AAPT PHYSICS EDUCATION | AMERICAN JOURNAL of PHYSICS

Alternative form of the hydrogenic wave functions for an extended, uniformly charged nucleus

E. Ley-Koo, E. Castaño, D. Finotello, E. Nahmad-Achar, and S. Ulloa

Citation: American Journal of Physics **48**, 949 (1980); doi: 10.1119/1.12365
View online: http://dx.doi.org/10.1119/1.12365
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/48/11?ver=pdfcov
Published by the American Association of Physics Teachers

Alternative form of the hydrogenic wave functions for an extended, uniformly charged nucleus

E. Ley-Koo
Instituto de Física, Universidad Nacional Autónoma de México, Apdo. Postal 20-364, México 20, D.F., México

E. Castaño, D. Finotello, E. Nahmad-Achar, and S. Ulloa
Facultad de Ciencias, Universidad Nacional Autónoma de México Apdo. Postal 20-364, México 20, D.F., México
(Received 14 January 1980; accepted 8 April 1980)

An exact closed solution for the hydrogenic wave functions for an extended, uniformly charged nucleus was reported in this Journal some time ago. We present an alternative form of such wave functions which allows numerical results to be obtained more easily. We illustrate the use of this alternative form by its application to muonic atoms throughout the periodic table.

I. INTRODUCTION

An atomic system consisting of a particle of mass m and charge $-e$, and a nucleus of mass M and charge Ze uniformly distributed over its spherical volume of radius R, has an electrostatic potential energy

$$V(r) = -\frac{Ze^2}{2R}\left(3 - \frac{r^2}{R^2}\right) \quad 0 \leqslant r \leqslant R \tag{1a}$$

$$= -\frac{Ze^2}{r} \quad r \geqslant R, \tag{1b}$$

where r is the distance of the particle from the center of the nucleus. The Schrödinger equation for this system is known to have an exact, closed solution as already reported in this Journal.[1] It is easy to understand that such a solution exists upon recognition that the particle feels a harmonic oscillator attraction when it is inside the nucleus [Eq. (1a)] and a Coulomb attraction when it is outside the nucleus [Eq. (1b)]. In fact, the solution is obtained by matching the respective oscillator and Coulomb wave functions, and their derivatives, at the radius of the nucleus. In Ref. 1, the inside and outside solutions were presented through their integral representations; the inside solution was also given in its power series representation, but this was not done for the outside solution. Correspondingly, no numerical solutions were obtained.

In this paper we present alternative forms of the oscillator and Coulomb wave functions which can be explicitly constructed and lead to numerical results for the energy eigenvalues and eigenfunctions of the atomic system. In Sec. II we obtain the inside and outside solutions of the Schrödinger equation and match their logarithmic derivatives at the radius of the nucleus, setting up the equation for the energy eigenvalues in a form which is simple and explicit enough to be solved numerically. Some specific cases of muonic atoms throughout the periodic table are presented in Sec. III to illustrate how the numerical calculations can be carried out. Section IV contains the results of these calculations and a discussion of the finite nuclear size effect on the atomic energy levels.

II. SCHRÖDINGER EQUATION AND ITS SOLUTION

The spherical symmetry of the system allows the separation of the Schrödinger equation and its solutions into radial and angular parts. The radial equation is

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + \frac{Ze^2}{2R^3}r^2\right]F(r) = \left(E + \frac{3Ze^2}{2R}\right)F(r) \tag{2a}$$

inside the nucleus and

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) - \frac{Ze^2}{r}\right]F(r) = EF(r) \tag{2b}$$

outside the nucleus. Here $\mu = mM/(m+M)$ is the reduced mass of the system.

