Wigner-Kirkwood expansion of the phase-space density for semi-infinite nuclear matter

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The phase-space distribution of semi-infinite nuclear matter is expanded in an $\hbar$ series analogous to the low-temperature expansion of the Fermi function. Besides the usual Wigner-Kirkwood expansion, oscillatory terms are derived. In the case of a Woods-Saxon potential, a smallness parameter is defined, which determines the convergence of the series and explains the very rapid convergence of the Wigner-Kirkwood expansion for average (nuclear) binding energies.

I. INTRODUCTION

The density of semi-infinite degenerate Fermi systems exhibits oscillations which are interference effects close to the surface of the medium. These oscillations are also present in the Wigner transform of the density matrix[1] $\hat{\rho}$. In the case of semi-infinite matter, the Wigner distribution function $f(\mathbf{r},\mathbf{p})$ in the six-dimensional space actually depends only on one spatial coordinate, say, z, perpendicular to the surface of the medium which is infinite in the x and y directions, and on the components $p_\parallel$ and $p_\perp = p_z$ of the momentum $\mathbf{p}$, respectively, parallel and perpendicular to the surface:

$$\hat{\rho}_W = f(z,p_\parallel,p_\perp)\ , \tag{1}$$

where W stands for "Wigner transform."

In the special case of the ramp potential $V(\mathbf{r})=V(z)=\alpha z$, the Wigner transform f is a function of the classical Hamiltonian only $H_{\rm cl}=\varepsilon=p^2/2m+\alpha z$: It may be convenient to write it also, in the case of a general potential, as a function of the total energy ε and of some angles θ and φ. For example,

$$\hat{\rho}_W = f(\varepsilon,\theta,\varphi)\ ,$$

with

$$\varepsilon = p^2/2m + V(z),\quad \tan\theta = \frac{V(z)}{p^2/2m},\quad \tan\varphi = p_\parallel/p_\perp\ . \tag{2}$$

For given values (θ_0,φ_0) of the angular variables, the above-mentioned oscillations of the Wigner distribution function show up close to the Fermi energy ε_F: They are similar to the ones known for the ramp potential and shown in Fig. 1. The main features of $f(\varepsilon,\theta_0,\varphi_0)$ are, with increasing ε,

(i) it oscillates around the unit step function (Wigner distribution of the homogeneous infinite matter) when $\varepsilon \to -\infty$,

(ii) it exhibits oscillations with increasing amplitudes when approaching ε_F,

(iii) it falls off to zero within a certain thickness representing the uncertainty of the momenta close to the surface, and

(iv) its surface is asymmetric around ε_F as compared to the step function.

Keeping in mind the picture of the Wigner distribution as a function of ε and knowing that the purely classical limit of $f(\mathbf{r},\mathbf{p})$ is a step function $\Theta(\varepsilon_F-\varepsilon)$ of the classical energy ε, the oscillations appear to be quantal effects. They are contained in higher-order terms obtained, for example, by a formal Taylor expansion of the density operator:

$$\hat{\rho} = \Theta(\varepsilon_F - \hat{H}) \tag{3}$$

around the classical Hamiltonian $H_{\rm cl}=\varepsilon$:

$$\hat{\rho} = \sum_{n=0}^{\infty} \frac{1}{n!}(\varepsilon-\hat{H})^n \left[\frac{\partial^n \Theta(\varepsilon_F-\hat{H})}{\partial(\varepsilon_F-\varepsilon)^n} \right]_\varepsilon\ . \tag{4}$$

The Wigner transform of Eq. (4) for a local potential leads to the well-known Wigner-Kirkwood expansion of

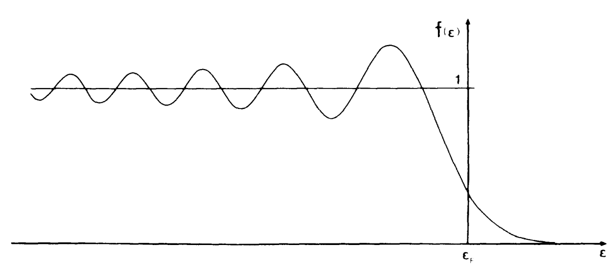

FIG. 1. The Wigner transform of the density matrix as a function of the classical energy ε in arbitrary units for the linear potential $V(\mathbf{r})=\alpha z$, as compared to the step function $\Theta(\varepsilon_F-\varepsilon)$ around the Fermi energy ε_F.

the density matrix:

$$\hat{\rho}_W = f(\mathbf{r},\mathbf{p})$$
$$= \Theta(\varepsilon_F - \varepsilon) - \frac{\hbar^2}{8m}\left\{ \Delta V\, \delta'(\varepsilon_F - \varepsilon) - \frac{1}{3}\left[(\nabla V)^2 + m\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2 V\right] \times \delta''(\varepsilon_F - \varepsilon)\right\} + O(\hbar^4) , \quad (5)$$

the Wigner transform $\hat{H}_W$ of the Hamiltonian being the classical energy ε and the derivatives being taken with respect to the Fermi energy ε_F. Equation (5) is an $\hbar$ expansion of the distribution function $f(\mathbf{r},\mathbf{p})$ by means of Dirac distributions but the derivation is completely formal and no statement with regard to its validity was made as yet.

For the purpose of obtaining some insight into the significance of this expansion, a comparison may be done with the low-temperature expansion of the Fermi function, which is known to be a good approximation.[2] In order to get clearly the conditions for this expansion to be valid and then to apply them to the case of expansion in Eq. (5), its derivation is briefly repeated.

If $h(\varepsilon)$ is an arbitrary continuous and continuously derivable function of the energy, its mean value with the Fermi function at temperature T, $F(\varepsilon) = \theta(\epsilon)\{1 + \exp[(\varepsilon - \varepsilon_F)/T]\}^{-1}$ is

$$\langle h \rangle = \int_{-\infty}^{+\infty} d\varepsilon\, h(\varepsilon) F(\varepsilon) . \quad (6)$$

If the temperature T is low enough, the unit step function is a first-order approximation for the Fermi distribution. It is thus reasonable to split it off in Eq. (6):

$$\langle h \rangle = \int_0^\infty d\varepsilon\, h(\varepsilon)\Theta(\varepsilon_F - \varepsilon) + \int_0^\infty d\varepsilon\, h(\varepsilon)[F(\varepsilon) - \Theta(\varepsilon_F - \varepsilon)] . \quad (6')$$

The following steps are now:

(i) The difference $[F - \Theta]$ is very small except around the Fermi energy: Thus a small error (which will be calculated later on) is made if the lower bound is extended from zero to $-\infty$ in the second integral.

