

also

$$\bar{\gamma} = -\alpha^{q_1} \alpha^{q_2}. \quad (69)$$

In (63) eingesetzt:

$$\bar{\lambda}_{p_1 p_2} = \alpha_{p_1} \alpha_{p_2} \alpha^{q_1} \alpha^{q_2} D^{-1} (\varepsilon + i o) (p_{10} + p_{20} - \varepsilon - i o)^{-1}. \quad (70)$$

In der Tat ist dann wegen (62) die Gl. (69) erfüllt. Damit ist λ völlig bestimmt. Es folgt:

¹ T. D. LEE, Phys. Rev. **95**, 1329 [1954].

² G. KÄLLÉN u. W. PAULI, Kgl. Danske Vidensk. Selskab, Mat.-Fys. Medd. **30**, 7 [1955].

³ R. D. AMADO u. R. P. KENSCHAF, J. Math. Phys. **5**, 1340 [1964].

⁴ A. PAGNAMENTA, J. Math. Phys. **6**, 955 [1965]; **7**, 356 [1966].

⁵ C. M. SOMMERFIELD, J. Math. Phys. **6**, 1170 [1965].

$$\psi^{q_1 q_2} = \chi^{q_1 q_2} + \alpha^{q_1} \alpha^{q_2} D^{-1} (q_{10} + q_{20} + i o) \int dp_1 dp_2 \alpha_{p_1} \alpha_{p_2} \chi^{p_1 p_2} (p_{10} + p_{20} - q_{10} - q_{20} - i o)^{-1}. \quad (71)$$

Wie in ¹² gezeigt wird, ist $\psi^{q_1 q_2}$ tatsächlich eine Lösung der Schrödinger-Gleichung. Im Falle eines instabilen V -Teilchens stellen die $\psi^{q_1 q_2}$ ein vollständiges orthonormiertes System im $N\Theta\Theta$ -Sektor dar.

⁶ E. KAZES, J. Math. Phys. **6**, 1172 [1965].

⁷ J. C. HOUARD, Ann. Inst. Henri Poincaré A II, 105 [1965].

⁸ G. L. TINDLE, Nuovo Cim. A **45**, 619 [1966].

⁹ D. I. FIVEL, J. Math. Phys. **11**, 699 [1970].

¹⁰ M. BOLSTERLI, Phys. Rev. **166**, 1760 [1968].

¹¹ H. v. DEWITZ u. K. HELMERS, Z. Naturforsch. **26 a**, 4 [1971].

¹² H. v. DEWITZ, Diplomarbeit.

The Energy-Density Functional of an Electron Gas in Locally Linear Approximation of the One-Body Potential *

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For a system of independent electrons moving in a common one-body potential $V(\mathbf{r})$ an integral representation of Dirac's density matrix is evaluated in the approximation that $V(\mathbf{r})$ at the point \mathbf{r} is replaced by a linear potential with a gradient equal to the gradient of V at \mathbf{r} . The particle density ρ , $\nabla \rho$ and the kinetic-energy density ε_k are derived from the density matrix. After eliminating the potential and its gradient a parametric representation for ε_k in terms of ρ and $y \equiv |\nabla \rho|^{1/2} \rho^{-2/3}$ is obtained. Explicit analytical expressions are given in the limits $y \rightarrow 0$ and $y \rightarrow \infty$ and compared with the inhomogeneity corrections of Kirzhnits and v. Weizsäcker.

1. Introduction

According to the original Thomas-Fermi theory the kinetic-energy density ε_k of electrons with particle density ρ moving independently in a common effective one-body potential $V(\mathbf{r})$ is given by

$$\varepsilon_k = \kappa \rho^{5/3} \quad [\kappa = 0.3 (3 \pi^2)^{2/3} \hbar^2 / m].$$

As is well-known, this relation is an insufficient approximation either when the potential varies rapidly in space or when the density is very low. For the general case of an inhomogeneous electron gas, Hohenberg and Kohn¹ have shown that the ground state kinetic energy is a unique functional of ρ whether or not the electrons are interacting. However, it seems difficult to gain valid explicit approximations to this functional beyond the TF-term.

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* Extracted from the author's doctoral thesis (D 84).

In a rather intuitive approach, v. WEIZSÄCKER² introduced an additive correction term $\sim (\nabla \rho)^2 / \rho$ to $\varepsilon_k^{\text{TF}}$ whereby qualitative improvements could be achieved. However, application to some specific potentials yields too high ground state energies³⁻⁵.

A systematic investigation of KIRZHITS⁶ starting from a reformulation of the Hartree-Fock equations in terms of Dirac's density matrix and expanding the latter in a power series of \hbar came to the result that for weak inhomogeneity the Weizsäcker correction term should be multiplied by a factor of $\gamma = 1/9$. Other authors⁷⁻⁹ using similar methods obtain the same factor. GOLDEN¹⁰ finds $\gamma = 13/45$. Using semiclassical arguments GOMBÁS¹¹⁻¹³ claims that not the Weizsäcker term but the TF term should be corrected by a factor dependent upon the number of electrons.

Several authors¹⁴⁻¹⁶ have pointed out that Kirzhnits' series expansion doesn't take into account the nonanalytical behaviour of Dirac's density matrix



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with respect to \hbar . Consequently, quantum oscillations are missing in that treatment. Furthermore, the Kirzhnits series appears to be merely asymptotic.

Concerning applications of the Kirzhnits correction, calculations of total energies of atoms¹⁷ and other atomic properties¹⁸ lead to rather disappointing results. Recently, JONES and YOUNG¹⁹ showed that in the case of a weakly perturbed extended system of noninteracting fermions the correct ground state energy is obtained if for very small perturbation wavelength the full Weizsäcker functional and for very large wavelength the Kirzhnits functional is used.

Starting from a free electron gas, STODDART and MARCH²⁰ have established a functional by perturbation theory to infinite order. Unfortunately, their expression is difficult to evaluate.

In the present paper, the author has treated this problem from a point of view somewhat different from previous work on this subject.

In deriving ϵ_k^{TF} it has been assumed that the whole space may be divided into volume cells each of which containing many electrons, but being yet so small that the potential inside a single cell can be replaced by a mean value V_0 . In this approximation the electrons in each cell are free and therefore occupy the planewave states of a local Fermi sphere whence the above expression for ϵ_k^{TF} is obtained after V_0 has been eliminated. As next approximation, it seems reasonable now to replace the potential in the cell by a linear one which has the same value and the same gradient as V at some point \mathbf{r}_0 within the cell. This approximation which has already been used by SWIATECKI²¹ for calculation of ϱ shall be adopted here in order to derive the energy-density functional. No further approximation shall be made. The plan of the work is as follows:

In Sect. 2 an integral representation of Dirac's density matrix $\varrho(\mathbf{r}, \mathbf{r}')$ is introduced which is evaluated in Sect. 3 after using the approximation described. In Sect. 4 ϱ and $\nabla\varrho$ are calculated from $\varrho(\mathbf{r}, \mathbf{r}')$ as functions of $\lambda - V(\mathbf{r})$ and $\nabla V(\mathbf{r})$ where λ is a constant necessary for normalizing ϱ . In Sect. 5 from $\varrho(\mathbf{r}, \mathbf{r}')$ the kinetic-energy density is obtained depending likewise upon $\lambda - V$ and ∇V . Eliminating the latter quantities by means of ϱ and $\nabla\varrho$ we arrive at a parametric representation of $\epsilon_k(\varrho, \nabla\varrho)$ which is evaluated numerically for general values in Section 6. In the limits $\varrho^{-1/3} |\nabla\varrho|^{1/3} \ll 1$ and $\gg 1$ explicit analytical expressions of ϵ_k can be given

(Sect. 7). In the last section the results are discussed.

