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Derivation of the differential equation for the Slater sum and of the differential virial theorem using the Wigner transform

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Abstract

Using the Wigner transform, we present an alternative derivation of the partial differential equation satisfied by the Slater sum, which is the diagonal element of the canonical Bloch density matrix. This is done in one dimension for the case of a general confining potential and also for the case of N independent fermions harmonically confined in d dimensions. We also present a simple proof of the so-called differential virial theorem for each of these cases.

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1. Introduction

The canonical or Bloch density matrix, defined as

$$C(\mathbf{r}, \mathbf{r}', \beta) := \langle \mathbf{r}|\widehat{C}|\mathbf{r}'\rangle = \langle \mathbf{r}|\exp(-\beta\widehat{H})|\mathbf{r}'\rangle, \tag{1.1}$$

plays an important role in the study of the properties of noninteracting fermions subjected to a one-body potential $V(\mathbf{r})$. Here, $\beta = (k_B T)^{-1}$ (where k_B is Boltzmann's constant and T the absolute temperature, although β can be considered just as a scaling parameter), $\widehat{C} = \exp(-\beta\widehat{H})$ is the Bloch density operator and $\widehat{H}$ is the one-particle Hamiltonian

$$\widehat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) = \sum_i \varepsilon_i |\Psi_i\rangle\langle\Psi_i|, \tag{1.2}$$

where ε_i are the energy eigenvalues and Ψ_i are the corresponding normalized wavefunctions of the Schrödinger equation

$$\widehat{H}|\Psi_i\rangle = \varepsilon_i|\Psi_i\rangle. \tag{1.3}$$

The Bloch density matrix is of particular interest since its knowledge enables the Dirac density matrix $\rho(\mathbf{r}, \mathbf{r}', \mu)$ to be found through an inverse Laplace transform of $C(\mathbf{r}, \mathbf{r}', \beta)/\beta$ [1]. This density matrix is obtained from the density operator, which, given the Fermi energy of the system μ, is

$$\widehat{\rho}_\mu = \sum_{\varepsilon_i<\mu} |\Psi_i\rangle\langle\Psi_i|, \qquad \rho(\mathbf{r},\mathbf{r}',\mu) = \langle\mathbf{r}|\widehat{\rho}_\mu|\mathbf{r}'\rangle. \tag{1.4}$$

Defining the so-called Slater sum as the diagonal element of the canonical density matrix

$$S(\mathbf{r},\beta) = C(\mathbf{r},\mathbf{r}',\beta)|_{\mathbf{r}=\mathbf{r}'}. \tag{1.5}$$

March and Murray [1] showed that, for central fields, such a quantity satisfies a set of partial differential equations for each orbital angular momentum quantum number ℓ, which in the one-dimensional case ($\ell = 0$) turns out to be precisely their equation (A1.6)

$$\frac{\hbar^2}{8m}\frac{\partial^3 S(x,\beta)}{\partial x^3} - \frac{\partial^2 S(x,\beta)}{\partial x\partial\beta} - V(x)\frac{\partial S(x,\beta)}{\partial x} - \frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}S(x,\beta) = 0. \tag{1.6}$$

Here $V(x)$ is a general confining potential in which an arbitrary number of independent fermions move.

For the case of N independent fermions in d dimensions which are confined by a spherical harmonic potential,

$$V(r) = \tfrac{1}{2}m\omega^2\mathbf{r}^2 \qquad \text{with} \qquad \mathbf{r}^2 = r^2 = x_1^2 + x_2^2 + \cdots + x_d^2, \tag{1.7}$$

it has also been shown [2, 3] that the corresponding Slater sum obeys the following partial differential equation:

$$\frac{\hbar^2}{8m}\frac{\partial}{\partial r}\nabla^2 S(r,\beta) - \left[V(r) + \frac{\partial}{\partial\beta}\right]\frac{\partial S(r,\beta)}{\partial r} - \left[1 - \frac{d}{2}\right]\frac{\mathrm{d}V(r)}{\mathrm{d}r}S(r,\beta) = 0. \tag{1.8}$$

