Influence-functional theory for a heavy particle in a Fermi gas

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We use Feynman's influence-functional theory to study the quantum dynamics of a heavy particle moving in a free Fermi gas with arbitrary average velocity. A semiclassical expansion yields a nonlinear Langevin equation with the exact friction coefficient as derived in an earlier publication. The fluctuations around a steady state far from equilibrium are due to a nonclassical state-dependent noise term and can be described by a diffusion constant. In the limit of zero average velocity, the Einstein relation is fulfilled for arbitrary temperatures. For finite velocities the diffusion around the steady state is different in longitudinal and transverse directions and can be expressed in terms of the transport cross section and a "diffusion" cross section. In the case where the frictional force exhibits a maximum as a function of velocity and thus an unstable branch for $v > v_c$, the longitudinal diffusion constant diverges on approaching v_c from below. Numerical results for the noise spectrum and the temperature and velocity dependence of the diffusion constants are presented for simple repulsive interaction potentials in one and three dimensions.

The theory of Brownian motion is a fundamental problem in nonequilibrium statistical mechanics which—for a classical particle—is usually treated in terms of simple Langevin or Fokker-Planck equations.[1] In quantum mechanics the standard model assumes that the particle is coupled linearly to a collection of harmonic oscillators.[2–4] Our aim in the present work is to investigate the problem of quantum Brownian motion for the more realistic case in which a heavy particle moves in a degenerate Fermi gas.[5] In particular we study the fluctuations around a steady state far from equilibrium with arbitrary average velocity. On the basis of the Feynman-Vernon influence-functional theory, which is appropriate to describe the quantum dynamics of a single particle in a dissipative environment,[6] we derive a semiclassical expansion that is valid for arbitrary velocities, temperatures, and strength of the interaction potential. Our main result is that the fluctuations are diffusive with state-dependent diffusion constants which are different in longitudinal and transverse directions.

As a model we use the Hamiltonian

$$H = H_S + H_B + H_{SB} - \mathbf{F}_{\text{ext}}\cdot\mathbf{q} \,, \tag{1}$$

where H_S is the heavy-particle kinetic energy and H_B is the Hamiltonian for the Fermion bath. The interaction between the heavy particle and the bath is described by

$$H_{SB} = \sum_i V(\mathbf{x}_i - \mathbf{q}) \tag{2}$$

with $\mathbf{x}_i$ the Fermion coordinates and V a localized potential which—for simplicity—we assume to be spherically symmetric and to have no bound states. In addition we have included a term corresponding to a constant external force $\mathbf{F}_{\text{ext}}$ which we expect to lead to a nonzero average velocity.

The complete information on the dynamics of the Brownian particle is contained in the reduced density matrix $\rho(t) = \mathrm{Tr}_B \rho_{\text{tot}}(t)$ which is obtained from the total density matrix by tracing out the bath variables. Its coordinate representation at time t can be related to the initial value at time t_0 (Ref. 6)

$$\langle \mathbf{q}|\rho(t)|\mathbf{q}'\rangle = \int d\mathbf{q}_0 d\mathbf{q}_0' \langle \mathbf{q}_0|\rho(t_0)|\mathbf{q}_0'\rangle J(\mathbf{q},\mathbf{q}',t|\mathbf{q}_0,\mathbf{q}_0',t_0) \tag{3}$$

with J expressed as a double path integral

$$J(\mathbf{q},\mathbf{q}',t|\mathbf{q}_0,\mathbf{q}_0',t_0) = \int_{\mathbf{q}_0}^{\mathbf{q}} \mathcal{D}\mathbf{q} \int_{\mathbf{q}_0'}^{\mathbf{q}'} \mathcal{D}^*\mathbf{q}' \exp\left[\frac{i}{\hbar}\{S[\mathbf{q}] - S[\mathbf{q}']\}\right] F[\mathbf{q},\mathbf{q}'] \,. \tag{4}$$

Here $S[\mathbf{q}]$ is the classical action for the particle moving along the path $\mathbf{q}(t)$ and $F[\mathbf{q},\mathbf{q}'] = \langle U^\dagger[\mathbf{q}']U[\mathbf{q}]\rangle$ the influence functional where $\langle \ldots \rangle$ means $\mathrm{Tr}_B[\rho_B(t_0)\ldots]$. $U[\mathbf{q}]$ is the time evolution operator under the influence of the Hamiltonian $H(t) \equiv H_B + H_{SB}(\mathbf{q}(t))$, i.e., the heavy particle acts like a time dependent *external* perturbation on the bath. In the semiclassical limit the dynamics of the heavy particle may be obtained from a quantum Langevin equation.[7] To derive this, it is convenient to introduce center-of-mass and relative coordinates $\mathbf{x} = (\mathbf{q}+\mathbf{q}')/2$ and $\mathbf{y} = \mathbf{q} - \mathbf{q}'$, such that

