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#### **LETTER**

### **Linear Response Relation between Charge Displaced in an Electron Liquid by Relativistic and Nonrelativistic Theory**

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For a linear response theory of the charge displaced in an electron liquid by the same, given, single-particle potential. the relativistic density is related directly to that derived from the Schrodinger equation.

**KEY** WORDS: Dirac equation, displaced charge.

We have recently treated<sup>1</sup> in relativistic quantum mechanics, the charge  $\Delta \rho_{\alpha}(x)$ displaced according to linear response theory of an electron liquid by a given potential *V(x), where the index*  $\alpha$  *denotes the fine-structure constant*  $e^{2}/(hc)$ *. The result was* shown to take the form

$$
\Delta \rho_a(\mathbf{x}) = \int F_a(|\mathbf{x} - \mathbf{x}'|) V(\mathbf{x}') d^3 x'
$$
 (1)

with

$$
F_{\alpha}(|\mathbf{x} - \mathbf{x}'|) \equiv -\frac{m}{\pi^3 \hbar^2 |\mathbf{x} - \mathbf{x}'|} \int_0^{k_F} \left[ j_0(2q|\mathbf{x} - \mathbf{x}'|) + \frac{\alpha^2 a_0^2 q}{|\mathbf{x} - \mathbf{x}'|} j_1(2q|\mathbf{x} - \mathbf{x}'|) \right] \frac{q^2 dq}{\left[1 + (\alpha a_0 q)^2\right]^{1/2}}
$$
(2)

 $a_0 = \frac{\hbar^2}{\text{me}^2}$ ,  $j_0$ , and  $j_1$  are the Bohr radius and the spherical Bessel functions of order 0 and **1,** respectively, and the electrons are supposed to occupy all positiveenergy free Dirac states up to the Fermi wave number  $k_F$ .

For the application below it is necessary to calculate the Fourier transform

$$
\widetilde{F}_a(\mathbf{k}) = \int e^{i\mathbf{k} \cdot \mathbf{x}} F_a(|\mathbf{x}|) d^3 x \tag{3}
$$

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of  $F_a(|x - x'|)$ . After expression (2) is inserted in Eq. (3) it is useful to interchange the order of integrations over x and over q. For the integrals over x we obtain with  $k \equiv |\mathbf{k}|$ 

$$
\int d^3x e^{i\mathbf{k}\cdot\mathbf{x}} \frac{j_0(2q|\mathbf{x}|)}{|\mathbf{x}|} = \frac{\pi}{kq} h\left(\frac{k}{2q}\right)
$$
 (4a)

and

$$
\int d^3x e^{i\mathbf{k}\cdot\mathbf{x}} \frac{j_1(2q|\mathbf{x}|)}{|\mathbf{x}|^2} = \frac{2\pi}{q} g\left(\frac{k}{2q}\right)
$$
 (4b)

where

$$
h(u) \equiv \ln \left| \frac{u+1}{u-1} \right| \tag{5}
$$

and

$$
g(u) \equiv \frac{1}{2} + \frac{1 - u^2}{4u} h(u).
$$
 (6)

Using Eqs (4a, b) the remaining integration over  $q$  may be performed subsequently yielding after a somewhat lengthy calculation

$$
\tilde{F}_a(\mathbf{k}) = -\frac{mk_F}{\hbar^2 \pi^2} \left\{ \frac{2}{3} \gamma_F - \frac{\kappa^2}{6\kappa_F} \ln(\kappa_F + \gamma_F) \right. \n+ \frac{\gamma_F - \gamma}{\kappa_F} \left[ \frac{1}{3\kappa} (2 + \kappa_F^2 + \gamma \gamma_F) - \frac{\kappa}{6} \right] \ln \left| \frac{2\kappa_F + \kappa}{2\kappa_F - \kappa} \right| \n+ \frac{\gamma}{\kappa_F} \left( \frac{1}{3\kappa} - \frac{\kappa}{6} \right) \ln \left( \frac{2 + 2\gamma \gamma_F - \kappa \kappa_F}{2 + 2\gamma \gamma_F + \kappa \kappa_F} \right) \right\} \n= \tilde{F}_a(\mathbf{k})
$$
\n(7)

In Eq. **(7),** the following abbreviations have been adopted

$$
\kappa_F \equiv \alpha a_0 k_F; \gamma_F \equiv (1 + \kappa_F^2)^{1/2} \tag{8a, b}
$$

$$
\kappa \equiv \alpha a_0 k; \gamma \equiv (1 + \frac{1}{4} \kappa^2)^{1/2}.
$$
 (8c, d)

It is important in what follows to relate the above relativistic treatment to the displaced charge  $\Delta \rho_0(x)$  due to the same potential  $V(x)$  in Eq. (1), as calculated from Schrödinger's equation. One can do this by taking the  $\alpha \rightarrow 0$  limit of Eqs (1), (2), and **(7)** when one is led to the result given by March and Murray2, namely

$$
\Delta \rho_0(\mathbf{x}) = \int F_0(|\mathbf{x} - \mathbf{x}'|) V(\mathbf{x}') d^3 x'
$$
 (9)

