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THE PAULI POTENTIAL IN RELATION TO THE DIFFERENTIAL VIRIAL THEOREM WITH APPLICATION TO EXPERIMENTS ON ULTRACOLD ATOMIC GASES OF FERMIONS

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Abstract

In early work by the writer introducing the Pauli potential $V_P(\mathbf{r})$ into density functional theory, the relation of $V_P(\mathbf{r})$ to the, as yet unknown, single-particle kinetic energy density functional was emphasized. Here, because of ongoing experiments on ultracold atomic gases of fermions, an explicit expression for the first derivative of $V_P(\mathbf{r})$ for an arbitrary number of closed shells generated by harmonic confinement is derived in terms of the spherically symmetric particle density $n(r)$ and the confining potential.

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With 'seeds' in the early work of March and Murray [1], the background to the introduction of the Pauli potential $V_P(\mathbf{r})$ into density functional theory (DFT) has been well reviewed by Levy and Görling [2; see also Herring and Chopra [3]]. As noted by the present writer [4, 5], the problem of finding an adequate approximation to the single-particle kinetic energy functional $T_S[n]$ can be viewed as that of finding an adequate representation of the Pauli potential $V_P(\mathbf{r})$. As set out especially in [2], there have been active studies of the Schrödinger equation for the density amplitude $\{n(\mathbf{r})\}^{1/2}$, with $n(\mathbf{r})$ the ground-state electron density. The one-body potential $V(\mathbf{r})$ in current usage in DFT [6] is then to be replaced by $V(\mathbf{r})+V_P(\mathbf{r})$ in the above-mentioned Boson-like differential equation for the density amplitude $\{n(\mathbf{r})\}^{1/2}$. Related work of Hunter [7] should also be noted here, which does not make a DFT connection [2]. In [5], $V_P(\mathbf{r})$ was specifically written in terms of $\delta T_S[n]/\delta n(\mathbf{r})$.

Here, the application we consider is motivated by ongoing experiments on ultracold atomic gases of fermions (e.g. vapors of ^{40}K and ^{6}Li isotopes populating hyperfine states inside magnetic traps) as in [8, 9, 10, 11]. This is intimately connected with harmonic confinement of fermions, which with arbitrary occupancy of closed shells is our main three-dimensional application below. However, we turn next to connect the above summary on the Pauli potential $V_P(\mathbf{r})$ with very recent work on the differential virial theorem [12, 13] by March and Nagy [14]. In this work, it was shown for spherical densities with arbitrary level occupancy that, given the differential virial theorem [DVT] in the form [13]

$$-\frac{\partial V(r)}{\partial r} = -\frac{\hbar^2}{4m\ n(r)}\frac{\partial}{\partial r}\nabla^2 n(r) + \frac{\hat{\mathbf{r}}\cdot\mathbf{z}_S(\mathbf{r})}{n(r)} \tag{1}$$

where $\hat{\mathbf{r}}$ is the unit radial vector $\mathbf{r}/r$, the last term could be replaced by [14]

$$\frac{\hat{\mathbf{r}}\cdot\mathbf{z}_s(\mathbf{r})}{n(r)} = \frac{4}{n(r)}\left[\frac{t_W(r)}{r} + \frac{1}{2}\frac{\partial t_W(r)}{\partial r}\right] + V_P'(r)\ . \tag{2}$$

In eqn.(2), the vector field $\mathbf{z}_s(\mathbf{r})$, following Holas and March [13], is defined via the single-particle (s) kinetic energy density tensor $t^{(s)}_{\alpha\beta}(\mathbf{r})$ as

$$\mathbf{z}_s(\mathbf{r}) = 2\sum_\beta \frac{\partial}{\partial r_\beta} t^{(s)}_{\alpha\beta}(\mathbf{r})\ . \tag{3}$$

Concerning eqn.(2), the first bracketed term on the right-hand side (RHS) was given by Akbari et al. [15] for single-level occupancy, the Pauli potential derivative $V_P'(r)$ being introduced by March and Nagy [14] for spherically symmetric densities with arbitrary occupancy. In eqn.(2), $t_W(r)$ is the von Weizsäcker [16] kinetic energy density defined generally in terms of the ground-state density $n(\mathbf{r})$ by

$$t_W(\mathbf{r}) = \frac{\hbar^2}{8m}\frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})}\ . \tag{4}$$

Next, we utilize the differential equation for the ground-state fermion density $n(r)$ given by Howard et al. [17] in d dimensions; namely

$$\frac{\hbar^2}{8m}\frac{\partial}{\partial r}\nabla^2 n + \{[M + (d+1)/2]\hbar\omega - V(r)\}\, n'(r) + \frac{d}{2}\left[\frac{\partial V}{\partial r}\right] n(r) = 0 \;, \tag{5}$$

where the confining potential energy $V(r)$ is $(1/2)m\omega^2 r^2$. Using eqns.(1) and (2) to remove $\partial V/\partial r$ from eqn.(5) then yields the result, but now specific to $d = 3$ (see below for $d = 1$, where a general treatment transcending harmonic confinement proves possible):

$$V_P'(r) = \frac{\hbar^2}{3m\; n(r)}\frac{\partial}{\partial r}\nabla^2 n(r) + \frac{2}{3}\{[M+2]\hbar\omega - V(r)\}\frac{n'(r)}{n(r)} - \frac{4}{n(r)}\left\{\frac{t_W(r)}{r} + \frac{1}{2}\frac{\partial t_W}{\partial r}\right\} \;. \tag{6}$$

Eqn.(6) is a central result of this Letter, and expresses the first derivative of the Pauli potential in terms of the density $n(r)$ and its low-order derivatives, given (a) harmonic confinement and (b) $M + 1$ closed shells, ensuring spherical symmetry. It is a straightforward matter to confirm eqn.(6) for the case $M = 0$ corresponding to single-shell occupancy by direct insertion of $V(r) = (1/2)m\omega^2 r^2$ and the corresponding ground-state density $n(r) = n(0)\exp(-\alpha r^2)$, where $\alpha = (m\omega)/\hbar$.

