eq}^{1/2} = \frac{\lambda}{i\hbar} \int_{t_0}^t F(s) V_\lambda(t, s) \widehat{A} \widehat{\rho}_{eq}^{1/2} U(s - t) ds \quad (3.9)$$

(and similarly for the adjoint) so the result follows since $\int_{-\infty}^t |F(s)| ds$ exists for any finite t .

Letting t_0 tend to $-\infty$, we then get:

$$\widehat{\rho}_{eq}(t, \lambda) := \widehat{\rho}_{eq} - \frac{\lambda}{i\hbar} \int_{-\infty}^t ds F(s) V_\lambda(t, s) [\widehat{A}, \widehat{\rho}_{eq}] V_\lambda(s, t) \quad (3.10)$$

A Taylor expansion near $\lambda = 0$ of $\widehat{\rho}_{eq}(t, \lambda)$ can be obtained by plugging in the Duhamel's formula in (3.10) :

$$V_\lambda(t, s) = U(t - s) + \frac{\lambda}{i\hbar} \int_s^t F(\sigma) V_\lambda(t, \sigma) \widehat{A} U(\sigma - t) d\sigma \quad (3.11)$$

This gives in the trace norm sense:

$$\widehat{\rho}_{eq}(t, \lambda) - \widehat{\rho}_{eq} = \frac{\lambda}{i\hbar} \int_{-\infty}^t dt' F(t') [\widehat{\rho}_{eq}, \widehat{A}_{t-t'}] + o(\lambda). \quad (3.12)$$

By this method the second term in λ (“quadratic response”) could also be explicitly written. ■

Equation (3.10) 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 “almost stationary” state $\widehat{\rho}_{eq}(t)$, the coefficient of the first order contribution in λ , as $\lambda \rightarrow 0$ to the result :

$$J_\lambda(t) = \text{tr} \left\{ \widehat{B} (\widehat{\rho}_{eq}(t, \lambda) - \widehat{\rho}_{eq}) \right\} \quad (3.13)$$

is of the form :

$$J_L(t) = \lambda \int_{-\infty}^t dt' F(t') \Phi(t - t') \quad (3.14)$$

where

$$\Phi(t) = \frac{1}{i\hbar} \text{tr} \left(\widehat{B} [\widehat{\rho}_{eq}, \widehat{A}_t] \right) = \frac{1}{i\hbar} \text{tr} \left(\widehat{\rho}_{eq} [\widehat{A}, \widehat{B}_{-t}] \right) \quad (3.15)$$

using the cyclicity of the trace.

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

$$\chi_{A,B}(\omega) = \int_{-\infty}^{+\infty} \Phi(t) e^{i\omega t} dt \quad (3.16)$$

which is the quantity that we shall study now. Given any function g whose Fourier Transform \tilde{g} is assumed to belong to $\mathcal{C}_0^\infty(\mathbb{R})$:

$$\int \chi_{A,B}(\omega) g(\omega) d\omega = \frac{1}{i\hbar} \int_{-\infty}^{+\infty} \text{tr} f(\beta(\widehat{H} - \mu)) [\widehat{A}, \widehat{B}_{-t}] \tilde{g}(-t) dt := I(\mu) \quad (3.17)$$

Our aim is to obtain a semiclassical expansion of $\chi_{A,B}(\omega)$ as $\hbar \rightarrow 0$, $\beta \rightarrow \infty$, namely a semiclassical expansion at low temperature.

It is useful to introduce the following parameter:

$$\sigma = \beta\hbar \quad (3.18)$$

which has the dimension of time. We also define the function f_σ as follows:

$$f_\sigma(x) = (1 + e^{\sigma x})^{-1} \quad (3.19)$$

so that $I(\mu)$ can be rewritten formally as:

$$I(\mu) = \frac{1}{i\hbar} \int \text{tr} \left(f_\sigma \left(\frac{\widehat{H} - \mu}{\hbar} \right) [\widehat{A}, \widehat{B}_t] \right) \tilde{g}(t) dt \quad (3.20)$$

