APPROXIMATIONS OF THE THOMAS-FERMI FUNCTION

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NUMEROUS articles have appeared recently (see reference 1, for example) concerning approximations to the solution of the Thomas-Fermi equation[2] for a free neutral atom:

$$\varphi'' = \varphi^{3/2}/\xi^{1/2}. \tag{1}$$

Here $\xi = r/\mu$, r is the distance from the center of the atom, $\mu = \nu a_0/Z^{1/3}$, a_0 is the Bohr radius, and $\nu = 0.8853$.

As a measure of the accuracy of an approximate solution, Umeda[3] has suggested using the numerical solution of an integral whose variation gives Eq. (1):

$$I(\varphi) = \int_0^\infty [\varphi'^2 + (^4/_5)\varphi^{5/2}\xi^{-1/2}]\, d\xi. \tag{2}$$

This functional has a minimum value[4] of 1.3612 when φ is an exact solution of (1). The deviation of I from the minimum value can serve as an estimate of the degree of accuracy of the approximate solution. Thus for Sommerfeld's approximation[5] $\varphi = [1 + (\xi/12^{2/3})^\lambda]^{-3/\lambda}$, I = 1.3670; for Kerner's form $\varphi = [1 + \lambda\xi]^{-1}$, I = 1.3679; for Tietz's solution $\varphi = [1 + \lambda\xi]^{-2}$, I = 1.3662; and for Rosenthal's solution[6] $\varphi = 0.7345e^{-0.562\xi} + 0.2655e^{-3.392\xi}$, I = 1.3636.

We can write φ in a new form for which I = 3.624, which is much closer to the minimum value:

$$\varphi(\xi) = e^{-x^{1/2}}(1 + {}^1/_2 x^{1/2})^2. \tag{3}$$

Here and hereinafter $x = \lambda\xi$, where λ is a parameter which can be determined in different ways. $\lambda = \lambda_{Um} = 6.119$ is determined by Umeda's method from the condition $\partial I/\partial\lambda = 0$.

Equation (3) can be derived by making the transition from the Lenz-Jensen approximate expression $\rho(r)$ for electron density in an atom to the function $\varphi(\xi)$. For this purpose let us consider the following relation between $\rho(r)$ and $\varphi(\xi)$:

$$\rho_I(r) = (Z/4\pi\mu^3)\varphi''/\xi, \tag{4}$$

$$\rho_{II}(r) = (Z/4\pi\mu^3)(\varphi/\xi)^{3/2}. \tag{4a}$$

When φ is an exact solution of (1), ρ_I and ρ_{II} will of course coincide. When φ is approximate, (4a) must be used because the function itself is a better approximation than its second derivative. But (4a) does not generally satisfy the normalization condition $\int_0^\infty \rho 4\pi r^2\, dr = Z$ for approximate φ and arbitrary λ. Therefore instead of ρ_{II} we must take

$$\rho = \rho_{II}(\lambda/\lambda_{Ma})^{3/2}, \tag{4b}$$

where λ_{Ma} is determined by the mean value method:

$$\int_0^\infty (\varphi'' - \varphi^{3/2}/\xi^{1/2})\,\xi d\xi = 0,$$

which has been proposed by March.[1,7] The transformation (4b) insures normalization of ρ for arbitrary λ as well as fulfillment of the virial theorem $2H_K + H_P = 0$. The advantage of (4a) and (4b) over (4) now also follows from energy considerations. Thus using Tietz's simple and convenient approximation of φ, (4) gives for the total energy of an atom by the Ritz method[2] H = −0.660 in the units $Z^{7/3}e^2/a_0$, whereas from (4a) and (4b) we obtain H = −0.768, which is much closer to the exact value H = −0.769. The value of ρ obtained from (4a) and (4b), with $\lambda = \lambda_{Ri}$ as determined by the Ritz method from $\partial H/\partial\lambda = 0$, may be regarded as the approximation that corresponds to a given approximate φ. For example, from Tietz's form ($\lambda_{Ma} = (\pi/8)^{2/3} = 0.536$), we obtain an expression which insures normalization and fulfillment of the virial theorem, and also gives a good value for the energy:

$$\rho_{TI} = \frac{Z}{4\pi\mu^3}\frac{8\lambda^3}{\pi}x^{-1/2}(1+x)^{-3}, \tag{5}$$

where $\lambda = \lambda_{Ri} = 0.527$.