The purpose of the present paper is twofold:

(i) to present an alternative derivation of (1.6) and (1.8) using the Wigner transform [4] and
(ii) to give a simple proof of the so-called differential virial theorem of March and Young [5, 6], which reads in one dimension

$$\frac{\partial\bar{t}(x,\mu)}{\partial x} = -\frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\rho(x,\mu). \tag{1.9}$$

Here, $V(x)$ is a general one-body potential and $\bar{t}(x,\mu) = (t(x,\mu) + t_G(x,\mu))/2$ is the average of the $(\Psi\nabla^2\Psi)$ and $(\nabla\Psi)^2$ wavefunction forms of the kinetic energy density. In the independent particle framework, these kinetic energy densities are given in terms of the single-particle wavefunctions (1.3) as

$$t(x,\mu) = -\frac{\hbar^2}{2m}\sum_{\epsilon_i<\mu}\Psi_i^*(x)\frac{\mathrm{d}^2\Psi_i(x)}{\mathrm{d}x^2}, \qquad t_G(x,\mu) = \frac{\hbar^2}{2m}\sum_{\epsilon_i<\mu}\left|\frac{\mathrm{d}\Psi_i(x)}{\mathrm{d}x}\right|^2, \tag{1.10}$$

$\rho(x,\mu)$ being the local single particle density obtained from the Dirac density matrix (1.4)

$$\rho(x,\mu) = \langle x|\widehat{\rho}_\mu|x\rangle = \sum_{\epsilon_i<\mu}|\Psi_i(x)|^2. \tag{1.11}$$

We shall also be concerned with the d-dimensional version of such a differential virial theorem, derived for the case of N-independent fermions moving in an isotropic harmonic confining potential [7], which using obvious notation reads

$$\frac{\partial\bar{t}(r,\mu)}{\partial r} = -\frac{d}{2}\frac{\mathrm{d}V(r)}{\mathrm{d}r}\rho(r,\mu). \tag{1.12}$$

2. The Bloch equation in phase space representation

Consider a system of N-noninteracting fermions whose one-body Hamiltonian is $\widehat{H}$ in (1.2). The corresponding Bloch density matrix can be expressed using (1.1) and (1.3)

$$C(\mathbf{r}, \mathbf{r}', \beta) = \sum_i \Psi_i(\mathbf{r})\Psi_i^*(\mathbf{r}') \exp(-\beta\varepsilon_i). \tag{2.1}$$

The derivative of the Bloch density operator $\widehat{C} = \exp(-\beta\widehat{H})$ with respect to β gives the Bloch equation

$$\frac{\partial\widehat{C}}{\partial\beta} = -\widehat{H}\widehat{C} = -\widehat{C}\widehat{H}, \tag{2.2}$$

subject to the initial condition $\widehat{C}(\beta = 0) = \widehat{I}$, where $\widehat{I}$ is the identity operator. In the following it is better to rewrite equation (2.2) in a symmetrized form, that is

$$\frac{\partial\widehat{C}}{\partial\beta} + \frac{1}{2}(\widehat{H}\widehat{C} + \widehat{C}\widehat{H}) = 0. \tag{2.3}$$

Next, to obtain the Bloch equation in phase space representation it is useful to introduce the Wigner transformation [4]. The Wigner transform of the canonical density matrix can be defined in d dimensions as follows:

$$C_W(\mathbf{q}, \mathbf{p}, \beta) = \int \exp\left(-\frac{\mathrm{i}\mathbf{p}\cdot\mathbf{s}}{\hbar}\right) C\left(\mathbf{q} + \frac{\mathbf{s}}{2}, \mathbf{q} - \frac{\mathbf{s}}{2}, \beta\right) \frac{\mathrm{d}\mathbf{s}}{(2\pi\hbar)^d}, \tag{2.4}$$

where C_W is a function of the phase space variables $\mathbf{q}$ and $\mathbf{p}$, and we have introduced the centre-of-mass and relative coordinates

$$\mathbf{q} = \frac{\mathbf{r} + \mathbf{r}'}{2}, \qquad \mathbf{s} = \mathbf{r} - \mathbf{r}'. \tag{2.5}$$

