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Kirzhnits gradient expansion for a *D*-dimensional Fermi gas

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Abstract

For an ideal D-dimensional Fermi gas under generic external confinement we derive the correcting coefficient $(D-2)/3D$ of the von Weizsacker term in the kinetic energy density. To obtain this coefficient we use the Kirzhnits semiclassical expansion of the number operator up to the second order in the Planck constant $\hbar$. Within this simple and direct approach, we determine the differential equation of the density profile and the density functional of the Fermi gas. In the case $D = 2$, we find that the Kirzhnits gradient corrections vanish to all order in $\hbar$.

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1. Introduction

At ultra-low temperatures macroscopic effects of quantum statistics are observable with bosonic vapors of neutral alkali–metal atoms [1, 2]. In the last few years quantum degeneracy has also been achieved with fermionic atoms [3–7]. For fermions, it has been predicted that a reduced dimensionality strongly modifies density profiles [8–11], collective modes [12] and stability of mixtures [13, 14]. In all these papers a Thomas–Fermi–von Weizsäcker density functional approach is used [15, 16].

Some years ago, Holas, Kozlowski and March [17] derived for a D-dimensional ideal Fermi gas a correcting coefficient to the von Weizsacker term in the kinetic energy density. They used a response-function approach based on the knowledge of the static susceptibility in a D-dimensional space [18]. The aim of this paper is to recover the result of [17] by using the Kirzhnits semiclassical expansion of the number operator [19]. We shall show that the Kirzhnits expansion in powers of $\hbar$ is a direct and simple approach to get the density profile and the energy of a D-dimensional ideal Fermi gas under generic external confinement.

2. Thomas–Fermi–von Weizsacker formulation

For an ideal D-dimensional spin-polarized Fermi gas in a hypercubic box of side L, the number of particles at zero temperature is given by

$$N = \int \frac{\mathrm{d}^D\mathbf{r}\,\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\Theta\left(\bar{\mu} - \frac{p^2}{2m}\right), \tag{1}$$

where $\Theta(x)$ is the Heaviside step function. The chemical potential $\bar{\mu}$, which is the Fermi energy, fixes the number of particles N. Into the formula we have substituted the discrete summation over box quantum numbers with the $2D$-dimensional integral over single-particle phase-space variables $(\mathbf{r}, \mathbf{p})$. This approximation becomes exact in the limit $L, N \to \infty$ and $n = N/L^D$ constant.

One can easily integrate over $\mathbf{r}$ and $\mathbf{p}$ in equation (1) and finds the following expression for the uniform density:

$$n = \left(\frac{m}{2\pi\hbar^2}\right)^{D/2}\frac{D}{2\Gamma\left(\frac{D}{2}+1\right)}F_D(\bar{\mu}), \tag{2}$$

where

$$F_D(\bar{\mu}) = \int_0^\infty \mathrm{d}y\, y^{D/2-1}\Theta(\bar{\mu}-y) = \frac{2}{D}\bar{\mu}^{D/2} \tag{3}$$

measures the number of states with the energy less than or equal to μ.

In many papers the inclusion of an external potential $U(\mathbf{r})$ is treated within the so-called local-density approximation, i.e. by simply using a local chemical potential

$$\mu(\mathbf{r}) = \bar{\mu} - U(\mathbf{r}) \tag{4}$$

in equation (2), which becomes

$$n(\mathbf{r}) = \left(\frac{m\mu(\mathbf{r})}{2\pi\hbar^2}\right)^{D/2}\frac{1}{\Gamma\left(\frac{D}{2}+1\right)}. \tag{5}$$