(ii) For the same reason, and due to the choice of the test function h, $h(\varepsilon)$ may be expanded in a power series of $(\varepsilon - \varepsilon_F)$.

(iii) With the new limits in the integral, the difference $(F - \Theta)$ being odd with respect to the variable $(\varepsilon - \varepsilon_F)$, only the odd moments of the distribution $(F - \Theta)$ are not vanishing. They are

$$\overline{(\varepsilon - \varepsilon_F)^{2n+1}} = \frac{2^{2n+1} - 1}{n+1}(\pi T)^{2n+2} \,|\, B_{2n+2} \,| , \quad (7)$$

where B_k are the Bernouilli numbers. Then

$$\langle h \rangle = \int_0^\infty d\varepsilon\, h(\varepsilon)\Theta(\varepsilon_F - \varepsilon) + \sum_n h^{(2n+1)}(\varepsilon_F)\frac{\overline{(\varepsilon - \varepsilon_F)^{2n+1}}}{(2n+1)!} . \quad (8)$$

In order to get an expansion for $F(\varepsilon)$ by comparison with Eq. (6), the derivatives $h^{(2n+1)}$ are written by means of the Dirac distribution:

$$h^{(2n+1)}(\varepsilon_F) = \int_0^\infty d\varepsilon\, h(\varepsilon)\delta^{(2n+1)}(\varepsilon_F - \varepsilon) , \quad (9)$$

which gives the low-temperature expansion:

$$F(\varepsilon) = \Theta(\varepsilon_F - \varepsilon) + \frac{\pi^2}{6}T^2\delta'(\varepsilon_F - \varepsilon) + \frac{7\pi^4}{360}T^4\delta'''(\varepsilon_F - \varepsilon) + O(T^6) . \quad (10)$$

The validity of this expansion depends on the smoothness of the function $h(\varepsilon)$, the mean value of which is to be calculated [second step in going from Eq. (6′) to Eq. (7)]: $h(\varepsilon)$ must not vary too strongly in the region around ε_F for the expansion to be rapidly converging. Thus, a first criterion for the convergency of expansion (10) is

$$h^{(2n+1)}(\varepsilon_F)/(\varepsilon_F^{2m} h^{(2n+2m+1)}) \gg 1, \quad \forall m > 0 \quad (11)$$

for $n \geq N$, where N is the maximum number of terms to be kept in the series.

On the other hand, Eq. (10) may be written with the dimensionless variables $e = \varepsilon/\varepsilon_F$ and $\eta = T/\varepsilon_F$,

$$F(e) = \Theta(1 - e) + \frac{\pi^2}{6}\eta^2\delta'(1 - e) + \frac{7\pi^4}{360}\eta^4\delta'''(1 - e) + O(\eta^6) , \quad (10')$$

which shows up a second criterion for the validity of this expansion: the width T of the region around ε_F where the difference $(F - \Theta)$ is not negligible must obey

$$\eta = T/\varepsilon_F \ll 1 . \quad (12)$$

Finally, the error introduced by replacing the lower limit by $-\infty$ [first step between Eqs. (6′) and (7)] can be evaluated:

$$\Delta h = -\int_{-\infty}^{0} d\varepsilon\, h(\varepsilon)\{[1 + \exp(\varepsilon - \varepsilon_F)/T]^{-1} - \Theta(\varepsilon_F - \varepsilon)\} . \quad (13)$$

Due to the condition (12), the difference in the bracket is equivalent to $\exp[(\varepsilon - \varepsilon_F)/T]$. Expanding again $h(\varepsilon)$ in a Taylor series around ε_F and with a relation analogous to Eq. (9), one gets the error ΔF on the Fermi distribution expanded following Eq. (10′):

$$\Delta F = e^{-1/\eta}[\eta\delta(1 - e) - \eta(1 + \eta)\delta'(1 - e) + \cdots] , \quad (14)$$

which is exponentially small as $\eta \rightarrow 0$.

We have thus obtained an expansion for the Fermi function which can be pushed to any desired order, according to the accuracy needed when calculating mean values of not too distorted functions $h(\varepsilon)$. The quality of the asymptotic expansion (10′) is fixed by the two constraints: Eq. (11) on $h(\varepsilon)$ and Eq. (12) on the temperature, and the error is measurable by ΔF [Eq. (14)]. The same method may now be used for the case of the Wigner distribution function [Eq. (5)].

II. ASYMPTOTIC EXPANSION OF THE WIGNER DISTRIBUTION FUNCTION

As previously, we are looking for an asymptotic expansion for the Wigner distribution function by means of Dirac function derivatives:

$$f(\varepsilon,\theta,\varphi)=\Theta(\varepsilon_F-\varepsilon)+\sum_{n=0}^{N} C_n(\theta,\varphi)\delta^{(n)}(\varepsilon_F-\varepsilon)\ , \tag{15}$$

where the limit N depends on the desired accuracy. The weights C_n may be obtained directly from inversion of (15):

$$C_n(\theta,\varphi)=\int_{-\infty}^{+\infty} d\varepsilon \frac{(\varepsilon-\varepsilon_F)^n}{n!}[f(\varepsilon,\theta,\varphi)-\Theta(\varepsilon_F-\varepsilon)]\ . \tag{16}$$

The Wigner function f which plays the role of the previous Fermi function is not in general an explicit function. It may be given as the inverse Laplace transform of the Bloch operator $\hat{C}^{(\beta)}=\exp[-\beta\hat{H}]$ in the phase space

$$f(\varepsilon,\theta,\varphi)=\mathcal{L}^{-1}_{\beta\to\varepsilon_F}\frac{C^{(\beta)}(\varepsilon,\theta,\varphi)}{\beta} \tag{17}$$

and now

$$C_n(\theta,\varphi)=\frac{1}{n!}\int_{-\infty}^{+\infty} d\varepsilon(\varepsilon-\varepsilon_F)^n\mathcal{L}^{-1}_{\beta\to\varepsilon_F} \times\left[\frac{C^{(\beta)}(\varepsilon,\theta,\varphi)-e^{-\beta\varepsilon}}{\beta}\right]\ . \tag{18}$$

The integrand in the inverse Laplace transform Eq. (18) is in general unknown. In order to get some preliminary insight before making any approximation for evaluating (18), the use of a simple potential, for which the exact Bloch density $C^{(\beta)}$ is available, will be chosen. This is the case for the linear potential: It will be treated as an example to follow in the same way as the Fermi function was an example in order to get Eqs. (15) and (18).

