Semiclassical expansion theory in phase space

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We study the $\hbar$ perturbation expansion of the quantum Wigner equation. It leads to a unified formulation of semiclassical approximations based on the phase-space representation of quantum mechanics. We derive the $O(\hbar^2)$ quantum corrections to the finite-temperature Bose and Thomas-Fermi phase-space distributions. Both reduce, in the high-temperature limit, to the known quantum corrections of the classical Gibbs-Boltzmann probability density. Within this approach, moreover, we obtain a very simple derivation of the extended Thomas-Fermi theory. Finally, the limits of applicability, the convergence problems, and the possibility of improving or defining new semiclassical approximations are discussed.

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In recent years a renewed interest has developed in the semiclassical formulations of quantum mechanics [1]. These approaches, indeed, combine a clearer interpretation of the results with very reduced computational efforts. One of the most utilized, especially in the context of the many-body theory, is based on the phase-space representation of quantum mechanics, proposed by Wigner in 1932 [2,3] while studying the quantum corrections to the Gibbs-Boltzmann statistical distribution. This formalism has been used in the development of a new approach to the quantum collision theory [4]. In conjunction with it, powerful numerical methods have been developed to solve nonequilibrium problems, first in the classical limit (that reduces to solve the Liouville equation) [5–8] and, recently, including $O(\hbar^2)$ quantum corrections [9–11].

Here we study the semiclassical expansion in $\hbar$ and the general solution up to second-order terms of the Wigner equation. This leads to a unified view of semiclassical approximations based on the Wigner representation of quantum mechanics. We derive the quantum corrections to the phase-space Thomas-Fermi and Bose distribution functions for fermions and bosons, respectively, and we show how both reduce, in the high-temperature limit, to the well-known quantum corrections to the Gibbs-Boltzmann distribution. We investigate, moreover, the relation that exists between the fermion phase-space distribution derived in this framework and the extended Thomas-Fermi (ETF) theory at zero and finite temperature. We discuss, finally, the limit of applicability of this method and the convergence problems and we give some hint to the possibility of improving or defining new semiclassical approximations.

The Wigner representation of quantum mechanics is based on a shifted Fourier transform of the quantum density matrix $\rho(\mathbf{r},\mathbf{r}')$:

$$f_w(\mathbf{r},\mathbf{p},t)=\frac{1}{(\pi\hbar)^3}\int d\mathbf{q}\; e^{-(2i/\hbar)\mathbf{q}\cdot\mathbf{p}}\rho(\mathbf{r}+\mathbf{q},\mathbf{r}-\mathbf{q},t). \quad (1)$$

The Wigner function Eq. (1) is real and can be interpreted as a phase-space distribution; nevertheless it can acquire negative values and cannot be interpreted as a probability density.

The von Neumann equation of motion for the density matrix is

$$i\hbar\frac{\partial}{\partial t}\rho=[H,\rho], \quad (2)$$

which in the Wigner formalism is expressed as

$$i\hbar\frac{\partial}{\partial t}f_w=H\star f_w-f_w\star H. \quad (3a)$$

The "$\star$" indicates the so-called twisted product [12], which is an operator product in the Schrödinger representation defined by

$$A\star B=A(\mathbf{r},\mathbf{p})\exp\left[\left(i\frac{\hbar}{2}\right)(\overleftarrow{\partial}_{\mathbf{r}}\,\overrightarrow{\partial}_{\mathbf{p}}-\overleftarrow{\partial}_{\mathbf{p}}\,\overrightarrow{\partial}_{\mathbf{r}})\right]B(\mathbf{r},\mathbf{p}). \quad (3b)$$

The twisted commutator has a well-known asymptotic expansion in even power of $\hbar$, hence the Wigner equation becomes

$$\frac{\partial f_w}{\partial t}+\frac{\mathbf{p}}{m}\frac{\partial f_w}{\partial \mathbf{r}}-\frac{\partial V}{\partial \mathbf{r}}\frac{\partial f_w}{\partial \mathbf{p}}=F_q,$$

$$F_q=\sum_{k=1}^{\infty}\frac{(-1)^k}{(2k+1)!}\left(\frac{\hbar}{2}\right)^{2k}H(\mathbf{r},\mathbf{p})\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{r}}\frac{\overrightarrow{\partial}}{\partial \mathbf{p}}\right)^{2k+1}f_w(\mathbf{r},\mathbf{p},t)$$
$$=-\frac{\hbar^2}{24}H(\mathbf{r},\mathbf{p})\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{r}}\frac{\overrightarrow{\partial}}{\partial \mathbf{p}}\right)^3 f_w(\mathbf{r},\mathbf{p},t)+O(\hbar^4)+\cdots, \quad (3c)$$

