Quantum response of finite Fermi systems and the relation of the Lyapunov exponent to transport coefficients

Klaus Morawetz

LPC-ISMRA, Boulevard Marechal Juin, 14050 Caen and GANIL, Boulevard Becquerel, 14076 Caen Cedex 5, France

(Received 12 March 1999; revised manuscript received 31 August 1999)

Within the frame of kinetic theory a response function is derived for finite Fermi systems that includes dissipation in relaxation time approximation and a contribution from additional chaotic processes characterized by the largest Lyapunov exponent. A generalized local density approximation is presented including the effect of many particle relaxation and the additional chaotic scattering. For small Lyapunov exponents relative to the product of wave vector and Fermi velocity, the largest Lyapunov exponent modifies the response in the same way as the relaxation time. Therefore the transport coefficients can be connected with the largest positive Lyapunov exponent in the same way as known from the transport theory in relaxation time approximation.

PACS number(s): 05.45.−a, 05.20.Dd, 05.60.Cd, 05.70.Ln

The problem of irreversibility is one of the still open questions. Two approaches basically can be distinct. One approach considers the many particle theory as a suitable starting point to understand the increase of entropy as a result of many random collisions leading to irreversible kinetic equations like the Boltzmann equation. The other approach considers the theory of deterministic chaos with the characteristic measure of Lyapunov exponent to understand the occurrence of irreversibility. While the many particle approach can be easily extended to quantum systems the quantum chaos is still a matter of debate about the correct term.

If both approaches describe some facet of irreversibility, what we will anticipate in the following; it should be possible to give relations between them. While the characteristic measure of many body effects is the relaxation time and the transport coefficients, the relevant measure for chaotic systems is the Lyapunov exponent as a measure of phase space spreading of trajectories. Considerable efforts have been made to connect the transport coefficients with the Lyapunov exponent [1–4]. In Refs. [1] and [4] the fact that the spreading of a small phase space volume is given by the sum of Lyapunov exponents $\delta V(t)=\delta V(0)\exp(\Sigma\lambda_i)t$, is used to give a relation between Lyapunov exponents and viscosity. This was possible to show with the help of the contact to a heat bath in the equation of motion ensuring constant internal energy. In Refs. [2] and [3] the relation between transport coefficients and Lyapunov exponents was presented in terms of Helfand's moments. The interlink was possible to establish by reinterpretation of the Helfand's moments as stochastic quantities such that the mean variance of the time derivatives represents just the transport coefficients. In Ref. [5] the authors derive a density expansion of largest Lyapunov exponent for hard sphere gases from a generalized Lorentz-Boltzmann equation. This has demonstrated the intimate relation between transport coefficients and dynamical quantities like the Lyapunov exponent.

Here we like to show that there exists a simple connection between the concept of Lyapunov exponent and the dissipation leading to irreversibility for interacting Fermi systems. It will be shown that if the largest positive Lyapunov exponent is smaller than the product of Fermi velocity times wavelength in a Fermi system, the Lyapunov exponent appears in the same way as the relaxation time of the system. Therefore all expressions known from kinetic theory, expressing the transport coefficients in terms of the relaxation time, can be considered as an expression in terms of the Lyapunov exponent.

The concept of response of an interacting many body system starts conveniently from the one-particle density distribution function $f(\mathbf{p},\mathbf{r},t)$ satisfying the appropriate kinetic equation. The space dependent density is then given by integration over momentum

$$n(\mathbf{r},t)=g\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}f(\mathbf{p},\mathbf{r},t), \tag{1}$$

where g is the spin, isospin,..., degeneracy of the system. The linearization of the kinetic equation for f yields the response to an external disturbance. First we discuss the semiclassical response and generalize later to quantum response. The starting semiclassical kinetic equation reads

$$\partial_t f(\mathbf{p},\mathbf{r},t)+\frac{\mathbf{p}}{m}\partial_{\mathbf{r}}\, f(\mathbf{p},\mathbf{r},t)-\partial_{\mathbf{r}}(V_{\rm ind}(\mathbf{r},t) + V_{\rm ext}(\mathbf{r},t))\partial_{\mathbf{p}}f(\mathbf{p},\mathbf{r},t)=\frac{f_0(\mathbf{p},\mathbf{r})-f(\mathbf{p},\mathbf{r},t)}{\tau}, \tag{2}$$

with the self-consistent mean-field potential given as a convolution between the two-particle interaction V_0 and the density $V_{\rm ind}=\int d\bar{\mathbf{r}}V_0(\mathbf{r},\bar{\mathbf{r}})n(\bar{\mathbf{r}},t)$, the external disturbance $V_{\rm ext}$ and a typical relaxation time τ. The relaxation time approximation serves here as the simplest form of collision integral to describe dissipative processes by internal collisions of the particles.