In any case, the $\delta^{(n)}$ will account for some details of the phase-space distribution close to the Fermi energy: The aim is not to reproduce them explicitly in the phase space, but to reproduce their effects when calculating mean values from the Wigner function.

A. Example of the linear potential

For the semi-infinite potential in the 3D space

$$V(\mathbf{r})=\alpha z \tag{19}$$

and constant in the direction parallel to the surface, the Bloch function is

$$C^{(\beta)}(\varepsilon)=\exp\left[-\beta\varepsilon+\frac{\beta^3}{3b^3}\right],\quad b=(8m/\hbar^2\alpha^2)^{1/3}\ . \tag{20}$$

The Wigner distribution function in the 6D-space $f(\mathbf{r},\mathbf{p})$ only depends on ε [Eq. (2)] and is an Airy function integral:[3]

$$f(\varepsilon)=\int_{b(\varepsilon-\varepsilon_F)}^{\infty} dx\ \mathrm{Ai}(x)\equiv I\mathrm{Ai}(b(\varepsilon-\varepsilon_F))\ . \tag{21}$$

For the Fermi distribution, the energy ε is restricted to positive values and the error in the low-temperature expansion stems from the extension of the integration range to negative energies [Eq. (13)]. For the Wigner distribution in a linear potential, the energy ε ranges from $-\infty$ to $+\infty$: In order to get a finite energy distribution, and also in order to approximate a finite depth V_0 to the potential, as in realistic cases, the potential energy will be limited to $V(\mathbf{r})\geq V_0$. Thus, we shall now consider the distribution function

$$f(\mathbf{r},\mathbf{p})=I\mathrm{Ai}(b(p^2/2m+\alpha z-\varepsilon_F))\Theta(\alpha z-V_0) \tag{22}$$

or

$$f(\varepsilon)=I\mathrm{Ai}(b(\varepsilon-\varepsilon_F))\Theta(\varepsilon-V_0)\ . \tag{22'}$$

It is clear that (22) is not the distribution function for a new potential which would be $V(z)=\alpha z$ if $z>z_0=V_0/\alpha$ and $V(z)=V_0$ if $z<z_0$, because the wave functions in such a potential are not simply obtained by cutting off the wave functions of the ramp potential beyond z_0. However, the limit of (22) when $V_0\to-\infty$ is (21), and everywhere in the following, this limit will give the result, eventually diverging, valid for the linear potential. The aim in defining (22) is to deal with a function which resembles realistic Wigner distributions, even if the corresponding potential is not precisely defined (at least it has a finite depth) and whose limit represents the known linear potential.

An exact calculation of the weights C_n [Eqs. (15) and (18)] is possible,

$$C_n=\sum_{k=0}^{n}\frac{(-1)^{n-k}n!}{(n-k)!(k+1)!}\frac{(\varepsilon_F-V_0)^{n-k}}{b^{k+1}} \times\{W(-b(\varepsilon_F-V_0);k+1)-[b(\varepsilon_F-V_0)]^{k+1}\} \tag{23}$$

with the function W defined by Balazs *et al.*,[4]

$$W(-y;n)=\int_{-y}^{\infty} dx(x+y)^n\mathrm{Ai}(x)\ . \tag{24}$$

By partial integrations and using the differential equation $x\mathrm{Ai}(x)=\mathrm{Ai}''(x)$, $W(-y,n)$ may be written by means of the Airy function, its first integral, and its first derivative.

Expression (23) can be simplified if the function W is replaced by its asymptotic expansion:[4]

$$W(-y;n)=y^n\left[1+\frac{\Gamma(n+1)}{3y^3\Gamma(n-2)}+O(y^{-6})\right]+\frac{1}{\pi^{1/2}}\frac{\Gamma(n+1)}{y^{(2n+3)/4}}\sin\left[\frac{2}{3}y^{3/2}-\frac{2n+1}{4}\pi\right][1+O(y^{-1})]\ . \tag{25}$$

(Higher-order terms may be obtained from the asymptotic expansions of Airy and related functions[3]). This is allowed in (23) if and only if

$$b(\varepsilon_F - V_0) \to +\infty \ . \tag{26}$$

It turns out that the actual variable in the asymptotic expansion of the Airy function $\mathrm{Ai}(x)$ is $x^{3/2}$, thus the smallness parameter is

$$\eta_0 = [b(\varepsilon_F - V_0)]^{-3/2} \ll 1 \ . \tag{27}$$

Due to (25), the asymptotic expansion of $f(\varepsilon)$ clearly splits into a smooth part f_{WK}, the subscript of which will be clarified later on, and an oscillatory part f_{oscil},

$$\lim_{\eta_0 \to 0} f(\varepsilon) = f_{\mathrm{WK}} + f_{\mathrm{oscil}} \ ,$$

$$f_{\mathrm{WK}} = \Theta(1-e) + \frac{\eta_0^2}{3}\delta''(e-1) + \frac{\eta_0^4}{18}\delta^{(5)}(e-1) + O(\eta_0^6) \ , \tag{28}$$

$$f_{\mathrm{oscil}} = -\frac{\eta_0^{3/2}}{\sqrt{\pi}} \sum_{n=0}^{5} \frac{1}{n!} \left[\sin\varphi_0 + (n - \tfrac{101}{48})\eta_0 \cos\varphi_0 - \left[\frac{35\,905}{4608} - \frac{233n}{48} + n^2 \right] \eta_0^2 \sin\varphi_0 \right] \delta^{(n)}(e-1) + O(\eta_0^{9/2}) \ ,$$

with

$$e = \frac{\varepsilon - V_0}{\varepsilon_F - V_0} \quad \text{and} \quad \varphi_0 = \frac{2}{3\eta_0} + \frac{\pi}{4} \ . \tag{29}$$

Note that even in the limit $\eta_0 \to 0$, $\sin\varphi_0$ and $\cos\varphi_0$ are finite. From Eq. (28) η_0 appears to be the convergence parameter, equivalent to $\eta = T/\varepsilon_F$ [Eq. (12)] for the Fermi distribution. Moreover, η_0 [Eq. (27)] also reads

$$\eta_0 = \hbar\alpha / [(8m)^{1/2}(\varepsilon_F - V_0)^{3/2}] \ll 1 \tag{29'}$$

and expansion (28) is at the same time an $\hbar$ expansion, the physical meaning of which is now clear: The slope α of the potential must be not too steep, for the expansion to converge.