The inverse Wigner transform reads

$$C(\mathbf{r}, \mathbf{r}', \beta) = C\left(\mathbf{q} + \frac{\mathbf{s}}{2}, \mathbf{q} - \frac{\mathbf{s}}{2}, \beta\right) = \int \exp\left(\frac{\mathrm{i}\mathbf{p}\cdot\mathbf{s}}{\hbar}\right) C_W(\mathbf{q}, \mathbf{p}, \beta)\, \mathrm{d}\mathbf{p}. \tag{2.6}$$

According to the definition of the Slater sum (1.5) one may write

$$S(\mathbf{r}, \beta) = \int C_W(\mathbf{r}, \mathbf{p}, \beta)\, \mathrm{d}\mathbf{p}. \tag{2.7}$$

Let us consider now the Bloch equation (2.3). In order to apply the Wigner transform to such an equation, one needs the transform of a product of two operators, which is given by the rule [4]

$$(\widehat{A}\widehat{B})_W = A_W \left[\exp\left(\frac{\mathrm{i}\hbar}{2}\widehat{\Lambda}\right)\right] B_W, \tag{2.8}$$

where A_W and B_W are the transforms of the operators $\widehat{A}$ and $\widehat{B}$, and $\widehat{\Lambda}$ is the operator

$$\widehat{\Lambda} = \frac{\overleftarrow{\partial}}{\partial\mathbf{r}}\frac{\overrightarrow{\partial}}{\partial\mathbf{p}} - \frac{\overleftarrow{\partial}}{\partial\mathbf{p}}\frac{\overrightarrow{\partial}}{\partial\mathbf{r}} = \sum_{i=1}^{d}\left[\frac{\overleftarrow{\partial}}{\partial x_i}\frac{\overrightarrow{\partial}}{\partial p_i} - \frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overrightarrow{\partial}}{\partial x_i}\right]. \tag{2.9}$$

In the above equation the arrows on the gradient operators indicate in which direction they act. Therefore, the transform of equation (2.3) reads

$$\frac{\partial C_W(\mathbf{r}, \mathbf{p}, \beta)}{\partial\beta} + \frac{1}{2}\left[H_W(\mathbf{r}, \mathbf{p}) \exp\left(\frac{\mathrm{i}\hbar}{2}\widehat{\Lambda}\right) C_W(\mathbf{r}, \mathbf{p}, \beta) + C_W(\mathbf{r}, \mathbf{p}, \beta) \exp\left(\frac{\mathrm{i}\hbar}{2}\widehat{\Lambda}\right) H_W(\mathbf{r}, \mathbf{p})\right] = 0, \tag{2.10}$$

where

$$H_W(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \tag{2.11}$$

is the Wigner transform of the quantum Hamiltonian (1.2). Now, if we perform a Taylor expansion of the operator $\left[\exp\left(\frac{i\hbar}{2}\widehat{\Lambda}\right)\right]$, equation (2.10) reduces to

$$\frac{\partial C_W(\mathbf{r}, \mathbf{p}, \beta)}{\partial \beta} + H_W(\mathbf{r}, \mathbf{p}) \left[\cos\left(\frac{\hbar}{2}\widehat{\Lambda}\right)\right] C_W(\mathbf{r}, \mathbf{p}, \beta) = 0, \tag{2.12}$$

where we have used the fact that the terms with odd powers of $\hbar$ or $\widehat{\Lambda}$ cancel. This is the Wigner translation of the Bloch equation [8]. We also want to quote a second equation satisfied by the Wigner function $C_W(\mathbf{r}, \mathbf{p}, \beta)$ which follows from the obvious fact that the operators $\widehat{H}$ and $\widehat{C}$ commute

$$[\widehat{H}, \widehat{C}] = \widehat{H}\widehat{C} - \widehat{C}\widehat{H} = 0. \tag{2.13}$$