Besides this chaotization by mutual collisions we want to discuss in the following how additional chaotic processes, e.g., caused by boundary conditions, surfaces etc., are influencing the response of the system to external perturbation $V_{\rm ext}$.

When the equation (2) is linearized with respect to the external perturbation, the self-consistent potential $V_{\rm ind}$ gives a linear density contribution δn via $\delta V_{\rm ind}=V_0\delta n$. Defining the total polarization function as the connection between induced density variation and external perturbation

1063-651X/2000/61(3)/2555(4)/$15.00 PRE 61

$$\delta n(\mathbf{x},\omega)=\int d\mathbf{x}'\,\Pi(\mathbf{x},\mathbf{x}',\omega)\,\delta V_{\rm ext}(\mathbf{x}',\omega), \tag{3}$$

one finds the relation between the polarization function including the effect of the self-consistent potential, Π, and the polarization without self-consistent potential, Π_τ, as

$$\Pi(\mathbf{x},\mathbf{x}')=\Pi_\tau(\mathbf{x},\mathbf{x}')+\int d\bar{\mathbf{x}}d\bar{\bar{\mathbf{x}}}\Pi_\tau(\mathbf{x},\bar{\mathbf{x}})V_0(\bar{\mathbf{x}},\bar{\bar{\mathbf{x}}})\Pi(\bar{\bar{\mathbf{x}}},\mathbf{x}'). \tag{4}$$

In other words it is sufficient to concentrate on the response function Π_τ to an external potential without self-consistent potential $V_{\rm ind}$. The self-consistent response Π is then given by the solution of the integral equation (4). The following derivation of Π_τ is adapted from Ref. [6].

Introducing the Lagrange picture by following the trajectory $\mathbf{x}(t),\mathbf{p}(t)$ of a particle in phase space

$$\frac{d}{dt}\mathbf{x}=\frac{\mathbf{p}}{m},\qquad \frac{d}{dt}\mathbf{p}=-\partial_{\mathbf{x}}V_{\rm ext} \tag{5}$$

we linearize the kinetic equation equation (2) around the stationary state f_0 according to $f(\mathbf{x},\mathbf{p},t)=f_0(\mathbf{x},\mathbf{p})+\delta f(\mathbf{x},\mathbf{p},t){\rm e}^{-t/\tau}$ and obtain

$$\frac{d}{dt}\delta f(\mathbf{x}(t),\mathbf{p}(t),t)=\partial_{\mathbf{p}}f_0\partial_{\mathbf{x}(t)}V_{\rm ext}. \tag{6}$$

This can be integrated to yield

$$\delta f(\mathbf{x},\mathbf{p},t)=-2m\int_{-\infty}^0 dt'\int_{-\infty}^{\infty}d\mathbf{x}'\frac{d}{dt'}\times\delta(\mathbf{x}'-\mathbf{x}(t'))\partial_{p^2}f_0(p^2,\mathbf{x}')V_{\rm ext}(\mathbf{x}',t+t'). \tag{7}$$

Integrating over $\mathbf{p}$, the density variation δn caused by varying the external potential is obtained as

$$\delta n(\mathbf{x},\omega)=-2mg\int d\mathbf{x}'\int\frac{d\mathbf{p}^3}{(2\pi\hbar)^3}\partial_{p^2}f_0(p^2,\mathbf{x}')\times\int_{-\infty}^0 dt'\,e^{-it'(\omega+i/\tau)}V_{\rm ext}(\mathbf{x}',\omega)\times\frac{d}{dt'}\delta(\mathbf{x}'-\mathbf{x}(t')), \tag{8}$$