Contrary to what was the case for the Fermi function, no change in the integration limit has been done and the only approximation in (28) lies in the limited number of terms in the asymptotic series for W. On the other hand, the oscillatory part is not a negligible correction and it may overcome the smooth part: Its contribution has to be considered[5] before being eventually neglected in the calculations of mean values.

An illustration of the role of the criterion (27) may be shown if the distribution function (22) is written by means of the convergence parameter η_0:

$$f(e) = I\,\mathrm{Ai}((e-1)\eta_0^{-2/3})\Theta(e) \ . \tag{30}$$

If $\eta_0 \ll 1$, the argument has almost always a very large modulus, even for $\varepsilon \sim \varepsilon_F$ ($e \sim 1$): The oscillations are concentrated close to the Fermi energy, as compared to the case $\eta_0 \sim 1$. This is schematically shown in Fig. 2. The expansion (28) of the Wigner function will be a better representation of the Airy function integral in the case of curve a than of curve b of Fig. 2. Expression (28) is now to be compared to the usual Wigner-Kirkwood expansion [Eq. (5)].

For a finite value $(\varepsilon_F - V_0)$ of the Fermi energy above the minimum of the energy scale, the criterion (26) allows expansion of the Bloch function Eq. (20) in powers of b^{-1}:

$$C^{(\beta)}(\varepsilon) = e^{-\beta\varepsilon} \left[1 + \frac{\hbar^2\alpha^2}{8m}\frac{\beta^3}{3} + \frac{1}{2!}\left[\frac{\hbar^2\alpha^2}{8m}\right]^2 \frac{\beta^6}{9} + O(\hbar^6) \right] \ . \tag{31}$$

By a formal inverse Laplace transform of $C^{(\beta)}/\beta$ with

$$\mathcal{L}^{-1}_{\beta \to \varepsilon_F} \left[\beta^n \frac{e^{-\beta\varepsilon}}{\beta} \right] = \frac{d^m}{d\varepsilon_F^m}\Theta(\varepsilon_F - \varepsilon) \ , \tag{32}$$

then, with the same condition $\eta_0 \ll 1$, only the first part of $f(\varepsilon)$ [Eq. (28)] is obtained, and the term f_{oscil} is missing. Thus the asymptotic expansion for the Wigner distribution consists in the Wigner-Kirkwood part f_{WK}

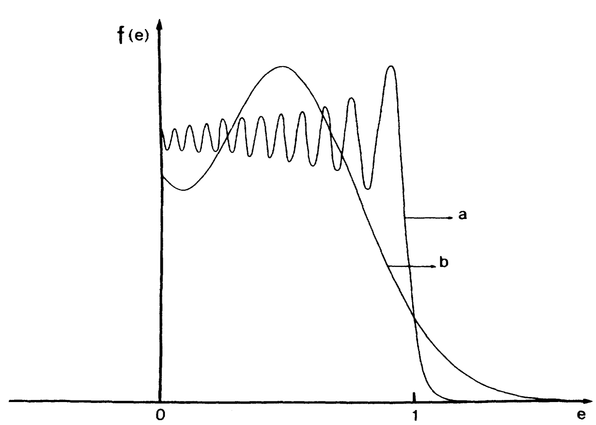

FIG. 2. Comparison between the exact distribution functions [Eq. (30)] corresponding to $\eta_0 \sim 0.1$ (curve a) and $\eta_0 \sim 1$ (curve b) as a function of the dimensionless energy variable e [Eq. (29)].

(the subscript of which is now clear) plus an oscillatory contribution: The latter measures the error when only the Wigner-Kirkwood series is taken into account.

The Wigner-Kirkwood part of the expansion may be obtained directly (and this method will be used for a more general potential) if, in the coefficients C_n [Eq. (18)] which now read

$$C_n = \frac{1}{n!}\int_{V_0}^{\infty} d\varepsilon(\varepsilon-\varepsilon_F)^n \frac{1}{2i\pi} \times \int_{c-i\infty}^{c+i\infty} d\beta\, e^{-\beta(\varepsilon-\varepsilon_F)} \frac{e^{\beta^3/3b^3}-1}{\beta} , \tag{33}$$

the β integration is performed along the imaginary axis ($\beta = it$, because no pole in β) and the ε integration is performed first with

$$\int_{V_0}^{\infty} d\varepsilon(\varepsilon-\varepsilon_F)^n e^{-it(\varepsilon-\varepsilon_F)} \sim 2\pi i^n \delta^{(n)}(t) . \tag{34}$$

From the previous study, it is now known that the series obtained by this method converges only if $\eta_0 \ll 1$ and that the error is the oscillatory part f_{oscil} [Eq. (28)] which is here neglected and which represents the approximation (34).

As an application, a "surface energy" may be defined:

$$\langle \varepsilon_S \rangle = \int d^3\mathbf{r} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \left[\frac{p^2}{2m} + \alpha z\right] \times [f(\mathbf{r},\mathbf{p}) - \Theta(\varepsilon_F - p^2/2m - \alpha z)] , \tag{35}$$

where the bulk phase-space density, represented by the step function in the bracket, is subtracted. $\langle \varepsilon_S \rangle$ is also the first moment of a "surface-energy distribution" $g_S(\varepsilon)$ obtained from the phase-space distribution function f after changes of variables:

$$f(\mathbf{r},\mathbf{p})d^3\mathbf{r}\frac{d^3\mathbf{p}}{(2\pi\hbar)^3} = \frac{1}{(2\pi\hbar)^3} f(\varepsilon)dx\, dy \frac{dV}{\alpha} m\, d\varepsilon\, d\varphi_{\parallel}\, dp_{\perp} \tag{36}$$

and integration over all variables except ε, giving

$$g_S(\varepsilon) = \frac{S}{(2\pi)^2}\frac{2}{3\alpha}k_F^3 \left[\frac{\varepsilon - V_0}{\varepsilon_F - V_0}\right]^{3/2} [f(\varepsilon) - \Theta(\varepsilon_F - \varepsilon)] \tag{37}$$

and

$$\langle \varepsilon_S \rangle = \int_{V_0}^{\infty} d\varepsilon\, \varepsilon g_S(\varepsilon) \tag{38}$$

by means of the Fermi momentum $k_F = [2m(\varepsilon_F - V_0)/\hbar^2]^{1/2}$ and the (infinite) surface S of the medium. The exact solution is

$$\langle \varepsilon_s \rangle_{\text{exact}} = \frac{S}{(2\pi)^2}\frac{2}{3\alpha}k_F^7 \eta_0^{7/3} \times \left[\tfrac{2}{7}W(-\eta_0^{-2/3};\tfrac{7}{2}) + \frac{2}{5}\frac{v_0}{\eta_0^{2/3}}W(-\eta_0^{-2/3};\tfrac{5}{2}) - \tfrac{2}{35}(5+7v_0)\right] , \tag{39}$$

with v_0 defined like e by $v_0 = V_0/(\varepsilon_F - V_0)$.