Translating this equation into phase space language by taking its Wigner transform, we get

$$H_W(\mathbf{r}, \mathbf{p}) \left[\exp\left(\frac{i\hbar}{2}\widehat{\Lambda}\right)\right] C_W(\mathbf{r}, \mathbf{p}, \beta) - C_W(\mathbf{r}, \mathbf{p}, \beta) \left[\exp\left(\frac{i\hbar}{2}\widehat{\Lambda}\right)\right] H_W(\mathbf{r}, \mathbf{p}) = 0, \tag{2.14}$$

where we have used the product rule (2.8). Expanding the exponential operator, equation (2.14) becomes

$$H_W(\mathbf{r}, \mathbf{p}) \left[\sin\left(\frac{\hbar}{2}\widehat{\Lambda}\right)\right] C_W(\mathbf{r}, \mathbf{p}, \beta) = 0, \tag{2.15}$$

since the terms with even powers of $\hbar$ or $\widehat{\Lambda}$ cancel. We emphasize that equations (2.12) and (2.15) are exact and hold in the multi-dimensional case. They constitute the basic relations for our analysis.

2.1. The partial differential equation for a general one-dimensional confining potential

We shall first examine the one-dimensional case for which $H_W(x, p) = p^2/(2m) + V(x)$. Expanding the cosine operator in equation (2.12) in Taylor series, with the use of definition (2.9), one can write explicitly

$$\frac{\partial C_W(x, p, \beta)}{\partial \beta} + H_W(x, p) C_W(x, p, \beta) - \frac{\hbar^2}{8m} \frac{\partial^2 C_W(x, p, \beta)}{\partial x^2} + \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k)!} \left(\frac{\hbar}{2}\right)^{2k} \frac{d^{2k} V(x)}{dx^{2k}} \frac{\partial^{2k} C_W(x, p, \beta)}{\partial p^{2k}} = 0.$$

If we integrate the above equation over the momentum p, taking into account equation (2.7) and the fact that, from equation (2.4), the terms containing derivatives with respect to p vanish by integration, we obtain

$$\frac{\partial S(x, \beta)}{\partial \beta} + \int_{-\infty}^{+\infty} dp \frac{p^2}{2m} C_W(x, p, \beta) - \frac{\hbar^2}{8m} \frac{\partial^2 S(x, \beta)}{\partial x^2} + V(x) S(x, \beta) = 0. \tag{2.16}$$

Taking the derivative with respect to x, we get

$$\frac{\partial^2 S(x, \beta)}{\partial x \partial \beta} + \frac{\partial}{\partial x} \int_{-\infty}^{+\infty} dp \frac{p^2}{2m} C_W(x, p, \beta) - \frac{\hbar^2}{8m} \frac{\partial^3 S(x, \beta)}{\partial x^3} + \frac{dV(x)}{dx} S(x, \beta) + V(x) \frac{\partial S(x, \beta)}{\partial x} = 0. \tag{2.17}$$

To simplify the second term in this equation we make use of (2.15) with (2.9), expanding in Taylor series the sine operator

$$\frac{\hbar}{2}\left(\frac{\mathrm{d}V(x)}{\mathrm{d}x}\frac{\partial C_W(x,p,\beta)}{\partial p}-\frac{p}{m}\frac{\partial C_W(x,p,\beta)}{\partial x}\right) +\sum_{k=1}^{\infty}\frac{(-1)^k}{(2k+1)!}\left(\frac{\hbar}{2}\right)^{2k+1}\frac{\mathrm{d}^{2k+1}V(x)}{\mathrm{d}x^{2k+1}}\frac{\partial^{2k+1}C_W(x,p,\beta)}{\partial p^{2k+1}}=0. \tag{2.18}$$