where g denotes the spin-isospin degeneracy. Comparing the expression (8) with the definition of the polarization function Π_τ in Eqs. (3) and (4), we are able to identify the polarization of finite systems including the relaxation time as

$$\Pi_\tau(\mathbf{x},\mathbf{x}',\omega)=\Pi_0\left(\mathbf{x},\mathbf{x}',\omega+\frac{i}{\tau}\right) \tag{9}$$

with

$$\Pi_0(\mathbf{x},\mathbf{x}',\omega)=-2mg\int\frac{d\mathbf{p}^3}{(2\pi\hbar)^3}\partial_{p^2}f_0(p^2,\mathbf{x}')\times\int_{-\infty}^0 dt'\,e^{-it'\omega}\frac{d}{dt'}\delta(\mathbf{x}'-\mathbf{x}(t')). \tag{10}$$

Further simplifications are possible if we focus on the ground state $f_0(p^2,\mathbf{x})=\Theta(p_f^2(\mathbf{x})-p^2)$ of the Fermi system with the local Fermi momentum $p_f(\mathbf{x})$. The modulus integration of momentum can be carried out and the Kirzhnitz-formula [6,7] appears

$$\Pi_0(\mathbf{x},\mathbf{x}',\omega)=-\frac{mgp_f(\mathbf{x})}{4\pi^2\hbar^3}\left[\delta(\mathbf{x}'-\mathbf{x}(0))+i\omega\int_{-\infty}^0 dt'\,e^{-it'\omega}\int\frac{d\Omega_{\mathbf{p}}}{4\pi}\delta(\mathbf{x}'-\mathbf{x}(t'))\right], \tag{11}$$

where the angular integration of $d\mathbf{p}$ remains as $d\Omega_p$. This formula represents the ideal free part and a contribution that arises by the trajectories $\mathbf{x}(t)$ averaged over the direction at the present time $\mathbf{n}_p p_f=m\dot{\mathbf{x}}(0)$. In principle, the knowledge of the evolution of all trajectories is necessary to evaluate this formula. Molecular dynamical simulations can perform this task but it requires an astronomical amount of memory to store all trajectories. Rather, we discuss two approximations, which will give us more insight into the physical processes behind. First the most radical one shows how the local density approximation emerges. In the next one we consider the influence of chaotic scattering.

The local density approximation appears from Eq. (11) when we perform two simplifications. Introducing Wigner coordinates $\mathbf{R}=(\mathbf{x}+\mathbf{x}')/2$, $\mathbf{r}=\mathbf{x}-\mathbf{x}'$ we have to assume

(1) gradient expansion

$$p_f\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)\approx p_f(\mathbf{R})+\mathcal{O}(\partial_{\mathbf{R}}); \tag{12}$$

(2) expansion of the trajectories to first order history

$$\mathbf{x}'-\mathbf{x}(t')\approx-\mathbf{r}-t'\dot{\mathbf{x}}+\mathcal{O}(t'^2)=-\mathbf{r}-t'\frac{p_f}{m}\mathbf{n}_p. \tag{13}$$

With these two assumptions we obtain from Eq. (11) after trivial integrations

$$\Pi_0^{\rm LDA}(\mathbf{q},\mathbf{R},\omega)=\int d\mathbf{r}\,{\rm e}^{-i\mathbf{qr}}\,\Pi_0^{\rm LDA}(\mathbf{r},\mathbf{R},\omega)=-\frac{mgp_f(\mathbf{R})}{4\pi^2\hbar^3}\left\{1+ik\int_0^\infty dy\;{\rm e}^{iky}\frac{\sin y}{y}\right\}, \tag{14}$$

where $k=m\omega/(qp_f(\mathbf{R}))$. This can be further integrated with the help of

$$\int_0^\infty dy{\rm e}^{iky}\frac{\sin y}{y}=\arctan({\rm Im}\,k-i\,{\rm Re}\,k)^{-1}=2i\ln\left(\frac{1+k}{1-k}\right)+\pi[{\rm sgn}(1+k)+{\rm sgn}(1-k)]|_{{\rm Im}\,k\to 0} \tag{15}$$