where $H(\mathbf{r},\mathbf{p})=\mathbf{p}^2/2m+V(\mathbf{r})$ is the classical Hamiltonian of the system and the arrows on the partial derivatives indicate the function on which they act. Note that for a harmonic potential all terms in the $\hbar$ expansion disappear and the corresponding quantum equation of motion is identical to the classical one: all quantum effects are in the initial conditions. However, in some cases (such as for potentials with sharp edges or systems at low entropy), the series might not be convergent, and a partial resummation [13–15] or a smoothing procedure [10,16,17] is necessary. The technique of expanding Eq. (3a) in an asymptotic series, collecting terms, and then obtaining quantum corrections has been studied in detail in [18]. Results on the asymptotic expansion Eq. (3c) and its classical limit can be found in [12].

In the following we will address our discussion to the one-body problem in a local mean-field potential. Our goal will be to solve perturbatively the quantum Wigner equation (QWE) Eq. (3c) in the stationary case ($\partial f_w/\partial t=0$), neglecting $O(\hbar^4)$ terms.

Let us expand formally the Wigner function Eq. (1) in a power series in $\hbar^2$:[1]

$$f(\mathbf{r},\mathbf{p})=f_0(\mathbf{r},\mathbf{p})+\hbar^2 f_2(\mathbf{r},\mathbf{p})+O(\hbar^4). \tag{4}$$

Replacing f_w in Eq. (3c) by its expansion Eq. (4) and ordering the $O(\hbar^0)$ and $O(\hbar^2)$ terms, we obtain

$$\frac{\mathbf{p}}{m}\cdot\frac{\partial f_0}{\partial \mathbf{r}}-\frac{\partial V}{\partial \mathbf{r}}\cdot\frac{\partial f_0}{\partial \mathbf{p}}=0, \tag{5a}$$

$$\frac{\mathbf{p}}{m}\cdot\frac{\partial f_2}{\partial \mathbf{r}}-\frac{\partial V}{\partial \mathbf{r}}\cdot\frac{\partial f_2}{\partial \mathbf{p}}=-\frac{1}{24}V\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{r}}\frac{\vec{\partial}}{\partial \mathbf{p}}\right)^3 f_0. \tag{5b}$$

Equation (5a) implies that f_0 can be an arbitrary function of all constants of motion of the system, but here we will assume it to be a function of the Hamiltonian alone, $f_0=f_0(H(\mathbf{r},\mathbf{p}))$.

It is not difficult to figure out that the solution of Eq. (5b), imposing as boundary conditions that the distribution vanishes for large distances, must be written in the form

$$f_2(\mathbf{r},\mathbf{p})=f_0'' g_1(\mathbf{r})+f_0''' g_2(\mathbf{r})+f_0'''\sum_{n,m} p_n p_m g_3^{(n,m)}(\mathbf{r}), \tag{6}$$

where p_i represents the components of momenta and the primes indicate the derivatives of $f_0(E)$ with respect to the energy.

Replacing Eq. (6) in Eq. (5b), we can solve the resulting equations for the $g_i(\mathbf{r})$ obtained by ordering and equaling to zero the terms with the same power in the momenta. The general solution of Eqs. (5a) and (5b) becomes

$$f(\mathbf{r},\mathbf{p})=f_0(E)+\frac{\hbar^2}{8m}\left\{-\frac{\partial^2 V(\mathbf{r})}{\partial \mathbf{r}^2}f_0''(E)-\left[\frac{1}{3}\left(\frac{\partial V(\mathbf{r})}{\partial \mathbf{r}}\right)^2+\frac{1}{3m}\left(\mathbf{p}\cdot\frac{\partial}{\partial \mathbf{r}}\right)^2 V(\mathbf{r})\right]f_0'''(E)\right\}+O(\hbar^4). \tag{7}$$

It is interesting to note that for a central potential it is possible to solve Eq. (5b) by simple quadratures, as we will show in the Appendix. The resolution of Eqs. (5) including high-order terms on $\hbar$ is a bit more intricate but does not present any special difficulty.