Multiplying the above equation by $p/2$ and then integrating over p, we get

$$\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}\frac{p^2}{2m}C_W(x,p,\beta)\,\mathrm{d}p=\frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\int_{-\infty}^{+\infty}p\frac{\partial C_W(x,p,\beta)}{\partial p}\,\mathrm{d}p, \tag{2.19}$$

since every term in the series vanishes upon integration on p, as follows easily from equation (2.4). The integral in the right-hand side term of (2.19) can be performed, upon using (2.4), as follows:

$$\begin{aligned}\int_{-\infty}^{+\infty}p\frac{\partial C_W(x,p,\beta)}{\partial p}\,\mathrm{d}p&=\int_{-\infty}^{+\infty}p\frac{\partial}{\partial p}\left(\int_{-\infty}^{+\infty}\exp\left(-\frac{\mathrm{i}ps}{\hbar}\right)C\left(x+\frac{s}{2},x-\frac{s}{2},\beta\right)\frac{\mathrm{d}s}{2\pi\hbar}\right)\mathrm{d}p\\&=\int_{-\infty}^{+\infty}sC\left(x+\frac{s}{2},x-\frac{s}{2},\beta\right)\frac{\mathrm{d}}{\mathrm{d}s}\left(\int_{-\infty}^{+\infty}\exp\left(-\frac{\mathrm{i}ps}{\hbar}\right)\frac{\mathrm{d}p}{2\pi\hbar}\right)\mathrm{d}s\\&=\int_{-\infty}^{+\infty}C\left(x+\frac{s}{2},x-\frac{s}{2},\beta\right)s\delta'(s)\,\mathrm{d}s=-C(x,x,\beta)=-S(x,\beta),\end{aligned}$$

where we have used the definition of the Slater sum (1.5). Therefore equation (2.19) becomes

$$\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}\frac{p^2}{2m}C_W(x,p,\beta)\,\mathrm{d}p=-\frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}S(x,\beta). \tag{2.20}$$

Now, if we insert equation (2.20) into (2.17), we obtain the partial differential equation given by (1.6).

2.2. *The partial differential equation for the case of harmonic confinement in d dimensions*

Let us now move to the case of spherical harmonic potential in d dimensions (1.7), for which

$$H_W(\mathbf{r},\mathbf{p})=\frac{\mathbf{p}^2}{2m}+\frac{1}{2}m\omega^2\mathbf{r}^2. \tag{2.21}$$

We note that, as the classical Hamiltonian H_W is of maximal degree two in position and momentum, we may reduce equations (2.12) and (2.15) by expanding in Taylor series the cosine and sine operators, because the terms in $\hbar^3,\hbar^4\ldots$ vanish and therefore one may write these equations as

$$\frac{\partial C_W(\mathbf{r},\mathbf{p},\beta)}{\partial\beta}+H_W(\mathbf{r},\mathbf{p})\left[1-\frac{\hbar^2}{8}\widehat{\Lambda}^2\right]C_W(\mathbf{r},\mathbf{p},\beta)=0, \tag{2.22}$$

$$H_W(\mathbf{r},\mathbf{p})\widehat{\Lambda}C_W(\mathbf{r},\mathbf{p},\beta)=0. \tag{2.23}$$

Thus, equations (2.22) and (2.23) are exact for a harmonic oscillator Hamiltonian, with $\widehat{\Lambda}$ given in equation (2.9), from which we get

$$\widehat{\Lambda}^2=\sum_{i,j=1}^{d}\left[\frac{\overleftarrow{\partial}^2}{\partial x_i\partial x_j}\frac{\overrightarrow{\partial}^2}{\partial p_i\partial p_j}+\frac{\overleftarrow{\partial}^2}{\partial p_i\partial p_j}\frac{\overrightarrow{\partial}^2}{\partial x_i\partial xj}-2\frac{\overleftarrow{\partial}^2}{\partial x_i\partial p_j}\frac{\overrightarrow{\partial}^2}{\partial p_i\partial x_j}\right]. \tag{2.24}$$