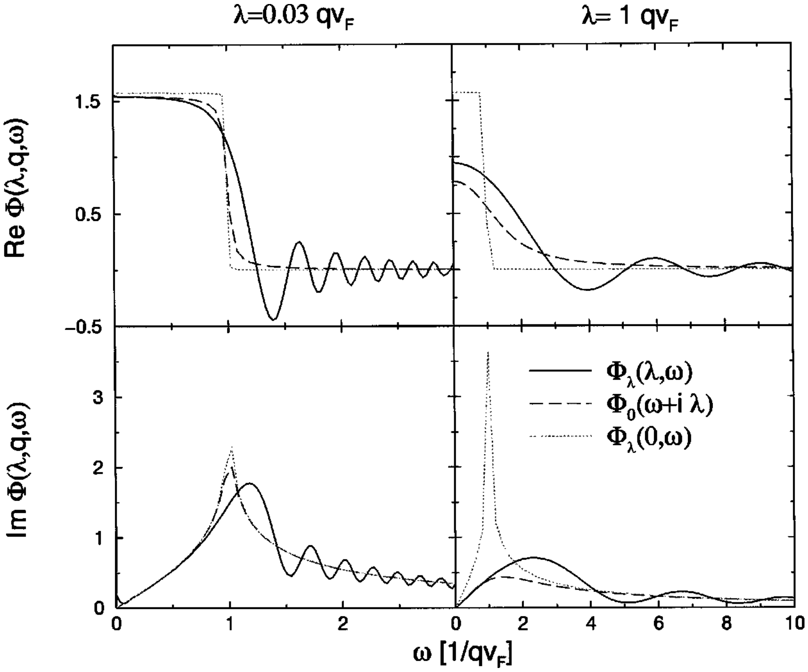

FIG. 1. The dimensionless polarization function $\Pi=-[mgp_f(\mathbf{R})/4\pi^2\hbar^3][1+ik\Phi(\lambda,k,\omega)]$ vs frequency for $q=1/v_F$ and two different Lyapunov exponents. The upper panel shows the real part and the lower the imaginary part of Φ. The result (21), solid line, is plotted together with the approximation (23), long dashed line. The result without Lyapunov exponents (15) is plotted as well for comparison, dotted line.

to yield the standard Lindhard result (28) in the classical limit

$$\Pi_0^{\rm inf}(\mathbf{q},p_f,\omega)=-\frac{mgp_f}{4\pi^2\hbar^3}\left\{1-2k\ln\left(\frac{1+k}{1-k}\right)+ik\pi\right.$$
$$\left.\times[\mathrm{sgn}(1+k)+\mathrm{sgn}(1-k)]\right\}, \qquad (16)$$

where $k=m\omega/(qp_f)$. We recognize the ground-state result for infinite matter except that the Fermi momentum $p_f(\mathbf{R})$ has to be understood as a local quantity corresponding to local densities so that we get with Eq. (9)

$$\Pi_\tau^{\rm LDA}(\mathbf{q},\mathbf{R},\omega)=\Pi_0^{\rm inf}\left(\mathbf{q},p_f(\mathbf{R}),\omega+\frac{i}{\tau}\right). \qquad (17)$$

For extensions beyond the local density approximation see Refs. [7] and [8].

Now we focus on the influence of an additional chaotic scattering, which will be caused e.g., by a surface boundary. In order to investigate this effect we add to the regular motion (13) a small irregular part $\Delta\mathbf{x}$

$$\mathbf{x}'-\mathbf{x}(t')\approx-\mathbf{r}-t'\frac{p_f}{m}\mathbf{n}_p+\Delta\mathbf{x}. \qquad (18)$$

The irregular part of the motion we specify in the direction of the current movement lasting a time Δ_t and given by an exponential increase in phase-space controlled by the largest Lyapunov exponent λ. Therefore we can assume $[t'<0]$

$$\Delta\mathbf{x}\approx\frac{p_f\mathbf{n}_p}{m}\Delta_t\,\exp[-\lambda(t'-\Delta_t)]+\mathrm{const}. \qquad (19)$$

Since we are looking for the largest Lyapunov exponent we can take Eq. (19) at the maximum $\Delta_t=-1/\lambda$. Further, we require, that in the case of vanishing Lyapunov exponent we should regain the regular motion (13). We have for Eq. (18) therefore

$$\mathbf{x}'-\mathbf{x}(t')\approx-\mathbf{r}-\frac{p_f}{m}\mathbf{n}_p\left[\frac{1-\exp(-\lambda t')}{\lambda}\right]. \qquad (20)$$

