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LETTER TO THE EDITOR

The Pauli potential in one-dimensional density functional theory: general result for two-level systems and specific example for *N* harmonically confined Fermions

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Abstract
There is ongoing interest in the kinetic energy functional $T_s[\rho]$ in density functional theory. The present study lies in this area and concerns the Pauli potential $V_P[\rho]$. A differential equation is obtained here for $V_P(x)$ in one dimension for a general two-level system. Also, as a specific example, such a functional of $\rho(x)$, the ground-state Fermion density, is given for the case of N Fermions which are harmonically confined.

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The purpose of this letter is to construct the Pauli potential, denoted by V_P and defined precisely below (see equation (15)), from the Fermion density and its derivatives. This sheds light on the study of the important kinetic energy functional. As special cases, the two-level system and the model of harmonic confinement for N levels, with N arbitrary, are then investigated in detail. It will be convenient to begin with the latter case in one dimension. For this model, Lawes and March [1] derived the differential equation

$$-\frac{1}{2}\rho\frac{\partial V}{\partial x} - \frac{\rho'''}{8} = (N - V(x))\rho' \tag{1}$$

for the Fermion density $\rho(x)$ for harmonic confinement with potential energy $V(x)$ given by

$$V(x) = \tfrac{1}{2}x^2. \tag{2}$$

N in equation (1) is the number of Fermions, the lowest state corresponding to $N = 1$. Here, instead of considering this equation in the manner proposed by Lawes and March, namely as a third-order linear homogeneous differential equation to be solved for the Fermion density $\rho(x)$, given $V(x)$ in equation (2) and N the total number of Fermions, we shall view equation (1) as a first-order differential equation to be integrated for $V(x)$ (of course given by equation (2)!).

Using an integrating factor, $V(x)$ is readily written in the form

$$V(x) = -\rho^2(x) \int_0^x \left[\frac{\rho'''(s)}{4\rho^3} + \frac{2N\rho'(s)}{\rho^3} \right] \mathrm{d}s \tag{3}$$

or

$$V(x) = -\rho^2(x) \int_0^x \frac{\rho'''(s)}{4\rho^3}\, \mathrm{d}s + N \left[1 - \frac{\rho^2(x)}{\rho^2(0)} \right]. \tag{4}$$

Since $N = \int_{-\infty}^{\infty} \rho(x)\, \mathrm{d}x$, this gives explicitly the form of the external potential $V(x)$ as a functional of the density. As will be detailed below, since $[V(x) + V_P(x)]$ is known explicitly as a function of $\rho(x)$ and its low-order derivatives (see equation (18)), knowledge of $V[\rho]$, as in equation (4) for the case of harmonic confinement, suffices to determine the Pauli potential from $\rho(x)$ and its derivatives.

In spite of the practical success of the so-called Slater–Kohn–Sham equations [2, 3], there is ongoing interest in the direct calculation of the single-particle kinetic energy functional $T_s[\rho]$ in density functional theory (DFT), examples being in the studies of [4, 5]. One route to calculate $T_s[\rho]$, as already noted, is via the Pauli potential V_P named by one of us ([6], see also [7]) and reviewed briefly by Levy and Görling [8]. One definition linking V_P with T_s is through functional derivatives, namely

$$V_P(\mathbf{r}) = \frac{\delta T_s}{\delta \rho(\mathbf{r})} - \frac{\delta T_W}{\delta \rho(\mathbf{r})} \tag{5}$$

where $\rho(\mathbf{r})$ is the ground-state Fermion density while T_W represents the von Weizsäcker inhomogeneity kinetic energy given by $T_w = \int t_W(\mathbf{r})\, \mathrm{d}\mathbf{r}$, where

$$t_W(\mathbf{r}) = \frac{1}{8} \frac{(\nabla \rho)^2}{\rho}. \tag{6}$$

Below, we shall first specialize to one dimension in order to exhibit results for V_P having some degree of generality; i.e., which are valid for any confining potential $V(x)$ in which independent Fermions move. Our starting point is the differential virial theorem of March and Young [9] for the positive definite kinetic energy density $t(x)$, namely

$$\frac{\partial t}{\partial x} = -\frac{1}{2} \rho \frac{\partial V}{\partial x} + \frac{1}{8} \frac{\partial^3 \rho}{\partial x^3}. \tag{7}$$

We now use the Euler equation of DFT, which is in fact an equation for the constancy of the chemical potential μ throughout the entire Fermion density distribution $\rho(x)$ [10, 11]:

$$\mu = \frac{\delta T_s}{\delta \rho(x)} + V(x). \tag{8}$$

Thus, we can replace $\partial V/\partial x$ in equation (7), using equation (8) plus the constancy of μ to find

$$\frac{\partial t}{\partial x} = \frac{1}{2} \rho \frac{\partial}{\partial x} \left[\frac{\delta T_s}{\delta \rho(x)} \right] + \frac{1}{8} \frac{\partial^3 \rho}{\partial x^3}. \tag{9}$$

