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Dirac density matrix and the Legendre transform of the kinetic energy generated by one-dimensional model potentials

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Abstract

In density functional theory, the single-particle kinetic energy is still not known in an orbital-free form. The natural tool to calculate such kinetic energy for a given one-body potential V is the Dirac density matrix γ. Here, by first taking solvable one-dimensional examples, and in particular the $\mathrm{sech}^2(x)$ potential, forms for the Dirac density matrix are exhibited in terms of the potential.This in turn generates the Legendre transform of the single-particle kinetic energy. Finally, one-dimensional perturbation theory for the kinetic energy density, summed to all orders in V, is presented in the appendix.

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1. Introduction

Current quantitative calculations using density functional theory (DFT) are based on single-particle Schrödinger equations into which a common one-body potential V is inserted, these equations, of symmetrized Hartree form, being associated with the names of Slater [1], Kohn and Sham [2]. Of course, a crucial problem for DFT is that the exchange-correlation contribution, V_{xc}, to the one-body potential V is not known. However, even with a given V, DFT is not directly employed to calculate the single-particle kinetic energy, this being obtained by standard wavefunction procedures from the Slater–Kohn–Sham one-electron wavefunctions generated by V. Numerous research groups continue the search for an orbital-free theory of this kinetic energy, and the present study is in this area.

It is, of course, amply recognized that the 'natural' tool for the calculation of kinetic energy is the first-order density matrix $\gamma(\mathbf{r}, \mathbf{r}')$. For a single Slater determinantal wavefunction

generated by orbitals $\psi_i(\mathbf{r})$, this goes back at least to Dirac [3] and is given by

$$\gamma(\mathbf{r}, \mathbf{r}') = \sum_{\text{occupied } i} \psi_i(\mathbf{r})\psi_i^*(\mathbf{r}') \tag{1.1}$$

with the central tool of DFT, namely the ground-state density $\rho(\mathbf{r})$, given immediately from equation (1.1) as $\gamma(\mathbf{r}, \mathbf{r})$. Already, in their early study, March and Young [4] proposed a variational approach in terms of $\rho(\mathbf{r})$ to approximate $\gamma(\mathbf{r}, \mathbf{r}')$. Of course, the single-particle kinetic energy density, say $t(\mathbf{r})$, is derivable directly from equation (1.1) as

$$t(\mathbf{r}) = -\frac{\hbar^2}{2m} \frac{\partial^2 \gamma(\mathbf{r}, \mathbf{r}')}{\partial \mathbf{r}^2}\bigg|_{\mathbf{r}'=\mathbf{r}}. \tag{1.2}$$

It is clear that, in order to obtain the single-particle kinetic energy functional $T[\rho]$ from equation (1.2),

$$T = \int t(\mathbf{r})\, \mathrm{d}\mathbf{r}, \tag{1.3}$$

one requires knowledge of $\gamma(\mathbf{r}, \mathbf{r}')$ in terms of its diagonal element $\rho(\mathbf{r})$. In turn, $\rho(\mathbf{r})$ is generated by the DFT potential $V(\mathbf{r})$, and $T[V]$ is referred to as the Legendre transform of $T[\rho]$. However, in order to present explicit examples in which the Dirac density matrix γ can be expressed directly in terms of V, then leading via equations (1.2) and (1.3) to the Legendre transform $T[V]$, we shall at first restrict ourselves here to one dimension, and to model choices of the one-body potential $V(x)$.

We clarify a few points on the presentation which follows, and especially the relation of this study to the Thomas–Fermi (TF) method, before passing to the treatment of one-dimensional model potentials. First, the leading kinetic TF term in the single-particle kinetic energy functional $t[\rho]$ has the density power $\rho^{1+2/D}$ in D dimensions. In the models discussed below we note that (i) $D = 1$, therefore (ii) $t_{\mathrm{TF}}[\rho] \propto \rho^3$ (not $\rho^{5/3}$ as in three dimensions) and (iii) $\rho \propto (\mu - V)^{1/2}$, where μ is the chemical potential and $V(x)$ is the one-body potential. Then, as a specific example of the Legendre transform referred to above, $t_{\mathrm{TF}}(V) \propto (\mu - V)^{3/2}$; but it is also relevant for what follows to note that there is an equivalent form of t_{TF}, namely, $t_{\mathrm{TF}} \propto \rho(\mu - V)$, in which both ρ and V now enter the kinetic energy. In this connection we also emphasize that one must interpret carefully some of the formulae in sections 2 and 3, e.g., equations (2.11) and (3.6). The point to be clarified here is that both these equations refer to small numbers of occupied levels generated by the one-body potential, whereas the TF method, having statistical origins, comes into its own when large numbers of energy levels are occupied. However, we emphasize in this context that section 4 is intimately connected to, and clearly transcends, the original TF method; the same being true of appendix C.

Returning to model potentials, we begin with a $\mathrm{sech}^2(x)$ form of $V(x)$, for which a number of analytic results are derivable.

