Semiclassical Results 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 for describing some of their thermodynamic properties, in particular through exact expansions in $\hbar$ (Planck constant) of their 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 order $\hbar$.

Consider a system of N 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, but near, its equilibrium state. The response of this quantum system to the external time-dependent perturbation is a subject of high physical interest, and 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 mechanics, and its link with the underlying chaotic dynamics [10, 11, 17, 18, 19].

A semi-empirical route which has been proposed and followed (see classical textbooks [14, 13]) consists, for small perturbations, to investigate the response function "to first order in the perturbation", i.e. the so-called "linear response theory". This semi-empirical route is being given a firmer foundation, in classical as well as quantum statistical mechanics, in terms of hyperbolicity properties of the dynamics, and the so-called KMS states [18, 19].

Here we are not following this line of research and do not address the question of validity of the linear response theory. 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 for it, assuming suitable "chaoticity assumptions" on the one-body classical underlying dynamics. These semiclassical expansions are developed in a similar spirit as previous studies on the "semiclassical magnetic response for non-interacting electrons" [16, 1, 4, 9, 7, 12, 15], 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.

Consider a system of N 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

$$H(q,p) = \frac{p^2}{2m} + V(q) \tag{H.1}$$

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

$$V(q) \geq c_0(1+|q|^2)^{s/2} \quad \text{some} \quad s, c_0 > 0\,. \tag{H.2}$$

Under these assumptions, $\widehat{H}$ is self-adjoint in $L^2(\mathbb{R}^n)$, and its spectrum is pure point and contained in $[0,\infty)$. Furthermore, if μ is the Fermi level at temperature T, and f the Fermi-Dirac distribution

$$f(x) \equiv f_\beta(x-\mu) = \left(1 + e^{\beta(x-\mu)}\right)^{-1} \tag{1}$$

where

$$\beta = 1/kT \quad (k \text{ being the Boltzmann constant}) \tag{2}$$

$$\rho_{eq} = f(\widehat{H}) \tag{3}$$

is a trace-class operator in $L^2(\mathbb{R}^n)$, which describes the fermionic equilibrium state, and

$$N = \operatorname{Tr} f(\widehat{H})\,. \tag{4}$$

Now assume that a one-body perturbation $\widehat{A}$ is switched adiabatically. The one-body perturbed Hamiltonian takes the form

$$\widehat{H}(t) = \widehat{H} + \widehat{A}F(t) \tag{5}$$

where $\widehat{A}$ is self-adjoint in $L^2(\mathbb{R}^n)$ (being the Weyl quantization of a symbol $A(q,p)$ that we shall make precise later), and

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

(In the usual Kubo formula for conductivity, $\widehat{A}$ is simply $\widehat{x} \cdot E$ where $\widehat{x}$ is the position operator in $\mathbb{R}^n$, and E an exterior electric field.) In the "linear response theory" we try to solve the following problem: find a "density matrix" $\rho(t)$ (i.e. a trace-class operator in $L^2(\mathbb{R}^n)$), which, to first order in the perturbation solves:

$$i\hbar \frac{\partial \rho}{\partial t} = [\widehat{H}(t), \rho] \tag{6}$$

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

$$\lim_{t\to-\infty} \rho(t) = \rho_{eq}\,.$$

Let $V(t,t_0)$ be the unitary evolution operator induced by $\widehat{H}(t)$ (with $V(t,t_0) =$ Identity), and

$$U(t) =: e^{-it\widehat{H}/\hbar}\,. \tag{7}$$

We can show that $\rho(t)$ solution of (6) is

$$\rho(t) = \lim_{t_0\to-\infty} V(t,t_0)\rho_{eq}\; V(t_0,t)\,. \tag{8}$$

From (5) it follows that:

$$V(t,t_0) = U(t-t_0) + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\; U(t-t')\; F(t')\; \widehat{A}\; V(t',t_0) \tag{9}$$

and the linear response density matrix $\rho_L(t)$ is obtained from $V(t,t_0)\rho_{eq}\;V(t_0,t)$ by

- retaining only the lowest order contributions with respect to perturbation $\widehat{A}$
- letting $t_0 \to -\infty$.

