

Spherical-Coordinate Analysis of Ground-State Energy Eigenfunctions for an Electron in the Field of a Finite Dipole*

W. R. Garrett, J. E. Turner, and V. E. Anderson[†]

Health Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

(Received 17 July 1969)

Ground-state energy eigenfunctions for an electron in the field of a stationary, finite dipole are obtained in spherical polar coordinates. The analysis is made in two systems, one with origin at the positive dipole charge and the other with origin at the dipole center. Results show the number of partial waves needed as a function of dipole moment D , and the structure of the radial functions throughout space. No regular nodal pattern in the radial functions for different angular momentum partial waves was noted. The functions expressed in spherical coordinates are available numerically for use in other calculations.

Previous calculations of the ground-state energy eigenfunctions ψ , for an electron and a stationary finite electric dipole were made in elliptic hyperbolic coordinates.¹ Though the variational calculation was greatly facilitated by the use of these coordinates, analysis of ψ in terms of spherical polar coordinates is more relevant to an understanding of the interaction of electrons with polar molecules. For example, one may be interested in negative-ion formation, electron scattering, or the influence of other forces on the interaction of electrons with polar molecules. The previous representation does not yield physical insight into these phenomena. In particular, a partial-wave analysis gives the number and relative importance of orbital angular momentum states in the electron wave function for different dipole moments D . A complete analysis of the wave functions of Ref. 1 has been made,² and we summarize the findings here.

With reference to Fig. 1 we use the coordinate systems (r_1, θ_1) and (r, θ) and write

$$\psi(\xi, \eta) = \sum_{l=0} F_l(r_1) P_l(\cos \theta_1) = \sum_{l=0} G_l(r) P_l(\cos \theta), \quad (1)$$

where (ξ, η) are the coordinates used previously.¹ The coordinates (r, θ) are convenient in a number of problems, particularly when other potentials are treated in addition to the dipole potential or when rotational excitation of the dipole about its center is considered. For large dipole moments and for comparisons with the properties of the hydrogen atom, (r_1, θ_1) are more convenient.

The functions F_l and G_l are found simply by taking inner products, e.g.,

$$F_l(r_1) = \int_{-1}^1 \psi(\xi, \eta) P_l(\cos \theta_1) d(\cos \theta_1). \quad (2)$$

The functions ψ given in Ref. 1 were transformed into (r_1, θ_1) and the integration in Eq. (2) performed numerically. A similar transformation yields

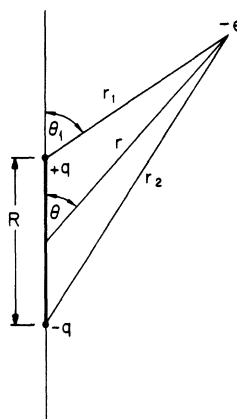


FIG. 1. Coordinate system for electron and finite dipole.

$G_l(r)$. Results thus found, agreed with those obtained independently by direct numerical integration of the coupled radial equations which result from expressing the Schrödinger equation in spherical coordinates.² Numerical values of the radial functions F_l and G_l are tabulated in Ref. 2 for the complete range of dipole moments.

Some of the results are illustrated in Figs. 2-4. In these calculations ten partial waves ($l=0, \dots, 9$) were used. As expected, when D is near D_{\min} , F_l and G_l are practically identical (Fig. 2), and the wave function is predominantly s and p . In the limit of zero binding energy the wave function goes smoothly into the continuum. This suggests that the description of low-energy electron scattering from polar molecules requires at least s and p waves. Since $\langle r_1 \rangle = \langle r_2 \rangle = 1.85435 \times 10^7$, the integrated probability density $\psi^* \psi$, from the origin to the region where F_l and G_l do not differ visibly, is $\ll 1$. Figures 3 and 4 shows the radial functions for $D=1.00002$. Generally, the functions are largest numerically near the dipole charges. Although oscillatory behavior occurs for the higher l values, no predictable node pattern was found.