Here

$$
F_0(|\mathbf{x} - \mathbf{x}'|) = -\frac{mk_F^2}{2\pi^3 \hbar^2} \cdot \frac{j_1(2k_F|\mathbf{x} - \mathbf{x}'|)}{|\mathbf{x} - \mathbf{x}'|^2}
$$
(10)

with Fourier transform

$$
\tilde{F}_0(k) = -\frac{mk_F}{\hbar^2 \pi^2} g\left(\frac{k}{2k_F}\right) \tag{11}
$$

The object of this work is to follow the proposal made in Ref. 3, namely to relate  $\Delta \rho_a(x)$  to  $\Delta \rho_0(x)$  in the present context. This is evidently equivalent to eliminating the given potential  $V(x)$  between Eqs (1) and (9). Going over to Fourier space one finds

$$
\Delta \tilde{\rho}_a(\mathbf{k}) = \frac{\tilde{F}_a(k)}{\tilde{F}_0(k)} \Delta \tilde{\rho}_0(\mathbf{k})
$$
\n(12)

(this is **Eq.** (3.4) of Ref. **3).** From **Eq.** (12) it follows formally that

$$
\Delta \rho_a(\mathbf{x}) = \int G_a(|\mathbf{x} - \mathbf{x}'|) \Delta \rho_0(\mathbf{x}') d^3 x'
$$
 (13)

with the kernel

$$
G_{\mathbf{x}}(|\mathbf{x} - \mathbf{x}'|) = \frac{1}{(2\pi)^3} \int \frac{\widetilde{F}_{\mathbf{x}}(k)}{\widetilde{F}_{0}(k)} e^{-i\mathbf{k}\cdot(\mathbf{x} - \mathbf{x}')} d^{3}k.
$$
 (14)

If, however, the ratio  $\tilde{F}_{\gamma}/\tilde{F}_{0}$  falls off more slowly than  $\sim k^{-2}$  as  $k \to \infty$ , the integral of **Eq.** (14) does not exist in the ordinary sense. An asymptotic analysis of this ratio yields that

$$
\frac{\tilde{F}_a(k)}{\tilde{F}_0(k)} = A_a + 0(k^{-2})
$$
\n(15)

as  $k \rightarrow \infty$ . The k-independent leading term is given by

$$
A_{\alpha} = \frac{3}{4\kappa_F^3} \left[ \kappa_F \gamma_F (1 + \frac{2}{3} \kappa_F^2) + \frac{1}{2} \ln \left( \frac{\gamma_F - \kappa_F}{\gamma_F + \kappa_F} \right) \right]
$$
(16)

Therefore, the kernel  $G_x$  is divergent for  $x' = x$ . It can be represented, however, as the sum of a convergent part and a part proportional to a  $\delta$ -function by writing

$$
G_x(|\mathbf{x} - \mathbf{x}'|) = D_x(|\mathbf{x} - \mathbf{x}'|) + A_x \delta(\mathbf{x} - \mathbf{x}') \tag{17}
$$

where the integrand of

$$
D_x(|\mathbf{x} - \mathbf{x}'|) \equiv \frac{1}{(2\pi)^3} \int \left[ \frac{\tilde{F}_x(k)}{\tilde{F}_0(k)} - A_x \right] e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} d^3k \tag{18}
$$

vanishes for  $k \rightarrow \infty$  rapidly enough, due to Eq. (15), to ensure convergence. By use of Eq. (17) it follows from **Eq.** (13) that

$$
\Delta \rho_a(\mathbf{x}) = \int D_a(|\mathbf{x} - \mathbf{x}'|) \Delta \rho_0(\mathbf{x}') d^3 x' + A_a \Delta \rho_0(\mathbf{x})
$$
(19)

We note that  $A_{\alpha} \to 1$  as  $\alpha \to 0$ , while  $D_{\alpha} \to 0$  in the same limit.

Equation (19), with the definitions (16) and (18), is the main result of the present work. We note that while, of course, the result (19) hinges on the two underlying assumptions of (i) a given potential  $V(x)$  and (ii) a linear response calculation, the relation exhibited in **Eq.** (19) is entirely non-perturbative in the fine-structure constant *c1.* Thus, it completes for this admittedly simple example, the proposal made in Ref. **3**  for calculating the relativistic electron density  $\rho_a$  from its non-relativistic limit  $\rho_0$ . Thus, using the tables of March and Murray<sup>2</sup>,  $\Delta \rho_a(x)$  could be computed using Eqs (7), (1 **I), (16), (18),** and (19), for a given electron liquid density characterized by wave number  $k_F$ .

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