$O(4)$ Symmetry of the Hydrogen Atom and the Lamb Shift*†

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The $O(4)$ symmetry of the nonrelativistic hydrogen atom is exploited in conjunction with Green's-function methods as a tool for the solution of Coulomb problems. The Bethe logarithm, the principal contribution to the Lamb shift, is treated by this means, and a rapidly convergent series is obtained. This is used to evaluate the Bethe logarithm of the $1S$, $2S$, and $2P$ states, and a discrepancy with the most precise previously published value for the $1S$ state is indicated. The new value is 2.9841285 with an estimated uncertainty of ± 3 in the last figure. The discrepancy is beyond the reach of experimental observation at present.

I. INTRODUCTION

THE "hidden symmetry" of the nonrelativistic Kepler problem,[1] which accounts for the accidental degeneracy of the hydrogen atom, has been known since 1926, when Pauli[2] showed that

$$\mathbf{A}=(1/2m)(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})-Z\alpha(\mathbf{r}/r) \tag{1}$$

is an additional conserved vector (a Hermitian form of the classical Runge-Lenz vector) for the system. Using the algebra containing $\mathbf{A}$, he was able to find the energy levels of the hydrogen atom and to analyze the Stark effect, within the framework of Heisenberg's matrix mechanics. Then, in 1935, Fock[3] showed that, working in momentum space, one could project that space stereographically onto the surface of the unit sphere in a four-dimensional space in such a way that Schrödinger integral equation becomes simply the eigenvalue equation for hyperspherical harmonics. This showed explicitly that the symmetry group of the hydrogen atom is not the obvious $O(3)$ but actually $O(4)$.

Except for some early applications based on Eq. (1), the hidden-symmetry group spent many years as a curiosity without much applicability. Then, in 1961, Biedenharn[4] published an analysis of the $O(4)$ group and advocated its application to Coulomb problems, a program he is currently persuing.[5] His methods are based upon developing an operator algebra involving both Eq. (1) and spin operators. The Fock representation was resuscitated by Schwinger[6] in deriving an explicit construction of the Coulomb Green's function.

It is a well-known experience in quantum mechanics that, from the point of view of applications, it is useful to translate the operator-algebraic (Heisenberg) formalism to the wave-function-analytic (Schrödinger) language. It is the essence of Fock's stereographic projection that it allows us to make use of the full symmetry inherent in Coulomb problems in combination with the powerful tools of analysis. The stumbling block which has caused the neglect of this method seems to be the dependence of the projection upon the energy of one given bound state, which makes working within this subspace much easier than going outside; this would appear to severely limit the scope of the method. However, combining the Fock projection with Green's-function techniques may offer a way out of this difficulty. For, while projected onto the sphere by making reference to a given energy level, the Green's function still retains information about all levels.

The purpose of this paper is to illustrate this idea by exploring the Lamb shift (in the lowest-order, nonrelativistic, dipole approximation) of a given energy level. After some preliminary remarks (Sec. II) to establish the problem (and notation) we separate the lowest terms which contain the divergent integrals (Sec. III), and convert the remainder to matrix form. In Sec. IV the mathematical structure of these matrices is analyzed. Finally, in Sec. V, the numerical results are obtained.

II. PRELIMINARIES

To establish notation and conventions we discuss the pure Coulomb Green's function briefly, following Schwinger.[6] Using units $\hbar=c=1$, the Green's function in momentum space is the solution to

$$(E-H)G=\left(E-\frac{p^2}{2m}\right)G(\mathbf{p},\mathbf{p}'|E)+\frac{Z\alpha}{2\pi^2}\int\frac{(d\mathbf{p}'')G(\mathbf{p}'',\mathbf{p}'|E)}{(\mathbf{p}-\mathbf{p}'')^2}=\delta(\mathbf{p}-\mathbf{p}'), \tag{2}$$

in which we make explicit the dependence of G upon the energy E. Restricting ourselves to $E<0$, we put

$$p_0=(-2mE)^{1/2} \tag{3}$$

and

$$\lambda(p)=p_0{}^2+p^2, \tag{4}$$

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so that

$$-\frac{\lambda}{2m}G+\frac{Z\alpha}{2\pi^2}\int\frac{(d\mathbf{p}'')G(\mathbf{p}'',\mathbf{p}')}{(\mathbf{p}-\mathbf{p}'')^2}=\delta(\mathbf{p}-\mathbf{p}')\,. \tag{5}$$

We project the three-dimensional momentum space onto the surface of the unit sphere in a four-dimensional space (the Fock sphere) via

$$\boldsymbol{\xi}=(2p_0/\lambda)\mathbf{p}\,,\quad \xi_0=(p_0^2-p^2)/\lambda\,, \tag{6}$$

so that the 4-vector $\xi=(\xi_0,\boldsymbol{\xi})$ is of unit length. It will be useful to introduce spherical coordinates (the angle α should not be confused with $\alpha=1/137$):

$$\begin{aligned}\xi_0&=\cos\alpha\,,\\ \xi_1&=\sin\alpha\,\cos\theta\,,\\ \xi_2&=\sin\alpha\,\sin\theta\,\cos\phi\,,\\ \xi_3&=\sin\alpha\,\sin\theta\,\sin\phi\,.\end{aligned} \tag{7}$$

The element of surface "area" is

$$d\Omega=\sin^2\alpha d\alpha\,\sin\theta d\theta\,d\phi=(8p_0^3/\lambda^3)d^3p \tag{8}$$

or, conversely,

$$(1/p_0^3)(d\mathbf{p})=d\Omega/(1+\xi_0)^3\,. \tag{9}$$

Defining a 4-vector ξ' corresponding to momentum $\mathbf{p}'$ (but still with the same p_0), we note that

$$(\xi-\xi')^2=(4p_0^2/\lambda\lambda')(\mathbf{p}-\mathbf{p}')^2\,, \tag{10}$$

with λ' defined for $\mathbf{p}'$ in analogy with (4). Making the further definitions

$$\nu=Z\alpha m/p_0\,, \tag{11}$$

$$D(\Omega,\Omega')=1/4\pi^2(\xi-\xi')^2\,, \tag{12}$$

and

$$\Gamma(\Omega,\Omega')=-(\lambda^2\lambda'^2/16mp_0^3)G(\mathbf{p},\mathbf{p}')\,, \tag{13}$$

we can rewrite (2):

$$\Gamma(\Omega,\Omega')-2\nu\int D(\Omega,\Omega'')\Gamma(\Omega'',\Omega')d\Omega''=\delta(\Omega,\Omega')\,, \tag{14}$$

where the points on the Fock sphere are denoted Ω, Ω' and the δ function is given, according to (9), by

$$\delta(\Omega,\Omega')=(\lambda^3/8p_0^3)\delta(\mathbf{p}-\mathbf{p}')\,. \tag{15}$$

