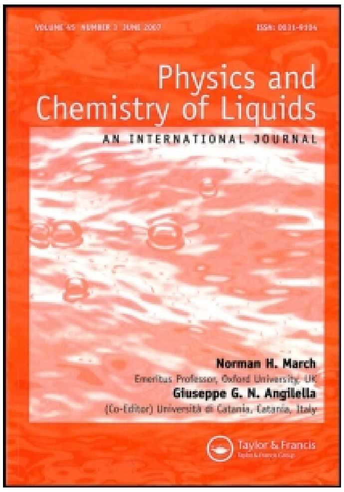

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LETTER
Relation between Kinetic and Exchange Energies in a Relativistic Inhomogeneous Electron Liquid

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The relativistic kinetic energy of a weakly inhomogeneous electron liquid can be calculated from Dirac's equation, as recently shown by Baltin and March. Here this result is combined with the relativistic exchange energy as given by MacDonald and Vosko to yield the exchange energy density in terms of kinetic energy and electron densities.

KEY WORDS: Dirac equation, electron density.

Using Dirac's one electron relativistic wave equation, Baltin and March[1] have obtained an explicit form for the kinetic energy density t of a weakly inhomogeneous electron liquid in terms of the electron density ρ. The relativistic treatment of, for example, an atom embedded in a dense plasma[2] is a problem to which this approximation for $t(\rho)$ has relevance.

Recently, we have used a non-relativistic density matrix for a bare Coulomb field to argue for an intimate relation between exchange, kinetic and electron densities[3]. The purpose of the present work is to display an explicit form of such a relationship for a weakly inhomogeneous relativistic electron liquid.

The result of Ref. 1 for the kinetic energy density t is

$$t = a\{\beta(\tfrac{1}{2} + \beta^2)(1 + \beta^2)^{1/2} - \tfrac{4}{3}\beta^3 - \tfrac{1}{2}\ln[\beta + (1 + \beta^2)^{1/2}]\} \quad (1)$$

where $a = (1/4\pi^2)(mc/\hbar)^3 mc^2$, $\beta = b\rho^{1/3}$, $b = (3\pi^2)^{1/3}(\hbar/mc)$.

Using the work of MacDonald and Vosko[4], the relativistic exchange energy density ε_x can similarly be written as[5]

$$\varepsilon_x = -\tfrac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\rho^{4/3}F(\beta) \quad (2)$$

where

$$F(\beta) = 1 - \tfrac{3}{2}\{(1 + \beta^2)^{1/2} - \ln[\beta + (1 + \beta^2)^{1/2}]\}^2/\beta^4.$$

It is now to be noted that the term $\ln[\beta + (1 + \beta^2)^{1/2}]$ is a common element between ε_x *and* t. Therefore we shall proceed by eliminating this term between Eqs. (1) and (2). The resulting relation may be expressed in the form

$$\varepsilon_x = -c_e\rho^{4/3} + \frac{3}{2}\frac{c_e}{b^4}\left[\frac{2t}{a} + (1 + \beta^2)^{1/2}\{1 - \beta - 2\beta^3\} + \tfrac{8}{3}\beta^3\right]^2 \qquad (3)$$

with $\beta = b\rho^{1/3}$, and $c_e = \frac{3}{4}e^2(3/\pi)^{1/3}$.

In the non-relativistic limit, the Dirac–Slater $\rho^{4/3}$ exchange energy density is recovered. Thus, near the non-relativistic limit, Eq. (3) can only be used to connect relativistic corrections to the nonrelativistic energy densities $t_0 = (3h^2/10m)(3/8\pi)^{2/3}\rho^{5/3}$ and $\varepsilon_{x0} = -c_e\rho^{4/3}$.

While Eq. (3) is certainly true in a weakly inhomogeneous electron liquid treated by Special Relativity, it is to be anticipated that, for more rapidly varying electron desities, $\varepsilon_x(\mathbf{r})$ will be related to $t(\mathbf{r})$ and $\rho(\mathbf{r})$ by a non-local theory. Any such non-local relation which may be set up in the future must clearly reduce to a form equivalent to Eq. (3) in the limit when $\rho(\mathbf{r})$ varies by but a small fraction of itself over a characteristic electron wavelength.

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