An asymptotic expansion for $g_S(\varepsilon)$ may be obtained in the same way as for $f(\varepsilon)$ [Eq. (15)],

$$g_S(\varepsilon) = \frac{S}{(2\pi)^2}\frac{2}{3\alpha}\left[\frac{2m}{\hbar^2}\right]^{3/2} \sum_n \frac{D_n}{n!}\delta^{(n)}(\varepsilon_F - \varepsilon), \tag{40}$$

and up to η_0^4 (or equivalently $\hbar^4$) order:

$$g_S(\varepsilon) = \frac{S}{(2\pi)^2}\frac{1}{6\alpha}k_F^3\eta_0^2 \left\{ \sum_{n=0}^{5} [(1-5n) - \tfrac{5}{16}(1+n)\eta_0^2] \frac{\delta^{(n)}(e-1)}{n!} + 3\eta_0 \sum_{n=0}^{5} \left[\cos\left[\frac{2}{3\eta_0}\right] - \frac{5n}{2}\eta_0 \sin\left[\frac{2}{3\eta_0}\right]\right] \frac{\delta^{(n)}(e-1)}{n!} + O(\eta_0^5) \right\} . \tag{41}$$

The semiclassical surface energy is then

$$\langle \varepsilon_S \rangle_{\text{semicl}} = \frac{S}{(2\pi)^2}\frac{1}{6\alpha}\left[\frac{\hbar^2}{2m}\right]^2 k_F^7\eta_0^2 \left[5 + v_0 + \frac{\eta_0^2}{16}(5-5v_0) + 3\eta_0 v_0 \cos\left[\frac{2}{3\eta_0}\right] + \tfrac{15}{2}\eta_0^2 \sin\left[\frac{2}{3\eta_0}\right] + O(\eta_0^5)\right] , \tag{42}$$

which is exactly the limit when $\eta_0 \to 0$ of the exact result [Eq. (39)].

If instead of expanding g_S, the previous expansion of $f(\varepsilon)$ is used in Eq. (37), the asymptotic condition $\eta_0 \to 0$ is not taken into account in $e^{3/2}$ and the accuracy is weaker because $\langle \varepsilon_S \rangle$ is an exact moment of the distribution g_S and not of $(e^{3/2}f)$: The Wigner-Kirkwood contribution in $\langle \varepsilon_S \rangle$ is unchanged but the oscillatory part is slightly different.

Numerically, for realistic values,

$$V_0 = -50 \text{ MeV}, \quad \varepsilon_F = -8 \text{ MeV}, \quad \alpha = 20 \text{ MeV } fm^{-1} . \tag{43}$$

then $\eta_0 \simeq 0.2$ and the η_0^4 contribution is about 2.10^{-3} times the η_0^2 contribution to the "surface energy," showing the high convergence of the Wigner-Kirkwood series. However, the oscillatory contribution is about 10% of the η_0^2 one and is not always negligible:[5] It actually strongly depends on η_0 and these terms have to be evaluated carefully.

The local density $\rho(z)$ and the momentum distribution $n(p)$, both in a three-dimensional space, are obtained from the Wigner distribution [Eq. (22)] by integration over **p** and **r**, respectively:

$$\lim_{\eta_0\to 0}\rho(z)=\frac{m\alpha}{6\pi^2\hbar^2}t^{-1}\Theta(\varepsilon_F-\alpha z)\Theta(\alpha z-V_0)$$

$$\times\left\{1-\tfrac{1}{8}t^2+\tfrac{35}{128}t^4+\cdots-\tfrac{3}{2}t^{2/3}\frac{\eta_0^{5/6}}{\sqrt{\pi}}\sin\left[\frac{2}{3\eta_0}+\frac{\pi}{4}\right]\left[1-\sum_{n=1}^{5}\frac{1.3\cdots(2n-3)}{2^n n!}\left[\frac{t}{\eta_0}\right]^{2n/3}\right]+O(\eta_0^{3/2})\right\},$$

$$\lim_{\eta_0\to 0}n(p)=\frac{S}{\alpha}\left[\frac{\hbar^2\alpha^2}{8m}\right]^{1/3}u^{-2/3}\Theta\left[\varepsilon_F-\frac{p^2}{2m}-V_0\right]\left[1-u^{2/3}\frac{\eta_0^{5/6}}{\sqrt{\pi}}\sin\left[\frac{2}{3\eta_0}+\frac{\pi}{4}\right]+O(\eta_0^{3/2})\right],$$

$$t=t(z)=[b(\varepsilon_F-\alpha z)]^{-3/2},\quad u=u(p)=\left[b\left[\varepsilon_F-\frac{p^2}{2m}-V_0\right]\right]^{-3/2}. \tag{44}$$

It may be noted that the only dependence on **p** in $n(p)$ is quadratic, in the Wigner-Kirkwood term.

In spite of negative powers of η_0 in the sum entering the oscillatory contribution to $\rho(z)$, the expansion does not diverge because $\eta_0\to 0$ means $\alpha/(\varepsilon_F-V_0)\to 0$ or $\alpha\to 0$ because V_0 has been chosen finite on purpose. Then $(t/\eta_0)^{2/3}=(\varepsilon_F-V_0)/\varepsilon_F$ is finite. The same is not true for a really linear potential ($V_0\to-\infty$) for which the local density is infinite.