We now introduce spherical harmonics

$$Y_{nlm}(\Omega)=Z_{nl}(\alpha)Y_{lm}(\theta,\phi)\,, \tag{16}$$

where $Y_{lm}(\theta,\phi)$ is an ordinary spherical harmonic and n, l, m are integers: $n\geq 1$, $0\leq l\leq n-1$, $|m|\leq l$. The representation (16) makes explicit the three-dimensional rotation group $O(3)$ which acts on $\mathbf{p}$ (and $\boldsymbol{\xi}$, which is parallel to $\mathbf{p}$). The functions $Z_{nl}(\alpha)$ are

$$Z_{nl}(\alpha)=N_{nl}(\sin\alpha)^l C_{n-l-1}{}^{l+1}(\cos\alpha)\,, \tag{17}$$

where $C_{n-l-1}{}^{l+1}$ is a Gegenbauer polynomial, defined by

$$\frac{1}{(1-2tx+t^2)^{l+1}}=\sum_{j=0}^{\infty} t^jC_j{}^{l+1}(x) \tag{18}$$

and the normalization constant is

$$N_{nl}=\left[\frac{n(n-l-1)!}{(n+l)!}\frac{1}{K_l}\right]^{1/2}, \tag{19a}$$

where

$$K_l=\pi/2^{2l+1}(l!)^2\,. \tag{19b}$$

(The phases have been chosen to make N_{nl} real and positive; this is not the usual choice, nor from the group-theoretic point of view the most natural choice, but we find it convenient to avoid the factor i^l.) The functions $Z_{nl}(\alpha)$ satisfy

$$\int_0^\pi Z_{nl}(\alpha)Z_{n'l}(\alpha)\,\sin^2\alpha d\alpha=\delta_{nn'}\,, \tag{20}$$

which makes the $Y_{nlm}(\Omega)$ a complete orthonormal set on the sphere.

The expansion

$$D(\Omega,\Omega')=\sum_{nlm}\frac{1}{2n}Y_{nlm}(\Omega)Y_{nlm}(\Omega')^* \tag{21}$$

immediately gives the solution to (14):

$$\Gamma(\Omega,\Omega')=\sum_{nlm}\frac{Y_{nlm}(\Omega)Y_{nlm}(\Omega')^*}{1-\nu/n}\,; \tag{22}$$

the poles at $\nu=n$ give the spectrum via (11) and (3):

$$E_n=-p_n^2/2m=-(Z\alpha)^2m/2n^2 \tag{23}$$

and the residues in the E plane are the wave function

$$\psi_{nlm}(\mathbf{p})=\frac{4p_n^{5/2}}{\lambda_n^2}Z_{nl}\left(\tan^{-1}\left(\frac{p}{p_n}\right)\right)Y_{lm}(\theta,\phi)\,, \tag{24}$$

writing p_n whenever we mean p_0 corresponding to the energy level E_n, and λ_n correspondingly.

To turn now to the Lamb shift,[7] the displacement of the state $n_0l_0m_0$ to second-order perturbation theory, in the dipole approximation, is

$$\Delta E(n_0l_0m_0)=\frac{\alpha}{4m^2\pi^2}\sum_{\lambda=1}^{2}\int\frac{(d\mathbf{k})}{k}\times\langle n_0l_0m_0|\,\mathbf{p}\cdot\mathbf{e}_\lambda\frac{1}{E_{n_0}-k-H}\mathbf{p}\cdot\mathbf{e}_\lambda\,|n_0l_0m_0\rangle\,, \tag{25}$$

where k is the intermediate photon energy, H is the Hamiltonian operator for the hydrogen atom, and $\mathbf{e}_\lambda$ is

[7] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson, and Co., Elmsford, N. Y., 1961).

the photon polarization vector. In momentum space this becomes

$$\Delta E(n_0l_0m_0)=\frac{\alpha}{4m^2\pi^2}\int\frac{(d\mathbf{k})}{k}(d\mathbf{p})(d\mathbf{p}')\sum_{\lambda=1}^{2}(\mathbf{p}\cdot\mathbf{e}_\lambda)(\mathbf{p}'\cdot\mathbf{e}_\lambda)$$
$$\times\psi_{n_0l_0m_0}(\mathbf{p})^*\psi_{n_0l_0m_0}(\mathbf{p}')G(\mathbf{p},\mathbf{p}'|E_{n_0}-k)\,,\quad(26)$$

where the Green's function G satisfies, instead of (2),

$$(E_{n_0}-k-H)G=\delta(\mathbf{p}-\mathbf{p}')\,.\quad(27)$$

Using $\mathbf{e}_\lambda\cdot\mathbf{k}=0$ and integrating over angles in k space (26) becomes

$$\Delta E(n_0l_0m_0)=\frac{2\alpha}{3\pi m^2}\int_0^K kdk(d\mathbf{p})(d\mathbf{p}')\mathbf{p}\cdot\mathbf{p}'\psi_{n_0l_0m_0}(\mathbf{p})^*$$
$$\times\psi_{n_0l_0m_0}(\mathbf{p}')G(\mathbf{p},\mathbf{p}'|E_{n_0}-k)\,,\quad(28)$$

where we have introduced a cutoff K, since the integral diverges. Note that the only k dependence is in G.