This expression of the local density $n(\mathbf{r})$ can be obviously obtained from equation (1) by inserting into it equation (4) and integrating over momenta $\mathbf{p}$. Equation (5), also called the Thomas–Fermi formula of the density profile[15], can be written in the following form,

$$\frac{2\pi\hbar^2}{m}\Gamma\left(\frac{D}{2}+1\right)^{2/D} n(\mathbf{r})^{2/D} + U(\mathbf{r}) = \bar{\mu} \tag{6}$$

to make explicit the dependence of the chemical potential $\bar{\mu}$ on the local density $n(\mathbf{r})$. It is important to stress that equation (5), and also equation (6), is semiclassical because it is derived by neglecting the fact that in quantum mechanics the kinetic operator $\hat{T} = -\hbar^2\nabla^2/(2m)$ and the operator $\hat{\mu} = \mu(\mathbf{r}) = \bar{\mu} - U(\mathbf{r})$ do not commute. Historically, it was von Weizsäcker [16] the first to introduce a gradient correction (in the case $D = 3$), which takes into account phenomenologically the increase of kinetic energy due spatial variation of the density. Including the gradient correction of von Wiezsäcker in equation (6) one has

$$\frac{\hbar^2}{2m}\left[\frac{1}{4}\frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})^2} - \frac{1}{2}\frac{\nabla^2 n(\mathbf{r})}{n(\mathbf{r})}\right] + \frac{2\pi\hbar^2}{m}\Gamma\left(\frac{D}{2}+1\right)^{2/D} n(\mathbf{r})^{2/D} + U(\mathbf{r}) = \bar{\mu}. \tag{7}$$

Remarkably, the gradient correction of von Weizsäcker does not depend on the dimensionality of the system, as shown in [17].

3. Kirzhnits gradient expansion

Let us now consider a full quantum-mechanical treatment. In quantum mechanics the number operator is

$$\hat{N} = \Theta(\hat{\mu} - \hat{T}). \tag{8}$$

The exact local density $n(\mathbf{r})$ can be written by using the number operator $\hat{N}$, the eigenstate $|\mathbf{r}\rangle$ of the position operator and the eigenstate $|\mathbf{p}\rangle$ of the momentum operator in the following way:

$$n(\mathbf{r}) = \langle \mathbf{r}|\hat{N}|\mathbf{r}\rangle = \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^{D/2}} \langle \mathbf{r}|\hat{N}|\mathbf{p}\rangle \, \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}, \tag{9}$$

where the last expression has been obtained by inserting the completeness

$$\int \mathrm{d}^D\,\mathbf{p}|\mathbf{p}\rangle\langle\mathbf{p}| = 1, \tag{10}$$

and the formula $\langle \mathbf{p}|\mathbf{r}\rangle = \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}/(2\pi\hbar)^{D/2}$. According to Kirzhnits [19, 20], one can expand the operator $\hat{N}$ at the second order of $\hbar$ in the following way:

$$\begin{aligned}\hat{N}|\mathbf{p}\rangle = \Theta(\hat{\mu} - \hat{T})|\mathbf{p}\rangle = \Theta(\hat{\mu} - T)|\mathbf{p}\rangle + \tfrac{1}{2}\Theta''(\hat{\mu} - T)[\hat{\mu}, \hat{T}]|\mathbf{p}\rangle \\ - \tfrac{1}{6}\Theta'''(\hat{\mu} - T)\{[\hat{\mu}, [\hat{\mu}, \hat{T}]] + [\hat{T}, [\hat{\mu}, \hat{T}]]\}|\mathbf{p}\rangle + \tfrac{1}{8}\Theta''''(\hat{\mu} - T)[\hat{\mu}, \hat{T}]^2|\mathbf{p}\rangle,\end{aligned} \tag{11}$$

where $[\hat{\mu}, \hat{T}] = \hat{\mu}\hat{T} - \hat{T}\hat{\mu}$ and $\hat{T}|\mathbf{p}\rangle = p^2/(2m)|\mathbf{p}\rangle = T|\mathbf{p}\rangle$. Here $\Theta'(x)$ is the first derivative of $\Theta(x)$ with respect to x, i.e. $\Theta'(x) = \delta(x)$ is the Dirac delta function, $\Theta''(x)$ is the second derivative of $\Theta(x)$ and so on. It is important to observe that equation (11) does not depend on the dimensionality of the system. Kirzhnits used equation (11) in the special case $D = 3$ [19], while here we consider it for a generic D. Note that higher order terms of the Kirzhnits expansion of the number operator $\hat{N}$ involve higher derivatives of the Heaviside function $\Theta(\hat{\mu} - T)$ [19, 20].