If the same functions were calculated from the exact Wigner distribution

$$\rho(z)=\frac{m\alpha}{6\pi^2\hbar^2}W(-b(\varepsilon_F-\alpha z);\tfrac{3}{2}),$$
$$n(p)=\frac{S}{\alpha}\left[\frac{\hbar^2\alpha^2}{8m}\right]^{1/3}W\left[-b\left[\varepsilon_F-\frac{p^2}{2m}-V_0\right];1\right], \tag{45}$$

and asymptotically expanded, the Wigner-Kirkwood contributions are the same as the semiclassical ones [Eq. (44)], but the oscillatory parts are different. The conditions for the asymptotic expansions of the exact densities (45) are, respectively, $t(z)\to 0$ and $u(p)\to 0$, but, for the semiclassical $\rho(z)$ and $n(p)$ they are $\eta_0\to 0$ and, respectively, $V(z)<\varepsilon_F$ and $p^2/2m<\varepsilon_F-V_0$, which is less restrictive. Thus the Wigner-Kirkwood expansion which is usually regarded as an $\hbar^2$ series is actually an η_0^2 series, which constraints the slope of the linear potential to not too large values.

As compared to the Fermi function expansion, the Wigner function expansion shows up some details of the shape: for example, the Fermi function being symmetrical around ε_F, its expansion contains only odd derivatives of $\delta(\varepsilon_F-\varepsilon)$, opposed to the Wigner function which is asymmetric around ε_F (Fig. 1) and for which, consequently, the first derivative of δ is missing. On the other hand, the correction to the Wigner-Kirkwood expansion is no longer exponentially decreasing with the convergence parameter, but it is an oscillation damped by η_0. All these results must now be extended to the case of a more realistic potential.

B. Case of a general local potential

As previously shown, the Wigner-Kirkwood expansion for the Bloch density,

$$C^{(\beta)}(\varepsilon,\theta,\varphi)=e^{-\beta\varepsilon}\left[1+\sum_{k=2}^{6}K_k(\varepsilon,\theta,\varphi)\beta^k\right]+O(\hbar^6), \tag{46}$$

the coefficients of which are given in Appendix A, may be used only if a condition analogous to Eq. (27) ($\eta_0\to 0$) is fulfilled.

For a general local potential $V(\mathbf{r})=V(z)$, the slope $V'(z)$ replaces the constant α of the linear potential in the definition (27) of the smallness parameter:

$$\eta(z)=\left[\left[\frac{8m}{\hbar^2}\frac{1}{V'^2(z)}\right]^{1/3}(\varepsilon_F-V_0)\right]^{-3/2}\ll 1. \tag{47}$$

For a smoothly increasing potential, like the Woods-Saxon one, $V'(z)$ has its largest value at the inflexion point z_0 and the convergence criterion now means

$$V'(z_0)\ll\left[\frac{8m}{\hbar^2}\right]^{1/2}(\varepsilon_F-V_0)^{3/2}. \tag{48}$$

The criterion for the convergence of the semiclassical expansion may be compared to the WKB constraint:

$$\eta_{\rm WKB}(\varepsilon,z)=\left[\left[\frac{8m}{\hbar^2}\frac{1}{V'^2(z)}\right]^{1/3}(\varepsilon-V)\right]^{-3/2}\ll 1, \tag{49}$$

which also reads

$$V'(z_0)\ll\left[\frac{8m}{\hbar^2}\right]^{1/2}(\varepsilon-V_0)^{3/2} \tag{50}$$

and (48) turns out to be a particular case of the WKB constraint, namely, $\varepsilon=\varepsilon_F$. Thus, if the condition for the WKB approximation to be valid is fulfilled, then the semiclassical one is fulfilled. On the opposite, the semiclassical condition does not imply any special range for the energy and therefore it is less severe than the WKB condition.

Forgetting for a while oscillatory terms, the weights C_n [Eq. (18)] of the $\delta^{(n)}(\varepsilon_F-\varepsilon)$ are calculated using the way of Eqs. (33) and (34):

$$C_n=\sum_{k=n}^{5}\frac{k!}{(n-k)!}K_{k+1}^{(k-n)}(\varepsilon_F,\theta,\varphi), \tag{51}$$

where the upper limit $k=5$ accounts for up to $\hbar^4$ order. Then

$$f(\varepsilon,\theta,\varphi)=\Theta(\varepsilon_F-\varepsilon)+\sum_{n=0}^{5}\left[\sum_{k=n}^{5}\binom{k}{n}K_{k+1}^{(k-n)}(\varepsilon_F,\theta,\varphi)\right]\times\delta^{(n)}(\varepsilon_F-\varepsilon)+O(\hbar^6)\ . \tag{52}$$

The derivatives of K_k are taken with respect to ε_F.

In order to calculate the oscillatory correction f_{oscil}, the approximated Bloch function (46) is partially resummed to look like the one which was already studied:

$$C^{(\beta)}(\varepsilon,\theta,\varphi)=\exp\left[-\beta\varepsilon+(\hbar^2\beta^3/24m)(V')^2\right]\times\left[1+\sum_{k=2}^{6}M_k(\varepsilon,\theta,\varphi)\beta^k\right]+O(\hbar^6)\ , \tag{53}$$

where the M_k are easily derived from the K_k (Appendix A).

It is known from the linear potential study that the asymptotic expansion is valid if the variable in the function W [Eq. (23)], which is now $\eta(z)^{-2/3}$, is very large—that means when $V'(z)\sim 0$. But in this case, the coefficients K_k and thus M_k are very small, because they all contain the derivatives of the potential and the sum in (53) plays the role of a correction to the linearized potential. If, on the other hand, the oscillatory part is considered like a correction to the Wigner-Kirkwood terms, the sum in (53) will bring only second-order oscillatory corrections, due to the weakness of the weights M_k.

The main approximation in the Wigner function [Eq. (50)] is therefore written as f_{oscil} [Eq. (28)] but with η_0 replaced by $\eta(z)$ [Eq. (47)].

C. Example: The Woods-Saxon potential

For this potential, in the 3D space:

$$V(\mathbf{r})=V_0[1+\exp(z-z_0)/a]^{-1}\ , \tag{54}$$

the criterion (48) for the validity of the Wigner-Kirkwood expansion connects the depth V_0 and the diffuseness a by

$$-V_0/a \ll 4\left[\frac{8m}{\hbar^2}\right]^{1/2}(\varepsilon_F-V_0)^{3/2}\ . \tag{55}$$

Defining a potential surface width Δ_S by

$$V'(z_0)=-V_0/\Delta_S\ , \tag{56}$$

with $\Delta_s=4a$ in the present case, the convergence parameter is ($p_F=\hbar k_F$)

$$\eta_0=\frac{\hbar}{\Delta_S p_F}\frac{V_0}{2(\varepsilon_F-V_0)}\ll 1\ . \tag{57}$$

For the numerical values already used with the ramp potential ($V_0=-50$ MeV and $\varepsilon_F=-8$ MeV) this leads to $a \gg 0.1$ fm, and the usual value $a\simeq 0.6$ fm obeys this condition, giving $\eta_0\sim 0.2$. In general, $V_0/(\varepsilon_F-V_0)\sim 1$ and hence the $\hbar^2$ correction to the Thomas-Fermi approximation will be proportional to $(\Delta_S k_F)^{-2}\sim 0.1$.