Inverting equation (5), we then have a differential equation for the Pauli potential $V_P(x)$, namely

$$\frac{\partial}{\partial x} V_P(x) = \frac{2}{\rho} \frac{\partial t}{\partial x} - \frac{1}{4\rho} \frac{\partial^3 \rho}{\partial x^3} - \frac{\partial}{\partial x} \left[\frac{\delta T_W}{\delta \rho(x)} \right]. \tag{10}$$

But from equation (6), one has almost immediately

$$\frac{\delta T_W}{\delta \rho(x)} = \frac{\rho'^2}{8\rho^2} - \frac{\rho''}{4\rho} \tag{11}$$

and hence it follows from equations (10) and (11) that

$$\frac{\partial}{\partial x} V_P(x) = \frac{2}{\rho}\frac{\partial t}{\partial x} - \frac{\rho''\rho'}{2\rho^2} + \frac{\rho'^3}{4\rho^3}. \tag{12}$$

Since $T_s = \int t \, \mathrm{d}x$, and $T_s = T_s[\rho]$, this gives V_P as a functional solely of the density $\rho(x)$.

While equation (12) is a quite general result in one dimension for an arbitrary confining potential energy $V(x)$ for an arbitrary number of Fermions, let us next apply it specifically to the case of a two-level system, for which Dawson and March [12] showed that

$$t(x) = t_W(x) + \tfrac{1}{2}\rho(x)\theta'^2(x). \tag{13}$$

Here $\theta(x)$ is the phase appearing in the two wavefunctions, $\psi_1(x)$ and $\psi_2(x)$ say, for the two levels, written as

$$\psi_1(x) = \sqrt{\rho(x)}\cos\theta \qquad \psi_2(x) = \sqrt{\rho(x)}\sin\theta. \tag{14}$$

In recent work, Gál *et al* [13] have written an explicit differential equation for essentially $\theta'^2/2$, i.e., from equation (13), for

$$\tau = \frac{t - t_W}{\rho}. \tag{15}$$

Using the differential equation for τ given in [13], equation (18), and utilizing the result that

$$\frac{\partial V_P}{\partial x} = \frac{2}{\rho}\frac{\partial}{\partial x}(\rho\tau) \tag{16}$$

one obtains after some calculation that $V_P(x)$ satisfies, to within an additive constant,

$$\frac{1}{16}\frac{\left(\rho V_P'\right)^2}{\left[\int_{-\infty}^{x}\rho V_P' \, \mathrm{d}x\right]^2} - \frac{1}{8}\frac{\left(\rho V_P'\right)'}{\left[\int_{-\infty}^{x}\rho V_P' \, \mathrm{d}x\right]} + \frac{1}{2\rho}\int_{-\infty}^{x}\rho V_P' \, \mathrm{d}x - V_P(x) + \left[\frac{3}{16}\left(\frac{\rho'}{\rho}\right)^2 - \frac{1}{8}\left(\frac{\rho''}{\rho}\right)\right] = 0. \tag{17}$$

We note also that from the definition of the Pauli potential, we can write

$$V_P'(x) = \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\nabla^2\sqrt{\rho(x)}}{2\sqrt{\rho(x)}}\right] - V'(x) \tag{18}$$

inserting equation (18) in equation (17) then yields a ρ–V relation for the general two-Fermion problem in one dimension. However, as the result is more complex in form than equation (17), we prefer to regard this density–potential relation as a consequence of solving equations (17) and (18) simultaneously. To illustrate the general two-level result for $V_P(x)$ in one-dimensional systems, we have found an analytical solution to date only for the harmonic confinement model summarized above in equations (1)–(4). For $N = 2$ we have therefore utilized this model to plot the solution $V_P(x)$ of equation (17) in figure 1 obtained from the harmonic two-level density $\rho(x)$. The corresponding kinetic energy density $t(x)$ can then be found from this form of Pauli potential using equations (16), (15) and (6), together again with the same two-level Fermion density $\rho(x)$, and $t(x)$ thus obtained is plotted in figure 2.