$$f(\mathbf{x},\mathbf{p},t)=\int \frac{d\mathbf{y}}{(2\pi\hbar)^d}\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{y}\right]\left\langle \mathbf{x}+\frac{\mathbf{y}}{2}\middle|\rho(t)\middle|\mathbf{x}-\frac{\mathbf{y}}{2}\right\rangle \tag{5}$$

is the standard Wigner distribution function which generalizes the classical phase space distribution to quantum systems. Introducing the influence phase $\Phi[\mathbf{q},\mathbf{q}']$ by $F=\exp(i\Phi)$ we expand F into powers of the off-diagonal components $\mathbf{y}$ up to order y^2. This is equivalent to separating $i\Phi$ into imaginary and real parts $i\Phi=i\Phi_1-\Phi_2$ where Φ_1 is linear in $\mathbf{y}$ and Φ_2 quadratic. There are several limits in which the expansion to order y^2 is expected to be a good approximation. (i) The classical limit is obtained from the Feynman-Vernon theory by an expansion to second order in the off-diagonal density matrix elements as was shown in Ref. 7 and 8. (ii) For large external force $\mathbf{F}_{\text{ext}}$ the term $(i/\hbar)\mathbf{F}_{\text{ext}}\cdot\int \mathbf{y}\,dt$ in the exponent of the path integral suggests a stationary phase expansion around $\mathbf{y}=0$ since the main contribution to the path integral is then obtained from paths for which $\int \mathbf{y}\,dt$ goes to zero. (iii) For large dissipation the quadratic term $\Phi_2\geq 0$ suppresses deviations from $\mathbf{y}=0$ exponentially.[7]

Using standard second-order time-dependent perturbation theory in $H_\pm(t)=H_{SB}[\mathbf{x}\pm\mathbf{y}/2]-H_{SB}[\mathbf{x}]$ the general form for Φ_1 and Φ_2 to order y and y^2 turns out to be

$$\begin{aligned}\Phi_1(t)&=-\frac{1}{\hbar}\int_{t_0}^{t}\mathbf{y}(t_1)\cdot\langle \mathbf{K}^{[\mathbf{x}]}(t_1)\rangle dt_1\ ,\\ \Phi_2(t)&=\frac{1}{\hbar^2}\int_{t_0}^{t}dt_1 y_\alpha(t_1)\int_{t_0}^{t_1}dt_2 y_\beta(t_2)\mathrm{Re}S_{\alpha\beta}^{[\mathbf{x}]}(t_1,t_2)\end{aligned} \tag{6}$$

with

$$S_{\alpha\beta}^{[\mathbf{x}]}(t_1,t_2)=\langle K_\alpha^{[\mathbf{x}]}(t_1)K_\beta^{[\mathbf{x}]}(t_2)\rangle-\langle K_\alpha^{[\mathbf{x}]}(t_1)\rangle\langle K_\beta^{[\mathbf{x}]}(t_2)\rangle$$

and the force operator

$$K_\alpha^{[\mathbf{x}]}(t)=-\sum_i U^\dagger[\mathbf{x}]\partial_\alpha V(\mathbf{x}_i-\mathbf{x}(t))U[\mathbf{x}]\ .$$

Physically ϕ_1 describes the systematic friction force exerted by the bath on the heavy particle while ϕ_2 corresponds to the associated fluctuating force. To see this we follow Schmid[7] and formally linearize the quadratic term Φ_2 by writing $\exp(-\Phi_2)$ as an average over a Gaussian stochastic process

$$e^{-\Phi_2}=\left\langle \exp\left[\frac{i}{\hbar}\int_{t_0}^{t}\mathbf{y}(t')\cdot\boldsymbol{\xi}(t')dt'\right]\right\rangle_\xi\ . \tag{7}$$

The fluctuating force ξ has zero average and covariance $[\mathbf{v}(t)\equiv\dot{\mathbf{x}}(t)]$

$$\langle \xi_\alpha(t)\xi_\beta(t')\rangle=\mathrm{Re}S_{\alpha\beta}^{[\mathbf{v}]}(t,t')\ . \tag{8}$$

Note that the spectrum of the random force depends on the complete history of the path $\mathbf{x}$ for times earlier than $\max(t,t')$.