We now wish to project this onto the Fock sphere. Although (27) is really identical to (2) with $E=E_{n_0}-k$, simply using (3) and (6) would have the effect of mixing up the photon energy k with the projection. For present purposes it is better to leave the k dependence explicit by using

$$p_{n_0}=(-2mE_{n_0})^{1/2}=Z\alpha m/n_0\quad(29)$$

in place of p_0 in (6). We get in this way

$$\Delta E_{(n_0,l_0,m_0)}=-(2\alpha p_{n_0}{}^4/3m^3\pi)\mathcal{L}(B,n_0l_0m_0)\,,\quad(30\text{a})$$

$$\Delta E_{(n_0,l_0,m_0)}=-\frac{2}{3\pi}\frac{Z^4\alpha^5 m}{n_0{}^4}\mathcal{L}(B,n_0l_0m_0)\,,\quad(30\text{b})$$

or, in rydbergs,

$$\frac{\Delta E(n_0,l_0,m_0)}{1\text{ Ry}}=-\frac{4}{3\pi}\frac{Z^4\alpha^3}{n_0{}^4}\mathcal{L}(B,n_0l_0m_0)\,.\quad(30\text{c})$$

Here

$$\mathcal{L}(B,n_0l_0m_0)=\int\int d\Omega d\Omega' Y_{n_0l_0m_0}(\Omega)^*$$
$$\times Y_{n_0l_0m_0}(\Omega')\xi\cdot\xi'\int_0^B\beta d\beta\,\Gamma(\Omega,\Omega'|\beta)\,,\quad(31)$$

where we have introduced the dimensionless photon energy

$$\beta=mk/p_{n_0}{}^2\quad(32)$$

with corresponding cutoff B. The projected Green's function Γ satisfies, instead of (14), the equation obtained from (27) using (29) in the projection

$$\Gamma(\Omega,\Omega'|\beta)-2\nu\int d\Omega''D(\Omega,\Omega'')\Gamma(\Omega'',\Omega'|\beta)$$
$$=\delta(\Omega,\Omega')-\beta(1+\xi_0)\Gamma(\Omega,\Omega'|\beta)\,,\quad(33)$$

where the last term is the extra term due to k, and where $\nu=n_0$.

In the following sections we shall analyze Eqs. (30)–(33) in detail. It should be emphasized that, so far in the treatment, no intermediate states appear: Only the single energy level E_{n_0} enters. The other energy levels are explicitly contained in the Green's function $G(p,p'|E_{n_0}-k)$ which has poles in the k plane when $k=k_{n_0n'}=E_{n_0}-E_{n'}$, for all hydrogen eigenvalues $E_{n'}$ in the discrete or continuous spectrum. However, in going from G to Γ, we have discarded the continuous spectrum, which could be recovered only by analytic continuation. Thus the continuum states never appear in the remainder of this paper; the other discrete states *will* appear when we expand in hyperspherical harmonics.

III. LOWEST TERMS

Since we are interested in the behavior of (33) as $\beta\to\infty$, it is inadequate to treat the extra term as a perturbation of (14). It is better to rewrite (33) as

$$\Gamma(\Omega,\Omega'|\beta)=\frac{\delta(\Omega,\Omega')}{1+\beta(1+\xi_0)}+\frac{2\nu}{1+\beta(1+\xi_0)}\int D(\Omega,\Omega'')$$
$$\times\Gamma(\Omega'',\Omega'|\beta)d\Omega''\,,\quad(34)$$

which is better behaved at large β. It is also convenient to introduce a scale change in β:

$$\beta=2\rho/(1-\rho)^2\,,\quad(35)$$

so that the interval $\beta=0$ to ∞ is mapped onto $\rho=0$ to 1. The reason for this is that (34) becomes

$$\Gamma(\Omega,\Omega'|\rho)=\frac{(1-\rho)^2\delta(\Omega,\Omega')}{1+2\rho\xi_0+\rho^2}+\frac{2\nu(1-\rho)^2}{1+2\rho\xi_0+\rho^2}$$
$$\times\int D(\Omega,\Omega'')\Gamma(\Omega'',\Omega'|\rho)d\Omega''\,,\quad(36)$$

where the factor $(1+2\rho\xi_0+\rho^2)^{-1}$ is recognized to be the generating function of $l=0$ spherical harmonics [Eq. (18)]. We may symbolically abbreviate (36) as

$$\Gamma=\Delta+\nu K\Gamma\,.\quad(37)$$

It would seem logical to expand (37) about $\nu=0$, i.e., the Neumann (Born) series for Γ. However, we wish to set $\nu=n_0$, so that an alternative approach is needed.

We extract the lowest (divergent) terms by using the identity

$$\Gamma=\Delta+n_0K\Delta+(1-n_0K)^{-1}n_0{}^2KK\Delta$$
$$=\Delta+n_0K\Delta+\Gamma'\,,\quad(38)$$

where we have placed $\nu=n_0$. The first term

$$\Delta(\Omega,\Omega'|\rho)=\frac{(1-\rho)^2\delta(\Omega,\Omega')}{1+2\rho\xi_0+\rho^2}\quad(39)$$

contributes a linear and a logarithmic divergence in k

as $\beta\to\infty$ ($\rho\to 1$). This follows when we note that

$$\beta d\beta \to \frac{4\rho(1+\rho)}{(1-\rho)^5}d\rho. \tag{40}$$

Because of the additional $(1-\rho)^2$ in K the second term $n_0K\Delta$ contributes only a logarithmic divergence (in fact, it vanishes except for S states; see below). The simple manipulations leading to (38) correspond to much less evident manipulations of the ordinary-space Green's function (Appendix A). If we use (39) as a lowest-order approximation to Γ we obtain

$$\mathcal{L}^{(0)}=\int_0^P d\rho\frac{4\rho(1+\rho)}{(1-\rho)^5}\int\int d\Omega\, d\Omega' Y_{n_0l_0m_0}(\Omega)^* \times Y_{n_0l_0m_0}(\Omega')\boldsymbol{\xi}\cdot\boldsymbol{\xi}'\Delta(\Omega,\Omega'|\rho)$$

$$=\int_0^P d\rho\frac{4\rho(1+\rho)}{(1-\rho)^5}L(\rho,n_0l_0m_0), \tag{41}$$

where P is the cutoff in ρ corresponding to B in β and K in k, and where

$$L(\rho,n_0l_0m_0)=\int d\Omega\frac{|Y_{n_0l_0m_0}(\Omega)|^2|\boldsymbol{\xi}|^2}{1+2\rho\xi_0+\rho^2}$$

or, by $\boldsymbol{\xi}^2+\xi_0^2=1$,

$$L(\rho,n_0l_0m_0)=A_{l_0}(n_0,n_0,\rho)-\int d\Omega\frac{\xi_0^2|Y_{n_0l_0m_0}(\Omega)|^2}{1+2\rho\xi_0+\rho^2}. \tag{42}$$

