Rigorous semiclassical results for the magnetic response of an electron gas

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Abstract

Consider a free electron gas in a confining potential and a magnetic field in arbitrary dimensions. If this gas is in thermal equilibrium with a reservoir at temperature $T > 0$, one can study its orbital magnetic response (omitting the spin). One defines a conveniently "smeared out" magnetization M, and the corresponding magnetic susceptibility χ, which will be analyzed from a semiclassical point of view, namely when $\hbar$ (the Planck constant) is small compared to classical actions characterizing the system. Then various regimes of temperature T are studied where M and χ can be obtained in the form of suitable asymptotic $\hbar$-expansions. In particular when T is of the order of $\hbar$, oscillations "à la de Haas-van Alphen" appear, that can be linked to the classical periodic orbits of the electronic motion.

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1 Introduction

The magnetic response theory for a free electron gas is an old problem considered by Landau [15], Fock [10] and Peierls [20]. The revival of interest in physics arose from the advances of recent experiments that made possible measurements of the magnetic response on small 2-dimensional electronic devices. These devices are so "pure" that the classical as well as quantum motion inside them can be considered as "ballistic", i.e. is uniquely determined by the confining potential. (Taking into account impurities would consist in adding the random potential created by random point scatterers inside the material). The bi-dimensional structure of such electron-gas is realized through semi-conductor heterostructures whose size, and shape can be controlled experimentally, together with the number N of confined electrons. The system being in contact with a reservoir at temperature T, and submitted to a magnetic field B perpendicular to the surface, the magnetic response can be measured : say, the magnetization M or magnetic susceptibility χ as a function of the thermodynamic parameters T, N, B. [22]. These experiments manifest the sensitivity of the magnetic response to the integrable versus non-integrable character of the classical dynamics of one electron in the system. Numerical experiments on two-dimensional magnetic billards have confirmed this observation, and suggested that the quantum magnetic response is an experimentally accessible criterion for distinguishing classically integrable versus chaotic dynamics [17]. A number of theoretical studies have analyzed the magnetic response from a "semi-classical" point of view, namely as properties manifesting themselves in the limit when $\hbar$ (the Planck constant) is small compared to classical actions characterizing the system (say $h \ll a^2 eB/c$ where a is a typical size of the system, e the charge of the electron, c the velocity of light and B the magnetic field size) [3]. In these studies, the Coulomb interactions between the electrons in the system are neglected, so that the system is a "free electron gas" to which the usual thermodynamic formalism is applied.

The thermodynamic functions in the grand-canonical ensemble can be expressed through the density of states of the quantum Hamiltonian for one electron in the system. This quantum density of states, in the semi-classical limit, splits into a mean part and a strongly oscillating one, according to the well known semi-classical trace formula. This formula is known in mathematics as Poisson formula (Colin de Verdière [4] , Duistermaat-Guillemin [9]) and in physics as the Gutzwiller trace formula in the chaotic case [12], or the Berry-Tabor trace formula in the integrable case [2]. This splitting provides a similar splitting in the magnetic response, which allows to understand the oscillations "à la de Haas-van Alphen" of the magnetic susceptibility and their link with the classical periodic orbits of the electronic motion.

The aim of the present paper is to reconsider these questions from a mathematical point of view, in the following two directions (for non-interacting electron gases in arbitrary dimension, and not necessarily homogeneous magnetic fields)

- examine the regimes of temperature in which the magnetic response can be obtained semi-classically in the form of asymptotic $\hbar$ expansions

- investigate a "mesoscopic" regime of low temperatures where the periodic orbits of the classical one-electron dynamics manifest themselves as highly oscillating contributions, to the magnetic response.

In a recent work, Fournais [11] studies the semi-classics of the quantum current for a non-interacting gas of electrons in dimension n and temperature T, confined in a potential V and subject to a suitable magnetic field B. For fixed non-zero temperature T, he obtains a complete asymptotic expansion of the quantum current in small $\hbar$, and for zero temperature, he obtains the dominant contribution plus an error term under suitable assumptions. J. Butler [3] has recently reexamined this last case using a "semi-classical trace formula" by Petkov and Popov [19].

We recall that in all these studies, the spin of the electron is omitted so that only the <u>orbital</u> magnetic response is considered.

The content of our paper is the following :

- In section 2 we consider the case when the temperature T is large compared to the Planck constant $\hbar$. We prove asymptotic expansion in $\hbar$ for the thermodynamical potential and we recover the Landau diamagnetic formula for 2-dimensional free electron gas.

- In section 3 we consider the case where the temperature T is of the same order as $\hbar$. Then we prove that the magnetization splits into two terms : an average part with a regular asymptotic expansion in $\hbar$ plus an oscillating part in $\hbar$ which is the contribution of the periodic orbits of the classical motion.

- In section 4 we come back to the regime T larger than $\hbar$ and prove that the contribution of non zero periods of the classical motion is exponentially small in $\hbar$.

2 The Landau magnetism

We shall first give the notations and assumptions that will hold all along this paper.

Given $\beta > 0$, we set :

$$F_\beta(x) = -\frac{1}{\beta}\,\mathrm{Log}\left(1 + e^{-\beta x}\right) \tag{2.1}$$

$$f_\beta(x) = F'_\beta(x) = \left(1 + e^{\beta x}\right)^{-1} \tag{2.2}$$

f_β is related with the Fermi-Dirac distribution.
These functions are meromorphic, with poles (or cuts for F_β) at :

$$x = \frac{2k+1}{\beta}\, i\pi \qquad k \in \mathrm{Z}$$

Let $\kappa \in I\!R$ be a real parameter (coupling constant with a magnetic field). We consider a family of Hamiltonians with magnetic fields given by :

$$H_\kappa(q,p) = \frac{1}{2}\,(p - \kappa a(q))^2 + V(q) \tag{2.3}$$

where $V : I\!R^n \mapsto I\!R$ and $a : I\!R^n \mapsto I\!R^n$ are $\mathcal{C}^\infty$ functions satisfying the following properties.

(H.1) $$\forall q \in \mathrm{R}^n,\ \ V(q) \geq 1\ ,\ |\partial_q^\alpha V(q)| \leq C_\alpha V(q)$$

(H.2) $$\forall q \in \mathrm{R}^n,\ \ |\partial_q^\alpha a(q)| \leq C_\alpha\ V(q)^{1/2}$$

(H.3) $$\forall q \in \mathrm{R}^n,\ \ V(q) \geq c_0 \left(1 + |q|^2\right)^{s/2} \quad \text{some } s,\ c_0 > 0$$

(confinement assumption).

Let now $\widehat{H}_\kappa$ be the Weyl quantization of H_κ. The previous assumptions ensure that $\widehat{H}_\kappa$ is self-adjoint and its spectrum $\sigma(\widehat{H}_\kappa) \subset [\varepsilon, \infty)$ is pure point for $|\kappa| \leq \kappa_0$ where $\varepsilon > 0$ ([23]). Let us call $(E_j)_{j\in \mathbb{N}}$ and $(\varphi_j)_{j\in \mathbb{N}}$ the set of corresponding eigenvalues and eigenstates.

In the grand-canonical ensemble, the thermodynamic potential Ω is given by :

$$\Omega(\beta,\mu,\kappa) = \sum_{j\in \mathrm{N}} F_\beta(E_j-\mu) = \mathrm{Tr}\left\{F_\beta\left(\widehat{H}_\kappa - \mu\right)\right\} \tag{2.4}$$

where $\mu > 0$ is the chemical potential, $\beta = 1/k_B T$, k_B being the Boltzmann constant, and $T > 0$ the temperature. (κ will be the size of the magnetic field). Furthermore, the mean-number of particles in the grand-canonical ensemble is given by :

$$N(\beta,\mu,\kappa) = \mathrm{Tr}\left(f_\beta\left(\widehat{H}_\kappa - \mu\right)\right) \tag{2.5}$$

Using the functional calculus [23], it is not difficult to see that $F_\beta(\widehat{H}-\mu)$ and $f_\beta(\widehat{H}-\mu)$ are trace-class and that the function : $\kappa \mapsto \Omega(\beta,\mu,\kappa)$ is $\mathcal{C}^\infty$ for $|\kappa| \leq \kappa_0$. We shall denote $\partial_\kappa = \frac{\partial}{\partial\kappa}$.