But using (9) we easily see that, up to highest orders in $\widehat{A}$:

$$V(t,t_0)\rho_{eq}\; V(t_0,t) = \rho_{eq} + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\; U(t-t')\; F(t')[\widehat{A},\rho_{eq}]U(t'-t) \tag{10}$$

so that, by the above prescription:

$$\rho_L(t) = \rho_{eq} + \frac{1}{i\hbar}\int_{-\infty}^{t} dt'\; F(t')\; U(t-t')[\widehat{A},\rho_{eq}]U(t'-t)\,. \tag{11}$$

Let $\widehat{B}$ be a suitable self-adjoint operator that we want to "measure" in the state $\rho_L(t)$, as compared to its mean-value in the stationary state ρ. Thus we consider

$$J(t) = \mathrm{Tr}\left[\widehat{B}(\rho_L(t)-\rho_{eq})\right] \tag{12}$$

which, according to (11) can be rewritten as

$$J(t) = -\frac{1}{i\hbar}\int_{-\infty}^{t} dt'\; F(t')\;\; \mathrm{Tr}\left\{\widehat{B}U(t-t')[\widehat{A},\rho_{eq}]U(t'-t)\right\} \tag{13}$$

(the norm convergence of the integral at $t=-\infty$ is ensured by the function $F(t')$, which allows to insert the trace operation inside the integral). If $\widehat{B}$ is the velocity operator $i[\widehat{H},\widehat{x}]$, and $\widehat{A} = \widehat{x}\cdot E$, $J(t)$ is the quantum current at time t (in the linear response framework).

(13) is therefore of the form

$$J(t) = \int_{-\infty}^{t} dt'\; F(t')\; \Phi(t-t') \tag{14}$$

where $\Phi(t)$ is by definition the "dynamical susceptibility" in the linear response framework. It is given by

$$\begin{aligned}\Phi(t) &= \frac{1}{i\hbar}\ \mathrm{Tr}\left\{\widehat{B}(t)[\rho_{eq},\widehat{A}]\right\}\\ &= \frac{1}{i\hbar}\,\mathrm{Tr}\left\{\rho_{eq}[\widehat{B}(t),\widehat{A}]\right\}\end{aligned} \tag{15}$$

where we have used the commutativity of the Trace, and we employ the usual notation for Heisenberg observables at time t evolved by the (unperturbed) Hamiltonian $\widehat{H}$:

$$\widehat{B}(t) = U(-t)\widehat{B}U(t) = e^{it\widehat{H}/\hbar}\ \widehat{B}e^{-it\widehat{H}/\hbar}\,. \tag{16}$$

Let now take the Fourier transform, in the distributional sense, of $\Phi(t)$: this gives the so-called generalized susceptibility:

$$\chi(\omega) = \int_{-\infty}^{+\infty} \phi(t)\ e^{i\omega t}\ dt \tag{17}$$

which is the quantity we shall study now, in the particular case where $\widehat{A} = \widehat{B}$.

Let $(E_n)_{n\in\mathbb{N}}$ and $(\varphi_n)_{n\in\mathbb{N}}$ denote respectively the eigenvalues and eigenstates of the one-particle hamiltonian $\widehat{H}$. It follows from (15)–(17) that

$$\chi(\omega) = \sum_{n,m\in\mathbb{N}} |\langle\varphi_n,\widehat{A}\varphi_m\rangle|^2\ \delta(\hbar\omega + E_n - E_m)\cdot[f(E_n) - f(E_m)]\,. \tag{18}$$