However this expression suffers from the singularity in 0 of f_σ as $\sigma \rightarrow 0$. In order to avoid this, we “regularize” it by using instead of f_σ :

$$f_{\sigma,\eta} = f_\sigma * \eta \quad (3.21)$$

where η is a function in $\mathcal{S}(\mathbb{R})$ such that its Fourier Transform $\tilde{\eta} \in \mathcal{C}_0^\infty(\mathbb{R})$. This amounts to study $\chi_{A,B}$ as a distribution on \mathbb{R}^2 in the variables s and ω in the following way:

$$\begin{aligned} & \int \int \chi_{A,B}(s, \omega) \tilde{\eta}(s) g(\omega) ds d\omega = \\ & \frac{1}{2i\pi\hbar} \int \int \text{tr} \left(e^{is(\widehat{H}-\mu)/\hbar} [\widehat{A}, \widehat{B}_t] \right) \tilde{f}_\sigma(s) \tilde{\eta}(s) \tilde{g}(t) ds dt \end{aligned} \quad (3.22)$$

Let us introduce the following test space functions on $\mathbb{R}^2 = \mathbb{R}_s \times \mathbb{R}_\omega$:

Definition 3.2 *We say that $\varphi \in \mathcal{K}_a$, $a > 0$, if φ is C^∞ on \mathbb{R}^2 and there exist $b > 0$, $c > 0$ such that $\varphi(s, \omega) = 0$ for $|s| \geq b$, $\omega \in \mathbb{R}$, and $|\tilde{\varphi}^{(2)}(s, t)| \leq ce^{-a|t|}$ for every $(s, t) \in \mathbb{R}^2$, where $\tilde{\varphi}^{(2)}(s, t)$ denotes the Fourier transform in the second argument.*

4 The results

In this section we first introduce the notations of the classical objects that will appear in the semiclassical expansions, together with the assumptions under which these expansions can be obtained.

Let ϕ^t be the classical flow induced by Hamiltonian (2.1). Consider Σ_μ the energy surface conserved by the flow:

$$\Sigma_\mu = \left\{ (q, p) \in \mathbb{R}^{2n} : H(q, p) = \mu \right\} \quad (4.1)$$

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:

$$C_{A,B,\mu}(t) = \int_{\Sigma_\mu} A \cdot B_t d\Sigma_\mu \quad (4.2)$$

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

$$c_{\gamma^*}(t) = \int_0^{T_{\gamma^*}} A_s(q, p) B_{s+t}(q, p) ds \quad (q, p) \in \gamma^* \quad (4.3)$$

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

$$c_{\gamma^*}(t) = \sum_{k=-\infty}^{k=+\infty} c_{\gamma^*,k} e^{2ikt\pi/T_{\gamma^*}} \quad (4.4)$$

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 [7]).

Let us assume that ϕ^t on Σ_μ satisfies the so-called 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 we shall be able to treat B obeying:

Assumption 3

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

Our result is as follows:

Theorem 4.1 *Under Assumptions 1,2,3, we have, in distributional sense in \mathcal{K}_a (see definition 3.2) :*

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

where μ_j and $\nu_{j,\gamma}$ are distributions in \mathcal{K}_a such that $\text{Supp}(\mu_j) \subseteq \{0\} \times \mathbb{R}$, $\text{Supp}(\nu_{j,\gamma}) \subseteq \{T_\gamma\} \times \mathbb{R}$, and γ_H is a non negative constant depending only on H and μ (not on a).

Proof:

As a distribution acting on $(\tilde{\eta} \otimes g)(s, \omega)$, $\chi_{A,B}$ is given by (3.22). We split the integral over t into two parts: $|t| < \gamma_H \text{Log}(1/\hbar)$ and its complement, where γ_H

is a constant obtained in Egorov-type estimates (see [4]) and only depending on Hamiltonian H .

Using the exponential decrease of $\tilde{g}(t)$, it is not difficult to estimate the contribution of the integration domain $|t| > \gamma_H \text{Log}(1/\hbar)$ as $O(\hbar^{a\gamma_H - \varepsilon - n})$, for any $\varepsilon > 0$. The larger is a (the exponential fall-off rate of \tilde{g}) the smaller is this “error term”.

In order to estimate the contribution of the integration domain $|t| < \gamma_H \text{Log}(1/\hbar)$ we shall use truncations in the spectral variable of Hamiltonian \widehat{H} in order to apply known results and usual methods.