As we have already stressed, the reference state $f_0(H(r,p))=f_0(E)$ is an arbitrary function of the classical Hamiltonian that we have to choose judiciously to approximate the *exact* stationary solution of the quantum Wigner equation (3).

Let us pick, as first example, a Thomas-Fermi distribution:

$$f_0(E)=f_{\mathrm{TF}}=\left[\exp\left(\frac{(H(\mathbf{r},\mathbf{p})-\mu_F)}{T}\right)+1\right]^{-1}, \tag{8}$$

where μ_F is the Fermi energy and T the temperature of the system.

Inserting Eq. (8) into Eq. (7) and noting that $\partial f(E-\mu_F)/\partial E=-\partial f(E-\mu_F)/\partial \mu_F$ we obtain

$$f(\mathbf{r},\mathbf{p})=f_0(H(\mathbf{r},\mathbf{p})-\mu_F)+\frac{\hbar^2}{8m}\left\{-\frac{\partial^2 V(\mathbf{r})}{\partial \mathbf{r}^2}f_0''(H-\mu_F)+\left[\frac{1}{3}\left(\frac{\partial V(\mathbf{r})}{\partial \mathbf{r}}\right)^2+\frac{1}{3m}\left(\mathbf{p}\cdot\frac{\partial}{\partial \mathbf{r}}\right)^2 V(\mathbf{r})\right]f_0'''(H-\mu_F)\right\}. \tag{9}$$

In this case, the derivatives of $f_0(H-\mu_F)$ have to be taken with respect to the chemical potential μ_F.

This fermion phase-space distribution, integrated over the coordinates or over the momenta, leads to a mass density and a momentum density that coincide with the one obtained in the ETF theory [15,19–23], which, then, is just a particular solution of Eqs. (5). Moreover, we can interpret the singularities that appear in ETF in the limit $T\to 0$: they arise from the derivatives of Eq. (8) which, at $T=0$, reduce to a step function $\Theta(E-\mu_F)$.

As a second application, we consider as a reference state the Bose distribution:

$$f_0(E)=f_B=\left[\exp\left(\frac{(H(\mathbf{r},\mathbf{p})-\mu_B)}{T}\right)-1\right]^{-1}. \tag{10}$$

Inserting this expression into Eq. (7) we have found out its quantum corrections in analogy with the previous case.

[1]When the boundary conditions are independent of $\hbar$, the odd powers of the $\hbar$ expansion Eq. (4) can be equal to zero [4].

This can allow us to calculate, for example, the corrections to the Bose-Einstein condensation temperature for a boson system in a mean-field potential. It can be defined imposing the normalization condition to Eq. (7) and reducing the chemical potential to zero.

Approaching the classical limit, the Thomas-Fermi Eq. (8) and the Bose Eq. (10) will be approximated by the classical Gibbs-Boltzmann statistical distribution $f_0 = \exp[(\mu - E)/T]$. In this case Eq. (7) will read

$$f = e^{(\mu - E)/T}\left(1 + \frac{\hbar^2}{8m}\left\{-\frac{1}{T^2}\frac{\partial^2 V(\mathbf{r})}{\partial \mathbf{r}^2} + \frac{1}{T^3}\left[\frac{1}{3}\left(\frac{\partial V(r)}{\partial \mathbf{r}}\right)^2 + \frac{1}{3m}\left(\mathbf{p}\cdot\frac{\partial}{\partial \mathbf{r}}\right)^2 V(\mathbf{r})\right]\right\}\right). \tag{11}$$

This last result was derived, first, by Wigner in his work of 1932 [2,24] studying the quantum corrections of the Gibbs-Boltzmann distribution. It is interesting to note that in Eq. (11) the quantum corrections associated with the gradients of the potential are still important, but that those coming from the statistical properties of identical particles disappear. This point was assumed by Wigner in the basis of some physical argument [2]. See also [24] for more discussions.