The term $\langle \mathbf{r}|\hat{N}|\mathbf{p}\rangle$ in equation (9) can now be calculated by using the Kirzhnits expansion. In this way, after straightforward but lengthy manipulations, at the second order in $\hbar$ equation (9) becomes

$$\begin{aligned}n(\mathbf{r}) = \left(\frac{m}{2\pi\hbar^2}\right)^{D/2} \frac{D}{2\Gamma\left(\frac{D}{2}+1\right)} \left\{F_D(\mu(\mathbf{r})) + \frac{\hbar^2}{2m}\left[\frac{1}{6}\nabla^2\mu(\mathbf{r})F_D''(\mu(\mathbf{r}))\right.\right. \\ \left.\left. + \frac{1}{12}(\nabla\mu(\mathbf{r}))^2 F_D'''(\mu(\mathbf{r}))\right]\right\},\end{aligned} \tag{12}$$

where $F_D'(\mu)$ is the first derivative of $F_D(\mu)$ with respect to μ, $F_D''(\mu)$ is the second derivative and so on. In the Kirzhnits expansion, after integration over momenta, each term containing a nth derivative of the Heaviside function $\Theta(\hat{\mu} - T)$ gives rise to a term containing a $(n-1)$th derivative of the function $F_D(\mu)$. As a consequence, in the special case $D = 2$, where $F_2(\mu) = \mu$, only the leading term of the Kirzhnits expansion is different from zero, i.e. with $D = 2$ the Kirzhnits gradient corrections vanish to all order in $\hbar$.

In the case $D = 3$, i.e. the three-dimensional Fermi gas, equation (12) becomes

$$n(\mathbf{r}) = \left(\frac{2m\mu(\mathbf{r})}{\hbar^2}\right)^{3/2} \frac{1}{6\pi^2}\left\{1 + \frac{\hbar^2}{2m}\left[\frac{1}{8}\frac{\nabla^2\mu(\mathbf{r})}{\mu(\mathbf{r})^2} - \frac{1}{32}\frac{(\nabla\mu(\mathbf{r}))^2}{\mu(\mathbf{r})^3}\right]\right\}, \tag{13}$$

which is exactly the formula reported in the book of Dreizler and Gross [20], which considers only the three-dimensional case. In the case $D = 2$, i.e. a two-dimensional Fermi gas, we have seen that all the quantum corrections are zero, while in the $D = 1$ case these corrections are in general finite, and in particular the $\hbar^2$ ones.

We observe that the vanishing of quantum corrections in the Kirzhnits expansion for the two-dimensional ideal Fermi gas is a consequence of the linear number of states, i.e. constant density of states, in this specific dimension. Obviously, this does not mean that with $D = 2$ the Thomas–Fermi formula of the density profile is exact; it simply means that the Kirzhnits expansion fails in the $D = 2$ case. For instance, recently Brack and van Zyl [21] have found that, for the a $2D$ ideal gas of fermions under harmonic confinement, the quantum kinetic energy is exactly reproduced by the Thomas–Fermi kinetic energy without gradient corrections, but only using the exact density of states, which is different from the Thomas–Fermi one [21].

Equation (12) has a serious turning point problem The local chemical potential $\mu(\mathbf{r}) = \bar{\mu} - U(\mathbf{r})$ becomes zero at the classical turning points, where $\bar{\mu} = U(\mathbf{r})$ Therefore, the gradient terms in equation (12) diverge at the turning points To overcome this problem we invert equation (12) finding $\mu(\mathbf{r})$ as a function of $n(\mathbf{r})$ Obviously, due to the gradients this inversion cannot be done exactly but only in a perturbative way First we note that equation (12) has the following structure:

$$n(\mathbf{r}) = A\mu(\mathbf{r})^{D/2}\left(1 + \frac{\hbar^2}{2m}B[\mu(\mathbf{r}), \nabla\mu(\mathbf{r})]\right), \tag{14}$$

where $A = (m/(2\pi\hbar^2))^{D/2}/\,\Gamma(D/2+1)$. Then from this expression we get