Proposition 2.1 *The function :* $\kappa \mapsto \Omega(\beta,\mu,\kappa)$ *is* $\mathcal{C}^\infty$ *on* R. *In particular we have*

$$\partial_\kappa\Omega = \mathrm{Tr}\left[f_\beta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa\widehat{H}_\kappa\right] \tag{2.6}$$

Now we have the following definitions of magnetization M and magnetic susceptibility χ :

$$\begin{aligned} M = \partial_\kappa\Omega &= \mathrm{Tr}\left[f_\beta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa\widehat{H}_\kappa\right] && (2.7)\\ \chi &= \partial_\kappa M && (2.8)\end{aligned}$$

<u>**Proof of proposition**</u>2.1 Since $\sigma(\widehat{H}_\kappa) \subset [\varepsilon_0, +\infty)$, we can draw a suitable curve Λ in the complex energy plane, around $\sigma(\widehat{H}_\kappa)$, with all branching points of $F_\beta(z-\mu)$ left outside. So using Cauchy formula we have

$$F_\beta\left(\widehat{H}_\kappa - \mu\right) = \frac{1}{2i\pi}\int_\Lambda dz\ F_\beta(z-\mu)\left(\widehat{H}_\kappa - z\right)^{-1} \tag{2.9}$$

Using Lebesgue convergence theorem and cyclicity of the trace, we get

$$\partial_\kappa\Omega = -\frac{1}{2i\pi}\mathrm{Tr}\int_\Lambda dz\ \left[F_\beta(z-\mu)\left(\widehat{H}_\kappa - z\right)^{-2}\partial_\kappa\widehat{H}_\kappa\right] \tag{2.10}$$

Integration by parts give

$$\partial_\kappa \Omega = \frac{1}{2i\pi} \mathrm{Tr} \int_\Lambda dz f_\beta(z-\mu) \left(\widehat{H}_\kappa - z\right)^{-1} \partial_\kappa \widehat{H}_\kappa \tag{2.11}$$

This procedure can be easily iterated to prove that Ω is C^∞-smooth in κ. Moreover in the semiclassical regime we can prove that the asymptotics for derivatives in κ of Ω can be computed using the following commutators formulas for derivatives of the resolvent. Starting from the well known identity :

$$[\hat{A}, (\hat{H}-z)^{-1}] = (\hat{H}-z)^{-1}[\hat{H}, \hat{A}](\hat{H}-z)^{-1}, \tag{2.12}$$

we get

$$\begin{aligned} \partial_\kappa(\hat{H}-z)^{-1} &= \partial_\kappa \hat{H}(\hat{H}-z)^{-2} - [\partial_\kappa \hat{H}, \hat{H}](\hat{H}-z)^{-3} \\ -[\hat{H}, [\hat{H}, \partial_\kappa \hat{H}]](\hat{H}-z)^{-4} &+ (\hat{H}-z)^{-1}[\hat{H}, [\hat{H}, [\hat{H}, \partial_\kappa \hat{H}]]](\hat{H}-z)^{-4}. \end{aligned} \tag{2.13}$$

Each commutator gives one $\hbar$ and we can compute in the same way higher derivatives in κ. So using Cauchy formula we can compute asymptotics in $\hbar$ of derivatives in κ of Ω. ∎

Theorem 2.2 *For any $\varepsilon > 0$ and $\kappa_0 > 0$, Ω admits an asymptotic expansion in $\hbar$, uniform in κ for $|\kappa| \leq \kappa_0$, and for $\beta \leq \hbar^{\varepsilon - 2/3}$. More explicitly, for any $N \in I\!N$ we have :*

$$\Omega = h^{-n} \sum_{j=0}^{N} \sum_{k \leq \frac{3j}{2}} \frac{(-1)^{k+1}}{k!} \hbar^j \ \Omega_{jk} + O\left(\hbar^{N+1-n} \ \beta^{\frac{3N}{2}+k(n)}\right) \tag{2.14}$$

with

$$\Omega_{jk} = \int_{I\!R^{2n}} dq \ dp \ d_{jk}(q,p) \ F_\beta^{(k)}(H_\kappa - \mu)$$

d_{jk} being a suitable linear combination of derivatives of H_κ with respect to q, p and $k(n)$ a constant depending only on the dimension n ($k(n) \leq 2n+1$). In particular :

$$\Omega_{00} = \int_{I\!R^{2n}} dq \ dp \ F_\beta \left(H_\kappa(q,p) - \mu\right) \tag{2.15}$$

$$\frac{1}{2}\Omega_{22} - \frac{1}{6}\Omega_{23} = -\frac{\beta}{48\pi^2} \int_{I\!R^{2n}} dq \ dp \frac{\kappa^2 \parallel B(q) \parallel^2 - \sum_{jk} \partial_{jk}^2 V}{\cosh^2\left[\frac{\beta}{2}\left(H_\kappa(q,p) - \mu\right)\right]} \tag{2.16}$$

where B_{jk} is the magnetic field

$$\| B \|^2 = \sum_{j<k} B_{jk}^2, \qquad B_{jk} = \frac{\partial a_j}{\partial q_k} - \frac{\partial a_k}{\partial q_j}, \; \partial_{jk}^2 V = \frac{\partial^2 V}{\partial q_j \partial q_k}. \tag{2.17}$$

and we have chosen the gauge so that $\partial a/\partial q$ is symmetric. Moreover, the asymptotic expansion can be derived term by term with respect to κ and yields an asymptotic expansion of the magnetization and the magnetic susceptibility.

Proof. We start with the following Cauchy formula as in the proof of proposition (2.1)

$$F_\beta\left(\widehat{H}_\kappa - \mu\right) = \frac{1}{2i\pi}\int_\Lambda dz\; F_\beta(z-\mu)\left(\widehat{H}_\kappa - z\right)^{-1} \tag{2.18}$$

Proceeding as in [23], good enough semi-classical approximations of $(\widehat{H}_\kappa - z)^{-1}$ (for $z \in \Lambda$) are obtained for any integer N of the following form :

$$\left(\widehat{H}_\kappa - z\right)^{-1} = \sum_{j=0}^{N} \hbar^j \widehat{b_j(z)} - h^{N+1}\left(\widehat{H}_\kappa - z\right)^{-1}\; \widehat{R}_N(z) \tag{2.19}$$

where $\widehat{A}$ denotes Weyl quantization, and $b_j(z)$ for $j \geq 2$ are obtained, from $b_0(z) = (H_\kappa(q,p) - z)^{-1}$ by the formula

$$b_j(z) = \sum_{2 \leq \ell \leq \left[\frac{3j}{2}\right]} d_{j\ell}\; b_0^{\ell+1}(z) \tag{2.20}$$

$d_{j\ell}$ being a symbol constructed through partial derivatives of $H_\kappa(q,p)$ and that can be computed explicitly. Furthermore, due to the particular form (2.3) of H_κ, $b_j \equiv 0$ for odd j's, and R_N obeys :

$$|R_N(z)| \leq C_N \left|\frac{z}{Im\ z}\right|^{\frac{3N}{2}+k(n)}, \tag{2.21}$$

$k(n)$ depending only on the dimension n. (for details see [8]).