In all that follows, the integration support in t variable is supposed to be $|t| < \gamma_H \text{Log}(1/\hbar)$, and we call $I_\eta(\mu)$ the resulting contribution to (3.22). Fix δ positive and small enough and let us introduce a C^∞ partition of unity as follows :

$$1 = \zeta_- + \zeta_0 + \zeta_+ \quad (4.5)$$

where

$$\zeta_0(t) = \begin{cases} 1 & |t| \leq \delta/2 \\ 0 & |t| \geq \delta. \end{cases} \quad (4.6)$$

and $\text{Supp}\zeta_- \subseteq]-\infty, -\delta/2]$, $\text{Supp}\zeta_+ \subseteq [\delta/2, +\infty[$.

Inserting in (3.22)

$$\mathbb{1} = \zeta_-(\widehat{H} - \mu) + \zeta_0(\widehat{H} - \mu) + \zeta_+(\widehat{H} - \mu)$$

we obtain, with obvious notations :

$$I_\eta(\mu) = I_\eta^0(\mu) + I_\eta^+(\mu) + I_\eta^-(\mu) \quad (4.7)$$

Let θ be a regular Schwartz function such that its Fourier Transform $\tilde{\theta}$ be in $C_0^\infty(\mathbb{R})$, and

$$\tilde{\theta}(t) \equiv \begin{cases} 1 & \text{if } |t| \leq 1 \\ 0 & \text{if } |t| \geq 2 \end{cases} \quad (4.8)$$

For any positive number τ , we set :

$$\tilde{\theta}_\tau(s) := \tilde{\theta}(s/\tau) . \quad (4.9)$$

and let us denote by θ_τ the inverse Fourier transform of $\tilde{\theta}_\tau$. Let τ_0 be a positive number, small enough in a sense to be made precise later. We shall now decompose $I_\eta^0(\mu)$ in two parts:

$$I_\eta^0(\mu) = I_{\eta,\tau_0}^0(\mu) + \frac{1}{2i\pi\hbar} \text{tr} \left[\int \int ds dt \tilde{f}_\sigma(s) \tilde{\eta}(s) \left(1 - \tilde{\theta}(s/\tau_0)\right) e^{is(\widehat{H}-\mu)/\hbar} [\widehat{A}, \widehat{B}_t] \zeta_0(\widehat{H} - \mu) \tilde{g}(t) \right] \quad (4.10)$$

Thus equ. (4.7) now becomes:

$$I_\eta(\mu) = I_{\eta,\tau_0}^0(\mu) + I_{\eta,\tau_0}^{osc}(\mu) + I_\eta^+(\mu) + I_\eta^-(\mu) \quad (4.11)$$

where each term can be estimated separately.

Estimate of $I_\eta^-(\mu)$:

Denote by :

$$\phi_\beta(E) := f(\beta(E - \mu)) \zeta_-(E - \mu)$$

We remark that $\phi_\infty = \zeta_-(E - \mu)$, and

$$\phi_\beta(\widehat{H}) = \phi_\beta(\widehat{H}) \chi(\widehat{H}) \quad (4.12)$$

for some $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ because the spectrum of \widehat{H} is bounded from below.

But $E \mapsto \phi_\beta(E) \chi(E)$ is a bounded family of functions in $\mathcal{C}_0^\infty(\mathbb{R})$ for β in $]0, +\infty]$. Therefore the \hbar -semiclassical functional calculus can be applied, yielding an asymptotic expansion of the following form :

$$I_\eta^-(\mu) \sim \hbar^{-n} \sum_{j \geq 0} c_j \hbar^j \quad (4.13)$$

uniformly in $\sigma \in]0, +\infty]$, where :

$$c_0 = (2\pi)^{-n} \int f(\beta(H(q,p) - \mu)) \zeta_-(H(q,p) - \mu) \{A, B_t\}(q,p) dq dp \quad (4.14)$$

and analogous formulae for $j \geq 1$, where we have used the known result that the principal symbol of:

$$\widehat{C}_t := \frac{i}{\hbar} [\widehat{A}, \widehat{B}_t] \quad (4.15)$$

is $\{A, B_t\}$, using Egorov's theorem in the form given in [4] for $|t| < \gamma_H \text{Log}(1/\hbar)$, and semiclassical calculus.

