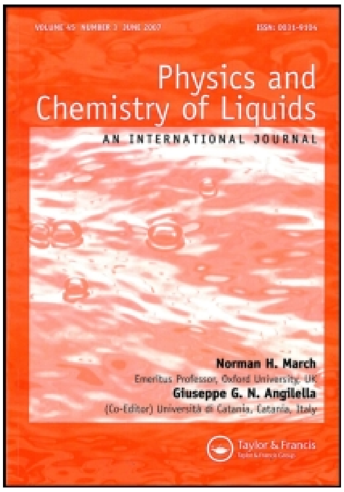

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

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To cite this Article Baltin, R. and March, N. H.(1989) 'Linear Response Relation between Charge Displaced in an Electron Liquid by Relativistic and Nonrelativistic Theory', Physics and Chemistry of Liquids, 19: 3, 189 — 192
To link to this Article: DOI: 10.1080/00319108908030619
URL: http://dx.doi.org/10.1080/00319108908030619

Phys. Chem. Liq., 1989, Vol. 19, pp. 189-192
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LETTER
Linear Response Relation between Charge Displaced in an Electron Liquid by Relativistic and Nonrelativistic Theory

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(Received 28 October 1988)

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 Schrödinger equation.

KEY WORDS: Dirac equation, displaced charge.

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

$$\Delta\rho_\alpha(\mathbf{x}) = \int F_\alpha(|\mathbf{x}-\mathbf{x}'|)V(\mathbf{x}')\,\mathrm{d}^3x' \tag{1}$$

with

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

$a_0 = \hbar^2/(me^2)$, 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 positive-energy free Dirac states up to the Fermi wave number k_F.

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

$$\tilde{F}_\alpha(\mathbf{k}) = \int e^{i\mathbf{k}\cdot\mathbf{x}}F_\alpha(|\mathbf{x}|)\,\mathrm{d}^3x \tag{3}$$

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

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

and

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

where

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

and

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

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

$$\begin{aligned} \tilde{F}_\alpha(\mathbf{k}) = &-\frac{mk_F}{\hbar^2\pi^2}\left\{\frac{2}{3}\gamma_F - \frac{\kappa^2}{6\kappa_F}\ln(\kappa_F + \gamma_F)\right. \\ &+ \frac{\gamma_F - \gamma}{\kappa_F}\left[\frac{1}{3\kappa}(2 + \kappa_F^2 + \gamma\gamma_F) - \frac{\kappa}{6}\right]\ln\left|\frac{2\kappa_F + \kappa}{2\kappa_F - \kappa}\right| \\ &\left. + \frac{\gamma}{\kappa_F}\left(\frac{1}{3\kappa} - \frac{\kappa}{6}\right)\ln\left(\frac{2 + 2\gamma\gamma_F - \kappa\kappa_F}{2 + 2\gamma\gamma_F + \kappa\kappa_F}\right)\right\} \\ = &\ \tilde{F}_\alpha(k) \end{aligned} \tag{7}$$

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

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

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

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

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

Here

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

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 $\Delta\rho_\alpha(\mathbf{x})$ to $\Delta\rho_0(\mathbf{x})$ in the present context. This is evidently equivalent to eliminating the given potential $V(\mathbf{x})$ between Eqs (1) and (9). Going over to Fourier space one finds

$$\Delta\tilde{\rho}_\alpha(\mathbf{k}) = \frac{\tilde{F}_\alpha(k)}{\tilde{F}_0(k)} \Delta\tilde{\rho}_0(\mathbf{k}) \tag{12}$$

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

$$\Delta\rho_\alpha(\mathbf{x}) = \int G_\alpha(|\mathbf{x}-\mathbf{x}'|)\Delta\rho_0(\mathbf{x}')\,\mathrm{d}^3x' \tag{13}$$

with the kernel

$$G_\alpha(|\mathbf{x}-\mathbf{x}'|) = \frac{1}{(2\pi)^3}\int \frac{\tilde{F}_\alpha(k)}{\tilde{F}_0(k)} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\,\mathrm{d}^3k. \tag{14}$$

If, however, the ratio $\tilde{F}_\alpha/\tilde{F}_0$ 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

$$\frac{\tilde{F}_\alpha(k)}{\tilde{F}_0(k)} = A_\alpha + 0(k^{-2}) \tag{15}$$

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

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

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

$$G_\alpha(|\mathbf{x}-\mathbf{x}'|) = D_\alpha(|\mathbf{x}-\mathbf{x}'|) + A_\alpha\delta(\mathbf{x}-\mathbf{x}') \tag{17}$$

where the integrand of

$$D_\alpha(|\mathbf{x}-\mathbf{x}'|) \equiv \frac{1}{(2\pi)^3}\int\left[\frac{\tilde{F}_\alpha(k)}{\tilde{F}_0(k)} - A_\alpha\right]e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\,\mathrm{d}^3k \tag{18}$$

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

$$\Delta\rho_\alpha(\mathbf{x}) = \int D_\alpha(|\mathbf{x}-\mathbf{x}'|)\Delta\rho_0(\mathbf{x}')\,\mathrm{d}^3x' + A_\alpha\Delta\rho_0(\mathbf{x}) \tag{19}$$

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 $V(\mathbf{x})$ and (ii) a linear response calculation, the relation exhibited in Eq. (19) is entirely non-perturbative in the fine-structure constant α. Thus, it completes for this admittedly simple example, the proposal made in Ref. 3 for calculating the relativistic electron density ρ_α from its non-relativistic limit ρ_0. Thus, using the tables of March and Murray[2], $\Delta\rho_\alpha(\mathbf{x})$ could be computed using Eqs (7), (11), (16), (18), and (19), for a given electron liquid density characterized by wave number k_F.

References

1. R. Baltin and N. H. March, *Phys. Rev. A*, **37**, 3942 (1988).
2. N. H. March and A. M. Murray, *Phys. Rev.*, **120**, 830 (1960); *Proc. Roy. Soc.*, **A261**, 119 (1961).
3. N. H. March, *Phys. Rev. A.*, **37**, 1869 (1988).