2. Dirac's Density Matrix in Integral Representation

Let us consider the ground state of an electron gas in Hartree-approximation where each electron (position vector \mathbf{r}) is assumed to move independently in a selfconsistent one-body potential $V(\mathbf{r})$. Then the state function of the whole system is a Slater determinant made up of one-electron wave functions obeying the Schrödinger equation

$$\hat{H} \psi_{n,\mu}(\mathbf{r}) = \epsilon_n \psi_{n,\mu}(\mathbf{r}), \quad n = 1, 2, \dots \quad (2.1)$$

with

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} + V(\mathbf{r}). \quad (2.2)$$

For simplicity, the spectrum is assumed to be discrete, so the energy levels may be labelled in ascending order, i. e., $\epsilon_1 < \epsilon_2 < \epsilon_3 \dots$. The index μ allows for distinction between wave functions belonging to a degenerate level. The $\psi_{n,\mu}$'s are supposed to satisfy the conditions of orthonormality and completeness. Let the level ϵ_n be $m(n)$ -fold degenerate. Then Dirac's density matrix is defined as

$$\varrho(\mathbf{r}, \mathbf{r}') = 2 \sum_{n=1}^{\infty} \sum_{\mu=1}^{m(n)} \psi_{n,\mu}^*(\mathbf{r}') \psi_{n,\mu}(\mathbf{r}). \quad (2.3)$$

In the ground state the electron density is given by $\varrho(\mathbf{r}, \mathbf{r})$ when all levels are occupied up to ϵ_n . Following the work of ALFRED²² and MACKIE and RENNERT²³ we now use an integral representation of $\varrho(\mathbf{r}, \mathbf{r}')$ where the individual wave functions are eliminated. By means of the step function $\theta(u)$ we can write

$$\varrho(\mathbf{r}, \mathbf{r}') = 2 \sum_{n=1}^{\infty} \sum_{\mu=1}^{m(n)} \theta(\lambda - \epsilon_n) \psi_{n,\mu}^*(\mathbf{r}') \psi_{n,\mu}(\mathbf{r}) \quad (2.4)$$

where the parameter λ satisfies the inequality

$$\epsilon_n < \lambda < \epsilon_{n+1}. \quad (2.5)$$

Since the $\psi_{n,\mu}$ are eigenfunctions of the real operator \hat{H} we may write

$$\begin{aligned} \theta(\lambda - \epsilon_n) \psi_{n,\mu}^*(\mathbf{r}') \psi_{n,\mu}(\mathbf{r}) \\ = \theta[\lambda - \tfrac{1}{2}(\hat{H} + \hat{H}')] \psi_{n,\mu}^*(\mathbf{r}') \psi_{n,\mu}(\mathbf{r}) \end{aligned} \quad (2.6)$$

where \hat{H}' acts upon functions of \mathbf{r}' .

Inserting this expression which is symmetric with respect to interchange of \mathbf{r} and \mathbf{r}' into Eq. (2.4) we are able to take the operator function out of the summation signs and to apply the closure condition

$$\varrho(\mathbf{r}, \mathbf{r}') = 2\theta[\lambda - \frac{1}{2}(\hat{H} + \hat{H}')] \delta(\mathbf{r} - \mathbf{r}'). \quad (2.7)$$

Using the well-known representations for $\theta(u)$ and for the δ -function

$$\theta(u) = \frac{1}{2\pi i} \int_{-\infty - i\eta}^{\infty - i\eta} \frac{d\omega}{\omega} e^{i\omega u}, \quad (2.8)$$

η being a positive infinitesimal, and

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{(2\pi)^3} \int_{-\infty}^{+\infty} d^3\mathbf{k} \cdot \exp\{-i\mathbf{k}(\mathbf{r} - \mathbf{r}')\} \quad (2.9)$$

we obtain

$$\varrho(\mathbf{r}, \mathbf{r}') = \frac{1}{i\pi(2\pi)^3} \int_{-\infty - i\eta}^{+\infty - i\eta} \frac{d\omega}{\omega} \int_{-\infty}^{+\infty} d^3\mathbf{k} \cdot \exp\{i\omega(\lambda - \frac{1}{2}[\hat{H} + \hat{H}'])\} \exp\{i\mathbf{k}(\mathbf{r}' - \mathbf{r})\}. \quad (2.10)$$

So we have shifted the problem of calculating and summing wave functions to the problem of evaluating and integrating an exponential operator acting upon a plane wave.

3. Density Matrix in locally linear Approximation of the Potential

For general $V(\mathbf{r})$ expression (2.10) can be evaluated only approximately because the kinetic energy operator $\hat{T} = (1/2m)\hat{p}^2$ and the potential do not commute. To proceed further we shall make an approximation to $V(\mathbf{r})$. Let us start with a Taylor series expansion of $V(\mathbf{r})$ about a fixed point

$$\mathbf{r}_0 = (x_1^{(0)}, x_2^{(0)}, x_3^{(0)})$$

and break off after the gradient term:

$$V(\mathbf{r}) \approx \bar{V}(\mathbf{r}_0) + \mathbf{r} \cdot \nabla V(\mathbf{r}_0) \quad (3.1)$$

with

$$\bar{V}(\mathbf{r}_0) = V(\mathbf{r}_0) - \mathbf{r}_0 \cdot \nabla V(\mathbf{r}_0). \quad (3.2)$$

Noting $[\hat{p}_i, x_j'] = [\hat{p}_i', x_j] = 0$ we can factorize the exponential in expression (2.10)

$$\begin{aligned} \exp\{i\omega(\lambda - \frac{1}{2}(\hat{H} + \hat{H}'))\} \\ = \exp\{i\omega(\lambda - \frac{1}{2}[\bar{V}(\mathbf{r}_0) + \bar{V}(\mathbf{r}_0')])\} \\ \cdot \prod_{i=1}^3 \{\hat{G}(\omega, \hat{p}_i, x_i) \hat{G}(\omega, \hat{p}_i', x_i')\} \end{aligned}$$

where

$$\hat{G}(\omega, \hat{p}_i, x_i) = \exp\left\{-\frac{i\omega}{2}\left(\frac{\hat{p}_i^2}{2m} + x_i \frac{\partial V}{\partial x_i} \Big|_{\mathbf{r}=\mathbf{r}_0}\right)\right\}.$$

$\hat{G}(\omega, \hat{p}_i, x_i)$ behaves as a c -number when acting upon a function which does not depend on x_i . Therefore we can write

$$\begin{aligned} \exp\{i\omega(\lambda - \frac{1}{2}(\hat{H} + \hat{H}'))\} \exp\{i\mathbf{k}(\mathbf{r}' - \mathbf{r})\} \\ = \exp\{i\omega(\lambda - \frac{1}{2}[\bar{V}(\mathbf{r}_0) + \bar{V}(\mathbf{r}_0')])\} \cdot D_1 D_2 D_3 \end{aligned} \quad (3.3)$$

with

$$\begin{aligned} D_i = [\hat{G}(\omega, \hat{p}_i, x_i) \exp\{-i k_i x_i\}] \\ \cdot [\hat{G}(\omega, \hat{p}_i', x_i') \exp\{i k_i x_i'\}] . \end{aligned} \quad (3.4)$$

Since D_i is independent of k_j for $j \neq i$ we are able to decompose in Eq. (2.10) the three-dimensional integral over \mathbf{k} -space into a threefold product of one-dimensional integrals over k_i :

$$\begin{aligned} \varrho(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi i (2\pi)^3} \int_{-\infty - i\eta}^{+\infty - i\eta} \frac{d\omega}{\omega} \\ \cdot \exp\{i\omega(\lambda - \frac{1}{2}[\bar{V}(\mathbf{r}_0) + \bar{V}(\mathbf{r}_0')])\} \\ \cdot \prod_{i=1}^3 \int_{-\infty}^{+\infty} dk_i D_i(\omega, x_i, x_i', k_i). \end{aligned} \quad (3.5)$$

The function D_i is a product of factors of the form $\exp\{a\hat{p}^2 + bx\} \cdot \exp\{ikx\}$, where $[\hat{p}, x] = -i\hbar$, and a, b, k are c -numbers. There are various methods for calculating expressions of this kind^{15, 23, 24} the result being

$$\begin{aligned} \exp\{a\hat{p}^2 + bx\} \cdot \exp\{ikx\} = \exp\{a\hbar^2 k^2 + bx \\ - i\hbar k a b - \frac{1}{3}\hbar^2 b^2 a\} \cdot \exp\{ikx\}. \end{aligned} \quad (3.6)$$