On the other hand, all derivatives $V^{(n)}$ can be written by means of the potential V and the first derivative $V'(z)$ factorizes in all coefficients M_k as in coefficients K_k (see Appendix A): They vanish at least as quickly as $V'(z)$ if $\eta(z)\ll 1$ and the correction Δf will mainly be due to the leading term in the Bloch density, as previously mentioned.

After a straightforward but tedious replacement of the derivatives of K_k in Eq. (52), the weights $C_n\ (\theta,\varphi)$ of the $\delta^{(n)}(\varepsilon_F-\varepsilon)$ are obtained: They are given in Appendix B for the $\hbar^2$ contribution. Actually, they have been computed and are available up to $\hbar^4$ order for any local half-infinite potential $V(z)$.

Due to the fact that the potential only depends on z, the phase-space distribution $f(\mathbf{r},\mathbf{p})$ in the 6D-space actually depends on three variables, as previously.

For the Woods-Saxon potential, the variables ε, $V(z)$, and $p_\perp$ are the most convenient because V and $p_\perp$ naturally arise in K_k, which are moreover independent of ε. Hence

$$f(\varepsilon,V,p_\perp)=\Theta(\varepsilon_F-\varepsilon)+\sum_{k=1}^{5}K_{k+1}(V,p_\perp)\delta^{(k)}(\varepsilon_F-\varepsilon)+O(\hbar^6)\ . \tag{58}$$

The surface-energy distribution function equivalent to (37) is now

$$g_S(\varepsilon)=\frac{S}{(2\pi)^2}\frac{m}{\hbar^3}\times\int_{V_0}^{\varepsilon}\frac{dV}{V'}\int_{-\sqrt{2m(\varepsilon-V)}}^{+\sqrt{2m(\varepsilon-V)}}dp_\perp[f(\varepsilon,V,p_\perp)-\Theta(\varepsilon_F-\varepsilon)]\ . \tag{59}$$

Its asymptotic expansion is obtained from Eq. (58), up to η_0^4:

$$g_S(\varepsilon)=\frac{m}{2\pi^2\hbar^2}k_F e^{1/2}\frac{32aS}{15v_0^3}\eta_0^2[A+B\eta_0^2+O(\eta_0^4)]\ , \tag{60}$$

with

$$A=\sum_{n=1}^{2}a_n(e)\delta^{(n)}(e-1)\ ,$$

$$B=\sum_{n=2}^{5}b_n(e)\delta^{(n)}(e-1)\ .$$

a_n and b_n are given in Appendix C, and S is the (infinite) surface. It gives for the surface energy previously defined [Eq. (38)]:

$$\langle\varepsilon_s\rangle=-\frac{4aS}{45\pi^2}\frac{\hbar^2}{2m}\frac{k_F^5}{v_0^3}\eta_0^2\times\left[12+25v_0+15v_0^2+\frac{8}{35}\frac{\eta_0^2}{v_0^4}(320+784v_0+560v_0^2+35v_0^3-35v_0^4)\right]. \tag{61}$$

For the numerical values previously used ($V_0=-50$ MeV, $\varepsilon_F=-8$ MeV, $a=0.6$ fm), the nonoscillatory η_0^4 term gives about 5.10^{-2} times the contribution of the η_0^2 term, which is much larger (~ 20 times) than for the linear potential.

However, the $\eta_0^3\cos\frac{2}{3}\eta_0$ and $\eta_0^4\sin\frac{2}{3}\eta_0$ [Eq. (40)] terms may reach, respectively, up to 12% and 0.5% the η_0^2 (or $\hbar^2$) contribution. This shows that the Wigner-Kirkwood expansion, or the partially resummed series, are accurate if the $\hbar^2$ correction is already very small and gives the mean energy with a good accuracy.

III. CONCLUSION

The Wigner-Kirkwood expansion of the phase-space distribution function was obtained in a way which differs from the usual ones. The method closely follows the derivation of the low-temperature expansion of the Fermi function, and thereby exhibits analogies and differences, with $\hbar$ playing now the role of the temperature. As a first example, the Wigner distribution function for the half-infinite Fermion matter bounded by a linear potential, which is an analytically solvable model, is investigated. Hence, oscillating terms are found to correct the usual Wigner-Kirkwood expansion, the meaning and the convergence properties of which are clarified. The same technique is then applied to a Woods-Saxon potential and a smallness parameter $\eta\sim\hbar/(\Delta_S p_F)$, where Δ_S is the surface thickness of the potential and p_F the Fermi momentum, is found to explain the rapid convergence of the Wigner-Kirkwood series for average nuclear binding energies. The expansion is actually a $\hbar^2$ (or equivalently a η^2) series and realistic values for the nuclear case give $\eta^2\simeq 0.1$: This confirms earlier empirical findings that the contribution of each higher order is smaller than the previous one by an order of magnitude.[6]

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APPENDIX A

The Bloch function $C^{(\beta)}(\mathbf{r},\mathbf{p})$ for a spherical local potential $V(\mathbf{r})=V(|r|)$ is, up to $\hbar^4$ order

$$C^{(\beta)}(\mathbf{r},\mathbf{p})=\exp\left[-\beta\left[\frac{p^2}{2m}+V\right]\right]\left[1+\sum_{k=2}^{6}K_k(\mathbf{r},\mathbf{p})\beta^k\right]+O(\hbar^6)\ ,$$

with

$$K_2=-\frac{\hbar^2}{8m}\Delta V\ ,$$

$$K_3=\frac{\hbar^2}{24m}\left[(\nabla V)^2+m\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2 V\right]-\frac{\hbar^4}{128m^2}\Delta^2 V\ ,$$

$$K_4=\frac{\hbar^4}{384m^2}\left[3(\Delta V)^2+2\nabla V\cdot\nabla\Delta V+\Delta(\nabla V)^2+2m\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2\Delta V\right]\ ,$$

$$K_5=-\frac{\hbar^4}{1920m^2}\left\{10\Delta V(\nabla V)^2+10m\,\Delta V\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2 V+4m\nabla V\cdot\nabla\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2 V\right.$$
$$\left.+8m\left[\nabla\left[\frac{\mathbf{p}}{m}\cdot\nabla V\right]\right]^2+m^2\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^4 V+4\nabla V\cdot\nabla(\nabla V)^2\right\}\ ,$$

$$K_6=\frac{\hbar^4}{1152m^2}\left[(\nabla V)^2+m\left[\frac{\mathbf{p}}{m}\cdot\nabla\right]^2 V\right]^2\ .$$

