Bare Coulomb field: Explicit solution

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(Received 4 February 1997)

The differential equation determining the nth-shell one-electron density of a bare Coulomb problem is solved explicitly. [S1050-2947(97)07108-4]

PACS number(s): 12.20.Ds, 31.15.Ew, 03.65.−w

It has been quite recently that Cooper [1] rederived Blinder's [2] (see also [3]) expression for the one-electron density ρ_n of the nth closed shell for a bare Coulomb problem, via applying the supersymmetric (SUSY) method, and obtained the following nonlinear differential equation:

$$r\rho_n'''(r)-(r/2)[\rho_n''(r)/\rho_n'(r)]^2\rho_n'(r)+2\rho_n''(r)+[4Z-2Z^2r/n^2]\rho_n'(r)=0. \tag{1}$$

The prime indicates the first derivative with respect to r. The integer $n\geqslant 1$ is the principal quantum number. He also showed that $\rho_n(r)$ fully determines the kinetic-energy density $t_n(r)=(1/4\pi)[Z/r-Z^2/2n^2]\rho_n(r)$ and the bound-state Slater sum $S(r,\beta)=(1/4\pi)\Sigma_n\rho_n(r)\exp(-\beta\varepsilon_n)$, where $\beta=(k_BT)^{-1}$ and $\varepsilon_n=-Z^2/2n^2$ are the eigenenergy of the nth shell electron in the Z-electron atom. As emphasized in Refs. [4,5], it makes sense to deal solely with ρ_n without routing to a wave function, if, of course Eq. (1) would be soluble. As derived by March [4], ρ_n obeys the spatial generalization of Kato's theorem [6] and besides, Eq. (1) and its analogs are of particular interest in the density-functional theory [4,7]. That is why it merits to solve this equation in analytical form.

Present work reports the explicit solution of Eq. (1). Under substitution $\rho_n'(r)=x^2(r)$, it becomes simplified [5],

$$rx''+2x'+\left(2Z-\frac{Z^2}{n^2}r\right)x=0, \tag{2}$$

that is, the square root of the first derivative of the nth-shell density obeys exactly the same differential equation that of the corresponding s-state radial wave function $R_{n0}(r)$ [5]. The related ratio $\rho_n'(r)/R_{n0}^2(r)=-2Z$ (see [1], Eq. (4.4)). Suggesting a solution of Eq. (2) as $x(r)=\exp(-\alpha r)\phi(r)$, with $\alpha=Z/n$, one converts this equation into a corresponding one for the unknown $\phi(r)$,

$$r\phi''+2\left(1-\frac{Z}{n}r\right)\phi'+2Z\left(1-\frac{1}{n}\right)\phi=0. \tag{3}$$

In the new variable, $R=2(Z/n)r$, Eq. (3) is simply transformed into the known equation for Kummer's function $\Phi(R)=\phi(r)$ ([8], Eq.(13.1.1)), with $a=1-n$ and $b=2$. Therefore, the regular solution of Eq. (2) is

$$x_n(r)=C_ne^{-(Z/n)r}M(1-n,2,2(Z/n)r)=C_ne^{-(Z/n)r}L_{n-1}^{(1)}(2Zr/n), \tag{4}$$

where Eq. (13.6.9) of Ref. [8] was applied to obtain the last equation, and where $L_n^{(\alpha)}$ is the generalized Laguerre polynomial and C_n the normalization constant. Further, one directly finds the nth-shell density,

$$\begin{aligned}\rho_n(r)&=C_n^2\int_\infty^r dy\ e^{-2Zy/n}[L_{n-1}^{(1)}(2Zy/n)]^2\\&=\frac{nC_n^2}{2Z}\sum_{m,l=0}^{n-1}\frac{(-1)^{m+l}}{m!l!}\binom{n}{n-m-1}\binom{n}{n-l-1}\int_\infty^{2Zr/n}d\alpha\ e^{-\alpha}\alpha^{m+l}\\&=\frac{nC_n^2}{2Z}\sum_{m,l=0}^{n-1}\frac{(-1)^{m+l}}{m!l!}\binom{n}{n-m-1}\binom{n}{n-l-1}\\&\quad\times\left[\frac{1}{m+l+1}(2Zr/n)^{m+l+1}\times e^{-2Zr/n}M(1,m+l+2,2Zr/n)-(m+l)!\right]\\&=\frac{nC_n^2}{2Z}e^{-2Zr/n}\sum_{m,l=0}^{n-1}(-1)^{m+l+1}\binom{m+l}{m}\binom{n}{n-m-1}\\&\quad\times\binom{n}{n-l-1}e_{m+l}(2Zr/n),\end{aligned} \tag{5}$$