Using this relation we obtain from Eq. (3.4)

$$D_i = A_i \cdot B_i \quad (3.7)$$

where

$$A_i = \exp\{-i\beta k_i^2 + i\gamma_i k_i\}, \quad (3.8a)$$

$$\begin{aligned} B_i = \exp\left\{-\frac{i\omega}{2}\left(x_i \frac{\partial V}{\partial x_i} \Big|_{\mathbf{r}_0} + x_i' \frac{\partial V}{\partial x_i'} \Big|_{\mathbf{r}_0'}\right) \right. \\ \left. - \frac{i\hbar^2 \omega^3}{48m} \left[\left(\frac{\partial V}{\partial x_i} \Big|_{\mathbf{r}_0}\right)^2 + \left(\frac{\partial V}{\partial x_i'} \Big|_{\mathbf{r}_0'}\right)^2\right]\right\} \end{aligned} \quad (3.8b)$$

$$\beta = \hbar^2 \omega / 2m, \quad (3.8c)$$

$$\gamma_i = x_i' - x_i + \frac{\hbar^2 \omega^2}{8m} \left\{ \frac{\partial V}{\partial x_i'} \Big|_{\mathbf{r}_0'} - \frac{\partial V}{\partial x_i} \Big|_{\mathbf{r}_0} \right\}. \quad (3.8d)$$

Since B_i does not depend upon k_i we get

$$\begin{aligned} \int_{-\infty}^{+\infty} D_i dk_i = B_i \int_{-\infty}^{+\infty} \exp\{-i\beta k^2 + i\gamma_i k\} dk \\ = B_i \cdot (i-1) \left(\frac{\pi}{2\beta}\right)^{1/2} \exp\left\{\frac{i\gamma_i^2}{4\beta}\right\}. \end{aligned} \quad (3.9)$$

Inserting this into Eq. (3.5) we find

$$\varrho(\mathbf{r}, \mathbf{r}') = \frac{(i-1)^3}{8\pi^4 i} \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega} \cdot \exp\{i\omega(\lambda - \frac{1}{2}[\bar{V}(\mathbf{r}_0) + \bar{V}(\mathbf{r}_0')])\} \cdot \left(\frac{\pi}{2\beta}\right)^{3/2} B_1 B_2 B_3 \exp\left\{\frac{i}{4\beta}(\gamma_1^2 + \gamma_2^2 + \gamma_3^2)\right\}$$

We now substitute expressions (3.8 b, c, d) for B_i , β , and γ_i , and then replace $\nabla V(\mathbf{r}_0)$ by $\nabla V(\mathbf{r})$ and $\nabla V(\mathbf{r}_0')$ by $\nabla V(\mathbf{r}')$ which amounts to neglecting higher derivatives of V corresponding to the approximation we have made in Equation (3.1). After some algebra we find

$$\varrho(\mathbf{r}, \mathbf{r}') = C \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{5/2}} \exp\left\{i\omega d_1 + \frac{i d_2}{\omega} + i\omega^3 d_3\right\} \quad (3.10)$$

with

$$C = (1-i) m^{3/2}/4 \pi^{5/2} \hbar^3, \quad (3.11)$$

$$d_1 = \lambda - \frac{1}{2}[V(\mathbf{r}) + V(\mathbf{r}')] + \frac{1}{8}(\mathbf{r} - \mathbf{r}') \cdot (\nabla V|_{\mathbf{r}} - \nabla V|_{\mathbf{r}'}), \quad (3.12a)$$

$$d_2 = m(\mathbf{r} - \mathbf{r}')^2/2 \hbar^2, \quad (3.12b)$$

$$d_3 = \frac{\hbar^2}{16m} \left\{ \frac{1}{8}(\nabla V|_{\mathbf{r}} - \nabla V|_{\mathbf{r}'})^2 - \frac{1}{8}[(\nabla V|_{\mathbf{r}})^2 + (\nabla V|_{\mathbf{r}'})^2] \right\} \quad (3.12c)$$

where Eq. (3.2) has been used. The density matrix does not contain \mathbf{r}_0 and \mathbf{r}_0' any longer, and the position vectors \mathbf{r} and \mathbf{r}' may vary unrestrictedly and independently from each other. Note that we have used the locally linear approximation to the given potential only to evaluate the integrand in Eq. (2.10), but afterwards, again the original potential has to be taken in the above expression for $\varrho(\mathbf{r}, \mathbf{r}')$.

4. The Electron Density and Density Gradient

From Eqs. (3.10), (3.11), and (3.12 a, b, c) we immediately obtain the electron density setting $\mathbf{r} = \mathbf{r}'$:

$$\varrho(\mathbf{r}) = \varrho(\mathbf{r}, \mathbf{r}) = C \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{5/2}} \cdot \exp\left\{i\omega(\lambda - V(\mathbf{r})) - \frac{i\omega^3 \hbar^2}{24m} |\nabla V|^2\right\}. \quad (4.1)$$

As we shall see below $\varrho(\mathbf{r})$ is always nonnegative.

To remain consistent with our approximation, we

have to keep $\nabla V(\mathbf{r})$ constant when calculating the gradient of $\varrho(\mathbf{r})$ because higher derivatives of V than the first have been already neglected in gaining ϱ . Thus

$$\nabla \varrho(\mathbf{r}) = -iC \nabla V(\mathbf{r}) \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{3/2}} \cdot \exp\left\{i\omega(\lambda - V(\mathbf{r})) - \frac{i\omega^3 \hbar^2}{24m} |\nabla V|^2\right\}. \quad (4.2)$$

Defining

$$\xi = \lambda - V(\mathbf{r}), \quad (4.3)$$

$$\zeta = \left(\frac{\hbar^2 |\nabla V|^2}{24m}\right)^{1/3} \geq 0, \quad (4.4)$$

$$R_\nu(z) = \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\tau}{\tau^{1+\nu}} \exp\{i\tau z - i\tau^3\}, \quad (4.5)$$

we may rewrite

$$\varrho(\mathbf{r}) = C \zeta^{3/2} R_{3/2}(\xi/\zeta), \quad (4.6)$$

$$\nabla \varrho(\mathbf{r}) = -iC \nabla V(\mathbf{r}) \zeta^{1/2} R_{1/2}(\xi/\zeta). \quad (4.7)$$

In order to improve convergence we introduce into Eq. (4.5) the identity

$$e^{-i\tau^3} = 3^{-1/3} \int_{-\infty}^{+\infty} \text{Ai}(3^{-1/3}t) e^{i\tau t} dt \quad (4.8)$$

where $\text{Ai}(-x)$ denotes Airy's function. Reversing the order of integration and using the relation

$$\int_{-\infty-i\eta}^{+\infty-i\eta} \exp\{i\tau(z+t)\} \frac{d\tau}{\tau^{1+\nu}} = \gamma_\nu(z+t)^\nu \theta(z+t) \quad (4.9)$$

$$\text{with } \gamma_\nu = -\frac{(1+i)\nu^{1/2}\pi^{1/2}}{\Gamma(1+\nu)} \quad (4.10)$$

we obtain

$$R_\nu(z) = 3^{-1/3} \gamma_\nu \int_{-z}^{\infty} \text{Ai}(3^{-1/3}t) (z+t)^\nu dt. \quad (4.11)$$

Let us express Airy's function by BESSEL functions²⁶ and distinguish the cases $z > 0$ and $z \leq 0$. Setting

$$\sigma = 2(|z|/3)^{2/3} \geq 0 \quad (4.12)$$

we get

$$R_\nu(z) = 3^{\nu-1} 2^{-(2\nu/3)} \gamma_\nu A_\nu^\pm(\sigma) \quad (4.13)$$

where

$$A_\nu^+(\sigma) = \int_0^\sigma (\sigma^{2/3} - u^{2/3})^\nu (J_{1/3}(u) + J_{-1/3}(u)) du + \frac{1/3}{\pi} \int_0^\infty (\sigma^{2/3} + u^{2/3})^\nu K_{1/3}(u) du, \quad (4.14a)$$

$$A_{\nu}^{-}(\sigma) = \frac{V^3}{\pi} \int_{\sigma}^{\infty} (u^{3/2} - \sigma^{3/2})^{\nu} K_{1/2}(u) du. \quad (4.14b)$$

In Eq. (4.13), the positive (negative) sign has to be taken for $z > 0$ ($z \leq 0$).