Since the phase Φ is now linear in $\mathbf{y}$ the functional integral over the relative coordinate $\mathbf{y}$ can be easily performed.[8] Integrating the kinetic energy term $M\dot{x}\dot{y}$ in the Lagrangian by parts, the discretized version of the integral $\mathcal{D}\mathbf{y}$ factorizes and leads to a product of delta functions for the $\mathbf{x}$ integrations, which force the path for the center-of-mass coordinate $\mathbf{x}$ to obey the nonlinear Langevin equation

$$\dot{\mathbf{v}}(t)+\frac{\langle \mathbf{K}^{[\mathbf{v}]}(t)\rangle}{M}=\frac{\mathbf{F}_{\text{ext}}}{M}+\frac{\xi^{[\mathbf{v}]}(t)}{M} \tag{9}$$

with a "state-dependent" noise where M is the mass of the heavy particle. The systematic friction force term $\langle \mathbf{K}^{[\mathbf{v}]}(t)\rangle$, as well as the spectrum of the random force cannot be explicitly calculated for arbitrary $\{\mathbf{v}(t)\}$ unless additional approximations like a weak potential or the adiabatic approximation are introduced. Here we study the limit of large mass M where the behavior should be nearly classical. If the external force $\mathbf{F}_{\text{ext}}$ is properly scaled (see below) only the neighborhood of the path $\mathbf{x}=\mathbf{v}_0 t$, i.e., $\mathbf{v}(t)=$const enters. For constant velocity $\mathbf{v}_0$ the friction force $\langle \mathbf{K}^{[\mathbf{v}_0]}(t)\rangle=\eta(v_0)\mathbf{v}_0$ was calculated previously for arbitrary velocities, temperatures and coupling strength[9,10] and—as will be shown below—$S_{\alpha\beta}^{[\mathbf{v}_0]}$ can also be explicitly calculated. Since the friction coefficient $\eta(v_0)$ is a function of velocity the Langevin equation (9) is nonlinear unless $v_0\ll v_F$ where $\eta(v_0)$ goes to a constant. For a three-dimensional hard sphere with constant mass density η increases like $M^{2/3}$. Therefore $\gamma(v)\equiv\eta(v)/M$ is proportional to $M^{-1/3}$, i.e., small in the large mass limit. In order for the external force $\mathbf{F}_{\text{ext}}$ to give a finite average drift velocity independent of M it has to scale like η and thus $\mathbf{F}_{\text{ext}}\sim M^{2/3}$ in our example. By contrast, as may be seen from the Einstein relation, the fluctuating force generally is expected to scale like $\sqrt{\eta}$, i.e., $|\xi|/M\sim M^{-2/3}$. Therefore to leading order in the large mass limit the term ξ/M representing the noise on the right-hand side (RHS) of (9) can be neglected. Then a path $\mathbf{x}(t)=\mathbf{v}_0 t+\mathbf{x}_0$, i.e., $\mathbf{v}(t)=$const is a solution and $v_0=|\mathbf{v}_0|$ is determined by

$$\mathbf{v}_0\eta(v_0)=\mathbf{F}_{\text{ext}}\ . \tag{10}$$

To obtain the fluctuations around this path we write $\mathbf{v}(t)=\mathbf{v}_0+\delta\mathbf{v}(t)$ and linearize (9)

$$M\delta\dot{v}_\alpha(t)+\int_0^t \chi_{\alpha\beta}^{[\mathbf{v}_0]}(t-t')\delta v_\beta(t')dt'=\xi_\alpha^{[\mathbf{v}_0]}(t)\ , \tag{11}$$

where

$$\chi_{\alpha\beta}^{[\mathbf{v}_0]}(t-t')=\delta\langle K_\alpha^{[\mathbf{v}]}(t)\rangle/\delta v_\beta(t')|_{\mathbf{v}(t)=\mathbf{v}_0}$$

and the derivative $\delta\xi_\alpha/\delta v_\beta$ has been neglected since it is of higher order. For variations of $\delta\mathbf{v}(t')$ on time scales large compared to the decay of $\chi_{\alpha\beta}(t)$ we may replace (11) by

$$M\delta\dot{v}_\alpha(t)+\tilde{\eta}_{\alpha\beta}(\mathbf{v}_0)\delta v_\beta(t)=\xi_\alpha^{[\mathbf{v}_0]}(t) \tag{12}$$

which describes a simple Ornstein-Uhlenbeck process[1] for the velocity fluctuations. Here we have introduced a friction *tensor*

$$\tilde{\eta}_{\alpha\beta}(\mathbf{v}_0)=\int_0^\infty \chi_{\alpha\beta}^{[\mathbf{v}_0]}(\tau)d\tau\ . \tag{13}$$