We are interested in the bound states of the atom, for which the energy is negative and can be written in the form

$$E = -Z^2e^2/2a_\mu\nu^2, \tag{3}$$

in terms of the Bohr radius of the system, $a_\mu = \hbar^2/e^2\mu$, and the dimensionless parameter ν. It is convenient to identify the frequency of the harmonic oscillator

$$\omega = \sqrt{Ze^2/\mu R^3},$$

to introduce the dimensionless radial coordinate

$$x = \sqrt{\mu\omega/\hbar}\, r = \sqrt{ZR/a_\mu}\,(r/R) = x_0 r/R \tag{4a}$$

and the dimensionless energy parameter

$$\epsilon(\nu) = \frac{E + 3Ze^2/2R}{\hbar\omega} = \sqrt{\frac{ZR}{a_\mu}}\left(\frac{3}{2} - \frac{ZR}{2a_\mu\nu^2}\right). \tag{4b}$$

Another useful dimensionless radial coordinate is

$$y = Zr/a_\mu\nu = x_0^4 r/R\nu. \tag{4c}$$

 0002-9505/80/110949-05$00.50

Then the radial equation becomes

$$\left(\frac{d^2}{dx^2}+\frac{2}{x}\frac{d}{dx}-\frac{l(l+1)}{x^2}-x^2+2\epsilon\right)F(x)=0 \quad (5a)$$

and

$$\left(\frac{d^2}{dy^2}+\frac{2}{y}\frac{d}{dy}-\frac{l(l+1)}{y^2}+\frac{2\nu}{y}-1\right)F(y)=0. \quad (5b)$$

For the solution inside the nucleus we propose a power series expansion

$$F_{\rm osc}(x)=A_{\nu l}x^l\sum_{s=0}^{\infty}a_s^{(l)}x^s, \quad (6a)$$

which has the proper behavior close to the origin. Substitution in Eq. (5a) leads to the recurrence relation for the coefficients,

$$a_{N+2}^{(l)}=\frac{-2\epsilon a_N^{(l)}+a_{N-2}^{(l)}}{(N+2)(2l+N+3)},\quad a_2^{(l)}=-\frac{\epsilon}{2l+3}. \quad (7a)$$

We take $a_0^{(l)}=1$, without any loss of generality. All coefficients with an odd subindex or a negative subindex are identically zero. Thus for a given value of ϵ or ν, the solution [Eq. (6)] is completely defined, except for the normalization constant $A_{\nu l}$. Notice that we do not have to worry about the asymptotic behavior of this solution, since it is valid only inside the nucleus. Of course, we could also separate a Gaussian exponential factor, as it is done for the normal harmonic oscillator and as it was done in Ref. 1; however, for the numerical solution of the problem at hand, it is to our advantage not to do so.

For the solution outside the nucleus we propose

$$F_{\rm coul}(y)=B_{\nu l}y^le^{-y}f(y), \quad (6b)$$

which has the proper asymptotic behavior. Substitution in Eq. (5b) leads to the equation satisfied by the last factor,

$$2y\frac{d^2f}{d(2y)^2}+(2l+2-2y)\frac{df}{d(2y)}-(-\nu+l+1)f=0. \quad (7b)$$

This is immediately identified as Kummer's equation,[2] whose solutions are Kummer's functions $M(-\nu+l+1,2l+2,2y)$ and $U(-\nu+l+1,2l+2,2y)$. The latter is chosen over the former in order to guarantee the proper asymptotic behavior in Eq. (6b). The structure of this solution coincides with that of Eq. (2) in Ref. 1; however, only the integral representation was presented there. It is worth examining the alternative forms of Kummer's functions, the relations between them, and the conditions for their validity. We do this in the Appendix, and recognize here that the logarithmic form Eq. (A4) is the relevant one for our problem.

The matching of the inside and outside solutions [Eqs. (6a) and (6b)] and of their derivatives, at the radius of the nucleus,

$$F_{\rm osc}(x_0=\sqrt[4]{ZR/a_\mu})=F_{\rm Coul}(y_0=ZR/a_\mu\nu), \quad (8a)$$

$$\sqrt[4]{Z/a_\mu R^3}\,F'_{\rm osc}(x_0)=(Z/a_\mu\nu)F'_{\rm Coul}(y_0), \quad (8b)$$

determines the energy eigenvalues. This is equivalent to matching the logarithmic derivatives, obtained by dividing Eq. (8b) by Eq. (8a), which has the advantage of being independent of the normalization constants:

$$\sqrt[4]{Z/a_\mu R^3}\left(\sum_{s=0}^{\infty}a_s^{(l)}(l+2s)x_0^{l+2s-1}\right)\left(\sum_{t=0}^{\infty}a_t^{(l)}x_0^{l+2t}\right)^{-1}$$

$$=(Z/a_\mu\nu)\{[(l/y_0)-1]U(-\nu+l+1,2l+2,2y_0)$$
$$-2(-\nu+l+1)U(-\nu+l+2,2l+3,2y_0)\}$$
$$\times[U(-\nu+l+1,2l+2,2y_0)]^{-1}. \quad (9)$$