With this ansatz one derives from Eq. (11) instead of Eq. (14) the result

$$\Pi_\lambda(\mathbf{q},\mathbf{R},\omega)=-\frac{mgp_f(\mathbf{R})}{4\pi^2\hbar^3}\left[1+ik\int_0^\infty dy\,\frac{\sin y}{y}\right.$$
$$\left.\times\left(1+\frac{ky}{\omega}\lambda\right)^{i\omega/\lambda-1}\right], \qquad (21)$$

which for $\lambda\to 0$ resembles exactly Eq. (14). The further integration could be given in terms of hypergeometric functions but this is omitted here.

With this formula (21) together with Eqs. (9) and (4) we have derived the main result of a polarization function including the influence of many particle effects and additional chaotic processes characterized by the Lyapunov exponent λ. In Fig. 1 the dimensionless integral of Eq. (21) is plotted and compared with the case without Lyapunov exponent. We see that an oscillating behavior is induced similar to the effect of an external electric field [9].

For the condition

$$\lambda\ll qv_F, \qquad (22)$$

with $v_f=p_f/m$ the Fermi velocity and q the wave vector we can use $\lim_{x\to\infty}(1+a/x)^x=\exp(a)$ under the integral of Eq. (21) and the final integration is performed with the result of Eq. (17) but a complex shift

$$\Pi_\lambda^{\rm LDA}(\mathbf{q},\mathbf{R},\omega)=\Pi_0^{\rm inf}\left(\mathbf{q},p_f(\mathbf{R}),\omega+i\left(\lambda+\frac{1}{\tau}\right)\right). \qquad (23)$$

We obtain by this way just the known Matthiessen rule, which states that the damping mechanisms are additive in the damping $\Gamma=(1/\tau)+\lambda$.

In Fig. 1 we compare the dimensionless integral of Eq. (21) for different approximations. The approximation of small x Lyapunov exponents which leads to the Matthiessen rule averages the oscillating behavior and reproduces the gross feature for the condition (22).

Next we discuss the quantum response function and we will see that all discussions outlined above can be straight forward applied to the quantum response function. Instead of the quasiclassical kinetic equation (2) we start now from the quantum kinetic equation [10]

$$\partial_t f(\mathbf{p},\mathbf{r},t)+\frac{\mathbf{p}}{m}\partial_{\mathbf{r}} f(\mathbf{p},\mathbf{r},t)-\frac{1}{i}\int d\mathbf{s}\,\frac{d\mathbf{p}'}{(2\pi\hbar)^3}\left[U\left(\mathbf{r}+\frac{\mathbf{s}}{2}\right)-U\left(\mathbf{r}-\frac{\mathbf{s}}{2}\right)\right]e^{i/\hbar\,\mathbf{s}(\mathbf{p}'-\mathbf{p})}f(\mathbf{p}',\mathbf{r},t)=\frac{f_0(\mathbf{p},\mathbf{r})-f(\mathbf{p},\mathbf{r},t)}{\tau}, \tag{24}$$

with $U=V_{\rm ind}+V_{\rm ext}$. The gradient expansion in U leads to first order the quasiclassical expression (2). We follow now exactly the same linearization as above and introduce the Lagrange picture. The trajectories are now described instead of Eq. (5) by the following set

$$\frac{d}{dt}\mathbf{x}=\frac{\mathbf{p}}{m},$$

$$\mathbf{s}\frac{d}{dt}\mathbf{p}=U\left(\mathbf{r}+\frac{\mathbf{s}}{2}\right)-U\left(\mathbf{r}-\frac{\mathbf{s}}{2}\right), \tag{25}$$

where the arbitrary vector $\mathbf{s}$ shows the infinite possibilities of trajectories by quantum fluctuations. The resulting polarization function for a finite quantum system reads now instead of Eq. (9)

$$\Pi_0(\mathbf{x},\mathbf{x}',\omega)=\frac{g}{\pi^2\hbar^3}\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}\times\int d\mathbf{s}\frac{\sin\left(\frac{1}{\hbar}\mathbf{sp}\right)}{s}\partial_s\left(\frac{\sin\left(\frac{1}{\hbar}sp_f\right)}{s}\right)\times\int_{-\infty}^{0}dt'\,e^{-it'\omega}\delta\left(\mathbf{x}'-\mathbf{x}(t')-\frac{\mathbf{s}}{2}\right). \tag{26}$$