The tensor $\tilde{\eta}_{\alpha\beta}(\mathbf{v}_0)$ is diagonal but has two independent components since $\mathbf{e}_0\equiv\mathbf{v}_0/v_0$ specifies a direction in the otherwise isotropic heat bath. If we decompose $\delta\mathbf{v}(t)=\delta\mathbf{v}_{\parallel}(t)+\delta\mathbf{v}_{\perp}(t)$ Eq. (12) becomes

$$M\delta\dot{\mathbf{v}}_{\sigma}(t)+\tilde{\eta}_{\sigma}(v_0)\delta\mathbf{v}_{\sigma}(t)=\xi_{\sigma}^{[\mathbf{v}_0]}(t) , \tag{14}$$

where σ stands for $\parallel$ or $\perp$. The relation between the two coefficients $\tilde{\eta}_{\sigma}(v_0)$ of the friction tensor describing the damping of velocity fluctuations around the nonequilibrium steady state and the usual friction coefficient $\eta(v_0)$ is obtained by replacing the random force on the RHS of (14) by a change $\delta\mathbf{F}_{\mathrm{ext},\sigma}$ of the constant external potential, which leads to

$$\begin{aligned}&\tilde{\eta}_{\perp}(v_0)=\eta(v_0) ,\\ &\tilde{\eta}_{\parallel}(v_0)=\frac{d}{dv}(v\eta(v))|_{v=v_0}=\eta(v_0)+v_0\eta'(v_0) .\end{aligned} \tag{15}$$

These two friction constants are identical with the inverse of the *differential* mobility defined by $B_{\sigma}^{[\mathbf{v}_0]}\equiv|\delta\mathbf{v}_{0,\sigma}|/|\delta\mathbf{F}_{\mathrm{ext},\sigma}|$. Obviously the transverse differential mobility $B_{\perp}^{[\mathbf{v}_0]}$ is simply given by the inverse friction coefficient $1/\eta(v_0)$ while $B_{\parallel}^{[\mathbf{v}_0]}$ has an additional term involving the derivative $\eta'(v_0)$, i.e., is not the same as the usual mobility $|\mathbf{v}_0|/|\mathbf{F}_{\mathrm{ext}}|$. In particular in a situation in which the product $v\eta(v)$ exhibits a maximum at some value v_c, which occurs for any finite interaction potential $V(\mathbf{x})$, the longitudinal differential mobility $B_{\parallel}^{[\mathbf{v}_0]}$ diverges linearly at v_c. The physical reason for this is that at high velocities $v \gg v_c$ the Fermi gas eventually always becomes transparent if the interaction V is finite. For a given external force $\mathbf{F}_{\mathrm{ext}}$ there is then more than one value of v_0 which fulfills the condition $\mathbf{F}_{\mathrm{ext}}=\langle \mathbf{K}^{[\mathbf{v}_0]}\rangle$. Only the solution with $B_{\parallel}^{[\mathbf{v}_0]}=\partial\langle|\mathbf{K}|\rangle/\partial v_0>0$ is stable, while solutions with $B_{\parallel}^{[\mathbf{v}_0]}<0$ are unstable with respect to an unlimited increase in velocity. As was pointed out by Thornber and Feynman[11] a similar situation occurs in the motion of polarons in high electric fields. Below we will see that the divergence of $B_{\parallel}^{[\mathbf{v}_0]}$ at v_c also implies a divergence of the associated longitudinal diffusion constant.

In order to derive the diffusive nature of the fluctuations around the nonequilibrium steady state the solution of (14)

$$\delta\mathbf{v}_{\sigma}(t)=\delta\mathbf{v}_{\sigma}(0)e^{-\tilde{\gamma}_{\sigma}(v_0)t}+\frac{1}{M}\int_0^t e^{-\tilde{\gamma}_{\sigma}(v_0)(t-t')}\xi_{\sigma}(t')dt' \tag{16}$$

with $\tilde{\gamma}_{\sigma}(v_0)\equiv\tilde{\eta}_{\sigma}(v_0)/M$ is averaged over the random force for $t>t'$ which leads to

$$\begin{aligned}&\langle\delta\mathbf{v}_{\sigma}(t)\cdot\delta\mathbf{v}_{\sigma}(t')\rangle_{\xi}-\langle\delta\mathbf{v}_{\sigma}(t)\rangle_{\xi}\cdot\langle\delta\mathbf{v}_{\sigma}(t')\rangle_{\xi}\\ &\quad=\frac{1}{M^2}\int_0^t dt_1\int_0^{t'}dt_2 e^{-\tilde{\gamma}_{\sigma}(v_0)(t-t_1)}e^{-\tilde{\gamma}_{\sigma}(v_0)(t'-t_2)}\\ &\qquad\qquad\times\langle\xi_{\sigma}(t_1)\cdot\xi_{\sigma}(t_2)\rangle_{\xi}\\ &\quad\approx\frac{S_{\sigma}^{[\mathbf{v}_0]}(\omega=0)}{2\tilde{\gamma}_{\sigma}(v_0)M^2}e^{-\tilde{\gamma}_{\sigma}(v_0)(t-t')}\end{aligned} \tag{17}$$

where $S_{\sigma}(\omega)$ is the Fourier transform of $\mathbf{S}_{\sigma}^{[\mathbf{v}_0]}(t-t')$. Here we have taken the limit $t\to\infty$ and have used that $\tilde{\gamma}\to 0$ in the limit $M\to\infty$ which means that the typical time scale for the motion of the heavy particle is much longer than characteristic times involved in the fluctuating force.