There is a further point to be remarked upon. The perturbative approach used here can be justified only if the higher-order terms in $\hbar$, in the semiclassical expansion of the quantum Wigner equation (3c), are much smaller than the lower-order ones. This is, clearly, not the case if we use a reference state $f_0(E)$ like, for example, the Thomas-Fermi distribution at very low temperature. However, surprisingly, even if the phase-space ETF distribution Eq. (9) at $T=$ contains singu-

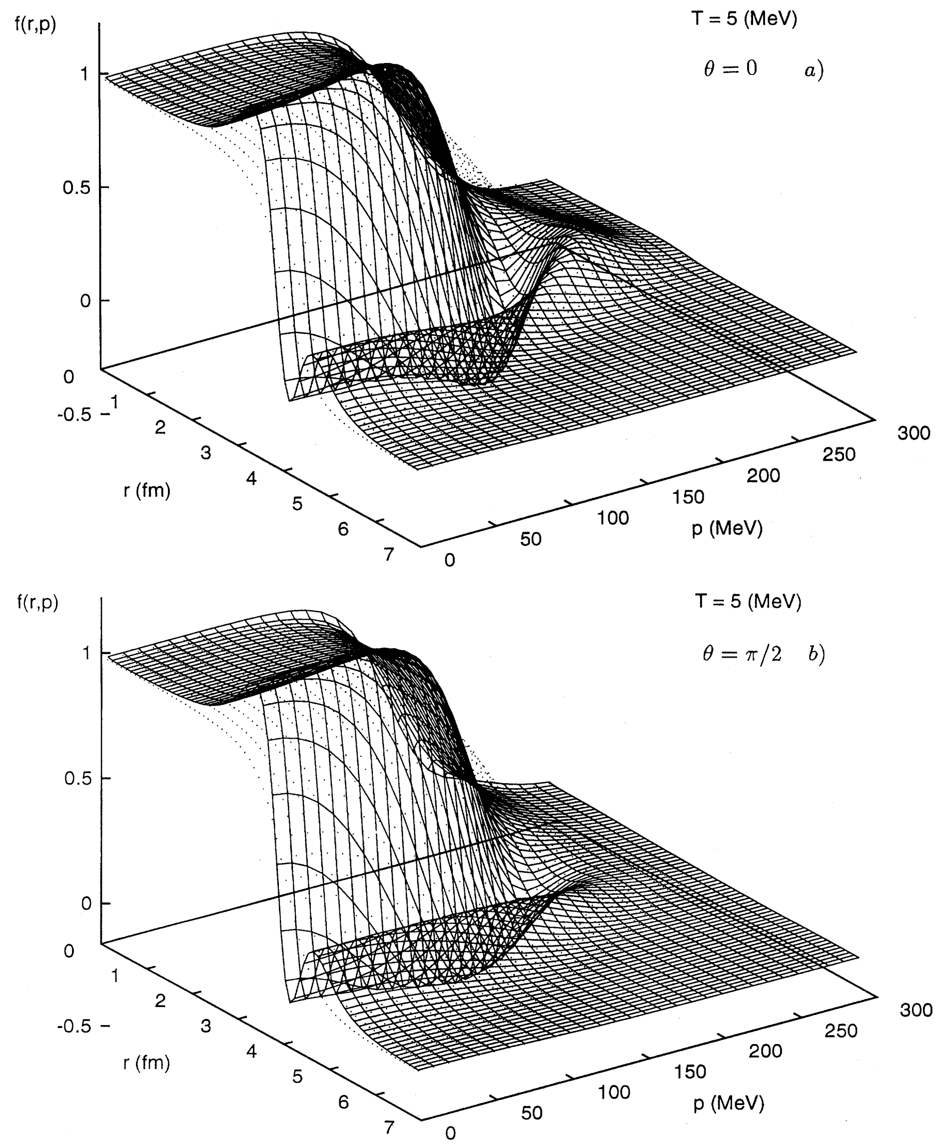

FIG. 1. The Thomas-Fermi (dotted mesh) and the phase-space ETF (lined meshed), Eqs. (8) and (9), for a hot nucleus in a Wood-Saxon potential $V = V_0\{1 + \exp[(r - r_0)/a]\}^{-1}$ with parameters $V_0 = -40$ MeV, $r_0 = 4$ fm, and $a = 0.65$ (^{40}Ca). The distribution is plotted as a function of the moduli of radius and momentum, at a fixed angle between these two vectors $\theta = 0$ (a) and $\theta = \pi/2$ (b). The temperature is $T = 5$ MeV. Note that the Wigner distribution acquires also negative values. The $\hbar^2$ quantum corrections act, mostly, on the tail of the distribution, becoming singular in the limit $T \to 0$.