2. One-dimensional potential $V(x)$ of $\mathrm{sech}^2(x)$ form

Though work on the $\mathrm{sech}^2(x)$ potential has a long history, we find the study of Hall [5] a valuable starting point. Given the potential

$$V(x) = -v(v+1)\,\mathrm{sech}^2(x), \tag{2.1}$$

the Schrödinger equation is

$$-\frac{\partial^2 \psi(x)}{\partial x^2} - v(v+1)\,\mathrm{sech}^2(x)\psi(x) + (v-n)^2\psi(x) = 0 \tag{2.2}$$

using Hall's expression for the eigenvalues, $F(n, v) = -(v - n)^2$. The solutions of equation (2.2) are of the form

$$\psi(x) = C_1 P_v^{v-n}(\tanh(x)) + C_2 Q_v^{v-n}(\tanh(x)),$$

where P and Q are the associated Legendre functions (as defined for instance in Abramowitz and Stegun [6]). The $Q's$ can be eliminated as non-physical solutions; n ranges from $0, 1, 2, \ldots$, and the nth eigenvalue appears only when $v > n$. The density for non-interacting particles can then be written as

$$\rho(x) = \sum_n C_{n,v} \left| P_v^{v-n}(\tanh(x)) \right|^2 \tag{2.3}$$

and the density matrix as

$$\gamma(x, x') = \sum_n C_{n,v}^2 P_v^{v-n}(\tanh(x)) P_v^{v-n*}(\tanh(x')), \tag{2.4}$$

or, in terms of the potential,

$$\gamma[V(x), V(x')] = \sum_n C_{n,v}^2 P_v^{n-v}\left(\sqrt{1 + V(x)/v(v+1)}\right) P_v^{n-v*}\left(\sqrt{1 + V(x')/v(v+1)}\right). \tag{2.5}$$

Thus, from (2.5), the kinetic energy density $t_g(x)$, defined (compare the wavefunction gradient (g) form $\propto (\nabla\psi)^2$) as

$$t_g(x) = \frac{\hbar^2}{2m} \frac{\partial^2 \gamma}{\partial x' \partial x}\bigg|_{x'=x} \tag{2.6}$$

can be written as

$$t_g[V] = \frac{v(v+1)}{8(v(v+1) + V(x))V(x)^2} \sum_{n=0}^{v-1} C_{n,v}^2 \Big[(n - 2v - 1) P_{v+1}^{n-v}\left(\sqrt{1 + V(x)/v(v+1)}\right) + (v+1)\sqrt{1 + V(x)/v(v+1)} P_v^{n-v}\left(\sqrt{1 + V(x)/v(v+1)}\right)\Big]^2 \tag{2.7}$$

provided that v is integral. Then P_v^{v-n} takes the form of a finite sum, and $\rho(x)$ is a finite sum of powers of $\tanh^2(x)$ (and so of $V(x)$); for instance, for $v = 4$, $n = 0 - 3$, the total density assuming singly occupied levels is

$$\rho(x) = 1.406\,25 - 5.468\,75 \tanh^8(x) + 8.75 \tanh^6(x) - 4.6875 \tanh^4(x), \tag{2.8}$$

which integrates to 4. The density matrix itself for this case can also be written, but is relegated to appendix A because of its lengthy form. However, figure 1 shows the density (solid line) obtained from equation (2.8) and $\gamma(x, x')|_{x'=x}$ (dots) from equation (A.1) as a function of x (Hall's scaled units [5] are used). As already mentioned, we can write the density as a function of the potential $V(x)$ here, the result being

$$\rho(x) = -0.341\,796\,875 \times 10^{-4} V^4 - 0.164\,0625 \times 10^{-2} V^3 - 0.028\,125 V^2 - V/4, \tag{2.9}$$

which is plotted in figure 2.

But a simpler example is that with $v = 2$, $n = 0 - 1$, i.e., two filled states in a potential $V(x) = -6\,\mathrm{sech}^2(x)$. Then the density (normalized to 2) is just

$$\rho(x) = \tfrac{3}{4}(1 - \tanh^4(x)) \tag{2.10}$$

or, in terms of the potential,

$$\rho = -\frac{V}{4}\left(1 + \frac{V}{12}\right). \tag{2.11}$$

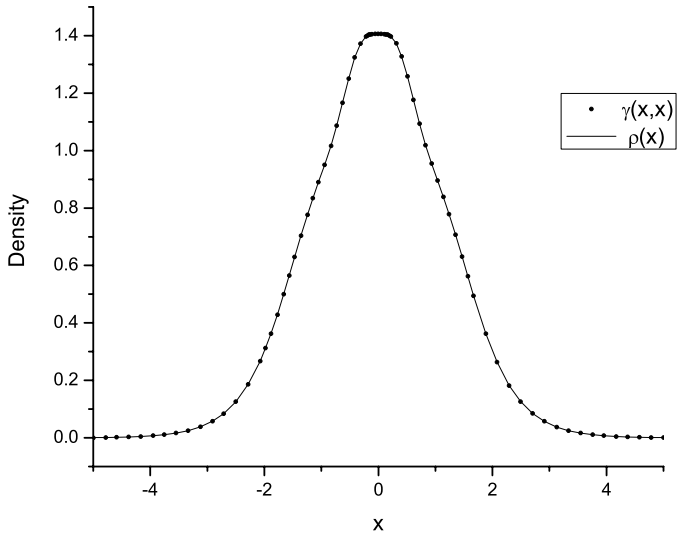

Figure 1. The total density $\rho(x)$, assuming singly occupied levels, for the case $v = 4, n = 0 - 3$ of the $\text{sech}^2(x)$ potential, compared to $\gamma(x, x')|_{x'=x}$, given in appendix A, equation (A.1). The density (solid line) is obtained from equation (2.8), and $\gamma(x, x')|_{x'=x}$ (dots) from equation (A.1).