Here we have made use of Eqs. (6a) and (6b) for the solutions and Eq. (A5) for the derivative of Kummer's function. It is convenient to recognize that for a given atom, the value of x_0, [Eq. (4a)] is fixed, while $y_0=x_0^4/\nu$ and the coefficients $a_s^{(l)}$ [Eqs. (4c), (7a), and (4b)] depend on ν, i.e., on the energy. Therefore, the solution of Eqs. (8a) and (8b) or (9) is equivalent to finding the zeros of

$$G_l(\nu)=\left(\sum_{s=0}^{\infty}a_{2s}^{(l)}(l+2s)x_0^{2s}\right)$$
$$\times U(-\nu+l+1,2l+2,2x_0^4/\nu)$$
$$-\left(\sum_{t=0}^{\infty}a_{2t}^{(l)}x_0^{2t}\right)[(l-x_0^4/\nu)U(-\nu+1+1,2l+2,2x_0^4/\nu)$$
$$-2(x_0^4/\nu)(-\nu+l+1)U(-\nu+l+2,2l+3,2x_0^4/\nu)]. \quad (10)$$

In practice, for a given l, it is convenient to carry out the numerical calculations by fixing first the value of ν. This fixes the energy parameter $\epsilon(\nu)$ [Eq. (4b)] which in turn allows the generation of the coefficients $a_s^{(l)}$ [Eq. (7a)]. Also, the parameters of Kummer's function are fixed and the latter can be evaluated by using Eq. (A4). The function $G_l(\nu)$ [Eq. (10)] can be determined numerically to the desired accuracy by including a finite number of terms in the summations. The values of ν can be varied until a zero of $G_l(\nu)$ is found. This corresponds to finding one of the solutions of the Schrödinger equation with the energy eigenvalue given by Eq. (3) and the eigenfunction of Eqs. (6a) and (6b).

III. MUONIC ATOMS

The importance of the finite nuclear size effect in muonic atoms has been well known for a long time.[3,4] In fact, such an effect is the basis for one of the methods to determine the radius of nuclei, which is given by

$$R=R_0A^{1/3}, \quad (11)$$

where $R_0=1.2\times10^{-13}$ cm and A is the mass number of the nucleus. The finite nuclear size effect is better appreciated by comparing the nuclear radius with the radius

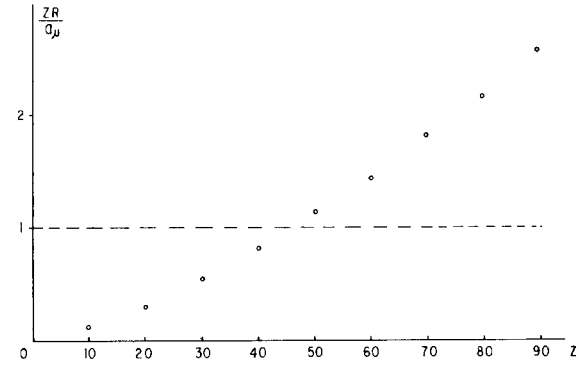

Fig. 1. Ratio of nuclear radius to first Bohr orbit radius for muonic atoms throughout the periodic table.

Table I. Numerical comparison of nuclear radii and first Bohr orbit radii for muonic atoms throughout the periodic table.