Having established a quite general result for the Pauli potential V_P for two-level systems, we continue with the specific example of N harmonically confined Fermions in one dimension, but generalized now to arbitrary N. We appeal to the recent work of Howard *et al* [14]. This is readily found to yield (their equation (19) written in one dimension)

$$\frac{\partial}{\partial x}\left[\frac{1}{\rho^2}\frac{\delta T_s}{\delta\rho(x)}\right] = \frac{1}{4\rho^3(x)}\frac{\partial^3\rho}{\partial x^3}. \tag{19}$$

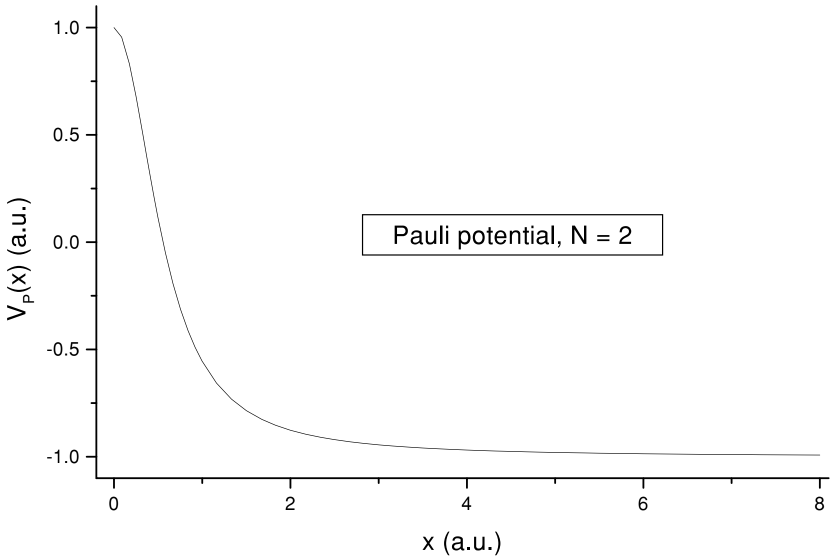

Figure 1. Pauli potential $V_P(x)$ for two-level harmonic confinement obtained from solution of general two-level equation (17) with $\rho(x)$, found from equation (1) with $N = 2$, as input.

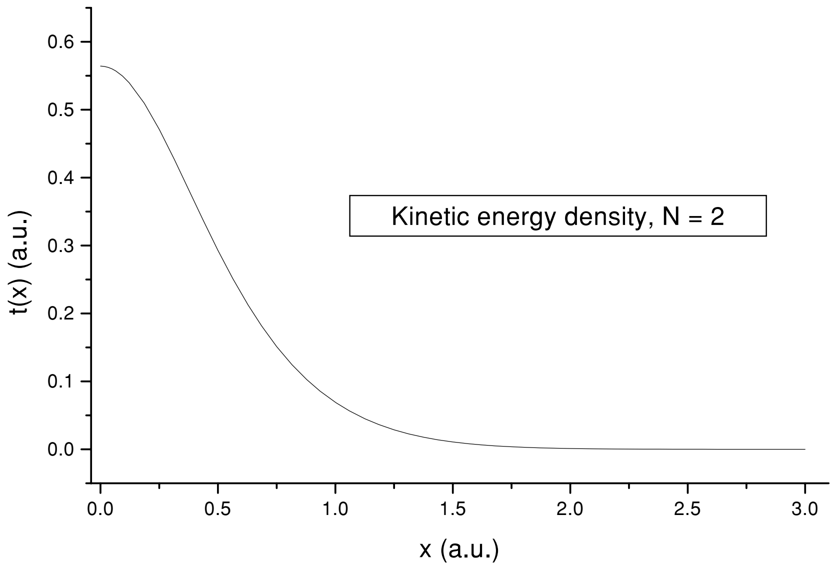

Figure 2. Kinetic energy density $t(x)$ obtained from Pauli potential $V_P(x)$ in figure 1, using same harmonic input density $\rho(x)$ for two levels, by means of equations (16), (15) and (6).

Using equation (5) for V_P, and the form of T_W represented by equation (6), it is a straightforward matter to obtain the following differential equation:

$$\frac{\partial}{\partial x}\left[\frac{V_P(x)}{\rho^2}\right] = \frac{1}{2\rho^3}\left[\rho''' + \frac{\rho'}{\rho}\left(\frac{\rho'^2}{\rho} - 2\rho''\right)\right] \tag{20}$$

where primes denote derivatives of $\rho(x)$ with respect to x. Omitting any additive constant, one obtains the result

