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Can a relativistic differential equation be set up to treat the angularity of the valence electron density in heavy atom clusters?

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ABSTRACT

This work provides an explicit relativistic non-linear differential equation to estimate the ground-state electron density, and especially its directionality dependence, for large clusters of heavy atoms, such as Pb, at their experimentally measured equilibrium geometry. The study embodies the early theory of Vallarta and Rosen, which seems to us to build a firm foundation on relativistic semi-classical many-electron theory. Assuming a finite nuclear radius for the heavy atoms would be advisable in subsequent numerical applications.

Theory

The earliest relativistic electron density theory goes back, at least, to Vallarta and Rosen [1]. These authors employed special relativity in the form of the relation between momentum and kinetic energy for an electron at the Fermi (F) level to write the constant chemical potential μ throughout the entire inhomogeneous electron density distribution $n(\vec{r})$ as

$$\mu = \left[c^2 p_F^2(\vec{r}) + m_0^2 c^4\right]^{1/2} - m_0 c^2 + V(\vec{r}), \tag{1}$$

where $V(\vec{r})$ is the self-consistent potential energy to be determined. The Fermi momentum $p_F(\vec{r})$ for, say, a cluster of atoms like Pb is related to $n(\vec{r})$ by phase space considerations [2], the result being

$$n(\vec{r}) = \frac{8\pi}{3h^3} p_F^3(\vec{r}). \tag{2}$$

Eliminating $p_F(\vec{r})$ from (1) by means of (2) readily yields

$$\mu = \left[Bc^2 n^{2/3}(\vec{r}) + m_0^2 c^4\right]^{1/2} - m_0 c^2 + V(\vec{r}), \tag{3}$$

where $B = (3/8\pi)^{2/3} h^2$. Adding the explicit requirement of self-consistency, we have that $V(\vec{r})$ is also related to $n(\vec{r})$ by the electrostatic Poisson equation, namely

$$\nabla^2 V(\vec{r}) = 4\pi n(\vec{r}) e^2. \tag{4}$$

We next form $\nabla V(\vec{r})$ entering the left-hand side of Eq. (4) by applying the gradient operator with respect to $\vec{r}$ to both sides of (3). This readily leads to

$$\nabla V(\vec{r}) = -\left[\frac{1}{3} Bc^2 n^{-1/3}(\vec{r}) \nabla n(\vec{r})\right]\left[Bc^2 n^{2/3}(\vec{r}) + m_0^2 c^4\right]^{-1/2}. \tag{5}$$

Inserting (5) into the left-hand side of (4) yields

$$\begin{aligned} -4\pi n(\vec{r}) e^2 &= \nabla \cdot \left\{\left[Bc^2 n^{2/3}(\vec{r}) + m_0^2 c^4\right]^{-1/2}\left[\frac{1}{3} Bc^2 n^{-1/3}(\vec{r}) \nabla n(\vec{r})\right]\right\} \\ &\quad + \left[Bc^2 n^{2/3}(\vec{r}) + m_0^2 c^4\right]^{-1/2}\left\{\frac{1}{3} Bc^2 n^{-1/3}(\vec{r}) \nabla^2 n(\vec{r}) \right. \\ &\quad \left. - \frac{1}{9} Bc^2 n^{-4/3}(\vec{r}) \left[\nabla n(\vec{r})\right]^2\right\}. \end{aligned} \tag{6}$$

Though somewhat complicated, to our knowledge this is the first time a relativistic non-linear differential equation has been derived explicitly in a form which may well be useful relative to the experimental equilibrium geometry for describing some aspects of the angularity of $n(\vec{r})$ in large clusters of heavy atoms, such as Pb.

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While Eq. (6) represents the main result of this letter, we wish to conclude by adding some brief comments in relation to linear response theory when the potential $V(\vec{r})$, but now assumed weak enough to allow one to work only to $O(V)$, is "switched on" to an originally uniform relativistic electron liquid of specified density n_0 [3]. Then one can generalize the non-relativistic linear response function $\vec{r}$-space theory of March and Murray [4] to read

$$n(\vec{r}) - n_0 = \int F_R\big(|\vec{r} - \vec{r}_0|\big) V(\vec{r}_0) d\vec{r}_0. \tag{7}$$

To date, the relativistic response function F_R entering (7) is not known in closed analytic form in $\vec{r}$-space, whereas, as $c \to \infty$, F in Eq. (7) is determined exactly by the first order spherical Bessel function j_1 [4]. Analytical progress in the relativistic case under discussion has proven tractable in $\vec{k}$ (Fourier transform) space [5].

Now, if we approximate the relativistic linear response formula (7) for the case of a slowly varying potential $V(\vec{r}_0)$ such that $V(\vec{r})$ is approximately equal to $V(\vec{r}_0)$, then we find

$$n(\vec{r}) - n_0 \approx V(\vec{r}) \int F_R\big(|\vec{r} - \vec{r}_0|\big) d\vec{r}_0. \tag{8}$$

In the non-relativistic limit, $c \to \infty$ the last expression is approximately $(4k_F/\pi e^2 a_0) d V(\vec{r})$, where k_F is the Fermi wave number, a_0 is the Bohr radius and d is a dimensionless geometrical factor.

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References

[1] M.S. Vallarta, N. Rosen, Phys. Rev. 41 (1932) 708.
[2] N.H. March, Electron Density Theory of Atoms and Molecules, Academic Press, NY, 1992.
[3] N.H. March, Phys. Chem. Liq. 35 (1997) 59.
[4] N.H. March, A.M. Murray, Phys. Rev. 120 (1960) 830.
[5] B. Jancovici, Nuovo Cimento 25 (1962) 428.