Since $K_{1/2}(u) \approx (2/(\pi u))^{1/2} \exp\{-u\}$ for $u \gg 1$ the corresponding integrals converge fast. The functions $A_{\nu}^{\pm}(\sigma)$ have been calculated numerically and are shown in Figs. 1, 2, and 3 for $\nu = -1/2, +1/2$,

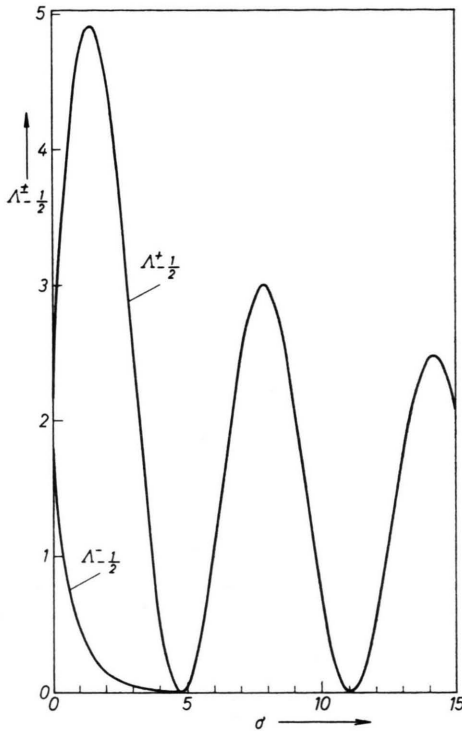


Fig. 1. The Functions $A_{1/2}^{\pm}(\sigma)$ for $0 \leq \sigma \leq 15$, see Eqs. (4.14 a, b).

+3/2, respectively. Some values of $A_{\nu}^{\pm}(\sigma)$ are given in the Tables 1 and 2 for the range $0 \leq \sigma \leq 14$.

Integrating by parts Eq. (4.5) the following recurrence relation can be established

$$R_{\nu}(z) = (i/\nu) [z R_{\nu-1}(z) - 3 R_{\nu-3}(z)].$$

Using Eq. (4.13) this may be rewritten in terms of $A_{\nu}^{\pm}(\sigma)$

$$A_{\nu}^{\pm}(\sigma) = \pm \sigma^{3/2} A_{\nu-1}^{\pm} + \frac{4}{3} (\nu-1)(\nu-2) A_{\nu-3}^{\pm} \quad (4.15)$$

which we shall need in connection with the calculation of the kinetic-energy density.

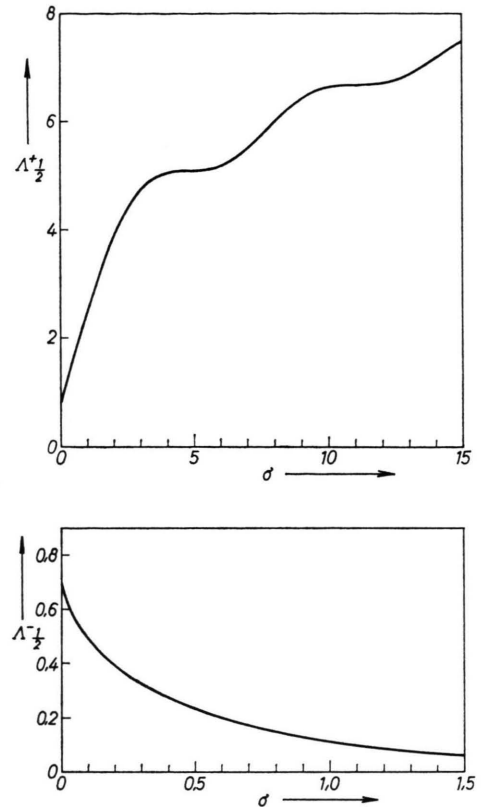


Fig. 2. The Functions $A_{1/2}^{+}(\sigma)$ (upper picture) and $A_{1/2}^{-}(\sigma)$ (lower picture), see Eqs. (4.14 a, b).

Table 1. Values of $A_{\nu}^{+}(\sigma)$, Eq. (4.14 a).

σ	$A_{-1/2}^{+}(\sigma)$	$A_{+1/2}^{+}(\sigma)$	$A_{+3/2}^{+}(\sigma)$
0	2.1586	0.6969	0.5774
1	4.7404	2.4639	2.7777
2	4.4624	3.8738	5.5755
3	2.4847	4.7539	8.7939
4	0.5337	5.0722	12.0587
5	0.0479	5.1013	15.1477
6	1.1125	5.1923	18.0555
7	2.5395	5.5236	20.9162
8	2.9786	6.0134	23.8609
9	2.0693	6.4412	26.9192
10	0.6653	6.6550	30.0204
11	0.0003	6.6907	33.0721
12	0.5811	6.7196	36.0399
13	1.7845	6.8885	38.9657
14	2.4708	7.1979	41.9206

Setting $z = \xi/\zeta$ we obtain from Eqs. (4.3), (4.4), and (4.12)

$$\sigma = \frac{4}{3} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{|\lambda - V(\mathbf{r})|^{3/2}}{|\nabla V(\mathbf{r})|} \quad (4.16)$$

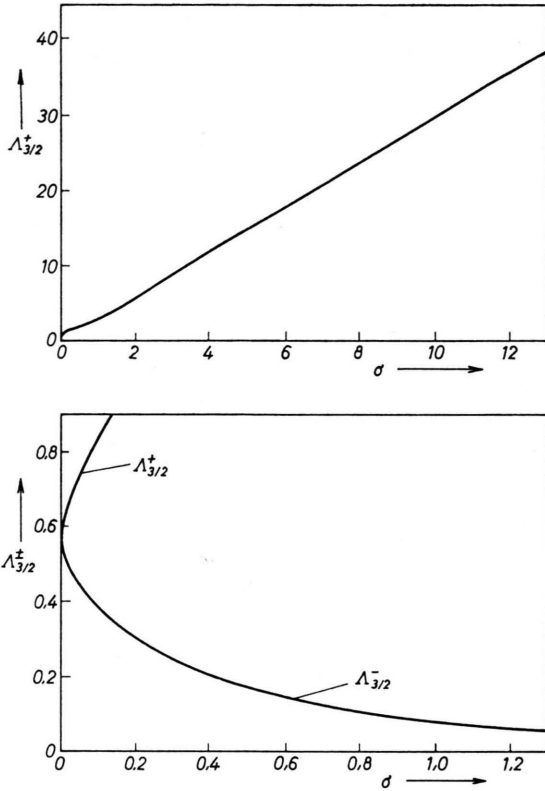


Fig. 3. The Functions $A_{3/2}^+(\sigma)$ (upper picture) and $A_{3/2}^-(\sigma)$ (lower picture), see Eqs. (4.14 a, b).

Table 2. Values of $A_{\nu}^-(\sigma)$, Eq. (4.14 b).