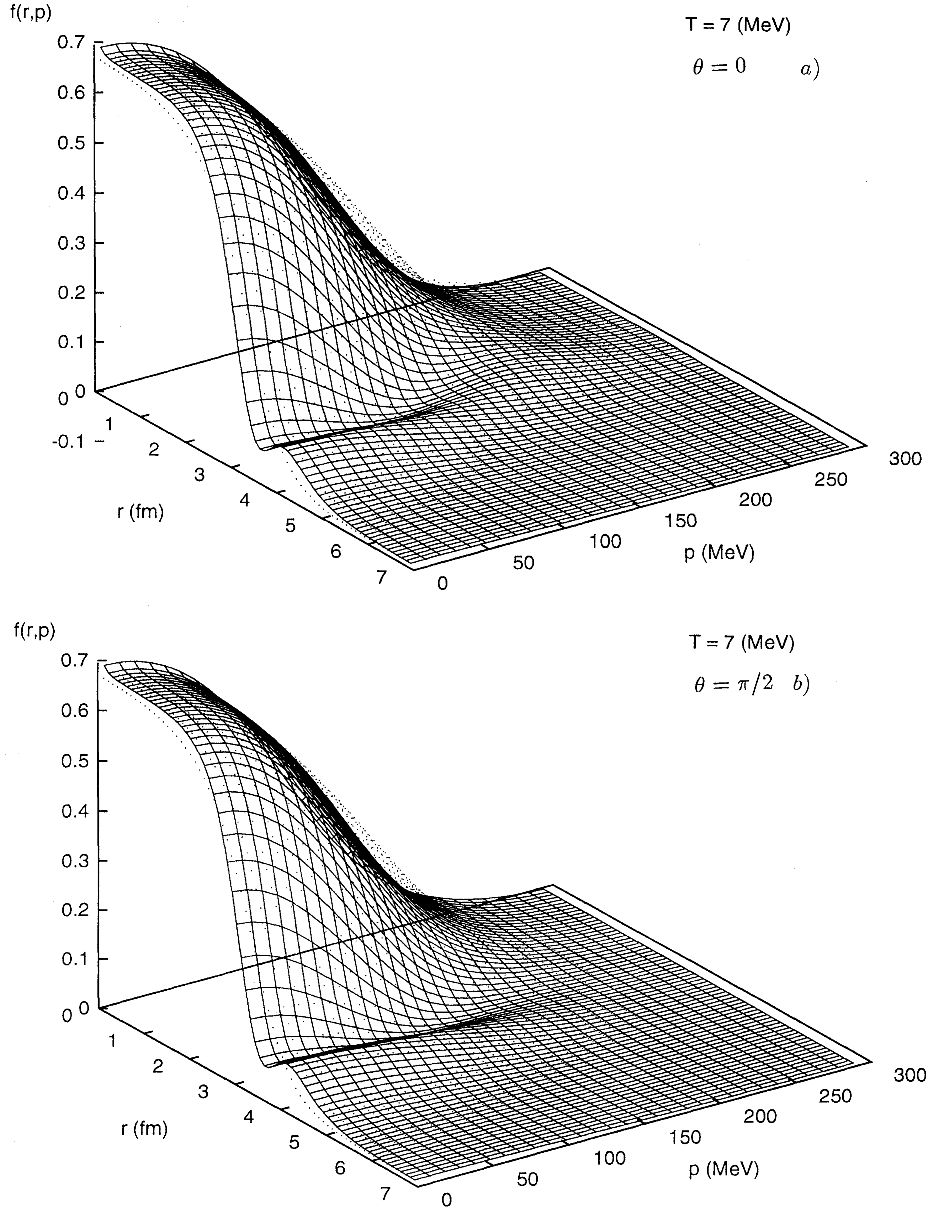

FIG. 2. The same as Fig. 1 at a temperature $T=7$ MeV. The oscillations are quite reduced and we can expect, in this case, that higher-order terms in the $\hbar$ expansion [Eq. (4)] become negligible.

larities, it has been demonstrated numerically, that, at least for some observables like the ground-state energy of nuclei, the $\hbar$ expansion is rapidly convergent, giving results in good agreement with static Hartree-Fock calculations [25].

Nevertheless, it is important to stress that we are free to choose $f_0(E)$ differently from that suggested in the Thomas-Fermi theory. One possibility is to consider the convolution of the TF distribution, Eq. (8), by some averaging function, in analogy with the Strutinsky method [26]. This could sufficiently smooth the TF distribution at low temperatures to improve considerably the convergence of the perturbative expansion, Eqs. (5a) and (5b). It is also interesting, in this regard, to investigate the properties of the Husimi function [16], obtained by a simple Gaussian smoothing of the Wigner distribution, Eq. (1). A further but equivalent smoothing method has been considered in the literature, calculating the phase-space ETF distribution at $T=0$ by the inverse Laplace transform of the semiclassical propagator with the saddle-point method [27].

