A long-term objective of density functional theory (DFT) has been to obtain the electronic kinetic energy density directly from the ground-state density, without recourse to wave functions. This is the more important in relativistic DFT since Dirac wave functions have four components. The above aim is here achieved for the admittedly specialized square barrier model of a one-dimensional inhomogeneous electron liquid.
1 Introduction

Density functional theory (DFT), having its origins in the pioneering studies of Thomas\(^1\), Fermi\(^2\) and Dirac\(^3,4\) and being formally completed by the theorem of Hohenberg and Kohn\(^5\), seeks to express the ground-state energy of an \(N\)-electron assembly as a functional of the electron density \(\rho\). One part of such a functional is the single-particle kinetic energy \(T[\rho]\), which is widely used in current applications of DFT, following the work of Slater\(^6\), which was formalized in the later study of Kohn and Sham\(^7\).

Though most applications at the present time return to one-electron wave functions (the so-called Slater-Kohn-Sham (SKS) orbitals) to calculate the single-particle kinetic energy \(T\), it is widely recognized that ‘orbital-free’ theory affords a very desirable longer-term objective\(^8\).

This situation is the more important in relativistic DFT, our dominant concern here, since in contrast to Schrödinger (or SKS) wave functions, Dirac spinors have four components. Hence to work with the ground-state density \(\rho\) alone, without recourse to individual Dirac one-electron wave functions, is an extremely attractive prospect for the future.

This is the motivation for the present study, but because of the complexity of the problem we shall approach the task of calculating the (single-particle) kinetic energy from the ground-state density via an admittedly very specialized model. This is chosen here as the square barrier model of a one-dimensional inhomogeneous electron liquid. Appeal can then be made to an earlier investigation of Baltin and March\(^9\), in which separate expressions were obtained for the kinetic energy per unit length (‘density’ in one-dimension) \(t(z)\), and for the ground-state electron density \(\rho(z)\).

2 Summary of non-relativistic results for kinetic energy and electron density of a semi-infinite electron liquid in \(d\) dimensions

Before appealing to this relativistic study of Baltin and March\(^9\) for a finite square barrier, of height \(V_0\) say, it will be useful for what follows to summarize earlier work in this Journal by the present writer\(^10\) pertaining to semi-infinite electron liquids in Schrödinger wave mechanics: i.e. in the limit when the barrier height \(V_0\) tends to infinity, but now in \(d\) dimensions. The passage to the limit \(V_0 \to \infty\) is straightforward in non-relativistic theory, as this theory already corresponds to the limiting case \(c \to \infty\), \(c\) being the velocity of light. As further emphasized below, one has to compare \(V_0\) with \(mc^2\) in relativistic theory, \(m\) being the rest mass of the electron. Then, one must take first the limit \(c \to \infty\), before proceeding to the infinite barrier case.

For this non-relativistic model when \(V_0 \to \infty\), the resulting semi-infinite electron liquid problem was solved by the writer\(^10\) in \(d\) dimensions. For singly occupied levels, the density
\( \rho_d(z) \) was then obtained as

\[
\rho_d(z) = \frac{k_f^d}{2\pi^{(d+1)/2}\frac{d}{2}} - \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{(2\pi)^{d/2}} \frac{j_{d-1/2}(2k_fz)}{2k_fz^{(d-1)/2}}
\]

where \( k_f \) is the Fermi wave number. This result (2.1), with \( j \) denoting the appropriate spherical Bessel function, is valid for \( d \) odd; if \( d \) even is needed then \( \rho_e(z) \) etc. can be calculated in terms of Bessel functions of a purely imaginary argument\(^{10}\).

The corresponding result for the kinetic energy density \( t_d(z) \) will also be quoted here, again for \( d \) odd\(^{10}\):

\[
t_d(z) = t_{d0} + \frac{k_f^d}{2} \left[ \rho_d(z) - \rho_{d0} \right] + \frac{k_f^d}{2\pi^2(2\pi)^{(d-3)/2}} \frac{j_{d-1/2}(2k_fz)}{(2k_fz)^{(d+1)/2}}
\]

where \( t_{d0} \) is the kinetic energy density of the homogeneous electron liquid of number density \( \rho_{d0} \). These non-relativistic results (2.1) and (2.2) will be appealed to later. Before that, the finite square barrier model will be treated in one-dimension, but now via Dirac’s relativistic wave equation.