where Eqs. (22.3.9), (6.5.3), and (6.5.12) of Ref. [8] were used successively. e_n is defined in [8] by Eq. (6.5.13). It follows from Eq. (5) that $\rho_n(r)$ falls to 0 as r goes to infinity. Normalizing $\rho_n(r)$ to unity, one easily obtains C_n, and thus, the final expression for the nth-shell one-electron density takes the form

$$\rho_n(r)=\frac{3}{4\pi\mathcal{N}_3^{(n)}}\left(\frac{2Z}{n}\right)^3e^{-2Zr/n}\sum_{m,l=0}^{n-1}(-1)^{m+l}\binom{m+l}{m}\times\binom{n}{n-m-1}\binom{n}{n-l-1}e_{m+l}(2Zr/n),$$

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where

$$\mathcal{N}_\alpha^{(n)}=\left[\sum_{k=0}^{2(n-1)}\frac{d}{dx^{k+\alpha}}x^\alpha[L_{n-1}^{(1)}(x)]^2\right]_{x=0}. \quad (6)$$

In particular, if $n=1$, $\rho_1(r)$ is merely the ground-state hydrogenic density, $(Z^3/\pi)\exp(-2Zr)$. Using Eq. (6), one then readily obtains the kinetic-energy density $t_n(r)$ and the bound-state Slater sum $S(r,\beta)$. Another quantity that might be of interest is the radial expectation value $<r^p>_n=\int d\mathbf{r}\ r^p\rho_n(r), p\geqslant -2$. With the help of Eq. (6) and Eq. (14) on p. 59 of Ref. [9], one gets

$$\langle r^{-2}\rangle_n=\frac{3\mathcal{N}_1^{(n)}}{\mathcal{N}_3^{(n)}},\quad \langle r^{-1}\rangle_n=\frac{3\mathcal{N}_2^{(n)}}{2\mathcal{N}_3^{(n)}},$$

$$\langle r^p\rangle_n=\frac{3\mathcal{N}_{3+p}^{(n)}}{\mathcal{N}_3^{(n)}(3+p)},\quad p\geqslant 0. \quad (7)$$

Summarizing, we have found the explicit solution of the differential equation for $\rho_n(r)$ in terms of generalized Laguerre polynomials that now makes it possible to apply a bare Coulomb model to a variety of many-body problems and density-functional theory, in particular, without routing to wave functions. This solution provides, in a straightforward manner, the analytical expressions for the kinetic-energy density, bound-state Slater sum, and radial expectation value.

[1] I. L. Cooper, Phys. Rev. A **50**, 1040 (1994).

[2] S. M. Blinder, Phys. Rev. A **29**, 1674 (1984).

[3] (a) R. Shakeshaft and L. Spruch, J. Phys. B **18**, 1919 (1985); (b) Rev. Mod. Phys. **51**, 369 (1979); (c) L. Spruch and R. Shakeshaft, Phys. Rev. A **29**, 2283 (1984).

[4] (a) N. H. March, Phys. Lett. **111A**, 47 (1985); (b) Phys. Rev. A **33**, 88 (1986); (c) N. H. March and R. Santamaria, *ibid.* **39**, 2835 (1989); (d) see also P. M. Kozlowski, J. Math. Chem. **9**, 291 (1992).

[5] S. Bhattacharyya, Phys. Rev. A **53**, 598 (1996).

[6] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).

[7] J. A. Flores and J. Keller, Phys. Rev. A **45**, 6259 (1991).

[8] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1972).

[9] V. Mangulis, *Handbook of Series for Scientists and Engineers* (Academic, New York, 1965).