Element	Z	A	$\mu(m_e)$	$R(10^{-13}\,\text{cm})$	$a_\mu/Z(10^{-13}\,\text{cm})$	ZR/a_μ
Ne	10	20	205.60	3.2573	25.738	0.1266
Ca	20	40	206.19	4.1039	12.832	0.3198
Zn	30	64	206.40	4.8000	8.546	0.5617
Zr	40	90	206.51	5.3777	6.406	0.8395
Sn	50	120	206.57	5.9189	5.123	1.1553
Nd	60	142	206.60	6.2605	4.269	1.4666
Yb	70	174	206.64	6.6993	3.658	1.8313
Hg	80	202	206.65	7.0410	3.201	2.1997
Pb	82	208	206.66	7.1100	3.123	2.2769
Th	90	232	206.67	7.3736	2.845	2.5918

a_μ/Z of the first Bohr orbit in the muonic atom. We take the muon mass to be 206.77 m_e and the nuclear mass to be 1822.84 $A\,m_e$, in terms of the electron mass m_e. Table I and Fig. 1 contain this information for some nuclei throughout the periodic table, and show explicitly the increasing importance of the finite nuclear size effect for heavier nuclei. Of course, this is easy to understand as it results from the combination of the increasing nuclear radius [Eq. (11)] and the decreasing radius of the first Bohr orbit.

We proceed next to obtain numerically the zeros of Eq. (10) for the above mentioned nuclei, which is equivalent to finding the energy eigenvalues and eigenfuctions of the corresponding muonic atoms. This is practically accomplished, by fixing first the nucleus, i.e., Z and A, we are interested in. From Table I we obtain ZR/a_μ, which through Eq. (4a) fixes the value of x_0. Next we have to choose the angular momentum l of the state of our interest. From here on, the discussion following Eq. (10) is valid and applicable. Of course, the set of zeros $\nu(l,n)$ of Eq. (10), where $n = 1,2,3,\ldots$, denotes the ordering of the zeros, determines the energy spectrum of the muonic atom [Eq. (3)].

IV. RESULTS AND DISCUSSION

Some of the results of our calculations are presented numerically in Tables II and III, and graphically in Figs. 2 and 3.

Table II consists of the lowest values of ν from Eq. (10) and the corresponding energy eigenvalues E from Eq. (3) for the $l = 0$, 1, and 2 states of the muonic atoms under consideration. We have included only the values of ν that differ from an integer by at least 0.001 and the blank spaces correspond to values of ν that differ from an integer by less than 0.001. We can immediately see that the departure of

Table II. Lowest energy eigenvalues for muonic atoms obtained from Eqs. (10) and (3). Only the values of ν differing by at least 0.001 from an integer are explicitly included.

Element	$\nu(l=0)$	E(MeV)	$\nu(l=1)$	E(MeV)	$\nu(l=2)$	E(MeV)
	1.005	−0.278				
$^{20}_{10}$Ne	2.005	−0.070				
	3.005	−0.031				
	1.027	−1.065				
$^{40}_{20}$Ca	2.027	−0.273				
	3.027	−0.123				
	1.064	−2.233				
$^{64}_{30}$Zn	2.064	−0.593				
	3.064	−0.269				
	1.112	−3.634				
$^{90}_{40}$Zr	2.111	−1.008	2.002	−1.121		
	3.110	−0.465	3.002	−0.499		
	1.166	−5.164				
$^{120}_{50}$Sn	2.164	−1.499	2.006	−1.745		
	3.163	−0.702	3.007	−0.777		
	1.219	−6.804				
$^{142}_{60}$Nd	2.214	−2.063	2.012	−2.500		
	3.213	−0.979	3.014	−1.113		
	1.279	−8.413				
$^{174}_{70}$Yb	2.270	−2.671	2.024	−3.359		
	3.268	−1.289	3.027	−1.502		
	1.336	−10.070				
$^{202}_{80}$Hg	2.324	−3.328	2.039	−4.323		
	3.321	−1.630	3.044	−1.940	3.001	−1.996
	1.348	−10.393				
$^{208}_{82}$Pb	2.335	−3.464	2.042	−4.529		
	3.331	−1.702	3.047	−2.034	3.001	−2.097
	1.394	−11.707				
$^{232}_{90}$Th	2.378	−4.023	2.058	−5.371		
	3.373	−1.999	3.065	−2.422	3.002	−2.524

Table III. Wave functions for the $1s$ state of muonic atoms obtained from Eqs. (6a) and (6b). The nuclear radius is the unit of length.