### 3 Relation between kinetic energy and electron densities in square barrier model of a one-dimensional inhomogeneous electron liquid treated relativistically

To the writer’s knowledge, results for \( \rho_d(z) \) and \( t_d(z) \) for the finite square barrier model via the Dirac equation have, as yet, only been obtained for the one-dimensional (\( d = 1 \)) case\(^9\). This study of Baltin and March gives \( t_1(z) \) and \( \rho_1(z) \) quite explicitly, for a finite square barrier of height \( V_0 \) and, as already anticipated in section 2 above, the ratio \( V_0/mc^2 \equiv \nu \) plays a significant role.

Their results for \( t_1(z) \) and \( \rho_1(z) \) are written as integrals over a variable \( \tau \) running from 0 to \( \tau_f \), where \( \tau = \hbar k/mc \). The result for \( \rho_1(z) \) will be written only for the region inside the containing energy barrier of height \( V_0 \), where the inhomogeneity in density disappears sufficiently far into the bulk electron liquid of uniform density \( \rho_{10} \) say. The form of \( \rho_1(z) \) is then subsumed in the dimensionless ‘displaced charge’ \( \Delta_1(z) \) (see eqn.(A1) with \( d = 1 \)), which is given by\(^9\)

\[
2\nu \tau_f \Delta_1(z) = \int_0^{\tau_f} \left( \frac{\tau^2}{\omega} - 2\nu \right) \cos(2\tau \zeta)d\tau + \int_0^{\tau_f} \left[ 1 - (\omega - 2\nu)^2 \right]^{1/2} \frac{\sin(2\tau \zeta)}{\omega} \frac{d\tau}{\tau}
\]

where \( \omega = (1 + \tau^2)^{1/2} \) and \( \zeta = \left( \frac{mc}{\hbar} \right) z \).

The corresponding result for the kinetic energy density \( t_1(z) \) is usefully expressed by writing

\[
t_1(z, k_f) = t^{\text{homo}}(k_f) + t^{\text{osc}}(z, k_f)
\]

3
where the oscillatory contribution $t^{osc}$ has the form:

$$t^{osc}(z,k_f) = \left(\frac{mc}{\pi\hbar}\right)\frac{mc^2}{\nu} \left[\int_0^{\tau_f} \cos(2\tau\zeta)(\omega - 1) \left(\frac{\tau^2}{\omega^2} - 2\nu\right) d\tau + \int_0^{\tau_f} \frac{\tau \sin(2\tau\zeta)}{\omega} \left[1 - (\omega - 2\nu)^2\right]^{1/2} d\tau \right]$$

(3.3)

and $\rho_{homo}$ is the homogeneous electron liquid kinetic energy density.

The basic step in relating eqns.(3.1) and (3.3) is now to differentiate both expressions with respect to $\tau_f$, to find first of all for the electron density the result

$$\frac{\partial}{\partial \tau_f} (2\nu \tau_f \Delta_1(z)) = \left(\frac{\tau_f^2}{\omega_f^2} - 2\nu\right) \cos(2\tau_f\zeta) + \left[1 - (\omega_f - 2\nu)^2\right]^{1/2} \tau_f \frac{\sin(2\tau_f\zeta)}{\omega_f}$$

(3.4)

By a similar procedure, one can derive from eqn.(3.3) the result

$$\frac{\pi h}{mc} \left(\frac{\nu}{mc^2}\right) \frac{\partial t^{osc}(z,k_f)}{\partial \tau_f} = (\omega_f - 1) \left(\frac{\tau_f^2}{\omega_f^2} - 2\nu\right) \cos(2\tau_f\zeta)$$

$$+ \left[1 - (\omega_f - 2\nu)^2\right]^{1/2} \tau_f \sin(2\tau_f\zeta).$$

(3.5)

If one now multiplies eqn.(3.4) throughout by $(\omega_f - 1)$ and subtracts from eqn.(3.5), the remarkably simple relation

$$\left[\frac{\pi h}{m^2c^3}\right] \frac{\partial t^{osc}(z,k_f)}{\partial \tau_f} = 2(\omega_f - 1) \left[\tau_f \frac{\partial \Delta_1(z)}{\partial \tau_f} + \Delta_1(z)\right]$$

(3.6)

emerges. Furthermore, it must be stressed that $\nu = V_0/mc^2$ has disappeared explicitly from the relation (3.6), even though, of course, $t^{osc}(z,k_f)$ and $\Delta_1(z)$ separately depend on the choice of barrier height. It is worthwhile, for taking the non-relativistic limit of eqn.(3.6), to use the definition of $\omega$ immediately below eqn.(3.1) to write

$$(\omega_f - 1) = \tau_f^2/(\omega_f + 1).$$

(3.7)

hence, using eqn.(3.7) in eqn.(3.6):

$$\frac{\pi h}{m^2c^3} (\omega_f + 1) \frac{\partial t^{osc}(z,k_f)}{\partial \tau_f} = 2\tau_f^2 \left[\tau_f \frac{\partial \Delta_1(z)}{\partial \tau_f} + \Delta_1(z)\right].$$

(3.8)

This eqn.(3.8) is then the desired connection between kinetic energy and electron densities in this square barrier model of an inhomogeneous relativistic electron liquid.