Now, using the analyticity of f:

$$f(E) - f(E+\hbar\omega) = -\sum_{k=1}^{\infty}\frac{(\hbar\omega)^k}{k!}\ f^{(k)}(E)$$

so that (18) is rewritten as

$$\chi(\omega) = -\sum_{n,m\in\mathbb{N}} |A_{nm}|^2\ \delta(\hbar\omega + E_n - E_m)\sum_{k=1}^{\infty}\frac{(\hbar\omega)^k}{k!}\ f^{(k)}(E_n) \tag{19}$$

where we use the notation

$$A_{nm} =: \langle\varphi_n,\widehat{A}\varphi_m\rangle\,. \tag{20}$$

After a careful justification of the commutation of various infinite summations, (19) yields:

$$\chi(\omega) = -\sum_{k=1}^{\infty}\frac{(\hbar\omega)^k}{k!}\int dE\ f^{(k)}(E)\sum_{n,m\in\mathbb{N}}|A_{nm}|^2\delta(E-E_n)\delta(\hbar\omega + E_n - E_m) \tag{21}$$

and we therefore have to study, semiclassically, the behaviour of distributions in E and ω of the form:

$$C(E,\omega) =: \sum_{n,m}|A_{nm}|^2\ \delta(E-E_n)\ \delta(\hbar\omega + E_n - E_m) \tag{22}$$

acting on suitable test functions, and in particular on derivatives of the Fermi-Dirac distribution f. However in all that follows, like in [7], we are only able to replace f_σ by $f_\sigma * \widetilde{\rho}_\tau$ for any fixed τ as large as we want, where

$$\sigma = \beta\hbar \tag{23}$$

is a fixed parameter which has the dimension of time and $\widetilde{\rho}_\tau$ is the Fourier transform of a $\mathcal{C}_0^\infty$ function ρ_τ:

$$\rho_\tau(t) = \rho(t/\tau)$$

where

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

$\int \rho(t)dt = 1$.

Let g be a $\mathcal{C}^\infty$ function such that its Fourier transform $\widetilde{g}$ has compact support contained in $[-T, T]$, for some $T > 0$. Then denote:

$$\ell(E) =: \left(f_\sigma^{(k)} * \widetilde{\rho}_\tau\right)(E) \tag{24}$$

(if $\tau \to \infty$, $\ell\left(\frac{E-\mu}{\hbar}\right)$ would be simply k^{th} derivative of the Fermi-Dirac function $k \geq 1$)

$$\langle C(E,\omega), g(\omega)\ell\left(\frac{E-\mu}{\hbar}\right)\rangle = \sum_{n,m\in\mathbb{N}} |A_{nm}|^2 \; g\left(\frac{E_n - E_m}{\hbar}\right) \; \ell\left(\frac{E_n-\mu}{\hbar}\right). \tag{25}$$

The RHS of (25) can be rewritten, using Fourier transform, as

$$\begin{aligned} &\frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\; \widetilde{g}(t) \sum_{n,m=0}^{\infty} |A_{nm}|^2 \; e^{it(E_n-E_m)/\hbar}\ell\left(\frac{E_n-\mu}{\hbar}\right) \\ =&\frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\; \widetilde{g}(t) \left\{ \operatorname{Tr} \widehat{A}(t)\widehat{A}\, \ell\left(\frac{\widehat{H}-\mu}{\hbar}\right)\right\}. \end{aligned} \tag{26}$$

Now since $\widetilde{g}$ is of compact support, and so is $\widetilde{\ell}$ (Fourier transform of ℓ) due to its definition (24), we can adapt our treatment of semiclassical trace formulae using coherent state decomposition [6] to this situation. Here the quantum observable appearing inside the Trace is the product of observable $\widehat{A}$ with its Heisenberg time translated $\widehat{A}(t)$ given by (16). We thus have also to make use of Egorov's theorem [8] to recognize, as a dominant classical symbol of $\widehat{A}(t)\widehat{A}$ simply $(A \circ \phi_t)(z)A(z)$ where $z = (x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n$ is the classical phase-space point.

We therefore define the various "classical objects" that will manifest themselves, in the limit as $\hbar \to 0$, in the semiclassical expansion of (26).