Substituting equation (2.24) into (2.22), and using

$$\frac{\partial^2 H_W(\mathbf{r},\mathbf{p})}{\partial x_i \partial x_j} = \delta_{ij} m\omega^2, \qquad \frac{\partial^2 H_W(\mathbf{r},\mathbf{p})}{\partial p_i \partial p_j} = \frac{\delta_{ij}}{m}, \qquad \text{and} \qquad \frac{\partial^2 H_W(\mathbf{r},\mathbf{p})}{\partial x_i \partial p_j} = 0,$$

one then obtains

$$\frac{\partial C_W(\mathbf{r},\mathbf{p},\beta)}{\partial \beta} + \frac{\mathbf{p}^2}{2m} C_W(\mathbf{r},\mathbf{p},\beta) + \frac{1}{2} m\omega^2 \mathbf{r}^2 C_W(\mathbf{r},\mathbf{p},\beta) - \frac{m(\hbar\omega)^2}{8}\left(\nabla_{\mathbf{p}}^2 C_W(\mathbf{r},\mathbf{p},\beta)\right) - \frac{\hbar^2}{8m}\left(\nabla_{\mathbf{r}}^2 C_W(\mathbf{r},\mathbf{p},\beta)\right) = 0, \qquad (2.25)$$

where $\nabla_{\mathbf{p}}^2$ stands for the Laplacian in the d-dimensional momentum space. Partial derivation with respect to the radial variable r leads to

$$\frac{\partial^2 C_W(\mathbf{r},\mathbf{p},\beta)}{\partial r \partial \beta} + \frac{\partial}{\partial r}\left(\frac{\mathbf{p}^2}{2m} C_W(\mathbf{r},\mathbf{p},\beta)\right) + \frac{1}{2} m\omega^2 \mathbf{r}^2 \left(\frac{\partial C_W(\mathbf{r},\mathbf{p},\beta)}{\partial r}\right) + m\omega^2 r C_W(\mathbf{r},\mathbf{p},\beta) - \frac{m(\hbar\omega)^2}{8}\frac{\partial}{\partial r}\left(\nabla_{\mathbf{p}}^2 C_W(\mathbf{r},\mathbf{p},\beta)\right) - \frac{\hbar^2}{8m}\frac{\partial}{\partial r}\left(\nabla_{\mathbf{r}}^2 C_W(\mathbf{r},\mathbf{p},\beta)\right) = 0. \qquad (2.26)$$

Integrating this equation over $\mathbf{p}$ and using (2.7) we obtain

$$\frac{\partial^2 S(\mathbf{r},\beta)}{\partial r \partial \beta} + \frac{\partial}{\partial r}\int \frac{\mathbf{p}^2}{2m} C_W(\mathbf{r},\mathbf{p},\beta)\,\mathrm{d}\mathbf{p} + m\omega^2 r S(\mathbf{r},\beta) + \frac{1}{2} m\omega^2 \mathbf{r}^2 \frac{\partial S(\mathbf{r},\beta))}{\partial r} - \frac{\hbar^2}{8m}\frac{\partial}{\partial r}(\nabla^2 S(\mathbf{r},\beta)) = 0. \qquad (2.27)$$

As in the previous case, the integrals of terms containing derivatives of $C_W(\mathbf{r},\mathbf{p},\beta)$ with respect to the variables $\mathbf{p}$ are zero. Now, we can express the second term in (2.27) with the help of equation (2.23), which using the definition (2.9), can be rewritten in the form

$$\frac{\mathbf{p}}{m}\cdot(\nabla_{\mathbf{r}} C_W(\mathbf{r},\mathbf{p},\beta)) = m\omega^2 \mathbf{r}\cdot(\nabla_{\mathbf{p}} C_W(\mathbf{r},\mathbf{p},\beta)). \qquad (2.28)$$