$r(R)$	$^{40}_{20}$Ca $F_{1s}(r)$	$^{208}_{82}$Pb $F_{1s}(r)$
0.0	1.0000	1.0000
0.2	0.9943	0.9739
0.4	0.9776	0.9000
0.6	0.9511	0.7906
0.8	0.9167	0.6625
1.0	0.8770	0.5331
1.5	0.7708	0.2788
2.0	0.6700	0.1359
2.5	0.5795	0.0641
3.0	0.4999	0.0297
3.5	0.4306	0.0135
4.0	0.3704	0.0061
4.5	0.3184	0.0028
5.0	0.2736	
6.0	0.2017	
7.0	0.1485	
8.0	0.1092	
9.0	0.0803	
10.0	0.0590	

the values of ν from integer values increases for heavier elements, which is a direct consequence of the increasing importance of the nuclear size effect. We can also see that for a given atomic system such a departure is more important for the lower angular momentum states, and for a given atom and a given angular momentum the relative value of such a departure is more important for the lower energy states. Both of these trends are directly related to the relative probabilities of finding the negatively charged particle in the region of the nucleus. Here the energies have been expressed in MeV in order to facilitate the comparison with experimental values. For example, the $2p \rightarrow 1s$ transition in $^{208}_{82}$Pb involves a γ ray with a calculated energy of 5.864 MeV to be compared with the observed value[4] of 5.8 MeV. Figure 2 consists of the energy spectra for different muonic atoms. The energies are expressed in units $Z^2e^2/2a_\mu$ and for the sake of clarity we have drawn only the $l = 0$ levels. The dashed horizontal lines correspond to the energy levels of atoms with point nuclei, and the $l = 1,2$ energy levels for the muonic atoms would be above these lines and below the $l = 0$ levels. The above mentioned trends of the energy levels can be globally appreciated in this graph.

Table III contains the radial wave functions for the $1s$ state of $^{40}_{20}$Ca and $^{208}_{82}$Pb obtained from Eqs. (6a) and (6b),

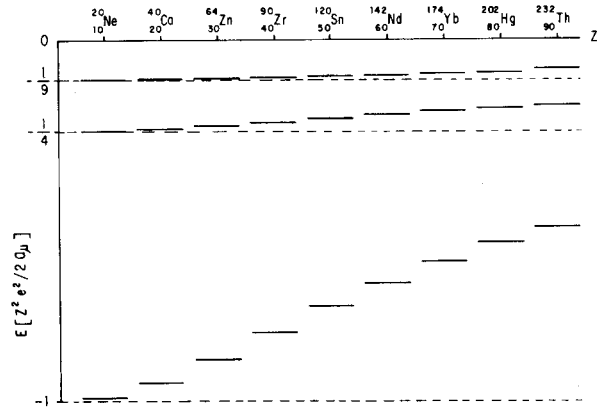

Fig. 2. Lowest ns energy levels for muonic atoms throughout the periodic table. Dashed lines correspond to point nucleus atom.

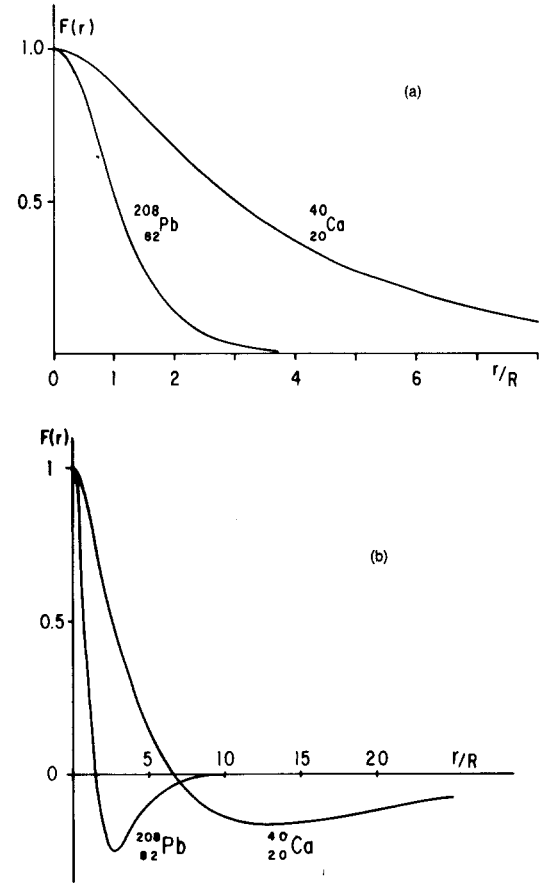

Fig. 3. (a) Radial wave function of the $1s$ state for $^{40}_{20}$Ca and $^{208}_{82}$Pb muonic atoms. (b) Radial wave function of the $2s$ state for $^{40}_{20}$Ca and $^{208}_{82}$Pb muonic atoms.