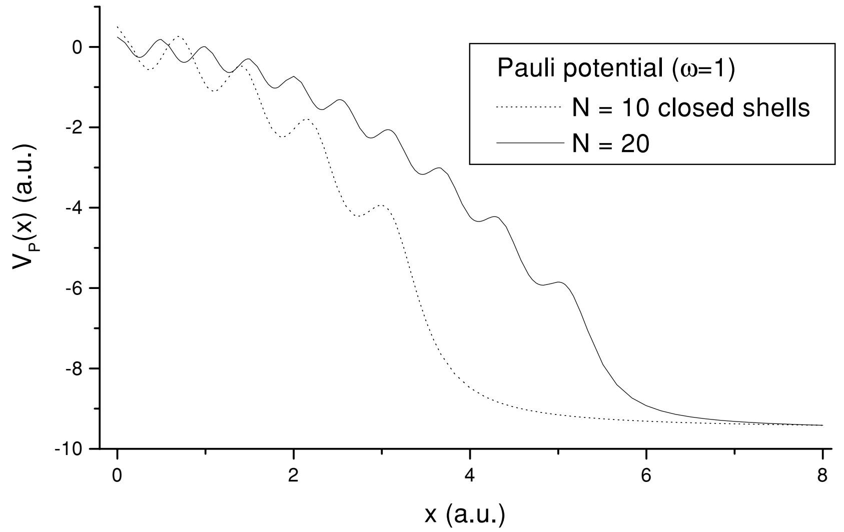

Figure 3. Form of the Pauli potential for the one-dimensional harmonic oscillator with $N = 10$ and 20 closed shells. The characteristic frequency ω is taken to be 1.

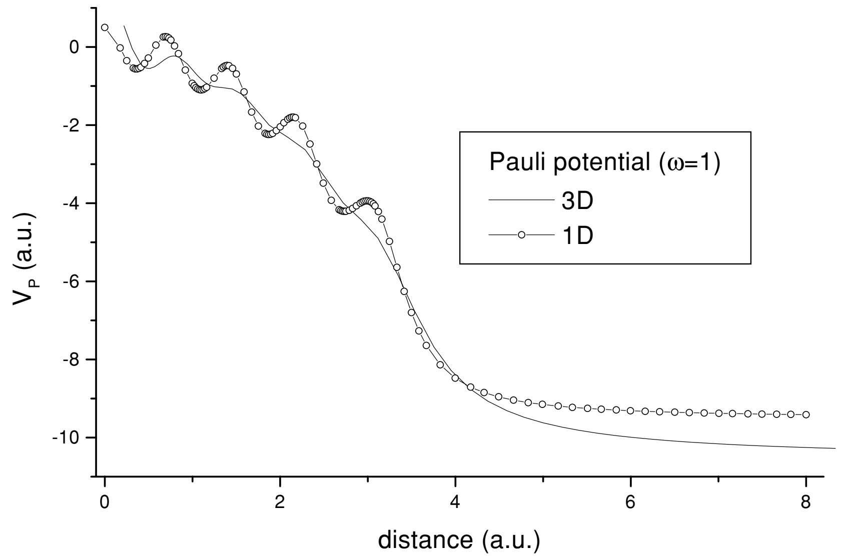

Figure 4. The Pauli potential for the harmonic oscillator with ten closed shells, in one dimension and in three dimensions. As in figure 1, we take $\omega = 1$.

$$V_P(x) = \rho^2(x) \int^x \frac{\rho'''(s)}{4\rho^3}\,\mathrm{d}s + \frac{1}{4}\frac{\rho''(x)}{\rho(x)} - \frac{1}{8}\left[\frac{\rho'(x)}{\rho(x)}\right]^2. \tag{21}$$

This result could alternately be obtained by integrating equation (18) of the work of March *et al* [15]. We have calculated $V_P(x)$ from equation (21) for $N = 10$ and 20 closed shells; results are shown in figure 3. We note here that since $\delta T_s/\delta\rho(x) = \mu - V(x)$, the oscillations in V_P come entirely from the form of $\delta T_W/\delta\rho(x)$.

Indeed, for isotropic harmonic confinement, a generalization to d dimensions can be readily effected using the results of [14]. We find then

$$\frac{\partial}{\partial r}\left[\frac{V_P(r)}{\rho^{2/d}}\right] = \frac{1}{4\rho^{1+2/d}}\left[\frac{1}{d}\frac{\partial}{\partial r}\nabla^2\rho + \rho''' + (1+1/d)\frac{\rho'}{\rho}\left(\frac{\rho'^2}{\rho} - 2\rho''\right)\right]. \quad (22)$$

For $d = 3$, we show in figure 4 the form of the Pauli potential for ten closed shells; the analogous quantity in one dimension is shown also for comparison.

In summary, the main results of this letter on the Pauli potential in DFT are embodied in equations (12), (17) and (20) in one dimension, and for the case of harmonic confinement in d dimensions in equation (22). Though in the most general of these results, namely equation (12), t is not known explicitly, no functional derivative of the kinetic energy functional $T_s[\rho]$ now appears. While equation (20) for the Pauli potential V_P for harmonic confinement is attractively compact, it must not be assumed to be the sought-after universal functional. However, this letter represents a step along the road to such a finding, equation (17) being a quite general one-dimensional form for two-level systems.

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