To better illustrate this argument, we compare in Figs. 1 and 2 the Thomas-Fermi Eq. (8) (dotted mesh) with the phase-space ETF Eq. (9) (lined mesh) at two different temperatures for a nucleus in a fixed Wood-Saxon potential. Due to the spherical symmetry of the system, the Wigner distribution depends only on three independent variables, which we choose to be the modulus of the radius, momentum, and the angle between these two vectors (see Appendix). At $T=5$ MeV (Fig. 1) we can observe strong oscillations on the tail of the ETF distribution that are originated by gradients of third order in Eq. (5b). We cannot interpret these oscillations as shells (that, in any case, should disappear at $T\simeq 2.5$ MeV [22]) or as the Friedel ones. Maybe, at this temperature, the higher-order $\hbar$ terms in Eq. (9) are still important, or the same expansion is not yet convergent. The smoothing is clearly necessary and it should increase the diffusivity in the tail of the momentum distribution on the nuclear surface [27], which could be important, for example, in the study of the subthreshold production of particles in heavy-ion reactions. However, we can see in Fig. 2 as the oscillations of the distribution at $T=7$ MeV are already quite reduced respect to the previous case. At high temperatures we can expect that the semiclassical expansion converges quite rapidly, though this depends both on the form of the reference state and the potential. It would be interesting, for this purpose, to compare the phase-space ETF Eq. (9) with the exact quantum Wigner distribution calculated numerically with the static Hartree-Fock wave functions using Eq. (1) [28].[2]

In summary, we have solved perturbatively the quantum Wigner equation including second-order terms in the $\hbar$ expansion. We have obtained a clear and unified view of the semiclassical methods based in the phase-space representation of quantum mechanics.

We have illustrated a very simple derivation of the extended Thomas-Fermi theory, discussing the origin of the unpleasant singularities that appear at zero temperature and suggesting their elimination through an appropriate smoothing procedure.

We have derived, for the first time, the quantum corrections to the phase-space boson distribution in a mean-field potential.

We have shown how, approaching the classical limit, both distributions reproduce the known quantum corrections to the Gibbs-Boltzmann probability density.

We have discussed, finally, the convergence of the semiclassical expansion studying the quantum corrections to the phase-space Thomas-Fermi distribution of a nucleus at different temperatures.

This method may open a route to new improvements of the actual semiclassical approximations, but it can also suggest new approaches, all of them based on the Wigner representation of quantum mechanics.

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[2]There is another interesting aspect associated with the smoothing procedure. Note that in Figs. 1(a) and 2(a) the phase-space ETF distribution acquires negative values. In general, with a smoothing over, for example, phase-space cells of volume $\geqslant(2\pi\hbar)^3$, the Wigner function Eq. (1) becomes positive everywhere and could be interpreted as a probability density [10,16].

APPENDIX

For a central potential it is possible to solve Eq. (5b) by simple quadrature. This will be useful if we consider as reference state f_0 a more complicated function of the constants of motion of the system.

Since we are considering a central potential, the term f_2 can depend only on three variables that we conveniently choose to be the radius r, the total energy E, and the modulus of the angular momentum $\mathbf{\Lambda}=\mathbf{r}\times\mathbf{p}$. Indeed, because the energy and the angular momentum are constants of the motion, two partial derivatives in Eq. (5b) disappear. This can be easily understood by writing

$$[H,f]_{(\mathbf{r},\mathbf{p})}=\sum_\alpha [H,c_\alpha]\frac{\partial f}{\partial c_\alpha}, \tag{A1}$$

where [ ] is the classical Poisson bracket and c_α is a new set of independent variables. If some of these are a constant of the motion, the corresponding Poisson bracket of right-hand side of (A1) is equal to zero.

The integral over the phase space can be transformed into integrals over the new variables by calculating the Jacobian of the transformation [29]:

$$\int d\mathbf{r}\,d\mathbf{p}=16\pi^2\int_0^\infty dr\int_0^\infty dE\int_0^\infty d\Lambda\,\frac{\Lambda}{v(r,E)}, \tag{A2}$$

where $v(r,E,\Lambda)$ is the radial velocity:

$$v(r,E,\Lambda)=\left[\frac{2}{m}\left(E-V(r)-\frac{\Lambda^2}{2mr^2}\right)\right]^{1/2}. \tag{A3}$$

A factor 2 has been added in Eq. (A2) to take in account that positive and negative momenta correspond to the same energy for a given value of the radius r.