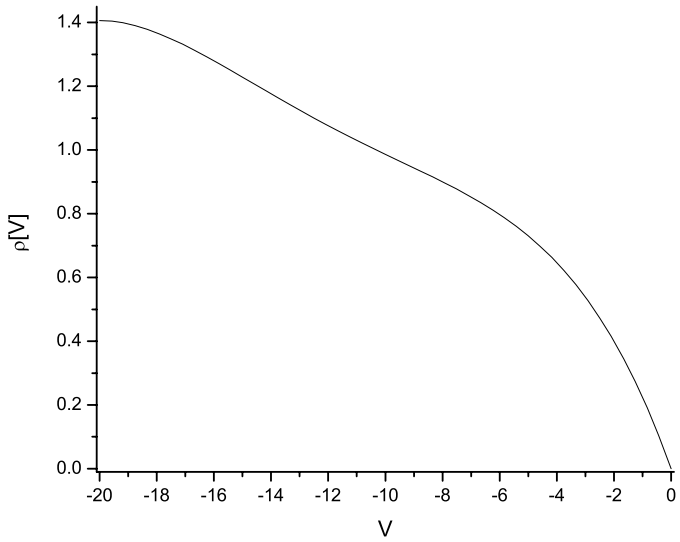

Figure 2. Density $\rho(x)$ for the case $v = 4, n = 0 - 3$ of the $\text{sech}^2(x)$ potential, as a function of the potential $V(x)$.

So here we can solve for $V[\rho]$ to get (only the physical solution being recorded here)

$$V[\rho] = -6.0 + 1.92(9.765\,625 - 13.020\,833\rho)^{1/2} \tag{2.12}$$

which is displayed in figure 3. The corresponding density matrix is

$$\gamma(x, x') = \tfrac{3}{2}\,\text{sech}^2(x)\,\text{sech}^2(x')\left(\tfrac{1}{2} + \sinh(x')\sinh(x)\right). \tag{2.13}$$

Figure 4 shows a plot of $\rho(x)$ (solid line) and $\gamma(x, x')|_{x'=x}$ (circles).

Having, thus, verified the equivalence of equation (2.10) for the ground-state density and the diagonal term $\gamma(x, x)$ of the Dirac density matrix (2.13), we turn to one major focus of the

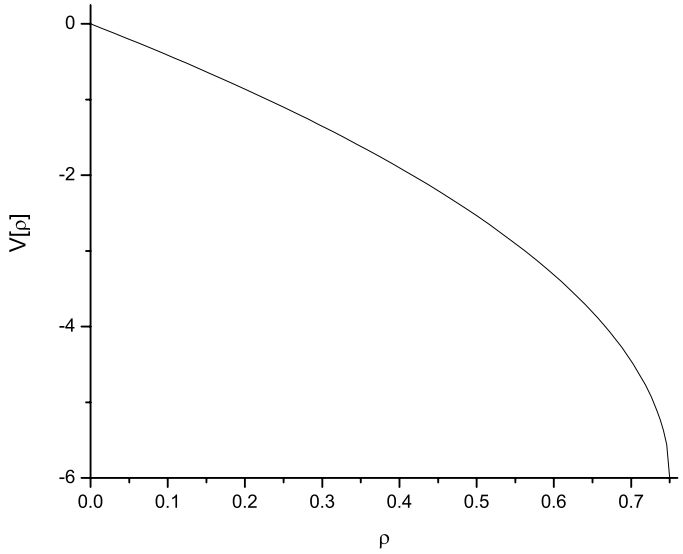

Figure 3. Potential $V[\rho]$ for two filled states in a potential $V(x) = -6\,\mathrm{sech}^2(x)$.

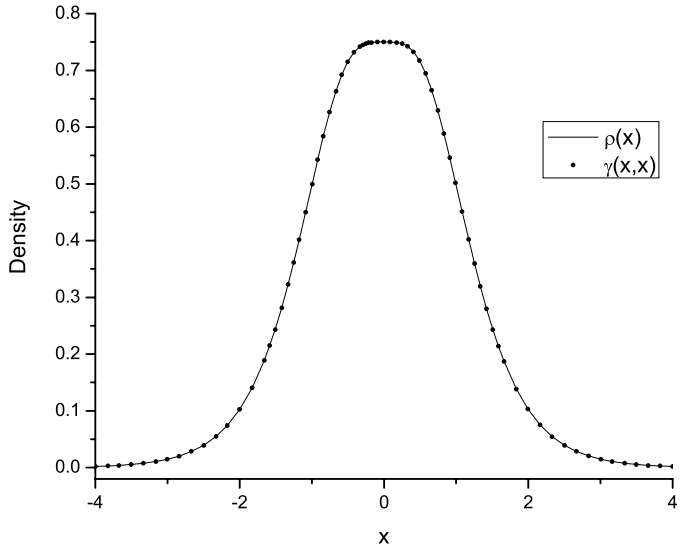

Figure 4. Density $\rho(x)$ (solid line) and $\gamma(x, x')|_{x'=x}$ (circles) compared for the $v = 2, n = 0, 1$ case of the $\mathrm{sech}^2(x)$ potential.

present study: namely to obtain this matrix (2.13) in compact form in terms of the one-body potential $V(x)$.