Here we have defined the basic matrix element (diagonal in l, m)

$$A_l(n,n',\rho)=\langle nlm|[1+2\rho\xi_0+\rho^2]^{-1}|n'lm\rangle$$

$$=\int d\Omega\frac{Y_{nlm}(\Omega)^*Y_{n'lm}(\Omega)}{1+2\rho\xi_0+\rho^2}$$

$$=\int_0^\pi\frac{Z_{nl}(\alpha)Z_{n'l}(\alpha)\sin^2\alpha\, d\alpha}{1+2\rho\cos\alpha+\alpha^2} \tag{43}$$

using (16). In (43) we have represented $Y_{nlm}(\Omega)$ by $\langle\Omega|nlm\rangle$, This shorthand will be occasionally convenient but $|nlm\rangle$ should be distinguished from the physical-space ket vector in, e.g., (25), which is connected with it by Eq. (24). The result (43) is independent of m_0 because the $O(4)$ symmetry-breaking ξ_0 dependence leaves $O(3)$ invariance intact. The matrix element $A_l(n,n',\rho)$ is evaluated in detail in Appendix B. Surprisingly, $A_l(n,n',\rho)$ is a *polynomial* in ρ (and therefore well-behaved as $\rho\to 1$). Also, by (20),

$$A_{l_0}(n,n',0)=\delta_{nn'}. \tag{44}$$

Returning to (42) we use the identity

$$4\rho^2\xi_0^2=(1+2\rho\xi_0+\rho^2)^2-2(1+\rho^2)(1+2\rho\xi_0+\rho^2)+(1+\rho^2)^2 \tag{45}$$

and the fact that (by symmetry)

$$\int\xi_0|Y_{n_0l_0m_0}(\Omega)|^2d\Omega=0 \tag{46}$$

to obtain

$$\int d\Omega\frac{\xi_0^2|Y_{n_0l_0m_0}(\Omega)|^2}{1+2\rho\xi_0+\rho^2}=-\frac{(1+\rho^2)}{4\rho^2}+\frac{(1+\rho^2)^2}{4\rho^2}A_{l_0}(n_0,n_0,\rho). \tag{47}$$

Thus

$$L(\rho,n_0l_0m_0)=\frac{(1+\rho^2)-(1-\rho^2)^2A_{l_0}(n_0,n_0,\rho)}{4\rho^2}. \tag{48}$$

Note that L is well behaved as $\rho\to 0$ in view of (44), so that there are no infrared divergences. Near $\rho=1$, L behaves like a constant ($\frac{1}{2}$), so that (41) is divergent like $(1-P)^{-2}$, which is the same as linearly in B or K.

The next term is

$$n_0K\Delta=\frac{2n_0(1-\rho)^4}{1+2\rho\xi_0+\rho^2}\int\frac{D(\Omega,\Omega'')\delta(\Omega'',\Omega')}{1+2\rho\xi_0''+\rho^2}d\Omega''$$

$$=\frac{2n_0(1-\rho)^4D(\Omega,\Omega')}{(1+2\rho\xi_0+\rho^2)(1+2\rho\xi_0'+\rho^2)}. \tag{49}$$

This contributes to $\mathcal{L}$

$$\mathcal{L}^{(1)}=2n_0\int_0^P d\rho\frac{4\rho(1+\rho)}{1-\rho}L'(\rho,n_0l_0m_0), \tag{50}$$

where

$$L'(\rho,n_0l_0m_0)=\int d\Omega d\Omega'\frac{Y_{n_0l_0m_0}(\Omega)^*Y_{n_0l_0m_0}(\Omega')\boldsymbol{\xi}\cdot\boldsymbol{\xi}'D(\Omega,\Omega')}{(1+2\rho\xi_0+\rho^2)(1+2\rho\xi_0'+\rho^2)}. \tag{51}$$

Since ξ, ξ' are unit 4-vectors, we have from (12)

$$1/4\pi^2D(\Omega,\Omega')=(\xi-\xi')^2=2(1-\xi\xi')=2(1-\xi_0\xi_0'-\boldsymbol{\xi}\cdot\boldsymbol{\xi}'), \tag{52}$$

so that

$$\boldsymbol{\xi}\cdot\boldsymbol{\xi}'=1-\xi_0\xi_0'-1/8\pi^2D(\Omega,\Omega') \tag{53}$$

and therefore

$$L'(\rho,n_0l_0m_0)=\int\frac{d\Omega d\Omega'(1-\xi_0\xi_0')Y_{n_0l_0m_0}(\Omega)^*Y_{n_0l_0m_0}(\Omega')D(\Omega,\Omega')}{(1+2\rho\xi_0+\rho^2)(1+2\rho\xi_0'+\rho^2)}-\frac{1}{8\pi^2}\left|\int\frac{d\Omega\, Y_{n_0l_0m_0}(\Omega)}{1+2\rho\xi_0+\rho^2}\right|^2. \tag{54}$$

The second integral is easily evaluated using $Y_{100}(\Omega)\equiv 2^{-1/2}/\pi$ (up to an unimportant phase factor):

$$\frac{1}{8\pi^2}\left|\int\frac{d\Omega\, Y_{n_0l_0m_0}(\Omega)}{1+2\rho\xi_0+\rho^2}\right|^2=\tfrac{1}{4}A_0(n_0,1,\rho)^2\delta_{l_00}\delta_{m_00}. \tag{55}$$

The first integral of (52) is evaluated using (21); calling the integral I,

$$I=\sum_{nlm}\frac{1}{2n}\int\frac{d\Omega d\Omega' Y_{n_0l_0m_0}(\Omega)^* Y_{nlm}(\Omega)Y_{n_0l_0m_0}(\Omega')Y_{nlm}(\Omega')^*(1-\xi_0\xi_0')}{(1+2\rho\xi_0+\rho^2)(1+2\rho\xi_0'+\rho^2)}$$

$$=\sum_{nlm}\frac{1}{2n}\{|\langle nlm|[1+2\rho\xi_0+\rho^2]^{-1}|n_0l_0m_0\rangle|^2-|\langle nlm|[1+2\rho\xi_0+\rho^2]^{-1}\xi_0|n_0l_0m_0\rangle|^2\}. \tag{56}$$