σ	$A_{-1/2}^-(\sigma)$	$A_{-1/2}^-(\sigma)$	$A_{-3/2}^-(\sigma)$
0	2.1586	0.6949	0.5774
1	0.4670	0.1137	0.07617
2	0.1457	0.0314	0.01908
3	0.0481	0.00955	0.00539
4	0.0163	0.00303	0.00162
5	0.00564	0.00099	0.00050
6	0.00196	0.00033	0.00016
7	0.00069	0.00011	$5.2 \cdot 10^{-5}$
8	$2.4 \cdot 10^{-4}$	$3.8 \cdot 10^{-5}$	$1.7 \cdot 10^{-5}$
9	$8.7 \cdot 10^{-5}$	$1.3 \cdot 10^{-5}$	$5.7 \cdot 10^{-6}$
10	$3.1 \cdot 10^{-5}$	$4.5 \cdot 10^{-6}$	$1.9 \cdot 10^{-6}$
11	$1.1 \cdot 10^{-5}$	$1.6 \cdot 10^{-6}$	$6.5 \cdot 10^{-7}$
12	$3.9 \cdot 10^{-6}$	$5 \cdot 10^{-7}$	$2.2 \cdot 10^{-7}$
13	$1.4 \cdot 10^{-6}$	$2 \cdot 10^{-7}$	$7 \cdot 10^{-8}$
14	$5 \cdot 10^{-7}$	$7 \cdot 10^{-8}$	$2 \cdot 10^{-8}$

and from Eqs. (3.11), (4.3), (4.4), (4.6), (4.7), (4.10), and (4.13) it follows

$$\varrho(\mathbf{r}) = \frac{m |\nabla V(\mathbf{r})|}{6 \hbar^2 \pi^2} A_{3/2}^+(\sigma), \quad (4.17)$$

$$\nabla \varrho(\mathbf{r}) = - \frac{(2m)^{4/3}}{2 \pi^2 6^{2/3} \hbar^{8/3}} \nabla V(\mathbf{r}) |\nabla V(\mathbf{r})|^{1/3} A_{1/2}^+(\sigma). \quad (4.18)$$

Here we have to take the positive (negative) sign for $\lambda - V > 0$ (≤ 0). Since $A_{3/2}^+(\sigma) \geq 0$ for all σ (see Fig. 3) the density cannot become negative.

5. Density of the Kinetic Energy as a Function of $V(\mathbf{r})$ and $\nabla V(\mathbf{r})$

The ground state kinetic energy of our system of independent electrons is given in coordinate representation by

$$2 \sum_{r=1}^n \sum_{\mu=1}^{m(r)} \langle \psi_{r,\mu} | \frac{\hat{p}^2}{2m} | \psi_{r,\mu} \rangle = \int \left\{ \frac{\hbar^2}{m} \sum_{r=1}^n \sum_{\mu=1}^{m(r)} |\nabla \psi_{r,\mu}|^2 \right\} d^3\mathbf{r} \quad (5.1)$$

where the factor 2 is due to the two spin orientations belonging to each $\psi_{r,\mu}$. The integrand on the right is regarded as the density ε_k of the total kinetic energy. Evidently, ε_k is positive definite in contrast to the usual definition

$$\varepsilon_k' \equiv - \frac{\hbar^2}{2m} 2 \sum_{r=1}^n \sum_{\mu=1}^{m(r)} \psi_{r,\mu}^* \Delta \psi_{r,\mu}. \quad (5.2)$$

The difference between ε_k and ε_k' is a divergence term. Since the kinetic energy itself is always positive it is convenient to choose the corresponding density positive definite too.

In terms of Dirac's density matrix, Eq. (2.3), ε_k may be written

$$\varepsilon_k = \frac{\hbar^2}{2m} \sum_{i=1}^3 \left[\frac{\partial^2}{\partial x_i \partial x_i'} \varrho(\mathbf{r}, \mathbf{r}') \right]_{\mathbf{r}'=\mathbf{r}}. \quad (5.3)$$

This expression is now evaluated on the basis of the linear potential approximation, Eq. (3.1). Thus we start from Eqs. (3.10), (3.11), (3.12 a, b, c) for the density matrix.

For infinitesimal $|\mathbf{r} - \mathbf{r}'|$, it is correct within our approximation to set $\nabla V(\mathbf{r}') = \nabla V(\mathbf{r})$. Thus

$$\varrho(\mathbf{r}, \mathbf{r}') = C \int_{-\infty - i\eta}^{+\infty - i\eta} \frac{d\omega}{\omega^{5/2}} \exp\{i K(\mathbf{r}, \mathbf{r}', \omega)\} \quad (5.4)$$

where

$$K(\mathbf{r}, \mathbf{r}', \omega) = \omega [\lambda - \frac{1}{2} \{V(\mathbf{r}) + V(\mathbf{r}')\}] + \frac{m(\mathbf{r} - \mathbf{r}')^2}{2 \hbar^2 \omega} - \frac{\hbar^2 \omega^3}{24m} \cdot |\nabla V(\mathbf{r})|^2. \quad (5.5)$$

Differentiating $\varrho(\mathbf{r}, \mathbf{r}')$ with respect to x_i and x_i' under the integral sign and then setting $\mathbf{r}' = \mathbf{r}$ we

find from Eq. (5.3)

$$\frac{2m}{\hbar^2} \varepsilon_k = -\frac{3imC}{\hbar^2} \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{7/2}} \exp\{iK(\mathbf{r}, \mathbf{r}, \omega)\} \\ - \frac{1}{4} C |\nabla V(\mathbf{r})|^2 \int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{1/2}} \exp\{iK(\mathbf{r}, \mathbf{r}, \omega)\}. \quad (5.6)$$

Using Eqs. (4.3), (4.4), (4.5), (4.12), (4.13), and (4.14 a, b) we get

$$K(\mathbf{r}, \mathbf{r}, \omega) = \omega \xi - \omega^3 \zeta^3 \quad (5.7)$$

$$\int_{-\infty-i\eta}^{+\infty-i\eta} \frac{d\omega}{\omega^{1+\nu}} \exp\{iK(\mathbf{r}, \mathbf{r}, \omega)\} = \zeta^\nu R_\nu(\xi/\zeta) \\ = 3^{\nu-1} 2^{-(2\nu/3)} \gamma_\nu \zeta^\nu A_\nu^\pm(\sigma). \quad (5.8)$$

In terms of $A_\nu^\pm(\sigma)$ we thus find

$$\varepsilon_k = \left(\frac{2m}{\hbar^2}\right)^{2/3} \frac{|\nabla V|^{5/3}}{8\pi^2 6^{1/3}} \left\{ \frac{3}{5} A_{5/2}^\pm(\sigma) + \frac{1}{3} A_{1/2}^\pm(\sigma) \right\}. \quad (5.9)$$

Applying the recurrence relation (4.15a) we eliminate $A_{5/2}^\pm$

$$\varepsilon_k = \left(\frac{2m}{\hbar^2}\right)^{2/3} \frac{|\nabla V|^{5/3}}{8\pi^2 6^{1/3}} \left\{ \pm \frac{3}{5} \sigma^{2/3} A_{3/2}^\pm(\sigma) + \frac{8}{15} A_{1/2}^\pm(\sigma) \right\}. \quad (5.10)$$

Since the positive (negative) sign has to be taken for $\lambda - V > 0$ (≤ 0) it follows from Eq. (4.16)

$$\pm \sigma^{2/3} = \pm |\lambda - V(\mathbf{r})| \left(\frac{4(2m)^{1/2}}{3\hbar |\nabla V|} \right)^{2/3} \\ = (\lambda - V(\mathbf{r})) \left(\frac{4(2m)^{1/2}}{3\hbar |\nabla V|} \right)^{2/3}. \quad (5.11)$$

Thus ε_k can be written

$$\varepsilon_k = \frac{m |\nabla V|}{10\pi^2 \hbar^2} \cdot (\lambda - V(\mathbf{r})) \cdot A_{3/2}^\pm(\sigma) \\ + \left(\frac{2m}{\hbar^2}\right)^{2/3} \frac{|\nabla V|^{5/3}}{15\pi^2 6^{1/3}} \cdot A_{1/2}^\pm(\sigma). \quad (5.12)$$

6. The Kinetic-Energy Density as a Function of ϱ and $\nabla\varrho$

Having derived expressions for ϱ , $\nabla\varrho$, and ε_k as functions of the potential and of its gradient, we shall now eliminate $\lambda - V$ and ∇V in order to obtain ε_k as a function of ϱ and of $\nabla\varrho$.