3. Dirac density matrix for two-level $\mathrm{sech}^2(x)$ potential in terms of $V(x)$ and derivatives

Since the Dirac density matrix $\gamma(x, x')$ in equation (2.10) is generated by the potential $V(x) = -6\ \mathrm{sech}^2(x)$, we can evidently write for γ the form

$$\gamma(x,x') = \frac{V(x)V(x')}{24}\left[\frac{1}{2} + \sinh(x)\sinh(x')\right]. \tag{3.1}$$

Forming $\rho(x) = \gamma(x,x')|_{x'=x}$ from equation (3.1) we can solve for the quantity $V(x)\sinh(x)$, which leads to the result

$$\gamma(x,x') = \frac{V(x)V(x')}{48} + \left[\rho(x) - \frac{V^2(x)}{48}\right]^{1/2}\left[\rho(x') - \frac{V^2(x')}{48}\right]^{1/2}. \tag{3.2}$$

But using next equation (2.11) for ρ in terms of V, we eliminate ρ from equation (3.2) to find

$$\gamma(x,x') = \frac{V(x)V(x')}{48} + \frac{1}{4}\left[-\left\{V(x) + \frac{V^2(x)}{6}\right\}\right]^{1/2}\left[-\left\{V(x') + \frac{V^2(x')}{6}\right\}\right]^{1/2}, \tag{3.3}$$

or in terms of V alone,

$$\gamma(x,x') = \frac{3}{2}\frac{V(x)}{6}\frac{V(x')}{6}\left(1/2 + \sqrt{-6/V(x) - 1}\sqrt{-6/V(x') - 1}\right). \tag{3.4}$$

This result (3.3) or (3.4), for this admittedly simplistic $\mathrm{sech}^2(x)$ for two levels, exemplifies a long-term aim which already had its origins in the variational density matrices proposed by March and Young [4]. However, they constructed $\gamma[\rho]$, whereas equation (3.3) is, of course, $\gamma[V]$.

3.1. Kinetic energy in Legendre transform

Inserting equation (2.13) into equation (2.6), we find the Legendre transform result for the kinetic energy to be

$$t_g[V] = \frac{[V'(x)]^2}{96} - \frac{1}{16}\frac{[V'(x)(1+V(x))/3]^2}{[V(x)(1+V(x)/6)]}, \tag{3.5}$$

or equivalently

$$t_g[V] = -\frac{V}{144}(V^2 + 6V + 18). \tag{3.6}$$

While equation (3.6) represents a quite explicit example of the Legendre transform of the kinetic energy density, we wish at this point to stress again the general Dirac density matrix $\gamma(x,x')$ in equation (2.5) for the $\mathrm{sech}^2(x)$ potential. Then we can justifiably claim that this equation (2.5) inserted into equation (2.6) leads to a Legendre transform-like expression for the kinetic energy density $t_g(x)$, as in equation (2.7).

4. Kinetic energy density $t(x)$ based on perturbation expansion in $V(x)$, with free electrons as the unperturbed problem

We follow in this section the three-dimensional perturbation study of March and Murray [7], who generated the Dirac density matrix $\gamma(\mathbf{r},\mathbf{r}')$ from a one-body potential $V(\mathbf{r})$ inserted into an originally uniform free Fermi gas, taken as the unperturbed problem. If we write the March–Murray series for the diagonal element $\rho(\mathbf{r}) = \gamma(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}$ as

$$\rho(\mathbf{r}) = \rho_0 + \sum_{j=1}^{\infty}\rho_j(\mathbf{r}), \tag{4.1}$$

where $\rho_j(\mathbf{r})$ is $\mathcal{O}(V^j)$ and ρ_0 is the constant unperturbed density, then these workers showed that when $V(\mathbf{r})$ varied sufficiently slowly in $\mathbf{r}$-space then equation (4.1) summed to the well-known Thomas–Fermi approximation [7] discussed briefly in the introduction.

Subsequently, Stoddart and March [8] used the March–Murray perturbation series for $\gamma(\mathbf{r}, \mathbf{r}')$ to derive the kinetic energy density $t(\mathbf{r})$ as

$$t(\mathbf{r}) = t_0 = -V(\mathbf{r}) \sum_j c_j \rho_j(\mathbf{r}), \tag{4.2}$$

$\rho_j(\mathbf{r})$ being as in equation (4.1). In the three-dimensional case, Stoddart and March [8] derived c_j as $j/(j+1)$, and since, as already mentioned $\rho_j(\mathbf{r})$ is already known as $\mathcal{O}(V^j)$, equation (4.2) is a Legendre transform result for $T[V] = \int t(\mathbf{r})\,\mathrm{d}\mathbf{r}$. Unfortunately to date the summation in equation (4.2) has not proved tractable.