Since completing the present Letter, it has come to the author's attention that Elliott et al. [18], in work on the semiclassical origins of density functionals, conclude 'how much simpler the kinetic energy is as a functional of the potential than of the density'. It is then, in the above context, worthy of note that the early study of Stoddart and March [19] of an exact Thomas-Fermi method in perturbation theory based on the homogeneous free-electron gas (HEG) with t_0 as the kinetic energy density of the HEG, and $t(\mathbf{r})$ that with the perturbation $V(\mathbf{r})$ 'switched on', gave

$$t(\mathbf{r}) - t_0 = -V(\mathbf{r})\sum_{j=1}^{\infty}\left(\frac{j}{j+1}\right) n_j(\mathbf{r}) \tag{7}$$

where the 'density' component $n_j(\mathbf{r})$ of $O(V^j)$ is given quite explicitly for arbitrary j also in terms of $V(\mathbf{r})$. However, using in eqn.(7) that $\frac{j}{(j+1)} = 1 - 1/j + 1$ plus the identity from [19] that $n - n_0 = \sum_{j=1}^{\infty} n_j(\mathbf{r})$, one can readily rewrite the RHS of eqn.(7) in terms of both $n(\mathbf{r})$ and $V(\mathbf{r})$. This latter form of $V_P'(\mathbf{r})$ is readily apparent in eqn.(6) above, and prompts us to conclude by reworking this equation for one dimension, following the early study of Lawes and March [20].

Again using the DVT, but now in one dimension [12]:

$$\frac{\partial t}{\partial x} = -\frac{1}{2}n(x)\frac{\partial V(x)}{\partial x} + \frac{\hbar^2}{8m}n'''(x) \tag{8}$$

which already shows quite generally that the kinetic energy density $t(x)$ is readily written in terms of n and V. Hence the total single-particle kinetic energy T_S is given also by

$$\begin{aligned} T_S &= \int_{-\infty}^{\infty} t(x)dx \\ &= \frac{1}{2}\int_{-\infty}^{\infty} n(x)x\frac{\partial V(x)}{\partial x}dx \end{aligned} \tag{9}$$

which, of course, is the integral virial theorem in quantum mechanics. Using next eqn.(5), but now for $d = 1$, one has, but now again for harmonic confinement:

$$\frac{\hbar^2}{8m} n'''(x) + \{[M+1]\hbar\omega - V(x)\} \, n'(x) + \frac{1}{2} n(x) \frac{\partial V}{\partial x} = 0 \; . \tag{10}$$

Utilizing eqn.(8) in eqn.(10) readily yields, by removing $\partial V/\partial x$ that

$$\frac{\hbar^2}{4m} n'''(x) - \frac{\partial t}{\partial x} + \{[M+1]\hbar\omega - V(x)\} \, n'(x) = 0 \tag{11}$$

where $V(x) = (1/2)m\omega^2 x^2$ in one-dimension. But the general Euler equation of DFT has the form [6]

$$\mu = \frac{\delta T_S}{\delta n(x)} + V(x) \; , \tag{12}$$

where μ is the chemical potential having a constant value throughout the inhomogeneous fermion density $n(x)$. Hence, one has the Pauli potential $V_P(x)$ in one dimension as [4, 5]

$$V_P(x) = \frac{\delta T_S}{\delta n(x)} - \frac{\delta T_W}{\delta n(x)} \tag{13}$$

where, from eqns.(11) and (12) it follows that

$$\begin{aligned} V_P(x) &= \mu - V(x) - \frac{\delta T_W}{\delta n(x)} \\ &= \left[-\frac{\hbar^2}{4m} \frac{n'''(x)}{n'(x)} + \frac{1}{n'(x)} \frac{\partial t}{\partial x} \right] + [\mu - \{M+1\}\hbar\omega] - \frac{\delta T_W}{\delta n(x)} \; . \end{aligned} \tag{14}$$

The functional derivative of the von Weizsäcker kinetic energy T_W is, of course, known explicitly in terms of $n(x)$ and its low-order derivatives from eqn.(4) and hence $V_P(x)$ is known from eqn.(14) without any functional differentiation of T_S to perform. Naturally level occupancy occurs in eqn.(14) via the chemical potential μ, the kinetic energy term $t(x)$ and the factor M, while the external potential $V = (1/2)m\omega^2 x^2$ enters through the characteristic energy $\hbar\omega$. To date, the kinetic energy per unit length $t(x)$ is only known explicitly for one-dimensional harmonic confinement [21] which then yields, after differentiation of eqn.(14), the one-dimensional analogue of eqn.(6).

In summary, a central result of this Letter is eqn.(6), which gives the first derivative of the Pauli potential $V(r)$ for spherically symmetric fermion densities corresponding to $(M+1)$ closed shells generated by harmonic confinement. A one-dimensional analogue of eqn.(6), but now for $V_P(x)$ itself, is also presented in eqn.(14), where the kinetic energy per unit length $t(x)$ is known from the study of March et al. [21] for the case of harmonic confinement under discussion here.

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