We now define nonequilibrium diffusion constants $D_{\sigma}(v_0)$ by

$$\begin{aligned}&2(d-1)D_{\perp}(v_0)\equiv\lim_{t\to\infty}\frac{d}{dt}\langle[\delta\mathbf{x}_{\perp}(t)-\delta\mathbf{x}_{\perp}(0)]^2\rangle_{\xi} ,\\ &2D_{\parallel}(v_0)\equiv\lim_{t\to\infty}\frac{d}{dt}\langle[\delta\mathbf{x}_{\parallel}(t)-\delta\mathbf{x}_{\parallel}(0)]^2\rangle_{\xi} ,\end{aligned} \tag{18}$$

where d is the number of spatial dimensions. Using (17) the diffusion constants can be related to the zero frequency limit of the force-force correlation function

$$\begin{aligned}&(d-1)D_{\perp}(v_0)=\frac{S_{\perp}^{[\mathbf{v}_0]}(\omega=0)}{2[\tilde{\eta}_{\perp}(v_0)]^2} ,\\ &D_{\parallel}(v_0)=\frac{S_{\parallel}^{[\mathbf{v}_0]}(\omega=0)}{2[\tilde{\eta}_{\parallel}(v_0)]^2}\end{aligned} \tag{19}$$

which is the central result of this paper. Since both $S_{\sigma}^{[\mathbf{v}_0]}(\omega=0)$ and $\tilde{\eta}_{\perp}(v_0)=\eta(v_0)$ are regular and finite functions of the average velocity v_0 the transverse diffusion constant $D_{\perp}(v_0)$ remains finite in any case. By contrast the linear divergence of $B_{\parallel}^{[\mathbf{v}_0]}=\eta_{\parallel}^{-1}(v_0)$ at v_c in the case of a nonmonotonic $v\eta(v)$ relation with a maximum at v_c leads to a quadratic divergence $D_{\parallel}(v_0)\sim(v_c-v_0)^{-2}$ of the longitudinal diffusion constant, signaling the approach to an unstable branch for $v>v_c$ as mentioned above. For nonzero average velocity there is no simple relation between the force-force correlation function $S^{[\mathbf{v}_0]}$ and the nonlinear friction coefficient $\eta(v)$ and thus there is no generalized fluctuation-dissipation theorem relating diffusion and friction in this case. It is only in the linear response limit $v_0\to 0$ that such a relation is valid. Indeed from (19) it is clear that the Einstein relation $D=k_BTB$ is fulfilled if the Kirkwood relation $S_{\parallel}^{[\mathbf{v}_0]}(\omega=0)=2\tilde{\eta}_{\parallel}(v_0)k_BT$, respectively, $S_{\perp}^{[\mathbf{v}_0]}(\omega=0)=2(d-1)\tilde{\eta}_{\perp}(v_0)k_BT$ which expresses the friction in terms of the zero frequency force-force correlation function holds in the limit $v_0\to 0$. To show this we explicitly calculate the correlation function $S_{\sigma}^{[\mathbf{v}_0]}(\omega)$ for the model of *noninteracting* Fermions. For an arbitrary path $\mathbf{x}(t)$ one obtains

$$\begin{aligned}S_{\alpha\beta}(t_1,t_2)=&\sum_{\mathbf{p},\mathbf{p}'}\langle\mathbf{p}|K_{\alpha}(t_1)|\mathbf{p}'\rangle\langle\mathbf{p}'|K_{\beta}(t_2)|\mathbf{p}\rangle\\ &\times f(\varepsilon_{\mathbf{p}})[1-f(\varepsilon_{\mathbf{p}'})]\end{aligned} \tag{20}$$

where $K_{\alpha}(t)$ is the single fermion version of the force operator defined following (6) and the $|\mathbf{p}\rangle$ are momentum states. For $\mathbf{x}=\mathbf{v}t+\mathbf{x}_0$ the time evolution operators can be calculated after a Galilean transformation[9,10] and one obtains for the Fourier transform