However, what we show below is that, in one dimension, the focus of the present study, the analogue of equation (4.2), can in fact be summed to all orders, though in doing so, as explained below, the density ρ enters the result, as well as the potential V. This is not especially surprising because in the summation $\sum_j c_j \rho_j$ appearing in equation (4.2) we can in three dimensions [8] write $c_j = j/(j+1) = 1 - (j+1)^{-1}$ and hence using equation (4.1) we have $\sum_j c_j \rho_j = \rho(\mathbf{r}) - \rho_0 - \sum_j \rho_j/(j+1)$.

The key result in achieving the summation of the one-dimensional analogue of equation (4.2) is the differential virial theorem derived by March and Young [9]. This reads

$$\frac{\partial t}{\partial x} = -\frac{1}{2}\rho\frac{\partial V}{\partial x} - \frac{\rho'''}{8}, \tag{4.3}$$

which follows from the equation of motion for $\gamma(x, x')$ by expansion of this matrix around the diagonal $x' = x$. We give the detail in appendix C, and merely summarize the result here. Writing the one-dimensional form of equation (4.2) as

$$t(x) - t_0 = -V(x)\Sigma(x) \tag{4.4}$$

we obtain in appendix C the form of Σ as

$$\Sigma(x) = \frac{1}{2V(x)} \int^x \rho(s) \frac{\partial V(s)}{\partial s}\,\mathrm{d}s + \frac{1}{8V(x)} \frac{\partial^2 \rho}{\partial x^2}. \tag{4.5}$$

Though the analogue of equation (4.1) can be derived in one dimension, we have not effected the summation required to allow $\rho(x)$ appearing in equation (4.5) to be written in closed form in terms of $V(x)$. Thus, combining equations (4.4) and (4.5), we have indeed an orbital-free theory of $t(x) - t_0$, where, as in section 1, $t_0 \propto \rho_0^3$ in one dimension, but not a Legendre transform $T[V]$ since, as discussed above, ρ also appears. Of course, one now has a problem in which the Fermi level lies in the continuum, in contrast to, for example, result (3.3) for $\gamma(x, x')$ for the $\mathrm{sech}^2(x)$ potential, in which the Fermi level is in the bound-state region of the spectrum.

While this section embodies our main findings for a general one-dimensional potential $V(x)$, in appendix D we summarize some results for the delta-function potential $V(x) = \lambda\delta(x)$, which we return to briefly in section 5.

5. Summary and future directions

The idempotent Dirac density matrix $\gamma(x, x')$ generated by a one-dimensional potential $V(x)$ has been studied for model potentials. Quite explicit results are presented for the lowest two, and four occupied levels generated by the potential $\mathrm{sech}^2(x)$ given in equation (2.1). The two-level result corresponding to the general result (2.5) has been written in equation (3.4) solely in terms of $V(x)$. This then leads to the result (3.6) for the positive definite form $t_g(x)$ in Legendre transform. In fact, one can rewrite the general form (2.4) for an arbitrary number of occupied energy levels generated by the $\mathrm{sech}^2(x)$ potential solely in terms of $V(x)$, though

the result is somewhat complicated, as seen in equation (2.7). Nevertheless, this example, admittedly simplistic, leads to an explicit orbital-free theory of single-particle kinetic energy, which is a long-term aim of numerous current workers in density-functional theory.

As a further example, dealt with quite briefly in appendix D, the repulsive delta-function potential $V(x) = \lambda\delta(x)$ is treated, the resultant ρ–V relation in this case being given in the form of a differential equation in which the λ (or V!) dependence is exhibited. Though we have, as yet, not found a solvable model example, section 4 and appendix C return to the theme of generating the kinetic energy density without recourse to orbitals for a general one-dimensional potential $V(x)$. This is already implicit in the March–Young [9] differential form of the virial theorem. But what appendix C demonstrates is that the Stoddart–March [8] three-dimensional perturbation series has an analogue in one dimension which can be summed. However, the sum presented involves both the ground-state density $\rho(x)$ and the potential $V(x)$ which generates it.

As to future directions, it will be, of course, of interest to study further models in which the Legendre transform of the kinetic energy can be generated. One which comes to mind is an exponentially decaying potential $V(x)$. In a central field context, this was found to be tractable analytically in the context of localized impurity scattering in a free-electron metal [10]. But clearly, the most important directions for the future will involve two- and three-dimensional problems. The summation of the Stoddart–March series (4.2) in three dimensions would be a major step, of course, in the search for an orbital-free single-particle kinetic energy density.