The first integral is then diagonal in l, m;

$$\langle nlm|[1+2\rho\xi_0+\rho^2]^{-1}|n_0l_0m_0\rangle=A_{l_0}(n_0,n,\rho)\delta_{ll_0}\delta_{mm_0}. \tag{57}$$

Similarly, using

$$\xi_0=\frac{1+2\rho\xi_0+\rho^2}{2\rho}-\frac{1+\rho^2}{2\rho}, \tag{58}$$

the second term is

$$\langle nlm|[1+2\rho\xi_0+\rho^2]^{-1}\xi_0|n_0l_0m_0\rangle =(1/2\rho)[\delta_{nn_0}-(1+\rho^2)A_{l_0}(n,n_0,\rho)]\delta_{ll_0}\delta_{mm_0}; \tag{59}$$

so that

$$I=\frac{(1+\rho^2)}{4n_0\rho^2}A_{l_0}(n_0,n_0,\rho)-\frac{1}{8n_0\rho^2}-\frac{(1-\rho^2)}{8\rho^2}\sum_{n=l_0+1}^{\infty}\frac{A_{l_0}(n,n_0,\rho)^2}{n}. \tag{60}$$

A little care shows that (60) is well behaved[8] as $\rho\to 0$ [cf. Eq. (44)]; in the evaluation of the ρ integrals it is best to separate the $n=n_0$ term of the sum in (60) and combine it with the preceding terms to make the behavior at $\rho=0$ explicitly smooth). Combining (60) with (55),

$$L'(\rho,n_0,l_0m_0)=-\tfrac{1}{4}A_0(n_0,1,\rho)^2\delta_{l_00}+\frac{(1+\rho^2)}{4n_0\rho^2}A_{l_0}(n_0,n_0,\rho)-\frac{1}{8n_0\rho^2}-\frac{(1-\rho^2)^2}{8\rho^2}\sum_{n=l_0+1}^{\infty}\frac{A_{l_0}(n,n_0,\rho)^2}{n}. \tag{61}$$

Noting (50) we see that the first three terms all contribute $\log(1-P)$, i.e., $\log K$ divergences. When $\mathcal{L}^{(0)}$ is combined with $\mathcal{L}^{(1)}$, only the S-state log divergence survives (together with the linear K divergence from $\mathcal{L}^{(0)}$).

[8] Actually, we have not shown here that the infinite series in (60) converges. In fact, it is shown in the author's thesis (unpublished) that it converges at least as fast as n^{-3}. Furthermore, it can always be summed *exactly* as will be seen in Sec. V. No closed form for the sum has been found although for $l=0$ the sum has been converted to an integral which can be evaluated directly for $n=1$, 2 but not in general.

$$\mathcal{L}^{(0)}+\mathcal{L}^{(1)}=\int_0^P d\rho\Bigg(\frac{2(1+\rho)}{(1-\rho)^3}-\frac{2n_0(1+\rho)\rho}{1-\rho}\times A_0(n_0,1,\rho)^2\delta_{l_00}+\frac{(1-\rho^2)}{\rho}A_{l_0}(n_0,n_0,\rho)-\frac{n_0(1+\rho)^2(1-\rho^2)}{\rho}\sum_{n=l_0+1}^{\infty}\frac{1}{n}A_l(n,n_0,\rho)^2\Bigg). \tag{62}$$

The first term of (62) can be directly integrated to give B, the linear divergence. The second, which occurs only for S states, is evaluated using Eq. (B8):

$$A_0(n_0,1,\rho)=(-\rho)^{n_0-1}, \tag{63}$$

which gives directly

$$-4n_0\ln(1-P)+4n_0h(2n_0)-1, \tag{64}$$

where we have defined

$$h(j)=\sum_{k=1}^{j}\frac{1}{k}. \tag{65}$$

The expression (64) can be rewritten by using

$$-2\ln(1-P)=\ln(B/2P)\to\ln B-\ln 2, \tag{66}$$

where $-\ln P$ has been replaced by 0 as $P\to 1$. The result of this rearranging is

$$\mathcal{L}^{(0)}+\mathcal{L}^{(1)}=B+[-2n_0\ln B+2n_0\times\ln 2+4n_0h(2n_0)-1]\delta_{l_00}+\mathcal{L}_{\text{finite}}, \tag{67}$$

with $\mathcal{L}_{\text{finite}}$ containing the last two terms of (62). The term B is removed completely by renormalization. Using (30) and (32) we see that the term B contributes

$$\Delta E(n_0l_0m_0,\,B\text{ term})=-\frac{2}{3\pi}\frac{Z^4\alpha^5m}{n_0^4}\frac{mK}{p_{n_0}^2}=-(2/3\pi)Z^2\alpha^3K/n_0^2; \tag{68}$$

on the other hand, the electromagnetic self-energy correction for the state $n_0l_0m_0$ is[9]

$$\Delta E_0(n_0l_0m_0)=-\frac{2}{3\pi}\int_0^K kdk\frac{\langle n_0l_0m_0|v^2|n_0l_0m_0\rangle}{k}=-(2\alpha K/3m^2\pi)\langle n_0l_0m_0|p^2|n_0l_0m_0\rangle, \tag{69}$$

[9] H. A. Bethe, Phys. Rev. 72, 339 (1947).

which is identical to (68) on observing that, by the virial theorem,

$$\langle n_0l_0m_0|p^2|n_0l_0m_0\rangle = -2mE_{n_0} = p_{n_0}{}^2. \quad (70)$$

It is only $\Delta E - \Delta E_0$ which is measurable and thus the B term cancels.

The remaining part of (67), when the $\log B$ divergence is properly dealt with (Sec. V), contributes the major portion of the Bethe logarithm for S states (96% for $1S$, 90% for $2S$). Before discussing the evaluation of these shifts, we must deal with $\mathcal{L}_{\text{finite}}$ in (67) and with Γ'; this task will occupy the remainder of this and the next section. However, we wish to point out that the manipulations needed to extract this dominant S-state contribution have their counterpart in ordinary space (see Appendix A).