For a spherical harmonic oscillator $C_W(\mathbf{r},\mathbf{p},\beta) = C_W(r,p,\beta)$, i.e., it depends only on the moduli $r = |\mathbf{r}|$ and $p = |\mathbf{p}|$ [8], that is

$$C_W(\mathbf{r},\mathbf{p},\beta) = \frac{1}{\cosh^d(\beta\hbar\omega/2)} \exp\left[-\frac{2\tanh(\beta\hbar\omega/2)}{\hbar\omega} H_W(\mathbf{r},\mathbf{p})\right], \qquad (2.29)$$

a fact that immediately allows us to write (2.28) in the form

$$\frac{p}{m}\frac{\partial C_W(r,p,\beta)}{\partial r} = m\omega^2 r \frac{\partial C_W(r,p,\beta)}{\partial p}. \qquad (2.30)$$

Multiplying by $p/2$ and integrating with respect to $\mathbf{p}$, we get

$$\frac{\partial}{\partial r}\int \frac{p^2}{2m} C_W(r,p,\beta)\,\mathrm{d}\mathbf{p} = \frac{1}{2} m\omega^2 r \int p \frac{\partial C_W(r,p,\beta)}{\partial p}\,\mathrm{d}\mathbf{p} = -\frac{d}{2} m\omega^2 r \int C_W(r,p,\beta)\,\mathrm{d}\mathbf{p} = -\frac{d}{2} m\omega^2 r S(r,\beta). \qquad (2.31)$$

We have taken into account that the integration on the $\mathbf{p}$-space can be reduced, in this case, to a 'radial' integral, with

$$\mathrm{d}\mathbf{p} = \frac{2\pi^{\frac{d}{2}} p^{d-1}\,\mathrm{d}p}{\Gamma\left(\frac{d}{2}\right)}, \qquad (2.32)$$

where $\Gamma(z)$ represents the Gamma function and we have also used the fact that $p^d C_W(r,p,\beta) \to 0$ as $p \to \infty$, a property which is satisfied by using (2.29). Finally, inserting (2.31) into (2.27), we easily get the result given in equation (1.8). Remark that no analytical expression of the Wigner function $C_W(\mathbf{r},\mathbf{p},\beta)$ was needed, only the fact that it depends on r and p.

3. The differential virial theorem

To prove the differential virial theorem, we start with the equation of motion

$$\widehat{H}\widehat{\rho}_\mu - \widehat{\rho}_\mu\widehat{H} = 0. \tag{3.1}$$

This relation is similar to equation (2.13) and therefore we follow the same procedure used in obtaining (2.15) to get the equation of motion in Wigner phase space:

$$H_W(\mathbf{r},\mathbf{p})\left[\sin\left(\frac{\hbar}{2}\widehat{\Lambda}\right)\right]\rho_W(\mathbf{r},\mathbf{p},\mu) = 0, \tag{3.2}$$

where $\rho_W(\mathbf{r},\mathbf{p},\mu)$ is the Wigner transform of the density matrix (1.4).

3.1. The case of a general one-dimensional confining potential

Again, in a similar way as was done previously to obtain equations (2.18)–(2.20) from (2.15), equation (3.2) leads, for the one-dimensional case, to

$$\frac{\partial}{\partial x}\int_{-\infty}^{+\infty}\frac{p^2}{2m}\rho_W(x,p,\mu)\,\mathrm{d}p = -\frac{1}{2}\frac{\mathrm{d}V(x)}{\mathrm{d}x}\rho(x,\mu), \tag{3.3}$$

where we have used the fact that the local particle density $\rho(x,\mu)$ is given in terms of its Wigner transform $\rho_W(x,p,\mu)$ as

$$\rho(x,\mu) = \int_{-\infty}^{+\infty}\rho_W(x,p,\mu)\,\mathrm{d}p. \tag{3.4}$$

Next, it has been shown in [9] that

$$\int_{-\infty}^{+\infty}\frac{p^2}{2m}\rho_W(x,p,\mu)\,\mathrm{d}p = \bar{t}(x,\mu) = \frac{t(x,\mu)+t_G(x,\mu)}{2}, \tag{3.5}$$

represents exactly the arithmetical average between the usual forms of the kinetic energy density (1.10). Equation (3.5) holds also in the multi-dimensional case and, as noted in [9], it exhibits the connnection between the classical average of the kinetic energy and its quantum counterpart. Inserting equation (3.5) into (3.3), one finally finds the one-dimensional version of the differential virial theorem given by equation (1.9).