Compared with Eq. (10) we see that due to quantum fluctuations an additional integration $\mathbf{s}$ appears. Equation (26) is the quantum generalization of the quasiclassical Kirzhnitz formula (11) for the response function in finite systems.

Applying now the same gradient approximation (13) we derive from Eq. (26) with the help of

$$i\int d\mathbf{s}\frac{\sin\left(\frac{1}{\hbar}\mathbf{sp}\right)}{s}\partial_s\left(\frac{\sin\left(\frac{1}{\hbar}sp_f\right)}{s}\right)e^{i1/2\mathbf{qs}}=\pi^2\hbar^3\left[\Theta\left(p_f^2-\left(\mathbf{p}-\frac{\mathbf{q}}{2}\right)^2\right)-\Theta\left(p_f^2-\left(\mathbf{p}+\frac{\mathbf{q}}{2}\right)^2\right)\right] \tag{27}$$

the quantum Lindhard result

$$\Pi_0(\mathbf{q},\mathbf{R},\omega)=g\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}\times\frac{\Theta\left(p_f^2(\mathbf{R})-\left(\mathbf{p}-\frac{\hbar\mathbf{q}}{2}\right)^2\right)-\Theta\left(p_f^2(\mathbf{R})-\left(\mathbf{p}+\frac{\hbar\mathbf{q}}{2}\right)^2\right)}{\hbar\omega-\frac{\hbar\mathbf{pq}}{m}+i\epsilon} \tag{28}$$

in local density approximation.

The ansatz about additional chaotic processes Eq. (20) leads then to exactly the same expression (23) under the condition (22) but with the quantum response (28) instead of $\Pi_0^{\rm inf}$.

We like to point out that this result has far reaching consequences. With the assumption (22) we have shown by this way that the linear response behavior is the same if dissipation comes from the relaxation time via collision processes in many-particle theories or from the concept of chaotic processes characterized by the Lyapunov exponent. We can therefore state that for small Lyapunov exponent compared to the product of wave vector and Fermi velocity in a many particle system, the largest Lyapunov exponent behaves like the relaxation time in the response function.

Since the transport theory is well worked out to calculate the transport coefficients in relaxation time approximation we can express by this way the transport coefficients in terms of the Lyapunov exponent alternatively. This illustrates the mutual equivalence of the concept of Lyapunov exponent and dissipative processes in many-particle theories.

Pavel Lipavský and Václav Špička are thanked for many enlightening discussions and A. Dellafiore for bringing the Kirzhnitz formula to my attention.

[1] D.J. Evans, E. Cohen, and G.P. Morriss, Phys. Rev. A **42**, 5990 (1990).
[2] J. Dorfman and P. Gaspard, Phys. Rev. E **51**, 28 (1995).
[3] P. Gaspard and J. Dorfman, Phys. Rev. E **52**, 3525 (1995).
[4] E. Cohen, Physica A **213**, 293 (1995).
[5] J. Dorfman and H. van Beijeren, in *Proceedings of the Euroconference on The Microscopic Approach to Complexity in Non-Equilibrium Molecular Simulations CECAM, July 1996* (North-Holland, Amsterdam, 1997), Vol. 1/2, p. 12.
[6] D. Kirzhnitz, Y. Lozovik, and G. Shpatakovskaya, Usp. Fiz. Nauk **117**, 3 (1975) [Sov. Phys. Usp. **18**, 649 (1975)].
[7] A. Dellafiore, F. Matera, and D.M. Brink, Phys. Rev. A **51**, 914 (1995).
[8] A. Dellafiore and F. Matera, Phys. Rev. A **41**, 4958 (1990).
[9] K. Morawetz and A.P. Jauho, Phys. Rev. E **50**, 474 (1994).
[10] L. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Addison-Wesley, New York, 1962).