The remaining part of (38) is Γ', which is the solution to

$$\Gamma'(\Omega,\Omega') - \frac{2\nu(1-\rho)^2}{1+2\rho\xi_0+\rho^2}\int d\Omega'' D(\Omega,\Omega'')\Gamma'(\Omega'',\Omega')$$
$$= \frac{4\nu^2(1-\rho)^6}{1+2\rho\xi_0+\rho^2}\int \frac{d\Omega'' D(\Omega,\Omega'')D(\Omega'',\Omega')}{1+2\rho\xi_0''+\rho^2} \times \frac{1}{1+2\rho\xi_0'+\rho^2}. \quad (71)$$

We expand this in spherical harmonics by multiplying by $Y_{nlm}(\Omega)^* Y_{n'l'm'}(\Omega')$ and integrating over Ω, Ω' to get

$$\langle nlm|\Gamma'|n'l'm'\rangle - \nu(1-\rho)^2 \sum_{n''} A_l(n,n''\rho) \times \frac{1}{n''}\langle n''lm|\Gamma'|n'l'm'\rangle = \nu^2(1-\rho)^6 \sum_{n''n'''} A_l(n,n'',p) \times \frac{1}{n''}A_l(n'',n''',\rho)\frac{1}{n'''}A_l(n''',n',\rho)\delta_{ll'}\delta_{mm'}, \quad (72)$$

in which we have used (21) in the form

$$\langle nlm|D|n'l'm'\rangle = \frac{1}{2n}\delta_{nn'}\delta_{ll'}\delta_{mm'}. \quad (73)$$

If we set

$$\langle nlm|\Gamma'|n'l'm'\rangle = (nn')^{1/2}\Gamma_l(\rho)_{nn'}\delta_{ll'}\delta_{mm'} \quad (74)$$

and

$$B_l(\rho)_{nn'} = (nn')^{-1/2}A_l(n,n',\rho), \quad (75)$$

then (75) becomes the matrix equation

$$[1-\nu(1-\rho)^2 B_l(\rho)]\Gamma_l(\rho) = \nu^2(1-\rho)^6 B_l(\rho)^3, \quad (76)$$

so that

$$\langle nlm|\Gamma'|n'l'm'\rangle = \nu^2(1-\rho)^2(nn')^{1/2} \times [C_l(\rho)B_l(\rho)^3]_{nn'}\delta_{ll'}\delta_{mm'}, \quad (77)$$

with

$$C_l(\rho) = [1-\nu(1-\rho)^2 B_l(\rho)]^{-1}. \quad (78)$$

Observe that when $\rho=0$ we get from (44)

$$C_l(0)_{nn'} = \delta_{nn'}(1-\nu/n)^{-1}, \quad (79)$$

which, combined with (37), yields

$$\Gamma = (1-\nu K)^{-1}\Delta \quad (80)$$

and

$$\Delta(\Omega,\Omega'|0) = \delta(\Omega,\Omega'), \quad (81)$$

reproduces the pure Coulomb Green's function (22). Therefore,

$$\Gamma'(\Omega,\Omega') = \nu^2(1-\rho)^6 \sum_{n,n'lm} [C_l(\rho)B_l(\rho)^3]_{nn'} \times (nn')^{1/2} Y_{nlm}(\Omega) Y_{n'lm}(\Omega')^*. \quad (82)$$

If we evaluate (78) we then have Γ completely. This will be done in Sec. IV. First, let us see how (82) enters $\mathcal{L}$. To do this we rewrite (82) in partial-wave form using (16) and the ordinary spherical harmonics addition theorem:

$$\sum_m Y_{nlm}(\alpha,\theta,\phi) Y_{n'lm}(\alpha',\theta',\phi')^* = Z_{nl}(\alpha)Z_{n'l}(\alpha') \sum_{m=-l}^{l} Y_{lm}(\theta,\phi)Y_{lm}(\theta',\phi')^*$$
$$= Z_{nl}(\alpha)Z_{n'l}(\alpha')P_l(\cos\omega)(2l+1)/4\pi, \quad (83)$$

where

$$\cos\omega = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi'). \quad (84)$$

We can rewrite (82) by performing the m sum:

$$\Gamma'(\Omega,\Omega') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\cos\omega)\Gamma_l(\alpha,\alpha'), \quad (85)$$

with

$$\Gamma_l(\alpha,\alpha') = \nu^2(1-\rho)^6 \sum_{n,n'=l+1} (nn')^{1/2} \times [C_l(\rho)B_l(\rho)^3]_{nn'} Z_{nl}(\alpha)Z_{n'l}(\alpha'). \quad (86)$$

Replacing ν by n_0 and inserting into

$$\mathcal{L}' = \int_0^1 \frac{4\rho(1+\rho)}{(1-\rho)^5} d\rho\, L''(\rho,n_0l_0m_0), \quad (87)$$

where

$$L''(\rho,n_0l_0m_0) = \int d\Omega d\Omega' \times Y_{n_0l_0m_0}(\Omega)^* Y_{n_0l_0m_0}(\Omega')\xi\cdot\xi'\Gamma'(\Omega,\Omega'), \quad (88)$$

$$L''(\rho,n_0l_0m_0) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\int_0^{\pi} \sin^3\alpha \sin^3\alpha' Z_{n_0l_0}(\alpha) \times Z_{n_0l_0}\Gamma_l(\alpha,\alpha')d\alpha\, d\alpha' g_{ll_0m_0}, \quad (89)$$

with

$$g_{ll_0m_0} = \int d\bar{\Omega}d\bar{\Omega}' \cos\omega\, P_l(\cos\omega) Y_{l_0m_0}(\theta,\phi) \times Y_{l_0m_0}(\theta',\phi')^*. \quad (90)$$

The latter is evaluated using

$$xP_l(x)=\frac{l+1}{2l+1}P_{l+1}(x)+\frac{l}{2l+1}P_{l-1}(x) \qquad (91)$$

and the addition theorem, with the result

$$g_{ll_0m}=\frac{4\pi}{2l_0+1}\left(\frac{l_0}{2l_0-1}\delta_{l,l_0-1}+\frac{l_0+1}{2l_0+3}\delta_{l,l_0+1}\right). \qquad (92)$$

We thus split up (89);

$$L''=L^++L^-,$$

with $l=l_0+1$ or l_0-1, respectively:

$$L^-=\frac{l_0}{2l_0+1}\int_0^\pi \sin^3\alpha\,\sin^3\alpha'\,Z_{n_0l_0}(\alpha)Z_{n_0l_0}(\alpha')\times\Gamma_{l_0-1}(\alpha,\alpha')d\alpha d\alpha' \qquad (93a)$$

and

$$L^+=\frac{l_0+1}{2l_0+1}\int_0^\pi \sin^3\alpha\,\sin^3\alpha'\,Z_{n_0l_0}(\alpha)Z_{n_0l_0}(\alpha')\times\Gamma_{l_0+1}(\alpha,\alpha')d\alpha d\alpha'. \qquad (93b)$$

The form of (93) is exactly what one would expect from the dipole radiation selection rules.[10] This is the first instance in our calculation where the transitions from state $n_0l_0m_0$ to other states make their physical presence known.