Let us consider, first, the one-dimensional problem: in this case only two variables are independent and we can choose the coordinate x and the energy E. The gradients are expressed as

$$\left(\frac{\partial}{\partial x}\right)_p=\left(\frac{\partial}{\partial x}\right)_E+\left(\frac{\partial E}{\partial x}\right)_p\left(\frac{\partial}{\partial E}\right)_x, \tag{A4}$$

$$\left(\frac{\partial}{\partial p}\right)_x=v(E,x)\left(\frac{\partial}{\partial E}\right)_x,$$

$$\left(\frac{\partial^3}{\partial p^3}\right)_x=\frac{3}{m}v(E,x)\frac{\partial^2}{\partial E^2}+v(E,x)^3\frac{\partial^3}{\partial E^3},$$

and the resulting equation is

$$\frac{\partial f_2(x,E)}{\partial x}=-\frac{1}{24}\frac{d^3V(x)}{dx^3}\left[\frac{3}{m}\frac{d^2f_0}{dE^2}+v(x,E)^2\frac{d^3f_0}{dE^3}\right], \tag{A5}$$

which can be solved by a simple integration imposing as boundary condition that the distribution function vanishes at large distances:

$$\hbar^2 f_2(x,E) = -\frac{\hbar^2}{8m}\left\{\frac{d^2 f_0(E)}{dE^2}\frac{d^2V(x)}{dx^2} + \frac{1}{3}\frac{d^3 f_0(E)}{dE^3}\left[mv^2(x,E)\frac{d^2V(x)}{dx^2} + \left(\frac{dV(x)}{dx}\right)^2\right]\right\}. \tag{A6}$$

The calculation in the three-dimensional case is more involved but straightforward. Equation (5b) can be written as

$$\frac{\partial f_2(r,E,\Lambda)}{\partial r} = -\frac{\hbar^2}{8m}\left[\frac{d^2 f_0(E)}{dE^2}\left(-\frac{2}{r^2}\frac{dV(r)}{dr} + \frac{2}{r}\frac{d^2V(r)}{dr^2} + \frac{d^3V(R)}{dr^3}\right) + \frac{d^3 f_0(E)}{dE^3}\left(-\frac{\Lambda^2}{mr^4}\frac{dV(r)}{dr} + \frac{\Lambda^2}{mr^3}\frac{d^2V(r)}{dr^2} + \frac{m}{3}v^2(r,E,\Lambda)\frac{d^3V(r)}{dr^3}\right)\right] \tag{A7}$$

with the solution

$$\hbar^2 f_2(r,E,\Lambda) = -\frac{\hbar^2}{8m}\left\{\frac{d^2 f_0(E)}{dE^2}\left(\frac{d^2V(r)}{dr^2} + \frac{2}{r}\frac{dV(r)}{dr}\right) + \frac{d^3 f_0(E)}{dE^3}\left[\frac{1}{3}\left(\frac{dV(r)}{dr}\right)^2 + \frac{\Lambda^2}{3mr^3}\frac{dV(r)}{dr} + \frac{m}{3}v^2(r,E,\Lambda)\frac{d^2V(r)}{dr^2}\right]\right\}, \tag{A8}$$

which is the same as Eq. (7) expressed in new coordinates.

In Figs. 1 and 2, Eq. (9) is plotted as a function of the moduli of radius and momentum at a given angle θ between these two vectors. Using these coordinates, Eq. (A8) becomes

$$\hbar^2 f_2(r,E,\Lambda) = -\frac{\hbar^2}{8m}\left\{\frac{d^2 f_0(E)}{dE^2}\left(\frac{d^2V(r)}{dr^2} + \frac{2}{r}\frac{dV(r)}{dr}\right) + \frac{d^3 f_0(E)}{dE^3}\left[\frac{1}{3}\left(\frac{dV(r)}{dr}\right)^2 + \frac{p^2}{3m}\frac{d^2V(r)}{dr^2} + \frac{p^2\sin^2(\theta)}{3m}\left(\frac{1}{r}\frac{dV(r)}{dr} - \frac{d^2V(r)}{dr^2}\right)\right]\right\}. \tag{A9}$$

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