Now inserting (2.19) into the Cauchy formula and using

$$f^{(m)}(\lambda) = \frac{(-1)^m m!}{2i\pi}\int_\Lambda dz\; f(z)\; (z-\lambda)^{-m-1} \tag{2.22}$$

together with ($h = 2\pi\hbar$) :

$$\mathrm{Tr}\ \widehat{A} = h^{-n}\int_{\mathbb{R}^{2n}} dp\; dq\; A(q,p) \tag{2.23}$$

we get the result. Let us make explicit the calculus. We have to find $b_2(z)$ such that

$$\left(\widehat{H}_\kappa - z\right)\left(\widehat{b_0(z)} + \hbar^2\widehat{b_2(z)}\right) = 1 + O(\hbar^3) \tag{2.24}$$

which, according to the rule for the symbol of the product of two operators, yields

$$b_2(z) = d_{22}\ b_0^3(z) + d_{23}\ b_0^4(z) \tag{2.25}$$

with $b_0(z) = (H_\kappa - z)^{-1}$, and

$$\left\{\begin{array}{l} d_{22} = -\dfrac{1}{4}\displaystyle\sum_{|\alpha|+|\alpha'|=2}\left(\partial_p^\alpha\partial_q^{\alpha'}H_\kappa\right)\left(\partial_p^{\alpha'}\partial_q^\alpha H_\kappa\right)\frac{(-1)^{|\alpha'|}}{\alpha!\alpha'!} \\ \\ d_{23} = \dfrac{1}{2}\displaystyle\sum_{|\alpha|+|\alpha'|=2}\left(\partial_p^\alpha\partial_q^{\alpha'}H_\kappa\right)\left(\partial_p^{\alpha'}H_\kappa\right)\left(\partial_q^\alpha H_\kappa\right)\frac{(-1)^{|\alpha'|}}{\alpha!\alpha'!} \end{array}\right. \tag{2.26}$$

α being a multi-index $\alpha = (\alpha_1, \cdots \alpha_n) \in I\!N^n$, we denote as usually by ∂_p^α the multiple derivative $\frac{\partial^{\alpha_s}}{\partial p_1}\frac{\partial^{\alpha_2}}{\partial p_2}\cdots\frac{\partial^{\alpha_n}}{\partial p_n}$, by $|\alpha|$ the sum $\sum\limits_{j=1}^n \alpha_j$, and by $\alpha!$ the product $\prod\limits_{j=1}^n \alpha_j!$.

Now the calculi proceed as in [13] :

$$\begin{aligned} \Omega_{23} \ &= \ \frac{1}{4}\int_{I\!R^{2n}} dq\ dq\ F_\beta^{(3)}(H_\kappa - \mu)\left(\sum_{j,k=1}^n \left(\partial_{q_j}H_\kappa\right)\left(\partial^2_{p_jp_k}H_\kappa\right)\left(\partial_{q_k}H_\kappa\right)\right. \\ &\quad \left. -2\left(\partial_{q_j}H_\kappa\right)\left(\partial_{p_k}H_\kappa\right)\left(\partial^2_{p_jq_k}H_\kappa\right) + \left(\partial p_j H_\kappa\right)\left(\partial_{p_k}H_\kappa\right)\left(\partial^2_{q_jq_k}H_\kappa\right)\right) \end{aligned}$$

and integrating by parts (over q_j, or p_k) we get

$$\Omega_{23} = 2\int_{I\!R^{2n}} dq\ dp\ F_\beta^{(2)}(H_\kappa - \mu)d_{22}(q,p) = 2\Omega_{22} \tag{2.27}$$

and thus :

$$\frac{1}{2}\Omega_{22} - \frac{1}{6}\Omega_{23} = \frac{1}{6}\Omega_{22} \tag{2.28}$$

We now make d_{22} explicit :

$$\begin{aligned} d_{22} \ &= \ \frac{1}{4}\sum_{j,k}\left(\partial^2_{q_jp_k}H_\kappa\right)\left(\partial^2_{p_jq_k}H_\kappa\right) - \left(\partial^2_{q_jq_k}H_\kappa\right)\left(\partial^2_{p_jp_k}H_\kappa\right) \\ &= \ \frac{1}{4}\left\{\kappa^2 \parallel B \parallel^2 + \sum_{j\ell}\left(\kappa\left(p_j - \kappa a_j(q)\right)\cdot\partial^2_{j\ell}a(q) - \partial_{j_\ell}V(q)\right)\right\} \end{aligned} \tag{2.29}$$

Clearly the term $(p_j - \kappa a_j(q))\partial^2_{jk} a(q)$ does not contribute to Ω_{22} using the change of variable $p \to p - \kappa a(q)$, and the oddness of the integrand with respect to p variable. Thus we are left with

$$\Omega_{22} = \frac{1}{4}\int_{I\!R^{2n}} dq\ dp\ F^{(2)}_\beta(H_0-\mu)\left(\kappa^2 \parallel B(q) \parallel^2 - \sum_{jk}\partial^2_{jk}V(q)\right)$$

Now the uniformity of the asymptotic expansion in $\hbar$ with respect to $\beta \le \hbar^{\varepsilon-\frac{2}{3}}$ (for any $\varepsilon > 0$) comes from the fact that $F^{(k)}_\beta(x) = \beta^{k-1}F^{(k)}_1(\beta x)$, $(k \ge 1)$ so that $\hbar^j\beta^k \le \hbar^{j\varepsilon}$ for $k \le \frac{3j}{2}$. Furthermore, the error term in (2.14) follows from (2.21).

For the magnetization M, we start with formula (2.7) and we use the semiclassical expansion for the resolvant to get

$$M = \frac{1}{2i\pi}\mathrm{Tr}\int_\Lambda dz f_\beta(z-\mu)\left(\sum_{0\le j\le N}\hbar^j\hat{b}_j(z)\partial_\kappa\widehat{H_\kappa}\right) \tag{2.30}$$

$$-\frac{\hbar^{N+1}}{2i\pi}\mathrm{Tr}\int_\Lambda dz f_\beta(z-\mu)(\widehat{H_\kappa}-z)^{-1}\widehat{R_N}(z)\partial_\kappa\widehat{H_\kappa} \tag{2.31}$$

Then using integration by parts we can prove that the first term in (2.30) is

$$\hbar^{-n}\sum_{0\le j\le N}\sum_{k\le 3j/2}\frac{(-1)^{k+1}}{k!}\hbar^j\partial_\kappa\Omega_{j,k}, \tag{2.32}$$

and the second term in (2.30), using estimate (2.21), is

$$O\left(\hbar^{N+1-n}\beta^{3N/2+k(n)}\right), \tag{2.33}$$

uniformly in κ for $|\kappa| \le \kappa_0$.
The same method can be used to prove semiclassical asymptotics for the susceptibility χ and also for higher order derivatives in κ of Ω. ∎

Now let us denote by $\sum^\kappa_\mu$ the energy surface at energy μ.

$$\sum\nolimits^\kappa_\mu = \left\{(q,p) \in I\!R^{2n} : H_\kappa(q,p) = \mu\right\} \tag{2.34}$$

and by $d\sigma^\kappa_\mu$ the Liouville measure on $\sum^\kappa_\mu$:

$$d\sigma^\kappa_\mu(q,p) = \frac{d\sum^\kappa_\mu}{|\nabla H_\kappa|} \tag{2.35}$$

defined for any non-critical μ (i.e. $\nabla H_\kappa(q,p) \ne 0$ on $\sum^\kappa_\mu$) ($d\sum^\kappa_\mu$ Lebesgue Euclidean measure). Then we have

Corollary 2.3 (Landau diamagnetism) *Let χ be defined by (2.8), and μ be non-critical for H_0. Then for $n = 2$ and $\kappa = 0$ we have*

$$\lim_{\hbar \to 0, \beta \to \infty, \beta \leq \hbar^{\varepsilon - 2/3}} \chi = -\frac{1}{24\pi^2} \int_{\sum_\mu^0} \| B(q) \|^2 \, d\sigma_\mu^0 \tag{2.36}$$

which is nothing but Landau's result of the diamagnetism for a 2-dimensional free electron gas.