For the semi-infinite Woods-Saxon potential,

$$V=V_0\left[1+\exp\left[\frac{z-z_0}{a}\right]\right]^{-1},\quad V'=\frac{V}{a}\left[\frac{V}{V_0}-1\right]\ ,$$

$$K_2=-\frac{\hbar^2}{8m}\frac{V'}{a}\left[2\frac{V}{V_0}-1\right]\ ,$$

$$K_3=\frac{\hbar^2}{24m}V'\left[V'+\frac{p_\perp^2}{ma}\left[2\frac{V}{V_0}-1\right]\right]-\frac{\hbar^4}{128m^2}\frac{V'}{a^3}\left[24\frac{V^3}{V_0^3}-36\frac{V^2}{V_0^2}+14\frac{V}{V_0}-1\right],$$

$$K_4=\frac{\hbar^4}{384m^2}\frac{V'}{a^2}\left[V'\left[44\frac{V^2}{V_0^2}-44\frac{V}{V_0}+9\right]+2\frac{p_\perp^2}{ma}\left[24\frac{V^3}{V_0^3}-36\frac{V^2}{V_0^2}+14\frac{V}{V_0}-1\right]\right],$$

$$K_5=-\frac{\hbar^4}{1920m^2}\frac{V'}{a}\left[18V'^2\left[2\frac{V}{V_0}-1\right]+2\frac{V'}{a}\frac{p_\perp^2}{m}\left[48\frac{V^2}{V_0^2}-48\frac{V}{V_0}+11\right]+\frac{p_\perp^4}{m^2a^2}\left[24\frac{V^3}{V_0^3}-36\frac{V^2}{V_0^2}+14\frac{V}{V_0}-1\right]\right],$$

$$K_6=\frac{\hbar^4}{1152m^2}V'^2\left[V'+\frac{p_\perp^2}{ma}\left[2\frac{V}{V_0}-1\right]\right]^2.$$

Writing $C^{(\beta)}$ with a partial resummation,

$$C^{(\beta)}(\mathbf{r},\mathbf{p})=\exp\left[-\beta\left[\frac{p^2}{2m}+V\right]+\frac{\hbar^2}{24m}\beta^3V'^2\right]\left[1+\sum_{k=2}^{6}M_k(\mathbf{r},\mathbf{p})\beta^k\right]+O(\hbar^6),$$

gives

$$M_2=K_2,\quad M_3=K_3-\frac{\hbar^2}{24m}V'^2,\quad M_4=K_4,$$

$$M_5=K_5,\quad M_6=\frac{\hbar^4}{1152m^2}V'^2\left[\frac{p_\perp^2}{ma}\left[2\frac{V}{V_0}-1\right]\right]^2.$$

APPENDIX B

The weights C_n of the $\delta^{(n)}(\varepsilon_F-\varepsilon)$ in Eq. (15) are [Eq. (51)]

$$C_n=\sum_{k=n}^{5}\frac{k!}{(k-n)!}K_{k+1}^{(k-n)}(\varepsilon_F,\theta,\varphi)$$

and their $\hbar^2$ contribution for a Woods-Saxon potential is given by means of the angles θ and φ such as

$$\tan\theta=\frac{V(z)}{p^2/2m},\quad \tan\varphi=\frac{p_\parallel}{p_\perp},$$

by

$$C_0=\frac{\hbar^2}{24m}\frac{1}{a^2(1+\cot\theta)}\left[(6\lambda_F^2+6\lambda_F+1)\left[\frac{2}{1+\cot\theta}-3\right]+\frac{4\cos^2\varphi}{1+\tan\theta}(12\lambda_F^2+9\lambda_F+1)\right],$$

$$C_1=\frac{\hbar^2}{24m}\frac{\varepsilon_F}{a^2(1+\cot\theta)}\left[(2\lambda_F^2+3\lambda_F+1)\left[\frac{4}{1+\cot\theta}-3\right]+\frac{4\cos^2\varphi}{1+\tan\theta}(8\lambda_F^2+9\lambda_F+2)\right],$$

$$C_2=\frac{\hbar^2}{12m}\frac{\varepsilon_F^2}{a^2(1+\cot\theta)}\left[(\lambda_F+1)^2\frac{1}{1+\cot\theta}+\frac{2\cos^2\varphi}{1+\tan\theta}(2\lambda_F^2+3\lambda_F+1)\right],$$

with $\lambda_F=\varepsilon_F/[V_0(1+\cot\theta)]$ and $C_n=O(\hbar^4)$ if $n\geq 3$.

APPENDIX C

The surface-energy distribution function for a Woods-Saxon potential is, up to $\hbar^4$ order,

$$g_S=\frac{m}{\hbar^2}\frac{k_F}{2\pi^2}e^{1/2}\frac{32aS}{15v_0^3}\eta_0^2[A+B\eta_0^2+O(\eta_0^4)],$$

$$A=e(4e+5v_0)\delta'(e-1)+\frac{4e^2}{21}(4e+7v_0)\delta''(e-1),$$

$$B=-\frac{8}{7v_0^4}\left\{e(128e^3+288e^2v_0+196ev_0^2+35v_0^3)\delta''(e-1)+\frac{2e^2}{99}(3584e^3+9856e^2v_0+8844ev_0^2+2541v_0^3)\delta'''(e-1)\right.$$
$$+\frac{4e^3}{19\,305}(56\,448e^3+183\,456e^2v_0+203\,060ev_0^2+78\,507v_0^3)\delta^{(4)}(e-1)$$
$$\left.+\frac{8e^4}{57\,915}(3968e^3+14\,880e^2v_0+19\,500ev_0^2+9295v_0^3)\delta^{(5)}(e-1)\right\}.$$

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