From Eqs. (4.16), (4.17), and (4.18) we obtain

$$y \equiv \frac{|\nabla\varrho|^{1/2}}{\varrho^{2/3}} = 2^{1/2} (3\pi)^{1/3} \frac{[A_{1/2}^\pm(\sigma)]^{1/2}}{[A_{3/2}^\pm(\sigma)]^{2/3}}, \quad (6.1)$$

$$|\nabla V| = \frac{6\hbar^2 \pi^2 \varrho}{m A_{3/2}^\pm(\sigma)}, \quad (6.2)$$

$$\lambda - V(\mathbf{r}) = \pm |\lambda - V(\mathbf{r})| = \pm \frac{\hbar^2 (3\pi)^{4/3}}{2m} \left(\frac{\sigma \varrho}{A_{3/2}^\pm(\sigma)} \right)^{2/3} \quad (6.3)$$

Substitution of Eqs. (6.2) and (6.3) into Eq. (5.12) yields ε_k as a product of the kinetic-energy density in TF-approximation and a variable correction factor

$$\varepsilon_k = \varepsilon_k^{\text{TF}} \cdot \chi(\sigma) \quad (6.4)$$

where

$$\varepsilon_k^{\text{TF}} = \frac{3}{5} (3\pi^2)^{2/3} \frac{\hbar^2}{2m} \varrho^{5/3} = \kappa \varrho^{5/3} \quad (6.5)$$

and

$$\chi(\sigma) = \left(\frac{3}{A_{3/2}^\pm(\sigma)} \right)^{2/3} \left(\frac{8}{9} \frac{A_{1/2}^\pm(\sigma)}{A_{3/2}^\pm(\sigma)} \pm \sigma^{2/3} \right). \quad (6.6)$$

The last step to be done is to solve Eq. (6.1) for σ and insert the solution $\sigma = \sigma(y) = \sigma(|\nabla\varrho|^{1/2} \varrho^{-2/3})$ into Eq. (6.6). We thus arrive at the wanted relation between ε_k , ϱ , and $\nabla\varrho$:

$$\varepsilon_k = \kappa \varrho^{5/3} \chi(\sigma(y)) = \kappa \varrho^{5/3} \bar{\chi}(|\nabla\varrho|^{1/2} \varrho^{-2/3}). \quad (6.7)$$

The function $y(\sigma)$, Eq. (6.1), has been computed numerically; it is shown in Figure 4. From the asymptotic behaviour of $y(\sigma)$, see Eqs. (7.1) and (7.7), and from Fig. 4 it is clear that σ and

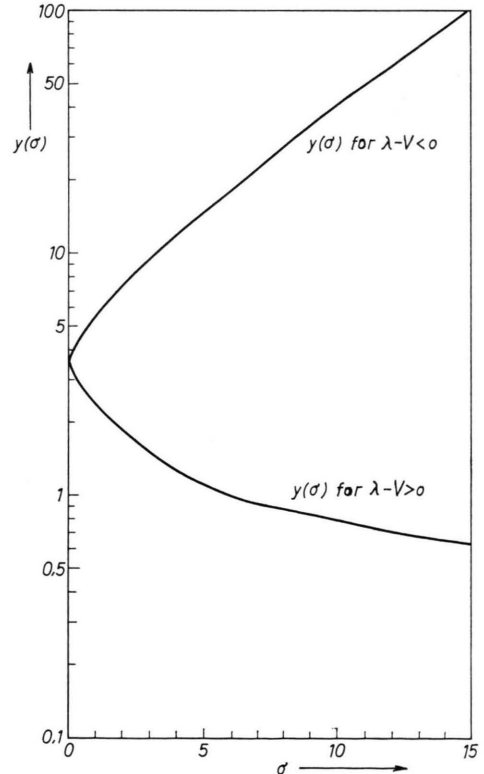


Fig. 4. The Function $y(\sigma)$ for both positive and negative values of $\lambda - V$, see Eq. (6.1).

$\text{sign}(\lambda - V)$ are determined uniquely by y . Then, according to Eq. (6.6), also χ is determined unambiguously by y , i. e., $\bar{\chi}$ defined by Eq. (6.7) is a unique function of y . However, it doesn't seem possible to eliminate σ and $\text{sign}(\lambda - V)$ in an analytical way except for the limits $\sigma \rightarrow \infty$; $\text{sign}(\lambda - V) = \pm 1$ which shall be treated in the next section. For general values of σ we must be satisfied with numerical evaluation of $\bar{\chi}(y)$, which is given as a parametric representation $y = y(\sigma, j)$; $\chi = \chi(\sigma, j)$ with the continuous parameter σ and the discrete parameter $j = \text{sign}(\lambda - V)$. Some values of $\bar{\chi}(y)$ are listed in Table 3. Figures 5 a, b show this function for different ranges of y .

Table 3. Values of $\bar{\chi}(y)$. Eq. (6.7).

y	$\bar{\chi}(y)$	y	$\bar{\chi}(y)$
0	1	2.8	4.32256
0.6	0.999407	3.0	5.39648
0.8	1.00427	3.5	9.10154
1.0	1.01154	4.0	14.6539
1.2	0.996981	4.5	22.5701
1.4	1.05822	5.0	33.4471
1.6	1.19679	6.0	66.8190
1.8	1.42045	7.0	120.911
2.0	1.74092	8.0	202.951
2.2	2.17289	9.0	321.243
2.4	2.73364	10.0	485.185
2.6	3.44295		

First of all, we note that $\bar{\chi}(y)$ is positive for all y (≥ 0). Therefore, according to Eq. (6.4), ε_k never becomes negative and vanishes only for $\varrho = 0$, i. e. ε_k is positive definite.

For $y = 0$ which means either $\varrho \rightarrow \infty$ or/and $\nabla\varrho = 0$ we have

$$\bar{\chi}(0) = 1 \quad (6.8)$$

or $\varepsilon_k = \kappa \varrho^{5/3} = \varepsilon_k^{\text{TF}} \quad (6.8a)$

as is expected. However, we also obtain oscillations of decreasing wavelength and amplitude when y approaches zero.

If $\varrho \ll |\nabla\varrho|^{3/4}$ or $y \gg 1$, $\bar{\chi}(y)$ becomes large compared with unity, thus

$$\kappa \varrho^{5/3} / \varepsilon_k = 1 / \bar{\chi}(y) \ll 1. \quad (6.9)$$

The TF-fraction to the whole kinetic-energy density is small for large y .

The quantitative behaviour of $\bar{\chi}(y)$ for $y \rightarrow 0$ and $y \rightarrow \infty$ is investigated in Section 7.

For comparison, Figs. 5 a, b also show $\bar{\chi}^{\text{TF}}(y) \equiv 1$ and $\bar{\chi}^{\text{TFW}}(y)$. The latter corresponds to the Thomas-

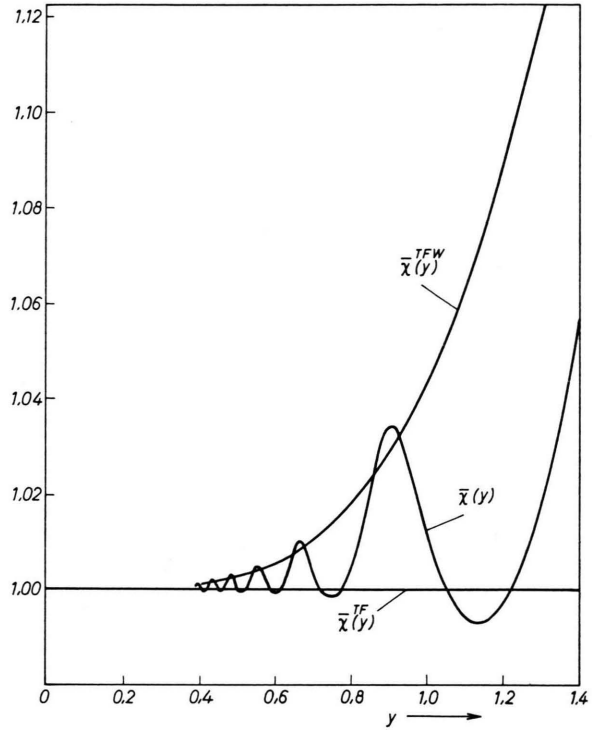


Fig. 5 a. The Functions $\bar{\chi}(y)$, $\bar{\chi}^{\text{TF}}(y)$, and $\bar{\chi}^{\text{TFW}}(y)$ in the range $0.4 \leq y \leq 1.4$, see Eqs. (6.7), (6.11).