$$S_{\alpha\beta}(\omega)=2\pi\hbar\int\langle\mathbf{p}+|K_\alpha|\mathbf{p}'+\rangle\langle\mathbf{p}'+|K_\beta|\mathbf{p}+\rangle \times f(\varepsilon_{\mathbf{p}+m\mathbf{v}})[1-f(\varepsilon_{\mathbf{p}'+m\mathbf{v}})] \times\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'}+\hbar\omega)d\mathbf{p}\,d\mathbf{p}' , \tag{21}$$

where we have taken the limit $t_0\to-\infty$. The $|\mathbf{p}+\rangle$ are one-particle scattering states with outgoing boundary conditions corresponding to the Hamiltonian $H_B+H_{SB}(\mathbf{q}=0)$ with the scattering potential centered at the origin. To check the validity of the Einstein relation for zero velocity we insert the completeness of the incoming scattering states $\int|\mathbf{p}'-\rangle\langle\mathbf{p}'-|d\mathbf{p}'=1$ instead of $\int|\mathbf{p}'+\rangle\langle\mathbf{p}'+|d\mathbf{p}'$ in (21) and use[12]

$$\langle\mathbf{p}\mp|\mathbf{K}|\mathbf{p}'\pm\rangle=\frac{i}{\hbar}(\mathbf{p}'-\mathbf{p})\langle\mathbf{p}|V|\mathbf{p}'\pm\rangle . \tag{22}$$

An expansion for small velocities then indeed shows that $S_{\alpha\beta}(\omega=0)=\delta_{\alpha\beta}2\tilde{\eta}k_BT+\mathcal{O}(v_0^2)$, i.e., the Einstein relation is valid for arbitrary temperatures even in the quantum limit $k_BT\ll\varepsilon_F$. Since the friction constant $\eta(v_0)$ behaves as $\eta(v_0)=\eta(v_0=0)+\mathcal{O}(v_0^2)$ in the low velocity limit, we have $\tilde{\eta}_\parallel=\eta$ as $v_0\to0$. For general velocities $\eta(v_0)$ is given by[9]

$$\eta(v_0)=\frac{1}{\pi\hbar m v_0}\int_{-\infty}^{\infty}f(\varepsilon_{p-mv_0})p|p|R(p)dp \tag{23}$$

for a one-dimensional system with the reflection coefficient $R(p)$ and for a three-dimensional system by[10]

$$\eta(v_0)=\frac{1}{(2\pi\hbar)^3 m v_0^2}\int f(\varepsilon_{\mathbf{p}-m\mathbf{v}_0})\mathbf{p}\cdot\mathbf{v}_0 p\sigma_{\mathrm{tr}}(p)d\mathbf{p} , \tag{24}$$

where $\sigma_{\mathrm{tr}}=\int(1-\cos\theta)\sigma(\theta)d\Omega$ is the transport cross section.

In order to discuss the behavior at $v_0\neq0$ we first consider the one-dimensional case where $S(\omega)$ can be given in closed form. According to our discussion above the limit $\omega=0$ determines the diffusion constant. Then the δ function in (21) restricts p' to $\pm p$ and in this case the force matrix elements can be expressed by the reflection coefficient[9]

$$\begin{aligned}|\langle p+|K|p+\rangle|^2&=\left[\frac{p^2}{\pi\hbar m}\right]^2R^2(p) ,\\ |\langle p+|K|(-p)+\rangle|^2&=\left[\frac{p^2}{\pi\hbar m}\right]^2R(p)[1-R(p)] .\end{aligned} \tag{25}$$

From time reversal invariance we have $R(-p)=R(p)$ and with the notation $f_\pm\equiv f(\varepsilon_{p\pm mv})$ we can write $S(\omega=0)$ as

$$S(\omega=0)=\frac{2}{\pi\hbar m}\int_0^\infty p^3R(p)[f_++f_--2f_+f_- -(f_+-f_-)^2R(p)]dp . \tag{26}$$

The case of very high velocity $v_0\gg v_F$ yields $S(\omega=0)=2mv^2\eta(v_0\to\infty)$. This corresponds to a replacement of the thermal energy $k_BT/2$ by the kinetic energy $mv_0^2/2$ which is clear from the fact that the bath Fermions in the latter case have a mean velocity v_0 relative to the particle. In the general case (26) has to be evaluated numerically. For simplicity the interaction is approximated by a rectangular potential with height V_0 and width L which we take as the unit length. In Fig. 1 the reduced dimensionless diffusion constant $D\eta(v_0=0)/\varepsilon_F$ is shown as a function of the temperature for different values of the average velocity v_0. In the limit $v_0\to0$ the diffusion constant is simply linear in the temperature as expected from the Einstein relation. At finite v_0 the diffusion constant no longer vanishes as $T\to0$, however the behavior is still roughly linear in T, as long as the velocity is smaller than v_F.