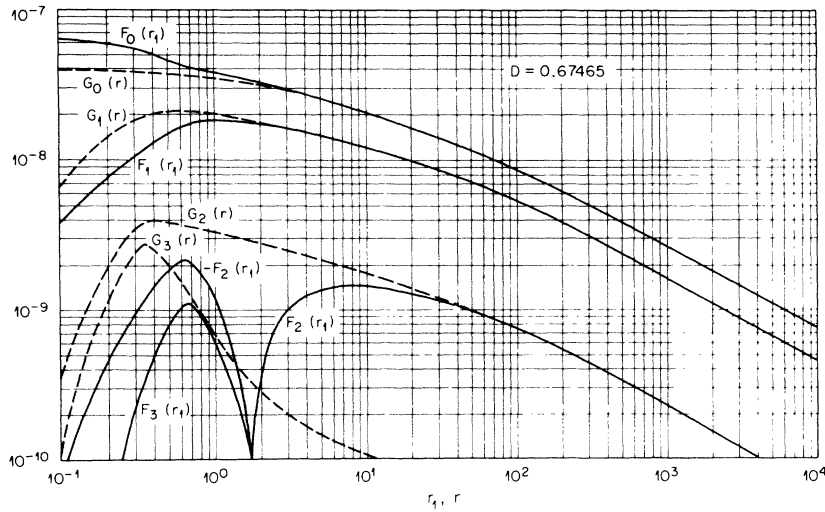


FIG. 2. Radial functions $F_l(r_1)$ and $G_l(r)$ for $D=0.67465$.

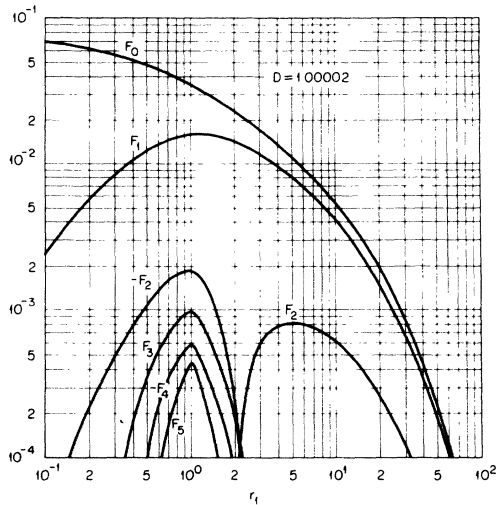


FIG. 3. Radial functions $F_l(r_1)$ for $D=1.00002$.

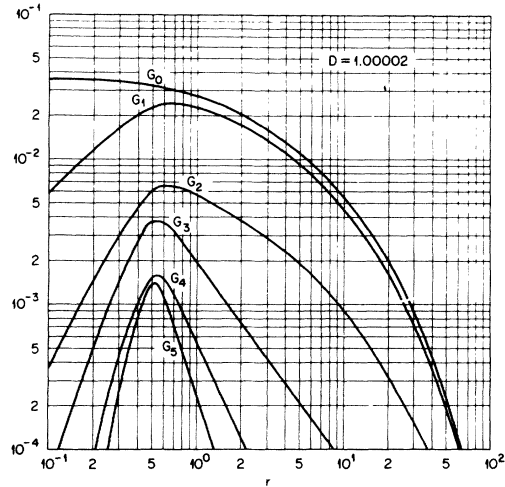


FIG. 4. Radial functions $G_l(r)$ for $D=1.00002$.

*Research sponsored by the U.S. Atomic Energy Commission under contract with Union Carbide Corporation.

†Computing Technology Center, Union Carbide Corporation, Nuclear Division, Oak Ridge, Tenn.

¹J. E. Turner, V. E. Anderson, and K. Fox, Phys. Rev. **174**, 81 (1968).

²W. R. Garrett, J. E. Turner, and V. E. Anderson, Oak Ridge National Laboratory Report No. ORNL-4431, 1969 (unpublished).