3 A "trace formula" for the magnetization

For a temperature regime $\beta \geq \hbar^{-\frac{2}{3}+\varepsilon}$ ($\varepsilon > 0$), in order to get information on the semi-classical limit of magnetization M, we shall use the Fourier inversion formula instead of Cauchy formula. First of all let us remark that f_β is not in the Schwartz space $\mathcal{S}(\mathrm{R})$ so it is more convenient to take its derivative, which is in $\mathcal{S}(\mathrm{R})$. We have explicitly

$$f'_\beta(x) = \frac{-\beta}{4\cosh^2(\beta x/2)}$$

So we have the following Fourier transform formula

$$f'_\beta(x) = -\frac{1}{2\pi} \int_{\mathrm{R}} dt \frac{\pi t/\beta}{\sinh(\pi t/\beta)} \mathrm{e}^{itx} \tag{3.1}$$

So we can write

$$f'_\beta(\widehat{H} - \mu) = h^{-1} \int_{-\infty}^{+\infty} dt \; e^{it(\widehat{H}-\mu)/\hbar} \; \frac{\pi t/\sigma}{\sinh \pi t/\sigma} \tag{3.2}$$

where

$$\sigma = \beta\hbar \tag{3.3}$$

The parameter σ, which has the dimension of a time, will be important in what follows. It plays a role in the Kubo-Martin-Schwinger condition (see[7]).
Because we cannot compute the semiclassical evolution for infinite time, we shall consider a "smeared out" magnetization defined as follows. Fix τ_0 and τ : $0 < \tau_0 < \tau$; given a $\mathcal{C}^\infty$ even function ρ such that :

$$\begin{aligned} &\rho(t) \equiv 1 \qquad \text{if} \quad |t| \leq 1 \\ &\rho(t) \equiv 0 \qquad \text{if} |t| \geq 2 \ \text{ and } \int_{\mathrm{R}} \rho(t) dt = 1 \end{aligned} \tag{3.4}$$

Let us define for $\tau > 0$,

$$\rho_\tau(t) = \rho(t/\tau) \tag{3.5}$$

and

$$M_\tau = \mathrm{Tr}\left\{ (f_\sigma * \widetilde{\rho}_\tau) \left(\frac{\widehat{H}_\kappa - \mu}{\hbar} \right) \partial_\kappa \widehat{H}_\kappa \right\} \tag{3.6}$$

where $\widetilde{g}$ denotes the inverse Fourier transform of g. Clearly $M_\tau \to M$ when $\tau \to \infty$. However we shall not be able to let $\tau \to \infty$ in this paper (see discussion at the end of this section), and we will only obtain results for finite τ.

Consider a cut-off function $\theta \in \mathcal{C}_0^\infty(I\!R)$ with supp $\theta \subset [-\delta, \delta]$, and $\theta \equiv 1$ on $[-\frac{\delta}{2}, \frac{\delta}{2}]$. It is a priori arbitrary but in the sequel, we will take δ so small that if μ is non-critical for H_κ, any $\lambda \in]\mu - 3\delta, \mu + 3\delta[$ will remain so.

Let us write the following decomposition

$$M_\tau = M_{\tau,\theta} + M_{\tau,1-\theta} \tag{3.7}$$

where

$$\begin{cases} M_{\tau,\theta} = \mathrm{Tr}\left\{ (f_\sigma * \widetilde{\rho}_\tau) \left(\frac{\widehat{H}_\kappa - \mu}{\hbar} \right) \theta \left(\widehat{H}_\kappa - \mu \right) \partial_\kappa \widehat{H}_\kappa \right\} \\ \\ M_{\tau,1-\theta} = \mathrm{Tr}\left\{ (f_\sigma * \widetilde{\rho}_\tau) \left(\frac{\widehat{H}_\kappa - \mu}{\hbar} \right) (1-\theta) \left(\widehat{H}_\kappa - \mu \right) \partial_\kappa \widehat{H}_\kappa \right\} \end{cases} \tag{3.8}$$

We now prove

Lemma 3.1 *Let us assume (H1-3) for $\widehat{H}_\kappa$, and let $\sigma > \sigma_0 > 0$. Then $M_{\tau,1-\theta}$ has a complete asymptotic expansion in $\hbar$.*

__Proof__. $(1-\theta)(x)$ is supported by the union of $(-\infty, -\delta]$ and $[\delta, +\infty)$, which yields two contributions to $M_{\tau,1-\theta}$ that we call $M^{\pm}_{\tau,1-\theta}$.

Since $f_\sigma * \widetilde{\rho}_\tau = -\int_x^\infty (f'_\sigma * \widetilde{\rho}_\tau)(y)dy$ is the primitive vanishing at $+\infty$ of a function in the Schwartz class $\mathcal{S}(\mathrm{R})$, we have for every N, uniformly for $\sigma > \sigma_0$ and $\hbar \in]0,1]$,

$$|\mathrm{Tr}\left\{ (f_\sigma * \widetilde{\rho}_\tau) \left(\frac{\widehat{H}_\kappa - \mu}{\hbar} \right) (1-\theta)^+ \left(\widehat{H}_\kappa - \mu \right) \partial_\kappa \widehat{H}_\kappa \right\}| \leq C_N \, \hbar^N$$

We now consider $M^-_{\tau,1-\theta}$.

Since $\int_{-\infty}^{+\infty} (f'_\sigma * \widetilde{\rho}_\tau)(y)dy = (\widetilde{f'_\gamma} \cdot \rho_\tau)(0) = 1$, we clearly have, uniformly for any $\lambda \in sp(\widehat{H}_\kappa - \mu) \cap (-\infty, -\delta]$, and any $\sigma > \sigma_0$:

$$f_\sigma * \widetilde{\rho}_\tau \left(\frac{\lambda}{\hbar}\right) = 1 + O(\hbar^N) \tag{3.9}$$

and, since $\widehat{H}_\kappa$ is semi-bounded from below, the contribution of 1 in (3.9) gives $\mathrm{Tr}\left\{(1-\theta)^-(\widehat{H}_\kappa - \mu)\partial\widehat{H}_\kappa\right\}$ and obviously has a complete $\hbar$ expansion by the functional calculus (in fact it is of the form $\mathrm{Tr}\left\{\theta_1(\widehat{H}_\kappa - \mu)\partial_\kappa\widehat{H}_\kappa\right\}$ for some $\theta_1 \in \mathcal{C}_0^\infty(I\!R)$.)
$\square$

The next step is to decompose ρ_τ in order to isolate the neighborhood of $t = 0$ of the rest :

$$\rho_\tau = \rho_{\tau_0}\ \rho_\tau + (1 - \rho_{\tau_0})\, \rho_\tau \equiv \rho_{\tau_0} + \rho_{1,\tau} \tag{3.10}$$

since $\rho_{\tau_0}\rho_\tau = \rho_{\tau_0}$ if $\tau > 2\tau_0$.