For arbitrary frequencies ω the matrix elements in (21) involve scattering states at different energies and can no longer be expressed by the reflection coefficient $R(p)$. Therefore we have numerically calculated $S(\omega)$ from (21) for the above mentioned model potential. Figure 2 shows $\phi(\omega)\equiv\frac{1}{2}[S(\omega)+S(-\omega)]$, i.e., the Fourier transform of $\mathrm{Re}S(t)$ for various velocities. It is only in the limit $V_0\gg(\varepsilon_p,\varepsilon_{p'})$ where simple expressions for the force matrix elements exist $(p,p'\geq0)$:

$$\begin{aligned}|\langle p+|K|p'+\rangle|^2&\to\left[\frac{pp'}{\pi\hbar m}\right]^2 ,\\ |\langle p+|K|(-p')+\rangle|^2&\to0 .\end{aligned} \tag{27}$$

Inserting this into (21) it follows that in the region $V_0\gg\hbar\omega\gg(\varepsilon_F,mv_0^2/2)$ the spectrum behaves like $\omega^{1/2}$. This is confirmed by the numerical calculations which are valid for arbitrary potential strength V_0. For $\hbar\omega\approx V_0$ the approximation (27) breaks down and $S(\omega)$ tends to zero. In our model the spectrum is obviously far from white noise.

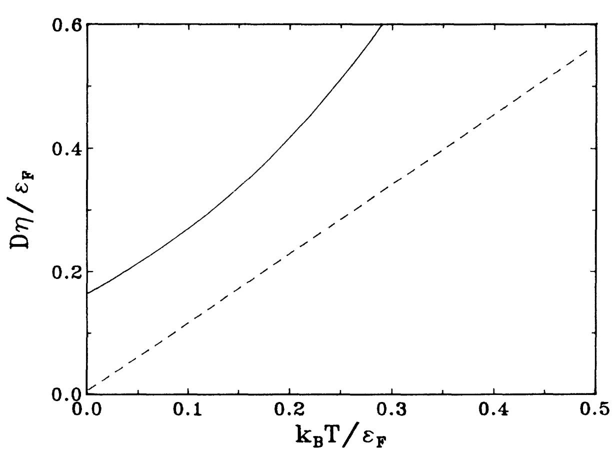

FIG. 1. The reduced diffusion constant $D\eta(v_0=0)/\varepsilon_F$ for a one-dimensional rectangular potential with height V_0 and width L is shown as a function of the temperature for velocities $v/v_F=2$ (solid curve) and $v/v_F=0.5$ (dashed). For the parameters we have chosen $k_FL=1$ and $V_0/\varepsilon_F=10$. Note that for any $v_0\neq0$ the diffusion constant is finite at $T=0$ which is however difficult to see on the scale chosen here if $v_0/v_F=0.5$.

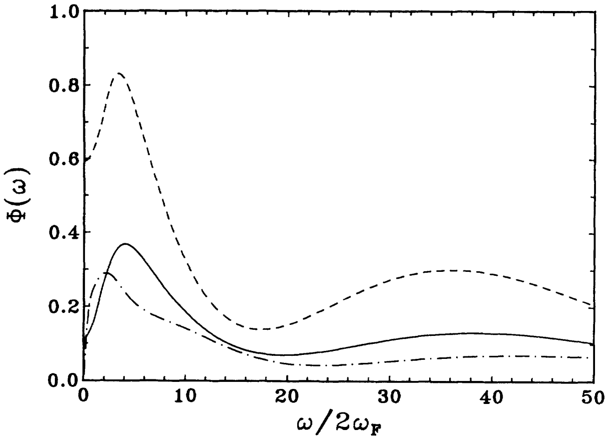

FIG. 2. For the one-dimensional model potential the spectrum $\phi(\omega)=\mathrm{Re}S(\omega)$ is shown in arbitrary units at zero temperature as a function of $\omega/2\omega_F$ where $\hbar\omega_F=\varepsilon_F$ for velocities $v/v_F=0.5$ (solid curve), $v/v_F=1$ (dashed) and $v=0$ (dashed dotted). We have chosen $k_FL=1$ and $V_0/\varepsilon_F=5$.