$$\begin{aligned}\mu(\mathbf{r}) &= \frac{A^{-2/D}n(\mathbf{r})^{2/D}}{\left(1 + \frac{\hbar^2}{2m}B[\mu, \nabla\mu(\mathbf{r})]\right)^{2/D}} \\ &= A^{-2/D}n(\mathbf{r})^{2/D}\left\{1 - \frac{2}{D}\frac{\hbar^2}{2m}B[\mu(\mathbf{r}), \nabla\mu(\mathbf{r})] + O(\hbar^4)\right\},\end{aligned} \tag{15}$$

where $O(\hbar^4)$ contains terms of order $\hbar^4$. Finally, we find, at the second order in $\hbar$, this expression

$$\frac{\hbar^2}{2m}\left(\frac{D-2}{3D}\right)\left[\frac{1}{4}\frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})^2} - \frac{1}{2}\frac{\nabla^2 n(\mathbf{r})}{n(\mathbf{r})}\right] + \frac{2\pi\hbar^2}{m}\Gamma\left(\frac{D}{2}+1\right)^{2/D} n(\mathbf{r})^{2/D} + U(\mathbf{r}) = \bar{\mu}. \tag{16}$$

This result differs from that of von Weizsäcker, equation (7), simply because there is a factor $(D-2)/3D$ in the gradient terms. We stress that the von Weizsäcker gradient terms are purely phenomenological, while the Kirzhnits gradient terms are based on a perturbative expansion of the exact number operator. In the scientific literature often the von Weizsäcker gradient terms are modified by inserting a coefficient c in front of them. For instance, with $D = 3$, March and Tosi [22] suggest $c = 1/3$, while Zaremba and Tso [23] suggest $c = 1/36$. Remarkably, both the phenomenological improvements disagree with the Kirzhnits result $c = 1/9$.

As previously discussed, the coefficient $(D-2)/3D$ was found some years ago by Holas, Kozlowski and March [17] by using a response–function approach based on the knowledge of the static susceptibility in a D-dimensional space [18]. Here we have instead applied the more direct Kirzhnits expansion. For $D = 3$ the factor gives the familiar coefficient $1/9$, for $D = 2$ the factor is zero and for $D = 1$ the factor is $-1/3$.

It is straightforward to show that the differential equation (16) is obtained by minimizing the energy density functional

$$E[n(\mathbf{r})] = \int \mathrm{d}^D\mathbf{r} \left\{ \left(\frac{D-2}{3D}\right) \frac{\hbar^2}{8m} \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})} + \frac{2\pi\hbar^2}{m} \frac{D}{D+2} \Gamma\left(\frac{D}{2}+1\right)^{2/D} n(\mathbf{r})^{(D+2)/D} + U(\mathbf{r}) n(\mathbf{r}) \right\} \tag{17}$$

with the constraint

$$N = \int \mathrm{d}^D\mathbf{r}\, n(\mathbf{r}), \tag{18}$$

which fixes the chemical potential $\bar{\mu}$. Equation (17) can be used as a starting point to investigate mixtures of interacting Fermi atoms and also electrons in nanotubes.

4. Conclusions

We have been able to determine the equations for the energy and the density profile of a D-dimensional ideal Fermi gas with external confinement by using the Kirzhnits expansion. These equations, which are correct at the second order in the Planck constant $\hbar$, can be improved by including higher order terms of the Kirzhnits expansion of the number operator [19]. In fact, in some cases, $\hbar$-expansions can be calculated to all orders and resumed to give the exact result [24]. In the special case $D = 2$ we have found, by using the Kirzhnits expansion, that all $\hbar$ corrections to the Thomas–Fermi formula of the density profile are zero. This is a direct consequence of the constant density of states in a two-dimensional ideal gas and it means that the Kirzhnits expansion is not reliable under these conditions. We recall that gradient corrections to the Thomas–Fermi formula of the density profile have been analyzed with different semiclassical techniques in previous studies [17, 25]. On the other hand, to our knowledge, this is the first time that the leading terms of the Kirzhnits expansion have been directly obtained for an ideal Fermi gas in a D-dimensional space and generic confining potential.

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