Estimate of $I_\eta^+(\mu)$:

$$|I_\eta^+(\mu)| \leq C \sum_{j \geq 1} |f(\beta(E_j - \mu)) \zeta_+(E_j - \mu)| \quad (4.16)$$

where C depends on \tilde{g} and A, B , and where $\{E_j\}_{j \geq 1}$ is the increasing sequence of the eigenvalues of \widehat{H}

$$|I_\eta^+(\mu)| \leq C \sum_{E_j \geq \delta/2} |f(\beta(E_j - \mu))| \quad (4.17)$$

We introduce the counting function :

$$N(E) := \#\{j : E_j \leq E\}$$

Using a ‘‘Lieb-Thirring-like’’ estimate, we get :

$$N(E) \leq \gamma \hbar^{-n} (1 + E)^m$$

We therefore deduce the existence of a positive constant c (depending on δ) such that :

$$|I_{\sigma, \infty}^+| \leq C \hbar^{-n} e^{-c\beta} \quad (4.18)$$

for any $\hbar \in]0, 1]$ and any positive σ .

Estimate of $I_{\eta, \tau_0}^0(\mu)$

Recall that :

$$I_{\eta, \tau_0}^0(\mu) = 1/i\hbar \int_{-\infty}^{+\infty} \text{tr} \left(f_{\sigma, \eta, \tau_0} \left(\frac{\widehat{H} - \mu}{\hbar} \right) \zeta_0(\widehat{H} - \mu) [\widehat{A}, \widehat{B}_t] \right) \tilde{g}(t) dt \quad (4.19)$$

where we have defined:

$$f_{\sigma, \eta, \tau_0} = f_\sigma * \eta * \theta_{\tau_0} \quad (4.20)$$

We want to estimate

$$L_{\mu, t} := \frac{1}{i\hbar} \text{tr} \left(f_{\sigma, \eta, \tau_0} \left(\frac{\widehat{H} - \mu}{\hbar} \right) \zeta_0(\widehat{H} - \mu) [\widehat{A}, \widehat{B}_t] \right) \quad (4.21)$$

Since :

$$f_{\sigma,\eta,\tau_0}(\nu) \rightarrow 0 \text{ as } \nu \rightarrow +\infty$$

we have :

$$f_{\sigma,\eta,\tau_0} \left(\frac{\widehat{H} - \mu}{\hbar} \right) = -1/\hbar \int_{-\infty}^{\mu} (f'_{\sigma} * \eta * \theta_{\tau_0}) \left(\frac{\widehat{H} - \lambda}{\hbar} \right) d\lambda \quad (4.22)$$

using equ. (4.11) we can write :

$$\begin{aligned} L_{\mu,t} &= \frac{-1}{\hbar} \text{tr} \int_{\mu-2\delta}^{\mu} (f'_{\sigma} * \eta * \theta_{\tau_0}) \left(\frac{\widehat{H} - \lambda}{\hbar} \right) \zeta_0(\widehat{H} - \mu) \widehat{C}_t d\lambda \\ &\quad - \hbar^{-1} \text{tr} \int_{-\infty}^{\mu-2\delta} (f'_{\sigma} * \eta * \theta_{\tau_0}) \left(\frac{\widehat{H} - \lambda}{\hbar} \right) \zeta_0(\widehat{H} - \mu) \widehat{C}_t d\lambda \end{aligned} \quad (4.23)$$

We have thus: $L_{\mu,t} = L_{\mu,t}^1 + L_{\mu,t}^2$, with

$$|L_{\mu,t}^2| \leq C \hbar^{-1} \int_{-\infty}^{\mu-2\delta} \sum_{j \geq 1} \left| (f'_{\sigma} * \eta * \theta_{\tau_0}) \left(\frac{E_j - \lambda}{\hbar} \right) \zeta_0(E_j - \mu) \right| d\lambda \quad (4.24)$$

where C is uniform with respect to $t \in \text{Supp} \tilde{g}$ and to \hbar .

By playing with localization and decay properties, one easily obtains that $L_{\mu,t}^2 = O(\hbar^{\infty})$ uniformly with respect to $t \in \text{Supp} \tilde{g}$, and with respect to $\sigma \in]0, +\infty[$.