To compare this exact result (3.8) derived via Dirac’s relativistic wave equation, with a non-relativistic (nr) Schrödinger counterpart, let us next note that $\omega_f \to 1$ as the velocity of light $c$ is allowed to tend to infinity. Then, replacing $\tau_f$ in eqn.(3.8) in favour of $k_f$, one finds the non-relativistic limit to be

$$\frac{\partial t^{osc}_{nr}(z)}{\partial k_f} = \frac{\hbar^2 k_f^2}{\pi m} \left[k_f \frac{\partial \Delta_1^{nr}(z)}{\partial k_f} + \Delta_1^{nr}(z)\right].$$

(3.9)

To conclude this section, let us check eqn.(3.9) in the infinite barrier non-relativistic limit.
3.1 Non-relativistic infinite barrier limit

One has almost immediately the dimensionless displaced charge in terms of the zero-order spherical Bessel function $j_0(x) = \sin x / x$ (compare eqn.(2.1)):

$$\Delta^{nr}_1(z) = -j_0(2k_f z) .$$  \hspace{1cm} (3.10)

The corresponding result for the non-relativistic kinetic energy in the same limit is given by

$$t^{nr}_{ec}(z) = \frac{k_f^3}{\pi} [\Delta^{nr}_1(z)] + \frac{2k_f^3}{\pi} \frac{j_1(2k_f z)}{2k_f z} .$$  \hspace{1cm} (3.11)

where the first-order spherical Bessel function $j_1(x)$ is simply $[\sin x - x \cos x] / x^2$. But now one has the mathematical identity

$$\frac{d}{dx} j_0(x) = -j_1(x) .$$  \hspace{1cm} (3.12)

Combining eqns.(3.10) and (3.12) immediately yields

$$j_1(2k_f z) = \frac{d}{d(2k_f z)} \Delta^{nr}_1(z) ,$$  \hspace{1cm} (3.13)

and hence one can substitute for $j_1(2k_f z)$ in eqn.(3.11) to obtain

$$t^{nr}_{ec}(z) = \frac{k_f^3}{\pi} \Delta^{nr}_1(z) + \frac{k_f z}{2\pi z} \frac{\partial}{\partial z} \Delta^{nr}_1(z) .$$  \hspace{1cm} (3.14)

Introducing the dimensionless change $\Delta t^{nr}(r)$ in the kinetic energy density induced by the barrier, defined by

$$\Delta t^{nr}(z) = t^{nr}_{ec}(z)/t_{10}$$  \hspace{1cm} (3.15)

and noting that the homogeneous electron liquid has $t_{10} = k_f^3/3\pi$ for the doubly filled level case under consideration, eqn.(3.14) is readily rewritten as

$$\Delta t^{nr}(z) = 3\Delta^{nr}_1(z) + \frac{3}{2k_f^2 z} \frac{\partial}{\partial z} \Delta^{nr}_1(z) .$$  \hspace{1cm} (3.16)

the $d$-dimensional generalization of this equation, using the results of section 2, being recorded in Appendix 1. It is worth stressing here that in non-relativistic theory, eqn.(3.16) affords a direct route to calculate the kinetic energy density from the ground-state electron density. In contrast, the relativistic theory of the inhomogeneous electron liquid generated by the one-dimensional square barrier model has the non-relativistic limit (3.9). It is apparent that, to check eqn.(3.9) in the infinite barrier limit, the LHS can be evaluated directly by inserting eqn.(3.11) while the RHS is determined solely by use of eqn.(3.10) for the displaced charge.