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Appendix A. Dirac density matrix for four occupied levels of the $\mathrm{sech}^2(x)$ potential

The purpose of this brief appendix is to give the explicit form of the Dirac density matrix $\gamma(x, x')$ for the $\mathrm{sech}^2(x)$ potential (2.1) with $v = 4$. Equation (2.4) can be calculated quite explicitly as

$$\begin{aligned}\gamma(x,x') = 20[&39\cosh(x+x') - 5\cosh(2x+4x') + 46\cosh(2x+2x') - 5\cosh(4x+2x')\\ &- 15\cosh(x'+3x) - 15\cosh(3x'+x) + 9\cosh(3x'+3x) + \cosh(4x+4x')\\ &+ 39\cosh(x'-x) - 15\cosh(3x'-x) - \cosh(-4x+4x')\\ &- 46\cosh(-2x+2x') + 5\cosh(-4x+2x') + 5\cosh(-2x+4x')\\ &+ 9\cosh(3x'-3x) - 15\cosh(x'-3x)]/[100\cosh(x+x') + 50\cosh(x'+3x)\\ &+ 50\cosh(3x'+x) + 25\cosh(3x'+3x) + \cosh(5x+5x') + 5\cosh(5x+3x')\\ &+ 5\cosh(3x+5x') + 10\cosh(5x'+x) + 10\cosh(5x+x') + 100\cosh(x'-x)\\ &+ 50\cosh(3x'-x) + 25\cosh(3x'-3x) + 50\cosh(x'-3x) + \cosh(-5x+5x')\\ &+ 10\cosh(-x+5x') + 10\cosh(-5x+x') + 5\cosh(-5x+3x')\\ &+ 5\cosh(-3x+5x')]. \end{aligned} \tag{A.1}$$

Two points to be made concerning this density matrix are that (a) it reduces to equation (2.8) on the diagonal $x' = x$ and (b) it is an idempotent matrix.

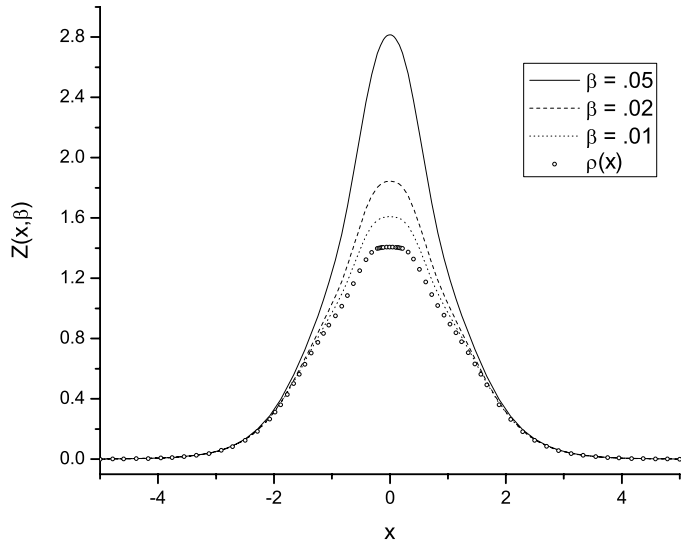

Figure 5. Slater sum $Z(x, \beta)$ over the bound states of the $\text{sech}^2(x)$ potential with $v = 4$, $n = 0-3$, plotted for several values of β. $Z(x, \beta)$ approaches the curve for the density as β decreases: here, the solid (top) curve is for $\beta = 0.05$, the second (dashed) is for $\beta = 0.02$ and the third (dots) for $\beta = 0.01$. The lowest curve (circles) is the density $\rho(x)$ itself. Hall's scaled units are used.

Appendix B. Bound-state Slater sum for two examples of the $\text{sech}^2(x)$ one-body potential

For the first case recorded in the main text for the $\text{sech}^2(x)$ potential, with $v = 4, n = 0 - 3$, we can sum over these bound states to find the Slater sum $Z(x, \beta)$ defined by

$$Z(x, \beta) = \sum_{\text{occupied bound states } i} \exp(-\beta\epsilon_i)|\psi_i(x)|^2, \tag{B.1}$$

where ϵ_i are the eigenvalues of the occupied states. Inserting these plus the corresponding eigenfunctions in equation (B.1) leads to explicit form (B.2):

$$\begin{aligned} Z(x, \beta) = \{&15.3125\exp(4\beta) + [-6.5625\exp(8\beta) - 15.3125 \\ &+ 1.093\,75\exp(15\beta)]\exp(\beta)\}\tanh^8(x) + \{-35\exp(4\beta) + [-4.375\exp(15\beta) \\ &+ 19.6875\exp(8\beta) + 28.4375]\exp(\beta)\}\tanh^6(x) + \{24.375\exp(4\beta) \\ &+ [6.5625\exp(15\beta) - 15.9375 - 19.6875\exp(8\beta)]\exp(\beta)\}\tanh^4(x) \\ &+ \{-5\exp(4\beta) + [2.8125 + 6.5625\exp(8\beta) \\ &- 4.375\exp(15\beta)]\exp(\beta)\}\tanh^2(x) \\ &+ 0.3125\exp(4\beta) + 1.093\,75\exp(16\beta). \end{aligned} \tag{B.2}$$

This is plotted for several values of β in figure 5. We see that it approaches the curve for the density: here (Hall's scaled units are used throughout this appendix), the solid (top) curve is Z for $\beta = 0.05$, the second (dashed) is for $\beta = 0.02$ and the third (dots) for $\beta = 0.01$. The lowest curve (circles) is the density $\rho(x)$ itself.