Finally, if we define

$$M_l(\rho)_{nn'}=(nn')^{1/2}[C_l(\rho)B_l(\rho)^3]_{nn'} \qquad (94)$$

and

$$D_l{}^{(\pm)}{}_{nn'}=\int_0^\pi \sin^3\alpha\,Z_{nl}(\alpha)Z_{n'\,l\pm1}(\alpha)d\alpha, \qquad (95)$$

then we may write $L^\pm$ in pure matrix form

$$L^-=\frac{l_0}{2l_0+1}n_0{}^2(1-\rho)^6[D_{l_0}{}^{(-)}M_{l_0-1}(\rho)D_{l_0}{}^{(-)T}]_{n_0n_0}, \qquad (96a)$$

$$L^+=\frac{l_0+1}{2l_0+1}n_0{}^2(1-\rho)^6[D_{l_0}{}^{(+)}M_{l_0+1}(\rho)D_{l_0}{}^{(+)T}]_{n_0n_0}. \qquad (96b)$$

The integrals $D_l{}^{\pm}{}_{nn'}$ are obtained from the identity

$$\sin\alpha\,Z_{n',l-1}(\alpha)=\frac{1}{2}\left(\frac{(n'+l+1)(n'+l)}{n'(n'+1)}\right)^{1/2}Z_{n'+1,l}(\alpha)-\frac{1}{2}\left(\frac{(n'-l)(n'-l-1)}{n'(n'-1)}\right)^{1/2}Z_{n'-1,l}(\alpha), \qquad (97)$$

which in turn follows from the Gegenbauer identity[11]

$$C_{n'-l}{}^l(x)=(l/n')[C_{n'-l}{}^{l+1}(x)-C_{n'-l-2}{}^{l+1}(x)]. \qquad (98)$$

The result is

$$D_l{}^{(-)}{}_{nn'}=\frac{1}{2}\left(\frac{(n'+l+1)(n'+l)}{n'(n'+1)}\right)^{1/2}\delta_{n,n'+1}-\frac{1}{2}\left(\frac{(n'-l)(n'-l-1)}{n'(n'-1)}\right)^{1/2}\delta_{n,n'-1}; \qquad (99)$$

the other matrix $D_l{}^{(+)}{}_{nn'}$ is obtained from

$$D_l{}^{(+)}{}_{nn'}=D_{l+1}{}^{(-)}{}_{n'n}. \qquad (100)$$

The matrix expressions will be further analyzed in Sec. IV.

IV. MATRIX TERMS

In this section we shall investigate the matrix inversion (78), which is equivalent to solving the integral equation for $\Gamma(\Omega,\Omega'|\rho)$. In a sense then, the matrix $C_l(\rho)$ contains all the information expressed by the Green's function for the system of hydrogen atom plus photon (in dipole approximation). When $\rho=0$ we know that $\nu=n_0$ is a singularity (or eigenvalue) corresponding to the bound state at n_0, and $C_l(0)$ does not exist. As ρ moves away from 0, $\nu=n_0$ is no longer a singularity. If $n_0\neq1$, we will reach further singularities corresponding to the dipole transitions. Thus we see that the matrix (78) has a very complex structure.

To perform the inversion we will diagonalize the matrix $B_l(\rho)$. Since $B_l(\rho)$ is real symmetric, we seek a real orthogonal matrix $U_l(\rho)$ such that

$$\tilde{B}_l(\rho)=U_l(\rho)B_l(\rho)U_l(\rho)^T, \qquad (101)$$

where $\tilde{B}_l(\rho)$ is the diagonal matrix made of the eigenvalues of $B_l(\rho)$. Let $\mu(\rho)$ be an eigenvalue of $B_l(\rho)$ and $\{Y_m(\rho)\}$, $m=l+1, l+2, \cdots$ be the corresponding eigenvector. Suppressing the index l, we write

$$\sum_{m=l+1}^\infty B(\rho)_{nm}Y_m(\rho)=\mu(\rho)Y_n(\rho). \qquad (102)$$

The left-hand side is, by (75),

$$\sum_{m=l+1}^\infty B(\rho)_{nm}Y_m(\rho)=\frac{1}{n^{1/2}}\int_0^\pi d\alpha\frac{\sin^2\alpha\,Z_{nl}(\alpha)\sum_{m=l+1}^\infty m^{-1/2}Y_m(\rho)Z_{ml}(\alpha)}{1+2\rho\cos\alpha+\rho^2}. \qquad (103)$$

If we define a new vector

$$\chi_m(\rho)=m^{-1/2}N_{ml}Y_m(\rho), \qquad (104)$$

[10] H. A. Bethe and E. E. Salpeter, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. XXXV/1.

[11] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, Inc., New York, 1966).

then the normalization factors on the Z_{nl} are removed and we get

$$\int_0^\pi d\alpha \frac{\sin^{2l+2}\alpha\, C_{n-l-1}{}^{l+1}(\cos\alpha) \sum_{m=l+1}^\infty \chi_m(\rho) C_{m-l-1}{}^{l+1}(\cos\alpha)}{1+2\rho\cos\alpha+\rho^2} = \mu(\rho)\frac{n}{N_{nl}{}^2}\chi(\rho)\,, \tag{105}$$

i.e.,

$$\sum_{m=l+1}^\infty I_{nm}\chi_m(\rho) = \mu\frac{n}{N_{nl}{}^2}\chi_n(\rho)\,, \tag{106}$$

where I_{nm} is given by Eq. (B11). This indicates the use of generating functions, as described in Appendix C. The generating function for I_{nm} is simply the $G_l(x,y,\rho)$ of Appendix B. It is convenient to define