This yields $\widetilde{\rho}_\tau = \widetilde{\rho}_{\tau_0} + \widetilde{\rho}_{1,\tau}$ and correspondingly :

$$M_{\tau,\theta} = M_0 + M_{osc} \tag{3.11}$$

$$\left\{\begin{array}{l} M_0 = \mathrm{Tr}\left\{(f_\sigma * \widetilde{\rho}_{\tau_0})\left(\dfrac{\widehat{H}_\kappa - \mu}{\hbar}\right)\theta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa\widehat{H}_\kappa\right\} \\ \\ M_{osc} = \mathrm{Tr}\left\{(f_\sigma * \widetilde{\rho}_{1,\tau})\left(\dfrac{\widehat{H}_\kappa - \mu}{\hbar}\right)\theta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa\widehat{H}_\kappa\right\} \end{array}\right. \tag{3.12}$$

Finally M_τ is decomposed into

$$M_\tau = \overline{M} + M_{osc} \tag{3.13}$$

where M_{osc} is given by (3.11), and

$$\overline{M} = M_0 + M_{\tau,1-\theta} \tag{3.14}$$

We prove :

Lemma 3.2 *Assume also μ is non-critical for H_κ. Then for τ_0 small enough the classical flow induced by Hamiltonian H_κ on $\sum_\mu^\kappa$ has no periodic point of period $\leq \frac{\tau_0}{2}$ and M_0 admits an asymptotic expansion in $\hbar$, uniform for $\sigma = \beta\hbar \geq \sigma_0 > 0$.*

Proof. We have

$$\begin{aligned} M_0 &= \int_{+\infty}^{\mu} d\lambda \ \mathrm{Tr}\left\{ (f'_\sigma * \tilde{\rho}_{\tau_0}) \left(\frac{\widehat{H}_\kappa - \lambda}{\hbar} \right) \theta\left(\widehat{H}_\kappa - \mu\right) \partial_\kappa \widehat{H}_\kappa \right\} \\ &= -\int_{\mu}^{\mu+3\delta} d\lambda \ \mathrm{Tr}\left\{ (f'_\sigma * \tilde{\rho}_{\tau_0}) \left(\frac{\widehat{H}_\kappa - \lambda}{\hbar} \right) \theta\left(\widehat{H}_\kappa - \mu\right) \partial_\kappa \widehat{H}_\kappa \right\} + O(h^\infty) \end{aligned} \tag{3.15}$$

using the fact that $f'_\sigma * \tilde{\rho}_{\tau_0}$ is in the space $\mathcal{S}(\mathrm{R})$ and the support property of the cut-off function θ. Now, if μ is non-critical for $\widehat{H}_\kappa$, it will remain true for any $\lambda \in [\mu, \mu+3\delta]$ for small enough δ.

We can rewrite the Trace inside the integral in (3.15), using inverse Fourier transform,

$$M_0 = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dt \ \frac{\pi t/\sigma}{\sinh \ \pi t/\sigma} \rho\left(\frac{t}{\tau_0}\right) \mathrm{Tr}\left\{ e^{-it(\widehat{H}-\lambda)/\hbar} \ \theta\left(\widehat{H} - \mu\right) \partial_\kappa \widehat{H} \right\} \tag{3.16}$$

(omitting the index κ of $\widehat{H}_\kappa$ for simplicity). Now, using either WKB method (see for instance [23]), or the coherent state decomposition [5], a complete asymptotic expansion in $\hbar$ of M_0 can be obtained, of the form :

$$M_0 = \hbar^{-n+1} \left(C_0(\lambda) + \hbar C_1(\lambda) + \cdots + h^k C_k(\lambda) + \cdots \right) \qquad \mathrm{mod} \ O(h^\infty)$$

which can be further integrated with respect to λ on the interval $[\mu, \mu+3\delta]$, yielding the result. □

Remark 3.3 *Above Lemmas therefore imply that $\overline{M}$ has a complete asymptotic expansion in $\hbar$. It is, so to say, the analog of the (complete $\hbar$-expansion of) the "mean density of states" in the Gutzwiller trace formula. The other term M_{osc} will be the sum of highly oscillating terms, also in complete analogy with the oscillatory part of Gutzwiller trace formula. Before showing this now, let us remark that the dominant $\hbar$ contribution to $\overline{M}$ has not yet been shown to reduce to the well known "Landau diamagnetism". This will be postponed to the end of this section.*

Proposition 3.4 *Assume (H1-3) together with*

(H.4) μ is non-critical for H_κ ($|\kappa| < \kappa_0$)

(H.5) On $\sum_\mu^\kappa$, the set $(\Gamma_\mu)_\tau$ of classical periodic orbits denoted γ with period smaller than τ is such that the corresponding Poincaré maps P_γ do not have eigenvalue 1.

Then for any $\sigma_1 > 0$ and for $\kappa_0 > 0$ small enough, we have the following uniform asymptotics for $\beta\hbar = \sigma \in]0, \sigma_1]$ and $|\kappa| \le \kappa_0$,

$$M_{osc} = \sum_{\gamma \in (\Gamma_\mu)_\tau} e^{i(S_\gamma/\hbar + \nu_\gamma \frac{\pi}{2})} \left\{ \frac{\rho_{1,\tau}(T_\gamma)}{|\det(1-P_\gamma)|^{1/2}} \frac{im_\gamma/2\sigma}{\sinh(\pi T_\gamma/\sigma)} + \sum_{k\ge1} d_\gamma^{(k)} \hbar^k \right\} + O(\hbar^\infty) \tag{3.17}$$

where $m_\gamma = \int_0^{T_\gamma^*} dt \partial_\kappa \ H_\kappa(q_t, p_t)$.

T_γ^* is the primitive period of orbit γ,

S_γ (resp. ν_γ) is the classical action (resp. Maslov index) of orbit γ.

$d_\gamma^{(k)}$ are constants depending on orbit γ, on the function $\rho_{1,\tau}$, and on γ.

Moreover the different orbits γ can be choosen such that they depend smoothly on the parameter κ and the asymptotic expansion holds uniformly in κ for $|\kappa|$ small enough.

Proof. Since $\rho_{1,\tau}$ is supported away from zero, we can rewrite M_{osc} (defined in (3.12)) as the non-singular integral :

$$M_{osc} = \frac{1}{h} \int_{-\infty}^{+\infty} \frac{dt}{t} \rho_{1,\tau}(t) \frac{\pi t/\sigma}{\sinh \ \pi t/\sigma} \mathrm{Tr} \left\{ \theta\left(\widehat{H_\kappa} - \mu\right) e^{-it(\widehat{H_\kappa}-\mu)/\hbar} \ \partial_\kappa \widehat{H_\kappa} \right\} \tag{3.18}$$

Now the method that we have developed in [6] applies, and yields the desired result. □

Remark 3.5 *At zero magnetic field ($\kappa = 0$) the term m_γ is computed as follows. We have*

$$m_\gamma = \oint_\gamma \partial_\kappa H_\kappa(q_t, p_t) dt = -\oint_\gamma a dq = -\Phi_\gamma$$

where Φ_γ is the flux of the magnetic field through the closed curve γ.

We now come back to $\overline{M}$, and prove that the dominant contribution of the $\hbar$-expansion is indeed the well-known diamagnetic Landau term.