The same sum for the allowed bound states for the $v = 2, n = 0, 1$ case above gives

$$Z(x, \beta) = \{0.75[\tanh^4(x) - 2\tanh^2(x) + 1]\exp(3\beta) - 1.5\tanh^2(x)[\tanh^2(x) + 1]\}\exp(\beta), \tag{B.3}$$

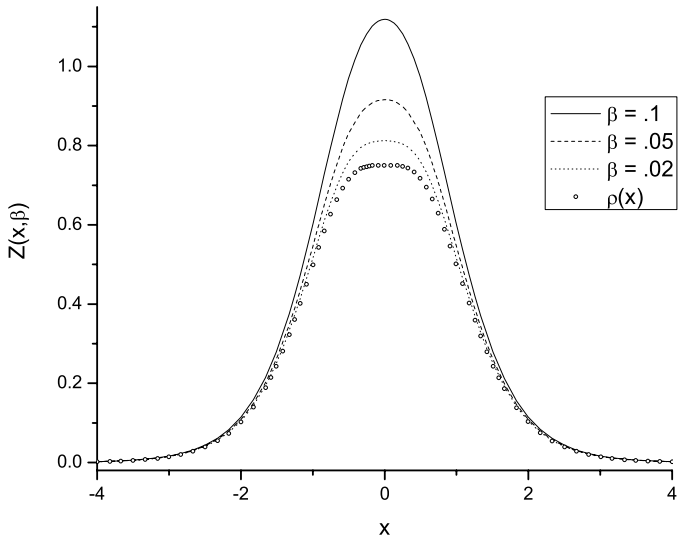

Figure 6. Slater sum $Z(x, \beta)$ for the bound states for the $v = 2, n = 0, 1$ case of the $\mathrm{sech}^2(x)$ potential: the top curve is for $\beta = 0.1$, the second (dashed) curve is for $\beta = 0.05$, while the third (dots) corresponds to $\beta = 0.02$. The lowest curve (circles) depicts the density $\rho(x)$. Hall's scaled units are used.

with a corresponding series of plots (figure 6) where the top curve is now for $\beta = 0.1$, the second (dashed) curve is for $\beta = 0.05$, while the third (dots) corresponds to $\beta = 0.02$. The lowest curve (circles) depicts the density $\rho(x)$. We also note that we can write the bound-state sum Z as a function(al) of ρ, when we obtain

$$Z[\rho] = \tfrac{3}{4}\big[\tfrac{7}{4} - \rho - 2\left(\tfrac{3}{4} - \rho\right)^{1/2}\big]\exp(3\beta) - \tfrac{3}{2}\left(\tfrac{3}{4} - \rho\right)^{1/2}\big[1 + \left(\tfrac{3}{4} - \rho\right)^{1/2}\big]\exp\beta. \tag{B.4}$$

It is true that the displayed eigenvalues in the exponential terms in equation (B.4) are naturally determined by the choice of one-body potential $V(x)$, or equivalently by the ground-state density $\rho(x)$. Both the Slater sum for $v = 2$ and $v = 4$ satisfy the differential equation

$$\frac{1}{4}\frac{\partial^3 Z}{\partial x^3} - \frac{\partial^2 Z}{\partial x \partial \beta} - V(x)\frac{\partial Z}{\partial x} - \frac{1}{2}\frac{\partial V}{\partial x}Z = 0. \tag{B.5}$$

Appendix C. Kinetic energy density of one-dimensional Fermi gas perturbed by potential $V(x)$

Stoddart and March [8] derived, for a localized potential $V(r)$ in three dimensions embedded in an initially uniform homogeneous electron gas, with density ρ_0 and kinetic energy density $t_0 = c_k \rho_0^{5/3}$, where $c_k = (3h^2/10m)(3/8\pi)^{2/3}$, an expression for the kinetic energy density change $t(\mathbf{r}) - t_0$, which had the form

$$t(\mathbf{r}) - t_0 = -V(\mathbf{r})\sum. \tag{C.1}$$

They obtained $\sum$ to all orders in V, but were not able to effect a summation analytically of this perturbation series.

A major advantage in one dimension is that March and Young [9] used the equation of motion of the density matrix $\gamma(x, x')$ to derive the differential form of the virial theorem,

quoted in equation (4.3). Assuming form (C.1) in one dimension also, we shall below derive a closed form for Σ. Writing $\Sigma = -(t - t_0)/V$, differentiating with respect to x, and using equation (4.3) readily yield

$$\Sigma' + \frac{1}{V(x)}\frac{\partial V(x)}{\partial x}\Sigma = \frac{\rho}{2}\frac{\partial \ln V}{\partial x} + \frac{\rho'''}{8V} \tag{C.2}$$

or equivalently

$$\frac{1}{V(x)}\frac{\partial(\Sigma V)}{\partial x} = \frac{\rho}{2}\frac{\partial \ln V}{\partial x} + \frac{\rho'''}{8V}. \tag{C.3}$$

Equation (C.3) then integrates to yield

$$\Sigma V = \frac{1}{2}\int^x V(s)\rho(s)\frac{\partial \ln V(s)}{\partial s}\,\mathrm{d}s + \frac{1}{8}\rho''(x). \tag{C.4}$$

Hence with the use of the differential form of the virial theorem in equation (C.2), which is however restricted to one dimension, the analogue of the three-dimensional result (C.1) can be formally summed to all orders to yield equation (4.5). However, this does not give the Legendre transform of $t(x)$ explicitly, after insertion in equation (4.4), since the density $\rho(x)$ is involved as well as the potential $V(x)$.