The term $L_{\mu,t}^1$ can be dealt with as in [8], using the fact that for δ small enough, λ is non critical for \widehat{H} for every $\lambda \in [\mu - 2\delta, \mu]$. Thus $L_{\mu,t}^1$ can be rewritten as:

$$L_{\mu,t}^1 = - \int_{\mu-2\delta}^{\mu} I(\lambda) d\lambda \quad (4.25)$$

where :

$$I(\lambda) = i\hbar^{-1} \int_{-\infty}^{+\infty} ds \frac{s\pi/\sigma}{\sinh s\pi/\sigma} \tilde{\theta}(s/\tau_0) \tilde{\eta}(s) \text{tr} \left\{ e^{-is(\widehat{H}-\lambda)/\hbar} \zeta_0(\widehat{H} - \mu) \widehat{C}_t \right\} \quad (4.26)$$

Then using a coherent states decomposition of the trace as in [7], we see, using the support property of $\tilde{\theta}_{\tau_0}$ that the dominant contribution in the stationary phase theorem comes from $s = 0$. Thus, provided that $2\tau_0$ is smaller than the smallest period of closed orbits on Σ_{μ} , equ. (4.26) provides an asymptotic expansion in \hbar , of the form:

$$I(\lambda) = \hbar^{-n}(C_0(\lambda) + \hbar C_1(\lambda) + \dots) \quad \text{mod } O(\hbar^\infty) \quad (4.27)$$

which is uniform in $\sigma \in]0, +\infty[$, and which can be further integrated with respect to λ on the interval $[\mu, \mu + 2\delta]$, yielding the result.

We shall now give the explicit form of the dominant $O(\hbar^{-n})$ contribution to $I_\eta(\mu)$ (equ. (4.6)) which comes from the sum of the contributions of $I_\eta^-(\mu)$ and $I_{\eta, \tau_0}^0(\mu)$; we obtain:

$$I_\eta(\mu) = h^{-n} \tilde{\eta}(0) \int \tilde{g}(t) \int_{[H \leq \mu]} \{A, B_t\}(q, p) dp dq dt + O(\hbar^{1-n}) \quad (4.28)$$

We have introduced the correlation in time of A and B on the energy surface $\Sigma_\mu = [H(q, p) = \mu]$ (see (4.2))

$$C_{A, B, \mu}(t) := \int_{[H=\mu]} AB_t \frac{d\sigma_\mu}{|\nabla H|} \quad (4.29)$$

Let φ be a \mathcal{C}^∞ function with compact support contained in $] -\infty, \mu + \delta]$. We have :

$$\int \{A, B_t\} \varphi(H(q, p)) dp dq = \int \{A\varphi(H), B_t\} dq dp - \int A \{\varphi(H), B_t\} dq dp \quad (4.30)$$

where the integration is over the full phase space \mathbb{R}^{2n} . $B\varphi(H)$ being a $\mathcal{C}_0^\infty(\mathbb{R}^{2n})$ function of (q, p) , we get by integration by part that :

$$\int \{A\varphi(H), B_t\} dq dp = 0$$

Moreover

$$\int \{A\varphi(H), B_t\} dq dp = \int \{H, B_t\} \varphi'(H) A dq dp = -\frac{d}{dt} \int AB_t \varphi'(H) dq dp$$

We now let φ tend to $\mathbb{1}_{]-\infty, \mu]}$, and find :

$$\int_{[H \leq \mu]} \{A, B_t\} dq dp = \frac{d}{dt} \left(\int_{[H=\mu]} A \cdot B_t \frac{d\sigma_\mu}{|\nabla H|} \right)$$

Therefore the dominant term of $I_\eta(\mu)$ is given by :

$$I_\eta(\mu) = h^{-n} \tilde{\eta}(0) \int C_{A, B, \mu}(t) \tilde{g}'(t) dt + O(\hbar^{1-n})$$

This completes the proof for the first term of the asymptotic expansion in Theorem (4.1).

Estimate of $I_{\sigma,\tau,\tau_0}^{osc}(\mu)$

We have :

$$I_{\eta,\tau_0}^{osc}(\mu) = h^{-1} \int dt \tilde{g}(t) \int \frac{1}{s} ds \frac{\pi s/\sigma}{\sinh \pi s/\sigma} \eta_{\theta,\tau_0}(s) \text{tr} \left\{ \zeta_0(\widehat{H} - \mu) e^{-is(\widehat{H} - \mu)/\hbar} \widehat{C}_t \right\} \quad (4.31)$$

where we have used the following notation :

$$\eta_{\theta,\tau_0}(s) := \tilde{\eta}(s) \left(1 - \tilde{\theta}_{\tau_0}(s) \right)$$