First of all, the classical flow induced by the classical Hamiltonian H is ϕ_t, since H does not depend explicitly on time, the classical flow lives on the energy surface

$$\sum_\mu = \left\{z = (x,\xi) \in \mathbb{R}^{2n} \colon H(x,\xi) = \mu\right\}$$

and we denote by $d\sigma_\mu$ the Liouville measure living on $\sum_\mu$. We call γ a generic periodic orbit living on $\sum_\mu$, i.e.

$$\gamma = \left\{z \colon \exists\, T_\gamma > 0 \colon \phi_{T_\gamma}(z) = z\right\} .$$

T_γ is therefore the classical period of orbit γ, which can be a repetition of a primitive orbit γ^*. The classical action along the closed orbit γ is called S_γ, σ_γ is the corresponding Maslov index, and P_γ the corresponding Poincaré map. (See [6].)

$$C_\mu(t) =: \int_{\sum_\mu} d\sigma_\mu(z)\ A(z)\ A \circ \phi_t(z) \tag{27}$$

is the classical autocorrelation of A on the energy surface at the Fermi level μ

$$c_\gamma(t) =: \int_0^{T_{\gamma^*}} ds\ A \circ \phi_s(z)\ A \circ \phi_{t+s}(z) \tag{28}$$

is the classical autocorrelation of A along the closed primitive orbit γ^*. It is independent of the point z of γ^* where we start the integration, and it is of course T_{γ^*} periodic, as a function of t. Therefore it can be expanded in Fourier series in the following form:

$$c_{\gamma^*}(t) = \sum_{p \in Z} c_{\gamma^*,p}\ e^{2i\pi pt/T_{\gamma^*}} . \tag{29}$$

Now we state the result

Theorem 1. *Assume (H1-2) together with*

(H.3) *μ is non-critical for H.*

(H.4) *On $\sum_\mu$, the set $(\Gamma_\mu)_\tau$ of classical periodic orbits γ with period smaller than τ is such that the corresponding Poincaré maps P_γ do not have eigenvalue 1.*

Then, as $\hbar \to 0$, (26) has a complete expansion in $\hbar$ of the following form:

$$\int dt\ \widetilde{g}(t) \Bigg\{ h^{-n}\ \widetilde{\ell}(0)\ C_\mu(t) + \sum_{j\geq 1} h^{-n+j}\ \lambda_j(\widetilde{\ell},t) \\ + \sum_{\gamma \in (\Gamma_\mu)_\tau} h^{-1} \frac{e^{iS_\gamma/\hbar + i\sigma_\gamma\pi/2}}{|\det(1-P_\gamma)|^{1/2}}\ \widetilde{\ell}(T_\gamma)\ c_\gamma(t) + \sum_{j\geq 0} h^j\ d_\gamma^j(\widetilde{\ell},t) \Bigg\}$$

where $\lambda_j(\cdot,t)$ and $d_\gamma^j(\cdot,t)$ are distributions supported respectively by $\{0\}$ and $\{T_\gamma\}$.

The proof of this theorem will be given elsewhere [5].

From this theorem, we can deduce an important result for $\chi(\omega)$, as a distribution, or rather to $\chi_\tau(\omega)$, a "regularized" version of it where the Fermi-Dirac function f is replaced by $f * \rho_{\tau/\hbar}$. This yields the following result:

Corollary 2. *Assume (H1-4) together with (H.5) and (H.6) below:*

(H.5) *the classical dynamics on $\sum_\mu$ is sufficiently mixing, in the sense that*

$$\int_{-\infty}^{+\infty} dt |C_\mu(t)| < \infty$$

(assuming A has been adjusted so that $\langle A \rangle_\mu = 0$).