Appendix D. Results for the repulsive potential $\lambda\delta(x)$ and in particular for the integrated density of states $\rho(x, E)$ as a function of coupling strength λ

In [10] it was found that the Slater sum $Z(x, \beta)$ for the potential $\lambda\delta(x)$ was given by

$$\begin{aligned} Z(x,\beta) = {} & \frac{1}{\sqrt{2\pi\beta}} - \lambda\exp(\lambda^2\beta/2)\operatorname{erfc}(\lambda\sqrt{2\beta}/2) + \frac{\lambda}{2}\operatorname{erf}(x\sqrt{2/\beta}) \\ & + \frac{\lambda}{2}\exp(\lambda^2\beta/2)\exp(2\lambda|x|)\operatorname{erfc}\left(\sqrt{2\beta}\left(\frac{\lambda}{2} + |x|\right)\right). \end{aligned} \tag{D.1}$$

Taking the inverse Laplace transform of $Z(x, \beta)/\beta$, we can write the density $\rho(x, E)$ as

$$\begin{aligned} \rho(x,E) = {} & \frac{\sqrt{2E}}{\pi} + \frac{\lambda}{\pi}\operatorname{Si}(2x\sqrt{2E}) + \frac{2\lambda}{\pi}[\exp(2\lambda x)/2 - 1]\arctan(\sqrt{2E}/\lambda) \\ & - \lambda\exp(2\lambda x)\int_0^{2^{3/2}x/\pi}\exp\left(-\frac{k\lambda}{\sqrt{2}}\right)\frac{\sin(k\sqrt{E})}{k}. \end{aligned} \tag{D.2}$$

With this expression for $\rho(x, E)$, we obtain

$$\frac{\partial^2\rho}{\partial x\partial E} = \frac{-2\lambda^2\sqrt{E}\sin(2x\sqrt{2E}) + \lambda^3\sqrt{2}\cos(2x\sqrt{2E})}{\pi\sqrt{E}(2E + \lambda^2)}. \tag{D.3}$$

If we write this in the form

$$\frac{\partial^2\rho}{\partial x\partial E} = f_1\sin(2x\sqrt{2E}) + f_2\cos(2x\sqrt{2E}), \tag{D.4}$$

we have evidently then

$$f_1 = \frac{-2\lambda^2}{\pi(2E + \lambda^2)}, \qquad f_2 = \frac{\lambda^3\sqrt{2}}{\pi\sqrt{E}(2E + \lambda^2)}. \tag{D.5}$$

It follows that

$$\frac{\partial^2}{\partial x^2}\left[\frac{\partial^2\rho}{\partial x\partial E}\right] + 8E\left[\frac{\partial^2\rho}{\partial x\partial E}\right] = 0, \tag{D.6}$$

and equation (D.6) can then be integrated with respect to x to give

$$\frac{\partial^2}{\partial x^2}\left[\frac{\partial \rho}{\partial E}\right] + 8E\left[\frac{\partial \rho}{\partial E}\right] - g(E) = 0, \tag{D.7}$$

or with respect to E, to give

$$\frac{\partial^3 \rho}{\partial x^3} + 8\int E\left[\frac{\partial^2 \rho}{\partial x \partial E}\right] \mathrm{d}E = h(x), \tag{D.8}$$

with $g(E)$ and $h(x)$ being unknown functions. However, $g(E)$ can be evaluated directly, using the expression for ρ, to give

$$g(E) = \frac{4\sqrt{2E}(2E - \lambda^2)}{\pi(2E + \lambda^2)}. \tag{D.9}$$

Recourse to the differential virial theorem (4.3) will allow the kinetic energy per unit length $t(x, E, \lambda)$ to be studied, but we shall not elaborate on the details.

References

[1] Slater J C 1951 *Phys. Rev.* **81** 385
[2] Kohn W and Sham L J 1965 *Phys. Rev.* A **140** 1133
[3] Dirac P A M 1930 *Proc. Camb. Phil. Soc.* **26** 376
[4] March N H and Young W H 1958 *Proc. Phys. Soc.* **72** 182
[5] Hall R L 1995 *Phys. Rev.* A **51** 1787
[6] Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* (New York: Dover) chapter 8
[7] March N H and Murray A M 1961 *Proc. R. Soc.* A **261** 119
[8] Stoddart J C and March N H 1967 *Proc. R. Soc.* A **299** 279
[9] March N H and Young W H 1959 *Nucl. Phys.* **12** 237
[10] Howard I A, March N H and Echenique P M 2003 *J. Phys. A.: Math. Gen.* **36** 11451