Proposition 3.6 *Assume (H1-4). Then for any $\sigma_1 > 0$ and for $\kappa_0 > 0$, uniformly for $\beta\hbar = \sigma \in]0, \sigma_1[$ we have, mod $O(h^\infty)$,*

$$\overline{M} = -\kappa \frac{\hbar^{2-n}}{24\pi^2} \int_{\sum_\mu^0} d\sigma_\mu^0 \parallel B(q) \parallel^2 \ + \sum_{k \geq 3-n} c_k(\mu, 0, \sigma, T)\hbar^k + O(\hbar^\infty). \tag{3.19}$$

<u>Proof</u>. Whereas the existence of a complete asymptotic expansion for $\overline{M}$ results immediately from lemmas (3.1) and (3.2), the explicit calculus of the dominant contribution in (3.19) is not an immediate consequence. It will be done through the functional calculus. In the previous section we have shown that the coefficients of the asymptotic $\hbar$-expansion are regular functions of κ, and can be differentiated with respect to κ. Thus, according to (3.14), we shall obtain the dominant contribution to $\overline{M}$ from two different contributions $\Omega_0(\lambda)|_{\lambda=\mu}$ and $\Omega_{\tau,1-\theta}(\lambda)|_{\lambda=\mu}$ by differentiating with respect to κ :

$$\begin{cases} \Omega_0(\lambda) = \mathrm{Tr}\left[(F_\beta * \tilde{\rho}_{\tau_0}) \left(\dfrac{\widehat{H}_\kappa - \lambda}{\hbar} \right) \theta \left(\widehat{H}_\kappa - \mu \right) \right] \\ \\ \Omega_{0,1-\theta}(\lambda) = \mathrm{Tr}\left[(F_\beta * \tilde{\rho}_{\tau}) \left(\dfrac{\widehat{H}_\kappa - \lambda}{\hbar} \right) (1-\theta) \left(\widehat{H}_\kappa - \mu \right) \right] \end{cases} \tag{3.20}$$

Let us consider the contribution of second derivatives in λ of $\Omega_0(\lambda)$:

$$\Omega_0''(\lambda) := G(\lambda) = h^{-n} c_0''(\lambda) + h^{-n+2} c_2''(\lambda) + O(h^{-n+3}) \tag{3.21}$$

and we shall identify $c_0(\lambda)$ and $c_2(\lambda)$ by the following trick (inspired from ref. [23] prop. V.8) : Take $\varphi \in \mathcal{C}_0^\infty(]\mu - 3\delta, \mu + 3\delta[)$ and integrate against (3.21) ; we get :

$$\int d\lambda \ \varphi(\lambda) \ G(\lambda) = h^{-1} \int \tilde{\rho}_{eff} \left(\frac{\lambda}{\hbar} \right) \mathrm{Tr}\left[\varphi_\theta \left(\widehat{H} - \lambda \right) \right] d\lambda \tag{3.22}$$

where

$$\rho_{eff}(t) = \rho_{\tau_0}(t) \frac{\pi t/\sigma}{\sinh{(\pi t/\sigma)}},$$

$\tilde{\rho}_{eff}(\lambda)$ is its Fourier transform, and

$$\varphi_\theta(E) := \varphi(E) \ \theta(E + \lambda - \mu) \tag{3.23}$$

(3.22) follows from :

$$G(\lambda) = \frac{1}{h} \int dt \ \rho_{eff}(t) \ \mathrm{Tr}\left[e^{-it(\widehat{H}_\kappa - \lambda)/\hbar} \ \theta \left(\widehat{H}_\kappa - \mu \right) \right]$$

Now (3.22) is rewritten as

$$\int d\lambda\ \varphi(\lambda)\ G(\lambda) = \frac{1}{2\pi}\int d\lambda\ \tilde{\rho}_{eff}(\lambda)\ \mathrm{Tr}\left[\varphi_\theta\left(\widehat{H_\kappa} - \lambda\hbar\right)\right] \tag{3.24}$$

which can be developed through Taylor's formula (since integration variable λ is in a compact interval), as :

$$\begin{aligned}\int d\lambda\ \varphi(\lambda)\ G(\lambda) \qquad &= \frac{1}{2\pi}\sum_{k=0}^{\infty}\frac{(-1)^k\hbar^k}{k!}\int d\lambda\ \lambda^k\ \tilde{\rho}_{eff}(\lambda)\mathrm{Tr}\left[\varphi_\theta^{(k)}(\widehat{H_\kappa})\right] \\ &= \sum_{k=0}^{\infty}\frac{i^k\hbar^k}{k!}\rho_{eff}^{(k)}(0)\ \mathrm{Tr}\left[\varphi_\theta^{(k)}(\widehat{H_\kappa})\right] \end{aligned}\tag{3.25}$$

Actually the term with $k = 0$ is absent since $\rho'_{eff}(0) = 0$ (ρ is an even function, and so is ρ_{eff}). We calculate the coefficients of $\hbar^{-n}$ and h^{2-n} by the functional calculus, like in section 2 :

$$\begin{aligned}\int d\lambda\varphi(\lambda)G(\lambda) = \qquad & h^{-n}\left(\int \varphi_\theta(H(q,p))dp\ dq - \frac{\hbar^2}{12}\int \varphi''_\theta(H(q,p))\left[\kappa^2 \parallel B \parallel^2 - \triangle V\right] dq\ dp\right. \\ & \left. -\frac{\hbar^2}{2}\rho''_{eff}(0)\int \varphi''_\theta\left[H(q,p)\right] dq\ dp + O(h^3)\right)\end{aligned}\tag{3.26}$$

Clearly the first and third terms in (3.26) are independent on κ (through the change of variable $p \mapsto p - \kappa a(q)$), and we are left with lower order term

$$\begin{aligned}& -\frac{h^{2-n}}{12\cdot 4\pi^2}\int dq\ dp\ \varphi''_\theta(H(q,p))\left[\kappa^2 \parallel B \parallel^2 - \sum_{1\le j,k\le n}\partial^2_{j,k}V\right] \\ &= \frac{-h^{2-n}}{12\cdot 4\pi^2}\int d\lambda\ \varphi_\theta(\lambda)\frac{d^2}{d\lambda^2}\int_{\sum_\lambda^\kappa}\left(\kappa^2 \parallel B \parallel^2 - \sum_{1\le j,k\le n}\partial^2_{j,k}V\right) d\sigma_\lambda^\kappa(q,p)\end{aligned}\tag{3.27}$$

where we have used integration by parts :

$$\int_{\mathbb{R}^{2n}} G(q,p)\ \varphi''((H_\kappa(q,p))dq\ dp = \int d\lambda\ \varphi(\lambda)\frac{d^2}{d\lambda^2}\left[\int_{\sum_\lambda^\kappa} d\sigma_\lambda^\kappa\ G(q,p)\right]$$

Therefore since the above calculation holds for an arbitrary test function φ, we can identify the functions c_0 and $c_2(\lambda)$ appearing in (3.21), modulo κ-independent terms as :

$$\begin{cases} c_0(\lambda) = 0 \\ \\ c_2(\lambda) = -\theta(\lambda) \dfrac{\kappa^2}{12 \cdot 4\pi^2} \displaystyle\int_{\sum_\lambda} \parallel B \parallel^2 d\sigma_\lambda(q,p) \end{cases} \tag{3.28}$$

We can do the same calculus for $\Omega_{\tau,1-\theta}$ instead of Ω_0 by replacing τ_0 by τ and θ by $1-\theta$. This yields a contribution to the magnetization which, added to that coming from $c_2(\lambda)$ in (3.28) gives the dominant Landau term in (3.19).

We shall extend now the above results to the magnetic susceptibility χ. The statement is the following

Theorem 3.7 *Let us assume H-1 to H-5 and $\sigma = \beta\hbar \in]0, \sigma_1]$ where $\sigma_1 > 0$ is fixed. For $\chi_\tau = \chi * \rho_\tau$, $\tau > 0$, we have the decomposition*

$$\chi_\tau = \overline{\chi} + \chi_{osc} \tag{3.29}$$

with

$$\overline{\chi} = -\frac{\hbar^{2-n}}{24\pi^2} \int_{\sum_\mu^\kappa} d\sigma_\mu^\kappa \parallel B(q) \parallel^2 + \sum_{k \geq 3-n} c_{\chi,k}(\mu,\kappa,\sigma,T)\hbar^k + O(\hbar^\infty) \tag{3.30}$$

$$\chi_{osc} = \sum_{\gamma \in (\Gamma_\mu)_\tau} e^{i(S_\gamma/\hbar + \nu_\gamma \frac{\pi}{2})} \left\{ \frac{\rho_{1,\tau}(T_\gamma)}{|\det(1-P_\gamma)|^{1/2}} \frac{r_\gamma m_\gamma^2/2\sigma}{\sinh(\pi T_\gamma/\sigma)} + \sum_{k \geq 1} d_{\chi,\gamma}^{(k)} \hbar^k \right\} + O(\hbar^\infty) \tag{3.31}$$

where we have used the notations in proposition (3.4) and $r_\gamma = \frac{T_\gamma}{T_\gamma^*}$, $c_{\chi,\gamma}$, $d_{\chi,\gamma}$ are smooth coefficients depending on the periodic orbit γ, on σ, and on function ρ.