3.2. The case of harmonic confinement in *d* dimensions

To obtain the differential virial theorem for an isotropic harmonic oscillator in d dimensions, we mimic the arguments developed in the previous section for such a potential (indeed equations (2.23), (2.28)–(2.31)). Thus, equation (3.2) can be rewritten as

$$H_W(\mathbf{r},\mathbf{p},\mu)\widehat{\Lambda}\rho_W(\mathbf{r},\mathbf{p},\mu) = 0, \tag{3.6}$$

and using the definition (2.9), we get

$$\frac{\mathbf{p}}{m}\cdot(\nabla_{\mathbf{r}}\rho_W(\mathbf{r},\mathbf{p},\mu)) = m\omega^2\mathbf{r}\cdot(\nabla_{\mathbf{p}}\rho_W(\mathbf{r},\mathbf{p},\mu)). \tag{3.7}$$

Next, it has been shown in [10] that for a degenerate system of fermions completely filling $(M+1)$ oscillator shells, the density in Wigner phase space, $\rho_W(\mathbf{r},\mathbf{p},\mu)$, depends only on the quantity $H_W(\mathbf{r},\mathbf{p})$ (2.21). Indeed

$$\rho_W(\mathbf{r},\mathbf{p},\mu) = \frac{1}{(\pi\hbar)^d}\left[\sum_{k=0}^{M}(-1)^k L_k^{d-1}(4H_W(\mathbf{r},\mathbf{p})/\hbar\omega)\right]\exp(-2H_W(\mathbf{r},\mathbf{p})/\hbar\omega). \tag{3.8}$$

Using such a dependence through the moduli r and p, equation (3.7) reduces to

$$\frac{p}{m}\frac{\partial\rho_W(r,p,\mu)}{\partial r} = m\omega^2 r\frac{\partial\rho_W(r,p,\mu)}{\partial p} \tag{3.9}$$

As this relation is similar to equation (2.30), we now follow the same derivation as was done there, to obtain here an equation similar to (2.31), satisfied by the density $\rho_W(r,p,\mu)$:

$$\frac{\partial}{\partial r}\int\left(\frac{p^2}{2m}\rho_W(r,p,\mu)\right)\mathrm{d}\mathbf{p} = -\frac{d}{2}m\omega^2 r\rho(r,\mu) = -\frac{d}{2}\frac{\mathrm{d}V(r)}{\mathrm{d}r}\rho(r,\mu). \tag{3.10}$$

In deriving the above equation, we have used that $p^d\rho_W(r,p,\mu)\to 0$ as $p\to\infty$. A property which is shown by invoking (3.8). Since equation (3.5) holds also in arbitrary dimension, one ends with the d-dimensional form of the differential virial theorem (1.12)

$$\frac{\partial\bar{t}(r,\mu)}{\partial r} = -\frac{d}{2}\frac{\mathrm{d}V(r)}{\mathrm{d}r}\rho(r,\mu). \tag{3.11}$$

Remark that again we did not use the precise analytical expression of the density $\rho_W(\mathbf{r},\mathbf{p},\mu)$, only the fact that it depends on the moduli r and p is needed.

4. Summary and future directions

The derivation presented in this paper can add to one's insight and may be useful in some future calculations. Although in this work we limited ourselves only to the local densities in the coordinate representation, for future directions it will be of interest to obtain, using the Wigner transform, equations for densities in momentum space. Equations for non-local quantities in coordinate representation, such as those given in [11–13], can also be worked out within the present treatement.

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