Again we proceed as in [7] by a ‘‘Gutzwiller type’’ estimate for the integral over s since the support of $\eta_{\theta,\tau_0}(s)$ doesn’t contain $s = 0$, but will only contribute by a finite number of closed classical orbits which we denote by γ . Furthermore due to the support properties of $\tilde{\theta}$, it is clear that $\eta_{\theta,\tau_0}(T_\gamma) = \eta(T_\gamma)$

Using the **Gutzwiller assumption**, and the compact integration support in variable t , we obtain the following asymptotic expansion of $I_{\eta,\tau_0}^{osc}(\mu)$, which is uniform in the parameter $\sigma \in]0, +\infty[$:

$$I_{\eta,\tau_0}^{osc}(\mu) = h^{-1} \int dt \tilde{g}(t) \sum_{\gamma \in \Sigma_\mu} \frac{\pi}{\sigma \sinh \pi T_\gamma / \sigma} \frac{e^{iS_\gamma/\hbar + i\nu_\gamma \pi/2}}{|\det(1 - P_\gamma)|^{1/2}} \times \quad (4.32)$$

$$\times \left(\sum_k \eta(T_\gamma) c_{\gamma^*,k} e^{2i\pi kt/T_\gamma^*} + \sum_{j \geq 1} h^j \nu_{j,\gamma}(t) \right)$$

This yields the following contribution of oscillating terms to $\chi_{A,B}(s, \omega)$, in the distribution sense, uniformly in $\sigma \in]0, +\infty[$:

$$\chi_{A,B,osc} = \sum_{\gamma: T_\gamma \neq 0} \frac{\pi e^{i(S_\gamma/\hbar + \nu_\gamma \pi/2)}}{\hbar \sigma \sinh(\pi T_\gamma / \sigma) |\det(1 - P_\gamma)|^{1/2}} \times$$

$$\times \left(\delta_{T_\gamma}(s) \otimes \sum_k c_{\gamma^*,k} \delta\left(\omega - \frac{2k\pi}{T_\gamma^*}\right) + \sum_{j \geq 1} \hbar^j \nu_{j,\gamma}(s, \omega) \right) \quad (4.33)$$

where $\nu_{j,\gamma}(s, \omega)$ are distributions supported in $\{T_\gamma\} \times \mathbb{R}$ ■

5 Concluding remarks

Theorem 4.1 is an extension of the well known Gutzwiller trace formulae for the spectral density of energy levels. The main difference is that here there are two real variables instead of one because in the “dynamical susceptibility” time and energy variables are mixed up in an intricated way. So we can put in a mathematical rigorous shape the main result of the paper [13].

As in the Gutzwiller trace formulae our formulae in Theorem 4.1 gives a semiclassical expansion with three different terms: the first line gives a regular expansion in h , which is the contribution of the period 0 of the classical flow; the second line is an oscillating part coming from the contributions of the non zero periods of the classical flow; the third line is the error term depending on the test functions considered.

So far we have shown that a semiclassical expansion, in the linear response theory, can be obtained for a regularized version of the “dynamical susceptibility”, i.e in a suitable distributional sense. The same is obviously true for the linear response function $J_L(t)$ defined by (3.15), as we shall establish now.

Formally, if φ is a $\mathcal{C}_0^\infty(\mathbb{R})$ function, we have, in distributional sense:

$$\langle J_L, \varphi \rangle = \int \widetilde{k}_1(\omega) \chi_{A,B}(\omega) d\omega$$

where $k_1(u) := \Theta(u)k(u)$,

(Θ being the Heavyside function)

and $k(u) := \int \varphi(s+u)F(s)ds$

However $\chi_{A,B}$ is only well defined mathematically as a semiclassical expansion in a “regularized” form:

$$\chi_{A,B,\eta} := \int \widetilde{\eta}(s) \chi_{A,B}(s, \omega) ds$$

where $\widetilde{\eta}$ is in $\mathcal{C}_0^\infty(\mathbb{R})$.