Fermi-Weizsäcker energy-density functional which is given by

$$\varepsilon_k^{\text{TFW}} = \kappa \varrho^{5/3} + \frac{\hbar^2}{8m} \frac{(\nabla\varrho)^2}{\varrho}. \quad (6.10)$$

Using the definition of y , Eq. (6.1), $\varepsilon_k^{\text{TFW}}$ can be rewritten as

$$\varepsilon_k^{\text{TFW}} = \kappa \varrho^{5/3} (1 + \frac{5}{12} (3\pi^2)^{-2/3} y^4) = \varepsilon_k^{\text{TF}} \cdot \bar{\chi}^{\text{TFW}}(y). \quad (6.11)$$

7. Asymptotic Behaviour of ε_k in the Limits

$y \rightarrow 0$ and $y \rightarrow \infty$

7.1. The Limit $y \rightarrow 0$

If ϱ is large and/or $\nabla\varrho \rightarrow 0$ y becomes small which implies $\sigma \rightarrow \infty$ and $\lambda - V > 0$. From Eqs. (6.1) and (A7a,b) we obtain

$$y = a \sigma^{-1/2} \left\{ 1 - \frac{\cos \sigma}{6\sigma} + O(\sigma^{-3/2}) \right\} \quad (7.1)$$

with

$$a = 2^{1/2} (3\pi^2)^{1/6}. \quad (7.2)$$

Let us solve Eq. (7.1) for σ by iteration. In zeroth order we find $y \approx a \sigma^{-1/2}$ or $\sigma \approx (a/y)^2$. Inserting

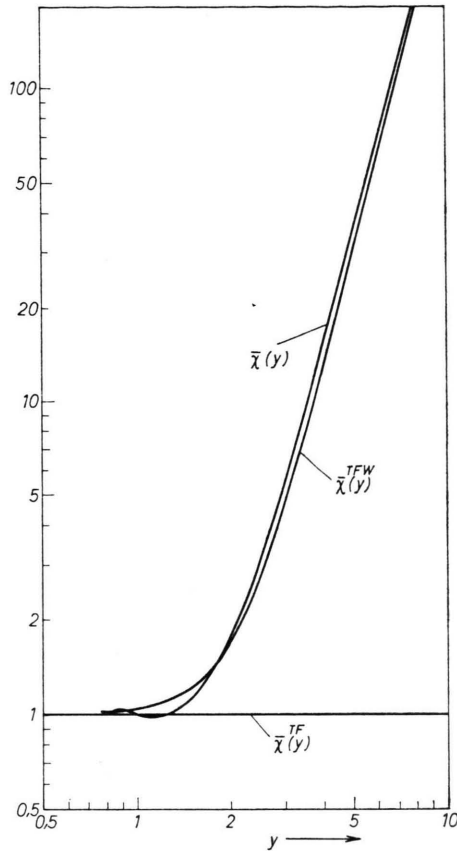


Fig. 5 b. The Functions $\bar{\chi}(y)$, $\bar{\chi}^{TF}(y)$, and $\bar{\chi}^{TFW}(y)$ in the range $0.8 \leq y \leq 8$, see Eqs. (6.7), (6.11).

this into the oscillating term of Eq. (7.1) we get in next approximation

$$\sigma \approx \left(\frac{a}{y}\right)^2 \left\{ 1 - \frac{1}{3} \left(\frac{y}{a}\right)^2 \cdot \cos\left(\frac{a}{y}\right)^2 \right\}. \quad (7.3)$$

The asymptotic expansion of $\chi(\sigma)$ for $\lambda - V > 0$ follows from Eqs. (6.6) and (A7a,c)

$$\chi(\sigma) = 1 + \frac{5}{9\sigma^2} \left(\frac{5}{3} + 2 \sin \sigma \right) + O(\sigma^{-5/2}). \quad (7.4)$$

Substitution of expression (7.3) yields

$$\bar{\chi}(y) = 1 + \frac{5}{9} \left(\frac{y}{a}\right)^4 \left\{ \frac{5}{3} + 2 \sin \sigma(y) \right\} + O(y^5) \quad (7.5)$$

Thus, for small $|\nabla \varrho|^{1/2} \varrho^{-2/3}$, ϵ_k is given by

$$\epsilon_k = \epsilon_k^{TF} + \frac{5}{9} \frac{\hbar^2}{8m} \frac{(\nabla \varrho)^2}{\varrho} + \frac{2}{3} \frac{\hbar^2}{8m} \frac{(\nabla \varrho)^2}{\varrho} \sin \left\{ \frac{2(3\pi^2)^{1/3} \varrho^{1/3}}{|\nabla \varrho|} \right\}. \quad (7.6)$$

7.2. The Limit $y \rightarrow \infty$

The case $y \rightarrow \infty$ which corresponds to $|\nabla \varrho| \gg \varrho^{1/3}$ implies $\sigma \rightarrow \infty$ and $\lambda - V < 0$. Using Eqs. (A11a, b, c) we obtain from (6.1)

$$y = (12\pi)^{1/3} \sigma^{1/3} e^{\sigma/6} \quad (7.7)$$

and from Eq. (6.6)

$$\chi(\sigma) = \frac{5}{3} 6^{2/3} (\sigma^{1/3} e^{\sigma/6})^4. \quad (7.8)$$

Hence we get

$$\chi(\sigma(y)) = \bar{\chi}(y) = \frac{5}{12} (3\pi^2)^{-2/3} y^4 \quad (7.9)$$

which shows that $\bar{\chi}(y)$ equals $\bar{\chi}^{TFW}(y)$ asymptotically for large y , see Equation (6.11). Finally, the kinetic-energy density becomes

$$\epsilon_k = \frac{\hbar^2}{8m} \frac{|\nabla \varrho|^2}{\varrho}. \quad (7.10)$$

8. Conclusion

The kinetic-energy density functional ϵ_k based upon the approximation of locally linear potential ad given by Eqs. (6.1), (6.4), (6.5), and (6.6) covers the whole range between very high and very low density.

For small ϱ or high $|\nabla \varrho|$ such that

$$y = |\nabla \varrho|^{1/2} \varrho^{-2/3} \gg 1$$

the main contribution to ϵ_k is given by the Weizsäcker correction term alone, see Equation (7.10).

If $y \ll 1$ corresponding to a weakly inhomogeneous electron gas, ϵ_k is approximately given by Equation (7.6). This result differs from the Kirzhnits approximation in two points:

(a) The factor of 5/9 at the steady gradient correction term lies just in the middle between 1 (full Weizsäcker term) and 1/9 (Kirzhnits term). When KIRZHITS' calculation²⁷ is repeated using, however, the positive definite expression (5.3) for ϵ_k and neglecting all derivatives of V higher than the first, then our factor of 5/9 is recovered.

(b) The third term in Eq. (7.6) representing quantum oscillations which are missing in Kirzhnits' work is of same order of magnitude as the second one. When $|\nabla \varrho| \rightarrow 0$, also the oscillating term approaches zero. However, the number of oscillations becomes infinite which is unphysical, of course, provided that this limit is reached within a finite domain of space. Now, if V is exactly linear with $\nabla V \neq 0$ it follows from $\varrho^{1/3} |\nabla \varrho|^{-1} \sim y^{-2} \sim \sigma$ [see

Eq. (7.3)] and from the definition of σ , Eq. (4.16), that the limit $\nabla\varrho \rightarrow 0$ implies $\lambda - V \rightarrow \infty$ which is clearly impossible within a finite region. Since, however, each potential which is capable of bound states cannot be exactly linear over the whole space those unphysical accumulation of oscillations may appear within finite regions.