On the other hand, let us start with the well-known Lenz-Jensen approximation[8] for ρ:

$$\rho_{LJ} = \frac{Z}{4\pi\mu^3}\frac{\lambda^3}{4P}x^{-3/2}\exp(-x^{1/2})(1 + Cx^{1/2})^3 \tag{6}$$

and pass in reverse to φ using (4a) and (4b) [$\lambda_{Ma} = (4P)^{2/3}$]. Letting $C = {}^1/_3$, we then obtain (3), where λ differs from the λ of (6) by the factor $^4/_9$. The selection of $C = {}^1/_3$, which differs somewhat from Jensen's value C = 0.265, is required to improve the form of φ at zero [$\varphi'(0) = -1.530$ instead of $\varphi'(0) = -\infty$ with the exact solution $\varphi'(0) = -1.588$]. When $C = {}^1/_3$, $\lambda_{Ri} = 11.41$ and H = −0.76 [for comparison $\lambda_{Ma} = 11.87$ and $\lambda_{Um} = (^9/_4)\,6.12 = 13.77$]. The form (3) which has been obtained is quite simple and convenient. In the principal range of variation, $0 < \xi < 1$, the

value of φ obtained from (3) differs on the average from the exact solution obtained numerically in reference 9 by less than 0.5%, and never differs by more than 1%. In the same region, φ' differs by less than 2.5% on the average and by not more than 5% from the exact value of φ'.

In conclusion it should be noted that any attempt to derive an extremely accurate approximation of the Thomas-Fermi function at small and at large distances from the nucleus is devoid of meaning, for there Eq. (1) does not correctly indicate the potential in the atom.

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PRODUCTION OF A STAR AND A FAST PROTON OR ANTIPROTON

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THE production of a star by a γ-quantum through an intermediate π-meson pair was investigated in reference 1. In the present work we consider an analogous process: a high-energy γ-quantum produces a proton-antiproton pair one particle of which is absorbed in the nucleus, producing a star. The other particle carries away energy of the order of the energy of the star. The study is carried out for the ultra-relativistic region where only small angles between the momentum of the γ-quantum and that of the emitted proton (or antiproton) are of importance. The strong interaction between the proton (and antiproton) and the nucleus is accounted for by using the optical model. The nucleus is regarded as an ideal black body of a given radius, as far as the proton and antiproton are concerned.

We shall assume that the behavior of nucleons is described by Dirac's equation. The anomalous magnetic moment of the nucleon is not of great importance for such high energies. Let us assume, for example, that the proton is absorbed and the antiproton is emitted to an infinite distance. Dirac's equation for such a process can be written as follows: ($\hbar = c = 1$)

$$(\gamma\nabla - \gamma_4 E_1 + m)\,\psi_{p_1}(\mathbf{r}) = \frac{ie}{V 2\omega}(\gamma\mathbf{e})\, e^{i\mathbf{kr}}\psi^{(-)}_{p_2}(\mathbf{r}). \qquad (1)$$

where $\mathbf{p}, E_1(\mathbf{p}_2, E_2)$ are the momentum and energy of the proton (or antiproton). We shall denote the momentum of a γ-quantum of frequency ω by $\mathbf{k}$, and its polarization vector by $\mathbf{e}$. The wave function of the antiproton, which is a free particle in its final state, is a superposition of a plane wave and of a wave diffracted on the black nucleus.[2]

We find the wave function ψ_{p_1} of the proton by means of the Green's function[3] of Eq. (1), under the condition that the antiproton is at infinity. We obtain the cross section for the process by calculating the total flux of protons incident upon the nucleus:

$$d\sigma = \int j(\mathbf{s}_1)\, d\mathbf{s}_1 |F|^2\, dp_2\, d\mathbf{k}_2/(2\pi)^3;$$

$$j(\mathbf{s}_1) = (\psi_{p_1}(\mathbf{s}_1)\frac{i\gamma p_1}{p_1}\psi_{p_1}(\mathbf{s}_1)),$$

where $\mathbf{k}_2$ is the transverse momentum of the emitted antiproton and F is in the nature of a nucleon form-factor.[4] Integration over $\mathbf{s}_1(\mathbf{s}_2)$ is carried out along a circle with radius R, perpendicular to $\mathbf{p}_1(\mathbf{p}_2)$ and passing through the center of the nucleus.

We obtain the following expression for the differential cross-section of the process, averaged over possible polarization of the γ-quantum:

$$d\sigma(E_2, \boldsymbol{\eta}) = \frac{e^2}{\omega^3}\frac{|F|^2 R}{(2\pi)^3 m}\{[E_2^2 + (\omega - E_2)^2]K(\varepsilon) + E_2(\omega - E_2)E(\varepsilon)\}\frac{dE_2 d\eta}{(1+\eta^2)^{3/2}}; \qquad (2)$$

$$\boldsymbol{\eta} = \mathbf{k}_2/m, \quad \varepsilon^2 = \eta^2/(1+\eta^2), \quad d\boldsymbol{\eta} = \eta d\eta d\varphi_\eta,$$

where $K(\epsilon)$ and $E(\epsilon)$ are complete elliptic in-