Taking first the RHS of eqn.(3.9), one readily obtains by using eqn.(3.12) the result

$$RHS = \frac{\hbar^2}{m} \left[ \frac{k_f^2}{\pi} j_0(2k_f z) + \frac{2k_f^3}{\pi} j_1(2k_f z) \right] .$$  \hspace{1cm} (3.17)
Turning to the evaluation of the LHS of eqn.(3.9), let us first insert eqn.(3.15) to find

\[
\left( \frac{m}{\hbar^2} \right) \frac{\partial}{\partial k_f} t_{\text{nr}}^{\text{osc}}(z) = k_f^2 \frac{1}{\pi} \Delta t_{\text{nr}}(z) + \frac{k_f^3}{3\pi} \frac{\partial \Delta t_{\text{nr}}(z)}{\partial k_f} .
\]  

(3.18)

One must now use the result (3.16) for \( \Delta t_{\text{nr}}(z) \) in eqn.(3.18). Some intermediate steps are supplied in Appendix 2, where two mathematical identities relating spherical Bessel functions, and their derivatives, of different orders are invoked. The first term on the RHS of eqn.(3.18) is then easily written in terms of \( j_0 \) and \( j_1 \) which are already present in eqn.(3.17):

\[
\frac{k_f^2}{\pi} \Delta t_{\text{nr}}(z) = \frac{3k_f^2}{\pi} j_0(2k_f z) + \frac{3k_f}{\pi z} j_1(2k_f z) .
\]  

(3.19)

The evaluation of the second term on the RHS of eqn.(3.18) after inserting eqn.(3.16) evidently involves second derivatives of \( j_0(x) \). After invoking the mathematical identities already referred to one finds (see Appendix 2)

\[
\frac{k_f^3}{3\pi} \frac{\partial \Delta t_{\text{nr}}(z)}{\partial k_f} = \frac{2k_f^2}{\pi} j_0(2k_f z) - \frac{3k_f}{\pi z} j_1(2k_f z) + \frac{2k_f^3}{\pi} j_1(2k_f z) .
\]  

(3.20)

after removing \( j_2(x) \) in favour of \( j_0 \) and \( j_1 \). Adding eqns.(3.19) and (3.20) leads back precisely to the quantity in the square bracket of eqn.(3.17). Thus, eqn.(3.9) is verified to hold in the limiting case of an infinite barrier.

4 Summary and future directions

For the finite square barrier model, solved via Dirac’s relativistic wave equation in the one-dimensional case, it has been demonstrated that the kinetic energy density and the ground-state electron density are related through eqn.(3.8). This finding is in the spirit of relativistic DFT, in which the calculation of the kinetic energy density directly from the electron density is a major aim, thereby avoiding four-component Dirac wave functions. Of course, it is recognized that eqn.(3.8) has been derived for a pretty specialized model, but it should be reiterated that in the relation (3.8) the barrier height has disappeared, even though the electron density and kinetic energy separately depend on \( V_0/mc^2 \).

It has then been shown that the non-relativistic limit of (3.9) can be checked for the infinite barrier model, where it emerges that kinetic and electron densities are related directly by eqn.(3.16), the \( d \)-dimensional version of which has also been derived in Appendix 1. Derivatives of eqn.(3.16) with respect to the Fermi wavenumber \( k_f \) lead back, after some manipulation, to eqn.(3.9).

In view of the above findings, it would seem to be of interest for the future if the results of Baltin and March on the one-dimensional relativistic square barrier model could be generalized to three dimensions using the Dirac equation. Such a generalization has already been given by these authors for (two and) three dimensions in the homogeneous electron liquid.
Acknowledgments

The writer is most grateful to Professor V.E. Van Doren for much support and encouragement and to Professor Yu Lu for generous hospitality at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy. It is pleasure also to thank Professor A. Holas for numerous valuable discussions over a long period on the general area embraced by the present study.

Appendix 1

d-dimensional generalization of non-relativistic relation between kinetic energy and electron densities for semi-infinite electron liquids

The purpose of this Appendix is to generalize the non-relativistic one-dimensional relation (3.16) between kinetic energy and electron densities to d dimensions. Eqns.(2.1) and (2.2) then afford the appropriate starting point.

Defining the dimensionless quantities

\[ A_{d}(z) = \frac{t_{d}(z) - t_{d0}}{t_{d0}}, \quad \Delta_{d}(z) = \frac{\rho_{d}(z) - \rho_{d0}}{\rho_{d0}}, \]

eqn.(2.1), valid for d odd, takes the form

\[ \Delta_{d}(z) = -2^{(d+1)/2} \left( \frac{1}{2}, \frac{3}{2}, \ldots, \frac{d}{2} \right) \frac{j_{(d-1)/2}(2kfz)}{(2kfz)^{(d-1)/2}}. \]

To relate this d dimensional expression to eqn.(3.11) of the main text, let us put d = 1 in eqn.(A1.2), when the spherical Bessel function part reduces to \( j_{0}(2kfz) \) while the multiplying constant is simply \((-1)\).