Similarly, a “regularized form” of J_L can be defined as:

$$J_{L,\eta}(t) := \int \widetilde{\eta}(s) J_L(t, s) ds$$

in the following sense:

$$\langle J_{L,\eta}, \varphi \rangle = \int \widetilde{k}_1(\omega) \chi_{A,B,\eta}(s, \omega) d\omega$$

So we have

$$\langle J_{L,\eta}, \varphi \rangle = \int \tilde{\eta}(s) \widetilde{k_1}(\omega) \chi_{A,B}(s, \omega) ds d\omega$$

It is not hard to see, using the definition of k_1 that $\tilde{\eta}(s) \widetilde{k_1}(\omega) \in \mathcal{K}_{\alpha-\varepsilon}$ for any $\varepsilon > 0$, so that our theorem applies. For example we can compute the leading term :

$$\langle J_{L,\eta}, \varphi \rangle = -2\pi h^{-n} \tilde{\eta}(0) \int_0^{+\infty} du C'_{A,B}(u) \int_{\mathbb{R}} ds \varphi(s+u) F(s) + O(h^{1-n})$$

References

- [1] O. Agam, *The magnetic response of chaotic mesoscopic systems*, J. Phys. I (France), **4** (1994), 697-730.
- [2] M. Aizenman, G. M. Graf, *Localization bounds for an electron gas*, J. Phys. A (Math. and Gen.), **31** (1998), 6783-6806.
- [3] R. Balian, *Du microscopique au macroscopique*, École Polytechnique, Ellipses (1982)
- [4] A. Bouzouina, D. Robert, *Uniform semiclassical estimates for the propagation of Heisenberg observables*, Duke Math. Journal, Vol.111, No.2 (2001) 223-252.
- [5] O. Bratelli and D. Robinson, *Operator Algebras and Quantum Statistical Mechanics*, Springer Verlag, vol II.
- [6] J. D. Butler, *Semiclassical counting function with application to quantum current*, 2000, Orsay preprint.
- [7] M. Combescure, J. Ralston, D. Robert, *A proof of the Gutzwiller semiclassical trace formula using coherent states decomposition*, Commun. Math. Phys., **202** (1999), 463-480.
- [8] M. Combescure, D. Robert, *Rigorous semiclassical results for the magnetic response of an electron gas*, Rev. in Math. Phys., Vol.13, No.9 (2001) 1055-1073.
- [9] Y. Egorov, *On canonical transformations of pseudodifferential operators*, Uspehi Mat. Nauk, **25** (1969), 235-236.
- [10] S. Fournais, *Semiclassics of the quantum current*, Commun. in PDE, **23** (1998), 601-628.

- [11] G. Gallavotti, E. G. Cohen, *Dynamical ensembles in stationary states*, J. Stat. Phys., **80** (1995), 931-970.
- [12] G. Gallavotti, D. Ruelle, *SRB states and nonequilibrium statistical mechanics close to equilibrium*, Commun. Math. Phys., **190** (1997), 279-285.
- [13] P. Gaspard, S. Jain, *Semiclassical theory for many-body fermionic systems*, Pramana Journal of Physics, **48** (1997), 503-516.
- [14] R. Kubo, M. Toda, N. Hashitsume, *Statistical Physics II*, (Nonequilibrium Statistical Mechanics), Springer-Verlag, Berlin, Heidelberg, New York, Tokyo (1978).
- [15] L. D. Landau, E. M. Lifshitz, *Statistical Physics*, Course of Theoretical Physics, vol. 5, Pergamon Press, Oxford, New York, Toronto, Sydney, Paris, Frankfurt (1980).
- [16] B. Mehlig, K. Richter, *Semiclassical linear response : far-infrared absorption in ballistic quantum systems*, Phys. Rev. Lett., **80** (1998), 1936-1939.
- [17] K. Richter, D. Ullmo, R. Jalabert, *Orbital magnetism in the ballistic regime : geometrical effects*, Phys. Rep., **276** (1996), 1-83.
- [18] D. Ruelle, *General linear response formula in statistical mechanics and the fluctuation-dissipation theorem far from equilibrium*, Phys. Lett., **A245** (1998), 220-224.
- D. Ruelle, *Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics*, J. Stat. Phys., **95** (1999), 393-468.
- D. Ruelle, *Natural nonequilibrium states in quantum statistical mechanics*, J. Stat. Phys., **98** (2000), 57-75.
- [19] K. Yajima, *Schrödinger evolution equations with magnetic fields*, Journ. Anal. Mathem., **56** (1991), 29-76