(H.6) $\sum\limits_{k=-\infty}^{+\infty} |c_{\gamma,k}| < \infty$ *(any γ so that $|T_\gamma| < \tau$).*

Then $\chi_\tau(\omega)$ admits, as a distribution, a complete asymptotic expansion of the form:

$$- \omega h^{1-n} \int dt\ C_\mu(t)\ e^{i\omega t} + \sum_{j \geq 2} h^{j-n}\ \mu_j(\omega)$$

$$+\omega \sum_{\gamma \in (\Gamma_\mu)_\tau} \frac{e^{iS_\gamma/\hbar + i\sigma_\gamma \pi/2}}{|\det(1-P_\gamma)|^{1/2}}\ \frac{\pi T_\gamma/\sigma}{sh\ \pi T_\gamma/\sigma} \left(\sum_{k=-\infty}^{+\infty} c_{\gamma,k}\ \delta\left(\omega - \frac{2\pi k}{T_{\gamma^*}}\right) + \sum_{j \geq 1} h^j\ \nu_j(\omega) \right)$$

where μ_j and ν_j are distributions.

References

[1] O. Agam, *The magnetic response of chaotic mesoscopic systems*, J. Phys. I (France), **4** (1994), 697–730.

[2] M. Aizenman and G. M. Graf, *Localization bounds for an electron gas*, J. Phys. A (Math. and Gen.), **31** (1998), 6783–6806.

[3] M. Berry, *Some quantum-to-classical asymptotics* in Chaos et Physique Quantique, Les Houches (1989) M. J. Giannoni, A. Voros and J. Zin-Justin, North Holland.

[4] J. D. Butler, *Semiclassical counting function with application to quantum current*, Orsay preprint (1999).

[5] M. Combescure and D. Robert, *Semiclassical results in linear response theory*, (in preparation).

[6] M. Combescure, J. Ralston and D. Robert, *A proof of the Gutzwiller semiclassical trace formula using coherent states decomposition*, Commun. Math. Phys., **202** (1999), 463–480.

[7] M. Combescure and D. Robert, *Rigorous semiclassical results for the magnetic response of an electron gas*, Orsay preprint (2000).

[8] Y. Egorov, *On canonical transformations of pseudodifferential operators*, Uspehi Mat. Nauk, **25** (1969), 235–236.

[9] S. Fournais, *Semiclassics of the quantum current*, Commun. in PDE, **23** (1998), 601–628.

[10] G. Gallavotti and E. G. Cohen, *Dynamical ensembles in stationary states*, J. Stat. Phys., **80** (1995), 931–970.

[11] G. Gallavotti and D. Ruelle, *SRB states and nonequilibrium statistical mechanics close to equilibrium*, Commun. Math. Phys., **190** (1997), 279–285.

[12] P. Gaspard and S. Jain, *Semiclassical theory for many-body fermionic systems*, Pramana Journal of Physics, **48** (1997), 503–516.

[13] R. Kubo, M. Toda and N. Hashitsume, *Statistical Physics II*, (Nonequilibrium Statistical Mechanics), Springer-Verlag, Berlin, Heidelberg, New York, Tokyo (1978).

[14] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Course of Theoretical Physics, vol. 5, Pergamon Press, Oxford, New York, Toronto, Sydney, Paris, Frankfurt (1980).

[15] B. Mehlig and K. Richter, *Semiclassical linear response : far-infrared absorption in ballistic quantum systems*, Phys. Rev. Lett., **80** (1998), 1936–1939.

[16] K. Richter, D. Ullmo and R. Jalabert, *Orbital magnetism in the ballistic regime : geometrical effects*, Phys. Rep., **276** (1996), 1–83.

[17] D. Ruelle, *General linear response formula in statistical mechanics and the fluctuation-dissipation theorem far from equilibrium*, Phys. Lett., **A245** (1998), 220–224.

[18] D. Ruelle, *Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics*, J. Stat. Phys., **95** (1999), 393–468.

[19] D. Ruelle, *Natural nonequilibrium states in quantum statistical mechanics*, J. Stat. Phys., **98** (2000), 57–75.

[20] M. Wilkinson, *A semiclassical sum rule for matrix elements of classically chaotic systems*, J. Phys. A : (Math. and Gen.), **20** (1987), 2415–2423.

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