using the nuclear radius as the unit of length. These wave functions are normalized in such a way that their value at the origin, $r = 0$, is one, which corresponds to the choice $A_{1s} = 1$ in Eq. (6a). Of course, the value of B_{1s} in Eq. (6b) is determined by the energy eigenvalue equation (8a), corresponding to the matching of the inside and outside solutions at the nuclear surface $r = R$. Figure 3(a) is a graph of these wave functions showing that there is indeed a smooth matching. As it is to be expected, the main difference of these wave functions with respect to the simple decreasing exponential wave function for a point-nucleus atom stands out in the region of the nucleus, starting out with a zero slope from the center $r = 0$. When going from the lighter to the heavier element, we can appreciate the increasing relative probability of finding the negatively charged particle inside the nucleus $r \leq R$. Similarly, Fig. 3(b) shows the graphs of the wave functions of the $2s$ state for the same muonic atoms.

In conclusion, the alternative form for the hydrogenic wave functions developed in this paper [Eqs. (6a) and (6b)] has allowed us to obtain numerical results for the energy spectra and eigenfunctions of muonic atoms, in which the finite nuclear size is very important.

APPENDIX

Kummer's differential equation

$$z\frac{d^2w}{dz^2} + (b - z)\frac{dw}{dz} - aw = 0 \qquad \text{(A1)}$$

has two independent solutions, $M(a,b,z)$ and $U(a,b,z)$.

The first one has the power series representation

$$M(a,b,z) = \sum_{n=0}^{\infty} \frac{(a)_n z^n}{(b)_n n!}, \tag{A2}$$

where $(a)_n = a(a+1)(a+2)\cdots(a+n-1)$; $(a)_0 = 1$. While its value at $z = 0$ is one, it diverges as $e^a z^{a-b}$ as $\mathrm{Re}z \to \infty$. This last property excludes its use in Eq. (6b).

The second Kummer's function is given by

$$U(a,b,z) = \frac{\pi}{\sin\pi b}\left(\frac{M(a,b,z)}{\Gamma(1+a-b)\Gamma(b)} - z^{1-b}\frac{M(1+a-b,2-b,z)}{\Gamma(a)\Gamma(2-b)}\right). \tag{A3}$$

It is obviously divergent at $z = 0$ for $b > 1$. Furthermore, for $b = n+1$ where $n = 0,1,2,\ldots$, which includes the case of Eq. (7b) with $b = 2l+2$, it takes the logarithmic form

$$U(a,n+1,z) = \frac{(-)^{n+1}}{n!\Gamma(a-n)}\left(M(a,n+1,z)\ln z + \sum_{r=0}^{\infty}\frac{(a)_r z^r}{(n+1)_r r!}[\psi(a+r) - \psi(1+r) - \psi(1+n+r)]\right) + \frac{(n-1)!}{\Gamma(a)} z^{-n} M(a-n,1-n,z)_n, \tag{A4}$$

where $\psi(a) = \Gamma'(a)/\Gamma(a)$. The last function is the sum to n terms, and it is taken to be zero when $n = 0$. The asymptotic behavior for $\mathrm{Re}z \to \infty$ is

$$U(a,b,z) \to z^{-a}.$$

This last property determines our choice of the second Kummer's function in Eq. (6b). Naturally, its divergence at $z = 0$ is of no importance since we intend to use it as the outside solution only.

Another useful property involving the derivative is

$$U'(a,b,z) = -aU(a+1,b+1,z). \tag{A5}$$

[1] A. F. Yano and F. B. Yano, Am. J. Phys. **40**, 969 (1972).

[2] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[3] R. D. Evans, *The Atomic Nucleus* (McGraw-Hill, New York, 1955), p. 43.

[4] H. Frauenfelder and E. Henley, *Subatomic Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1974), p. 152.