Turning to the d dimensional kinetic energy density and using the dimensionless ratio \( \Delta_{d} \) defined in eqn.(A1.1), one obtains

\[ \Delta_{d}(z) = \frac{k_{f}^{2} \rho_{d0}}{2 t_{d0}} \Delta_{d}(z) + \frac{k^{d+2}}{(2\pi)^{(d-3)/2} t_{d0}} \frac{j_{(d+1)/2}(2kfz)}{(2kfz)^{(d+1)/2}}. \]

One can readily calculate the ratio \( \rho_{d0}/t_{d0} \) appearing in eqn.(A1.3) from the results of ref.10 as

\[ \frac{\rho_{d0}}{t_{d0}} = \frac{2}{k_{f}^{2}} \left( \frac{d + 2}{d} \right), \]

and therefore the first term on the RHS of eqn.(A1.3) is simply \( \{(d + 2)/d\} \Delta_{d}(z) \), which again checks with the result for \( d = 1 \) in eqn.(3.16).

Thus it only remains to relate the final terms in eqn.(A1.3) to eqn.(A1.2). Using once again the identity (3.21), but now with \( \ell + 1 = (d + 1)/2 \) for d odd, one has immediately

\[ \frac{j_{(d+1)/2}(2kfz)}{(2kfz)^{(d-1)/2}} = \frac{1}{2k_{f}} \frac{\partial}{\partial z} \left[ \frac{j_{(d-1)/2}(2kfz)}{(2kfz)^{(d-1)/2}} \right]. \]
Substituting this result for $j_{(d+1)/2}$ in eqn.(A1.3) then leads to

$$\Delta t_d(z) = \left(\frac{d+2}{d}\right) \Delta_d(z) - \frac{k_f^{d+2}}{(2\pi^2)(2\pi)^{(d-3)/2}} \frac{1}{t_{d0}} \frac{1}{4k_f^2z}$$

\[ \times \frac{\partial}{\partial z} \left[ j_{(d-1)/2}(2k_fz) \right]. \quad (A1.6) \]

Differentiating eqn.(2.1) with respect to $z$ then allows the final term of eqn.(A1.6) to be replaced in favour of the derivative $\frac{\partial}{\partial z} \Delta_d(z)$. Using eqn.(2.1), in which the first term on the RHS is $\rho_{d0}$, and eqn.(A1.4), one can eliminate $t_{d0}$ from eqn.(A1.6) to obtain

$$\Delta t_d(z) = \left(\frac{d+2}{d}\right) \left[ \Delta_d(z) + \frac{1}{2k_f^2z} \frac{\partial \Delta_d(z)}{\partial z} \right]. \quad (A1.7)$$

This is the desired non-relativistic $d$ dimensional relation between kinetic energy and electron densities in this class of models. It immediately reduces to eqn.(3.16) of the main text in the special case when $d = 1$.

### Appendix 2

**Some details of derivation of eqn.(3.20) of main text**

This Appendix will supply some details used in obtaining eqn.(3.20) of the main text. Into the LHS, one first inserts the result (3.16) and then utilizes eqn.(3.13). In terms of the spherical Bessel function $j_1$, one then finds after a short calculation:

$$\frac{k_f^3}{3\pi} \frac{\partial}{\partial k_f} \Delta_{nr}(z) = \left[ \frac{2k_f^3z}{\pi} - \frac{k_f}{\pi z} \right] j_1(2k_fz) + \frac{2k_f^2}{\pi} j_1'(2k_fz). \quad (A2.1)$$

For the derivative $j_1'$, one now appeals to the mathematical identity\(^{11}\)

$$\frac{d}{dx} [x^{-\ell}j_k(x)] = -x^{-\ell}j_{k+1}(x) \quad (A2.2)$$

with $\ell = 1$, and evidently $j_2(2k_fz)$ then enters eqn.(A2.1). This equation then can be re-expressed readily as

$$\frac{k_f^3}{3\pi} \frac{\partial}{\partial k_f} \Delta_{nr}(z) = \frac{2k_f^3z}{\pi} j_1(2k_fz) - \frac{2k_f^2}{\pi} j_2(2k_fz). \quad (A2.3)$$

But one has the further identity\(^{11}\)

$$j_{k-1}(x) + j_{k+1}(x) = \frac{(2\ell + 1)}{x} j_k(x) \quad (A2.4)$$

and putting $\ell = 1, j_2(2k_fz)$ can be removed from eqn.(A2.3) in favour of $j_0$ and $j_1$. The resulting equation is identical to eqn.(3.20). Using this equation together with eqns.(3.19) and (3.17) verifies eqn.(3.9) for the infinite barrier model.
References


2 E. Fermi, Zeits für Phys. 48, 73 (1928).


11 See, for example, L.I. Schiff, Quantum Mechanics (McGraw-Hill, New York, 1955), 2nd ed., p.79.