<u>Proof</u> We use the same cut-off already introduced for the magnetization M. So we define in a natural way

$$\overline{\chi} = \partial_\kappa M_{\tau_0,\theta} + \partial_\kappa M_{\tau,1-\theta} \tag{3.32}$$

$$\chi_{osc} = \chi_\tau - \overline{\chi} \tag{3.33}$$

Compute first the term $\chi_{\tau_0,\theta} = \partial_\kappa M_{\tau_0,\theta}$. From the proof of proposition (3.4) we get

$$\chi_{\tau_0,\theta} = -\frac{1}{h} \int_0^\mu d\lambda \int_{-\infty}^{+\infty} dt \, \frac{\pi t/\sigma}{\sinh(\pi t/\sigma)} \rho\left(\frac{t}{\tau_0}\right) \partial_\kappa \mathrm{Tr}\left\{ \mathrm{e}^{-\frac{it}{\hbar}(\widehat{H_\kappa}-\lambda)} \, \theta\left(\widehat{H_\kappa} - \lambda\right) \partial_\kappa \, \widehat{H_\kappa} \right\} \tag{3.34}$$

We compute derivative in the parameter κ with the following easy consequence of the Duhamel formula

$$\partial_\kappa \mathrm{Tr}\left\{ \mathrm{e}^{-\frac{it}{\hbar}(\widehat{H}-\mu)}\ \theta\left(\widehat{H}-\mu\right)\partial_\kappa\ \widehat{H}\right\} = \mathrm{Tr}\left\{ \mathrm{e}^{-\frac{it}{\hbar}(\widehat{H}-\lambda)}\ \partial_\kappa[\theta\left(\widehat{H}-\lambda\right)\partial_\kappa\ \widehat{H}]\right\} + \frac{1}{i\hbar}\mathrm{Tr}\left\{ \int_0^t ds\left(\mathrm{e}^{\frac{is}{\hbar}\widehat{H}_\kappa}\partial_\kappa\widehat{H_\kappa}\mathrm{e}^{-\frac{is}{\hbar}\widehat{H_\kappa}}\right)\mathrm{e}^{-\frac{it}{\hbar}(\widehat{H_\kappa}-\lambda)}\theta\left(\widehat{H}-\mu\right)\partial_\kappa\ \widehat{H_\kappa}\right\} \quad (3.35)$$

Then due to the support property of τ_0, the only stationary points corresponds to the period $T=0$ and the leading term in $\hbar$ is given by the first term. The term $\chi_{\tau,1-\theta} = \partial_\kappa M_{\tau,1-\theta}$ is computed in the same way and the both term combines to yield the asymptotic expansion of $\overline{\chi}$.
For the term χ_{osc} we start from a formula like (3.34) replacing the time cut-off ρ_{τ_0} by the following $\rho_{1,\tau} = \rho_\tau(1-\rho_{\tau_0})$. Hence applying the methods of [6] we can compute with the stationary phase theorem the contributions of the periodic trajectories with period $T_\gamma \in (\Gamma_\mu)_\tau$.

Remark 3.8 *In the so-called "mesoscopic regime" examined in this section (i.e. $T = \frac{\hbar}{\sigma k_B}$ for some fixed σ having the dimension of time) , and in the special case of dimension 2, the dominant semi-classical contribution M_L to $\overline{M}$ and M_1 to M_{osc} are of the same order (apart from highly oscillating factors). A comparison of the corresponding contributions χ_L and χ_1 to the susceptibility is made in the physics literature, measuring a factor of 100 for χ_1/χ_L [22].*

Remark 3.9 *Thus the magnetic response is a measurable quantity where the skeleton of the periodic orbits of the classical motion manifests itself clearly ; we have investigated this effect rigorously and in great generality. Furthermore the oscillations in (3.17) are a generalization of the well-known de Haas-van Alphen oscillations of the magnetic response which are a result of the classical cyclotronic orbits demonstrated in dimensions 2 and 3, and which can be recovered from (3.17) in the limiting case where all classsical orbits are of cyclotronic nature ($V=0$ or quadratic).*

Now, we want to comment about the fact that we have only been able to give semi-classical expansions for "smeared out magnetizations" M_τ instead of the true one ($\tau=\infty$). For non-zero temperature $T \neq 0$, the exponential decrease of $\widetilde{f'_\beta}(t)$ when $k \to +\infty$ lets us expect that the Fourier inversion formula (3.1) combined with "trace formulas" will be enough to obtain Proposition (3.4) without the $\widetilde{\rho}_\tau$ which cuts off time at $|t| \leq \tau$. We expect that our method using semi-classical evolution estimates for coherent states [5] will allow to prove this for $\sigma = \beta\hbar > \sigma_0 > 0$ with suitable assumptions on the classical flow. This is presently under study. However for $T = 0$, the cut-off $\widetilde{\rho}_\tau$ will be necessary to make the sum over periodic orbits finite and thus convergent, and we cannot expect to get rid of it.

For the moment, using estimates proved in [5], we can see that it is sufficient to control the periods of the classical flow in the time interval $[\tau, c_0\log(\frac{1}{\hbar}])$. In [5] we have proved that the semi-classical propagation of coherent states is valid in time interval $[-c_0\log(\frac{1}{\hbar}), c_0\log(\frac{1}{\hbar})]$ for some $c_0 > 0$. So we can write down the operator $\mathrm{e}^{-\frac{it}{\hbar}(\widehat{H}-\lambda)}$ as a Fourier integral operator with a complex phase for $|t| \le c_0\log(\frac{1}{\hbar})$. So we have to compute two terms, $(H_\kappa = H)$,

$$F_1(\hbar,\sigma) := \int_{\mathbb{R}} dt \mathrm{Tr}\left\{\mathrm{e}^{-\frac{it}{\hbar}(\widehat{H}-\mu)}\,\theta\left(\widehat{H}-\mu\right)\hat{A}\rho\left(\frac{2t}{c_0\log(\frac{1}{\hbar})}\right)R_\sigma(t)\right\} \tag{3.36}$$

$$F_2(\hbar,\sigma) := \int_R dt \mathrm{Tr}\left\{\mathrm{e}^{-\frac{it}{\hbar}(\widehat{H}-\mu)}\,\theta\left(\widehat{H}-\mu\right)\hat{A}\left[1-\rho\left(\frac{2t}{c_0\log(\frac{1}{\hbar})}\right)\right]R_\sigma(t)\right\} \tag{3.37}$$

where $\hat{A}$ is some quantum observable and $R_\sigma(t) = \frac{\pi t/\sigma}{\sinh \pi t/\sigma}$. The term F_1 is difficult to check and we have nothing to say about it here except that for each time, it is a Fourier integral with a known complex phase but it is difficult to control the stationary phase argument for large times.

The term F_2 is easily controlled because it contains the damping factor R_σ. More precisely we have

Lemma 3.10 *There exists $C > 0$ such that for every $\hbar \in]0,1]$ and $\sigma > 0$ we have easily :*

$$F_2(\hbar,\sigma) \le Cc_0\log(\frac{1}{\hbar})\hbar^{(\pi/\sigma)c_0}. \tag{3.38}$$

So that $F_2(\hbar,\sigma)$ is negligible for $\frac{c_0}{\sigma}$ large enough.