From these considerations the author hopes that if the approximation scheme presented here is extended to include the second derivatives of V , one should be able to reproduce

- (1) the steady correction term of Kirzhnits in the limit of weak slowly varying inhomogeneity,
- (2) the Weizsäcker result in the limit of small ϱ or large $\nabla\varrho$,
- (3) oscillatory behaviour of ε_k which is reasonable also quantitatively.

Investigations in this direction are in progress.

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Appendix

The Asymptotic Behaviour of the Functions $\Lambda_\nu^\pm(\sigma)$

The rather lengthy calculation of the asymptotic form of $\Lambda_\nu^\pm(\sigma)$, Eqs. (4.14 a, b), can only be sketched here.

First, let us consider $\Lambda_\nu^+(\sigma)$ which may be written as the sum of two integrals

$$W_\nu(\sigma) = \sigma^{2\nu/3} \int_0^\sigma \left(1 - \left(\frac{u}{\sigma}\right)^{2/3}\right)^\nu (J_{1/3}(u) + J_{-1/3}(u)) du, \quad (A1)$$

$$L_\nu(\sigma) = \frac{1}{\pi} \sigma^{2\nu/3} \int_0^\infty \left(1 + \left(\frac{u}{\sigma}\right)^{2/3}\right)^\nu K_{1/3}(u) du. \quad (A2)$$

Since in $W_\nu(\sigma)$ an expansion of $(1 - (u/\sigma)^{2/3})^\nu$ in powers of $(u/\sigma)^{2/3}$ diverges at the upper limit $u = \sigma$ we divide the interval of integration into $I_1 \equiv [0, \theta\sigma]$ and $I_2 \equiv [\theta\sigma, \sigma]$ with $0 < \theta < 1$ and use the expansion in I_1 only. If σ is large enough we have also $\theta\sigma \gg 1$. Therefore, we may integrate termwise over I_1 using a relation for integrals of Bessel functions with large upper limits²⁹. In the integral over I_2 we substitute $u(v) = \sigma(1 - v^2)^{3/2}$ and replace the Bessel

functions by their asymptotic expansions. The asymptotic forms of the arising integrals may be found by repeated integration by parts and by applying the method of stationary phase³⁰. The result is

$$W_{3/2}(\sigma) = 2\sigma - \frac{3\sigma^{1/3}}{2^{1/3}\Gamma(\frac{3}{2})} - \frac{2^{1/3}}{4\Gamma(\frac{3}{2})\sigma^{1/3}} - \frac{1}{9\sigma} - \frac{\sin\sigma}{\sigma} + O(\sigma^{-3/2}), \quad (A3a)$$

$$W_{1/2}(\sigma) = 2\sigma^{1/3} - \frac{1}{2^{1/3}\Gamma(\frac{1}{2})\sigma^{1/3}} + \frac{2^{1/3}}{12\Gamma(\frac{1}{2})\sigma} - \frac{\cos\sigma}{\sigma^{7/3}} + O(\sigma^{-7/3}), \quad (A3b)$$

$$W_{-1/2}(\sigma) = \frac{2+3\sin\sigma}{\sigma^{1/3}} + O(\sigma^{-5/3}). \quad (A3c)$$

Denoting the integrand of $L_\nu(\sigma)$, Eq. (A2), with $f(u, \sigma, \nu)$ let us split the region of integration

$$L_\nu(\sigma) = L_{1,\nu}(\sigma, \theta) + L_{2,\nu}(\sigma, \theta), \quad (A4)$$

$$L_{1,\nu}(\sigma, \theta) = \int_0^{\theta\sigma} f(u, \sigma, \nu) du, \quad (A5a)$$

$$L_{2,\nu}(\sigma, \theta) = \int_{\theta\sigma}^\infty f(u, \sigma, \nu) du \quad (A5b)$$

with $0 < \theta < 1$. In $L_{2,\nu}$ we may replace $K_{1/3}$ by its asymptotic form if $\theta\sigma$ is large enough. Then it is estimated easily that $L_{2,\nu}$ falls off roughly as $\exp\{-\theta\sigma\}$ for all ν . In $L_{1,\nu}$ we may expand

$$\left(1 + \left(\frac{u}{\sigma}\right)^{2/3}\right)^\nu = \sum_{\mu=0}^\infty \binom{\nu}{\mu} \left(\frac{u}{\sigma}\right)^{2\mu/3}$$

and split up $\int_0^{\theta\sigma} = \int_0^\infty - \int_{\theta\sigma}^\infty$. The first integral is integrated exactly, term by term, while the second can be shown to fall off $\sim \exp\{-\theta\sigma\}$ due to the asymptotic behaviour of $K_{1/3}$. Neglecting all terms with exponential decay we find

$$L_{3/2}(\sigma) = \sigma + \frac{3\sigma^{1/3}}{2^{1/3}\Gamma(\frac{3}{2})} + \frac{2^{1/3}}{4\Gamma(\frac{3}{2})\sigma^{1/3}} - \frac{1}{18\sigma} + O(\sigma^{-5/3}), \quad (A6a)$$

$$L_{1/2}(\sigma) = \sigma^{1/3} + \frac{1}{2^{1/3}\Gamma(\frac{1}{2})\sigma^{1/3}} - \frac{2^{1/3}}{12\Gamma(\frac{1}{2})\sigma} + O(\sigma^{-5/3}), \quad (A6b)$$

$$L_{-1/2}(\sigma) = \sigma^{-1/3} - \frac{1}{2^{1/3}\Gamma(\frac{1}{2})\sigma} + O(\sigma^{-5/3}). \quad (A6c)$$

Combining Eqs. (4.14a), (A1), (A2), and (A3a-c) we thus arrive at

$$\Lambda_{3/2}^+(\sigma) = 3\sigma - 1/(6\sigma) - \sin\sigma/\sigma + O(\sigma^{-3/2}), \quad (A7a)$$

$$A_{1/2}^+(\sigma) = 3\sigma^{1/2} - \cos \sigma / \sigma^{2/3} + O(\sigma^{-7/6}), \quad (\text{A7b})$$

$$A_{-1/2}^+(\sigma) = 3\sigma^{-1/2}(1 + \sin \sigma) + O(\sigma^{-5/6}). \quad (\text{A7c})$$

Concerning $A_v^-(\sigma)$ we need only the leading terms of the asymptotic expansions. Setting as a new variable of integration $v = u/\sigma - 1$ we obtain from Equation (4.14b)

$$A_v^-(\sigma) = g_v(\sigma) \int_0^\infty e^{-\sigma v} h_v(v) dv \quad (\text{A8})$$

where

$$g_v(\sigma) = \left(\frac{3}{2\pi}\right)^{1/2} \sigma^{(2v/3 + 1/2)} e^{-\sigma}, \quad (\text{A9})$$

$$h_v(v) = (1+v)^{-1/2} \{ (1+v)^{2/3} - 1 \}^v. \quad (\text{A10})$$

Since $\int_0^\infty v^\gamma e^{-\sigma v} dv = \sigma^{-\gamma-1} \Gamma(1+\gamma)$ the leading term of $A_v^-(\sigma)$ is determined by the lowest order term $(2v/3)^v$ in the power series expansion of $h_v(v)$. Thus we get

$$A_v^-(\sigma) = g_v(\sigma) \int_0^\infty e^{-\sigma v} (2v/3)^v dv \quad (\text{A11})$$

or

$$A_{3/2}^-(\sigma) = \frac{1}{2} \sigma^{-1} e^{-\sigma}, \quad (\text{A11a})$$

$$A_{1/2}^-(\sigma) = \frac{1}{2} \sigma^{-2/3} e^{-\sigma}, \quad (\text{A11b})$$

$$A_{-1/2}^-(\sigma) = \frac{3}{2} \sigma^{-1/2} e^{-\sigma}. \quad (\text{A11c})$$

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