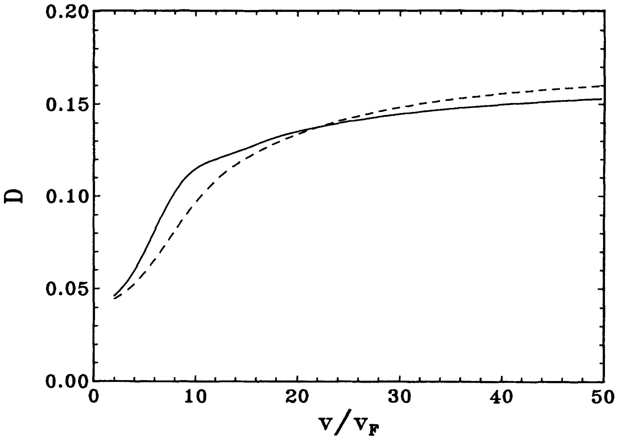

FIG. 3. The longitudinal (solid curve) and transversal (dashed) diffusion constants according to (28) are shown as a function of the renormalized velocity in the regime $v_0/v_F>2$ for a hard sphere potential with radius a and $k_Fa=0.1$. $D_\parallel$ and $D_\perp$ are divided by a factor $v_0/\pi a^2 n_0$ and are therefore dimensionless.

Since it does not seem possible to calculate the force matrix elements in (21) at energies $\varepsilon_p\neq\varepsilon_{p'}$ in closed form for a three-dimensional system we further restrict the discussion to $\omega=0$ and large velocities. As mentioned above the Einstein relation holds in the low velocity regime. In the opposite limit of high velocity it is advantageous to split (21) into two contributions where the first term without the extra Fermi function $f(\varepsilon_{\mathbf{p}'+m\mathbf{v}})$ can be simplified in the same manner as in the proof of the Einstein relation. Then the matrix element may be removed from the integrand. This is also true for the second contribution where the remaining integral containing two Fermi functions is exactly known at zero temperature. If we choose $\mathbf{v}_0=v_0\mathbf{e}_3$ we obtain $S_{\alpha\beta}(\omega=0)=\frac{1}{2}\delta_{\alpha\beta}[S_\perp+\delta_{\alpha 3}(2S_\parallel-S_\perp)]$ with the longitudinal and transversal components given by ($T=0, v_0\gg v_F$)

$$S_\perp=m^2v_0^3n\,\sigma_{\mathrm{diff}}(mv_0)\ ,$$
$$S_\parallel=m^2v_0^3n\left[2\sigma_{\mathrm{tr}}(mv_0)-\sigma_{\mathrm{diff}}(mv_0)-\frac{k_F^2}{5\pi}\sigma_{\mathrm{tr}}^2(mv_0)\right]\ , \tag{28}$$

where n is the Fermion density and $\sigma_{\mathrm{diff}}(p)=\int(1-\cos^2\theta)\sigma_p(\theta)d\Omega$ which we call the *diffusion cross section.* Obviously σ_{diff} is large if there is a strong scattering transverse to the incident direction $\theta=\pi/2,\ 3\pi/2$, leading to large transverse fluctuations $S_\perp$. Taking the average over different directions yields $\mathrm{Tr}S_{\alpha\beta}(0)=2mv^2\eta(v\to\infty)$ (Ref. 13) where σ_{diff} plays no role, i.e., one obtains an expression similar to one dimension. In the same manner as σ_{tr} the diffusion cross section may be expressed in terms of phase shifts δ_l of partial waves l by

$$\sigma_{\mathrm{diff}}(p)=8\pi\left[\frac{\hbar}{p}\right]^2\sum_{l=0}^{\infty}\frac{1}{2l+3}\left[\frac{(2l+1)(l^2+l-1)}{2l-1}\sin^2\delta_l-(l+1)(l+2)\cos(\delta_{l+2}-\delta_l)\sin\delta_l\sin\delta_{l+2}\right] \tag{29}$$

which we used in the numerical calculations. The resulting velocity dependence of the longitudinal and transversal diffusion constants derived from (28) are shown in Fig. 3 in the case of a hard-sphere potential. Since (28) is only valid in the limit $v_0\gg v_F$ we have chosen $k_Fa\ll 1$. In contrast to our one-dimensional potential the scattering cross sections for an infinitely hard potential do not tend to zero in the high energy limit, i.e., $\lim_{p\to\infty}\sigma_{\mathrm{tr}}(p)=\pi a^2$ and $\lim_{p\to\infty}\sigma_{\mathrm{diff}}(p)=2\pi a^2/3$ and therefore $D_\sigma\to v_0/6\pi a^2 n$ for $v_0\gg v_F$. The fact that the longitudinal and the transverse diffusion constants are equal in the high-velocity regime is an artifact of our hard sphere model potential and will not hold for finite potentials.

In conclusion we have studied the fluctuations in the motion of a heavy particle interacting with a free-Fermion gas by means of a semiclassical expansion. Our model may be considered as an example for a quantum system far from thermal equilibrium. No assumptions like a weak potential or linear response[14–16] were made. We have shown that the fluctuations around the nonequilibrium steady state are diffusive and have calculated the corresponding longitudinal and transverse diffusion constants explicitly for simple model potentials.

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