4 The regime of temperature $\hbar^{1-\varepsilon} \le T \le \hbar^{\frac{2}{3}-\varepsilon}$

In section 2 we have shown that the functional calculus applies to the thermodynamical functions in the grand-canonical ensemble and provided asymptotic expansions in the semi-classical limit provided $T \ge \hbar^{\frac{2}{3}-\varepsilon}$ (some $\varepsilon > 0$). In section 3 we have investigated a rather different temperature regime (called "mesoscopic") where $k_BT = \hbar/\sigma$ (some $\sigma > 0$ but finite) where a splitting of the magnetic response into a "mean part" and an "oscillating part" appears in the semi-classical limit. In order to be complete, the "in-between regime" is now considered.

Theorem 4.1 *Assume (H1.4). Then the magnetisation* $M = \partial_\kappa \Omega$ *has for any temperature* T *satisfying* $\hbar^{1-\varepsilon} \leq T \leq \hbar^{\frac{2}{3}-\varepsilon}$ *(some* $\varepsilon > 0$*) a complete asymptotic expansion in* $\hbar$ *obtained by taking the derivative in* κ *of the formal expansion in* $\hbar$ *for* Ω *given (2.14).*

Proof. As in section 3 take $\tau_0 > 0$ so small that, the classical flow induced by H_κ has no periodic point with non-zero period $\in [-2\tau_0, 2\tau_0]$, and take ρ_{τ_0} as in section 3. Futhermore let $\theta \in \mathcal{C}_0^\infty(I\!R)$ be, as in section 3 ($\theta \equiv 1$ on $\left[-\frac{\delta}{2}, \frac{\delta}{2}\right]$, and $\equiv 0$ on $I\!R \setminus [-\delta, \delta]$). We decompose M and

$$M = M_\theta + M_{1-\theta} \tag{4.1}$$

with

$$M_\theta = Tr\left\{ f_\beta\left(\widehat{H}_\kappa - \mu\right)\theta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa \widehat{H}_\kappa \right\} \tag{4.2}$$

and similarly for $M_{1-\theta}$.

Furthermore :

$$\begin{aligned} M_\theta &= -\int_\mu^\infty d\lambda \ \mathrm{Tr}\left\{ f'_\beta\left(\widehat{H}_\kappa - \lambda\right)\theta\left(\widehat{H}_\kappa - \mu\right)\partial_\kappa \widehat{H}_\kappa \right\} && (4.3) \\ &= -\int_\mu^\infty d\lambda \frac{1}{h}\int_{-\infty}^{+\infty} dt \frac{\pi t/\sigma}{\sinh\ \pi t/\sigma} \mathrm{Tr}\left\{ e^{-it(\widehat{H}-\lambda)}\theta\left(\widehat{H} - \mu\right)\partial_\kappa \widehat{H} \right\} \\ &= M_{\theta,\rho} + M_{\theta,1-\rho} && (4.4) \end{aligned}$$

where we insert, inside the integral over t, the partition of unity $1 = \rho_{\tau_0}(t) + (1-\rho_{\tau_0})(t)$, which yields, correspondingly a splitting of M_θ into the two contributions. ∎

Lemma 4.2 *Assuming (H.1-3),* $M_{1-\theta}$ *has a complete asymptotic expansion in* $\hbar$.

Proof. We can proceed as in the proof of Lemma (3.1), by splitting $(1-\theta)(x)$ into the sum of two disjoint functions $(1-\theta)^\pm$ supported respectively in $[\delta, +\infty)$ (for + sign) and $(-\infty, -\delta]$. Since f_β is the primitive vanishing at $+\infty$ of a function in the Schwartz class of $\mathcal{C}^\infty$ functions of rapid decrease, we have

$$|\mathrm{Tr}\left\{f_\beta\left(\widehat{H_\kappa}-\mu\right)(1-\theta)^+\left(\widehat{H_\kappa}-\mu\right)\partial_\kappa\widehat{H_\kappa}\right\}|\leq C_N\,\hbar^N \qquad \text{(for any } N\text{)}$$

and

$$|\mathrm{Tr}\left\{(1-f_\beta)\left(\widehat{H}-\mu\right)(1-\theta)^-\left(\widehat{H}-\mu\right)\frac{\partial\widehat{H}}{\partial\kappa}\right\}|\leq C_N\,\hbar^N \qquad \text{(for sany } N\text{)}$$

Finally, we know, like in the proof of Lemma (3.1), that $\mathrm{Tr}\left\{(1-\theta)^-(\widehat{H}-\mu)\partial_\kappa\widehat{H}\right\}$ has a complete asymptotic $\hbar$ expansion by the functional calculus. ∎

Lemma 4.3 *Assuming (H1-3), one has, for $\hbar^{1-\varepsilon}\leq T\leq\hbar^{\frac{2}{3}-\varepsilon}$*

$$M_{\theta,1-\rho}=O\left(e^{-c_1/\hbar^\varepsilon}\right)$$

where c_1 is a positive constant only depending on τ_0.

<u>**Proof**</u>. Using (4.3), the support property of θ, and the exponential decrease of f'_β, it is easy to show that :

$$M_\theta=-\int_\mu^{\mu+2\delta}d\lambda\;\mathrm{Tr}\left\{f'_\beta\left(\widehat{H_\kappa}-\lambda\right)\theta\left(\widehat{H_\kappa}-\mu\right)\partial\widehat{H_\kappa}\right\}+O\left(e^{-\delta/\sqrt{\hbar}}\right)$$

Therefore

$$M_{\theta,1-\rho}=-\int_\mu^{\mu+2\delta}d\lambda h^{-1}\int_{-\infty}^{+\infty}dt\,(1-\rho_{\tau_0}(t))\,\frac{\pi t/\sigma}{\sinh\ \pi t/\sigma}$$
$$\mathrm{Tr}\left\{\mathrm{e}^{-it(\widehat{H}-\lambda)/\hbar}\theta\left(\widehat{H}-\mu\right)\partial_\kappa\widehat{H_\kappa}\right\}+O\left(\mathrm{e}^{-\delta/\sqrt{\hbar}}\right)$$

and since, in the considered temperature regime

$$\left|\frac{\pi t/\sigma}{\sinh(\pi t/\sigma)}\right|\leq C\ \mathrm{e}^{-c_0|t|/\hbar^\varepsilon}$$

we have, using the support property of $1-\rho_{\tau_0}$:

$$|M_{\theta,1-\rho}|\leq C\ e^{-c_1/\hbar^\varepsilon}$$

c_1 being a positive constant depending on τ_0. ∎

Lemma 4.4 *Assuming (H.1-4), then $M_{\theta,\rho}$ has a complete asymptotic expansion in $\hbar$.*

Proof. As is the previous section, we take δ so small that, if μ is non-critical for H_κ, then any $\lambda \in [\mu, \mu + 2\delta]$ is also non-critical for H_κ.

Now, using the support property of ρ_{T0}, and either WKB method, or decomposition over coherent states, a complete asymptotic expansion can be obtained for

$$h^{-1} \int_{-\infty}^{+\infty} dt\ \rho_{T0}(t) \frac{\pi t/\sigma}{\sinh\ \pi t/\sigma} \mathrm{Tr} \left\{ e^{-it(\widehat{H}_\kappa - \lambda)/\hbar}\ \theta\left(\widehat{H}_\kappa - \mu\right) \widehat{H}_\kappa \right\}$$

for any $\lambda \in [\mu, \mu + 2\delta]$. Integrating with respect to λ in this interval yields the result.

∎

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