$$f(t,\rho) = \sum_{m=l+1}^\infty t^{m+l}\chi_m(\rho)\,, \tag{107}$$

so that $t^{-2l-1}f(t,\rho)$ is the generating function for $\chi_m(\rho)$ that starts with t^0. With these points in mind (106) becomes, using (19),

$$\frac{1}{2\pi i}\oint G_l(t,1/z,\rho)\frac{f(z,\rho)}{z^{2l+1}}\frac{dz}{z} = \mu(\rho)\sum_{n=l+1}^\infty \frac{n}{N_{nl}{}^2}t^{n-l-1}\chi_n(\rho)$$

$$= \mu(\rho)K_l\left(\frac{d}{dt}\right)^{2l+1} f(t,\rho)\,. \tag{108}$$

and so, using (B21b),

$$\mu(\rho)\left(\frac{d}{dt}\right)^{2l+1} f(t,\rho) = \frac{(2l+1)!}{l+1}\frac{(1-\rho^2)^l}{(1+t\rho)^{l+1}}\oint dz\frac{F(-l,\,l+1;\,l+2;\,-(t+\rho)(1+\rho z)/(1-\rho^2)(z-t))f(z,\rho)}{[(z+\rho)(z-t)]^{l+1}}\,. \tag{109}$$

This is an integro-differential equation for the generating function of the eigenvectors. In writing it we have assumed $f(t,\rho)$ analytic for all t inside the unit disk. It is this condition that determines the eigenvalues μ.

Since the treatment of (109) is complicated, we will illustrate here only the case $l=0$ and refer the reader to the author's thesis for the details of the general case. However, we will give the general result.

For $l=0$, F reduces to unity and (109) becomes

$$\mu\frac{df}{dt} = \frac{1}{1+t\rho}\frac{1}{2\pi i}\oint\frac{dz\, f(z,\rho)}{(z-t)(z+\rho)}$$

$$= \frac{f(t,\rho)-f(-\rho,\rho)}{(1+t\rho)(t+\rho)}\,. \tag{110}$$

If we set $g(t,\rho)=f(t,\rho)-f(-\rho,\rho)$, we can integrate (110) immediately, with constant of integration c.

$$g(t,\rho) = c\left(\frac{t+\rho}{1+t\rho}\right)^{1/\mu(1-\rho^2)}\,. \tag{111}$$

Now $g(t,\rho)$ differs from $f(t,\rho)$ only by a constant and so is equally satisfactory as a generator for $\chi_m(\rho)$. We see that since $\rho<1$, $g(t,\rho)$ will have a branch point unless $[\mu(1-\rho^2)]^{-1}$ is an integer n. Thus the eigenvalues are

$$\mu^{(n)}(\rho) = 1/n(1-\rho^2) \tag{112}$$

and the generator of the corresponding eigenvector

$$g^{(n)}(t,\rho) = c_n(\rho)\left(\frac{t+\rho}{1+t\rho}\right)^n\,. \tag{113}$$

The constant $c_n(\rho)$ must be chosen to normalize $\{Y_m\}$ and make $U_l(\rho)$ an orthogonal matrix:

$$\sum_{m=\rho}^\infty Y_m{}^{(n)}(\rho)^2 = 1 = K_0\sum_{m=1}^\infty m\chi_m{}^{(n)}(\rho)^2$$

$$= K_0\frac{1}{2\pi i}\oint g^{(n)}(1/y,\rho)\frac{d}{dy}$$

$$\times g^{(n)}(y,\rho)dy\,, \tag{114}$$

where we have recognized that $\{m\chi_m{}^{(n)}(\rho)\}$ is generated by $(d/dy)g^{(n)}(y,\rho)$. Then (114) gives

$$c_n(\rho) = \pm(nK_0)^{-1/2} \tag{115}$$

(in this case independent of ρ but not for $l\neq0$); the plus sign must be taken in order that $U_l(\rho)\to1$ as $\rho\to0$.

The result for arbitrary l is stated as a theorem:

Theorem: The eigenvalues $\mu(\rho)$ of (109) are

$$\mu_{(m)}(\rho) = 1/m(1-\rho^2) \quad (m=l+1,\, l+2,\, \cdots) \tag{116}$$

and the corresponding eigenfunction is, correctly normalized,

$$f_{(m)}(t,\rho)=c_{(m)}(\rho)g_{(m)}(t,\rho)+q_{(m)}(t,\rho)\,, \quad (117)$$

where

$$g_{(m)}(t,\rho)=(t+\rho)^{m+l}/(1+t\rho)^{m-l}\,, \quad (118)$$

$$c_{(m)}(\rho)=N_{ml}/[m^{1/2}(1-\rho^2)^l]\,, \quad (119)$$

and $q_{(m)}(t,\rho)$ is a polynomial of degree $2l$ in t needed to bring f_m to the form (107).

Finally, we can write the results:

$$\tilde{B}_l(\rho)_{n'n''}=\delta_{n'n''}[n''(1-\rho^2)]^{-1} \quad (120)$$

and

$$U_l(\rho)_{n'n''} = Y_{n''}^{(n')}(\rho) = \frac{(n'+n''-1)!(-1)^{n+l+1}\rho^{n'+n''-2l-2}(1-\rho^2)^{l+1}}{(n''+l)!(n''-l-1)!(n'+l)!(n'-l-1)!} \times F(l+1-n',\, l+1-n'';\, 1-n'-n'';\, 1/\rho^2)\,, \quad (121)$$

where the latter has been obtained by expanding $g^{(n')}(\rho)$, picking out the coefficient of $t^{n''+l}$ and transforming via (B16). The hypergeometric function appearing in (121) is a *polynomial* of degree $\min(n',n'')-l-1$ in $1/\rho^2$ and so we see that the elements of U_l are polynomials in ρ, a surprising result.

The matrix $C_l(\rho)B_l(\rho)^3$ occurring in (94) is also diagonalized by $U_l(\rho)$:

$$C_l(\rho)B_l(\rho)^3=U_l(\rho)^T\tilde{C}_l(\rho)\tilde{B}_l(\rho)^3U_l(\rho)\,, \quad (122)$$

where

$$\tilde{C}_l(\rho)_{n'n''}=\frac{\delta_{n'n''}}{1-n_0(1-\rho)^2\tilde{B}_l(\rho)_{n'n'}} =\frac{n'(1+\rho)}{n'+n_0}\left(\rho+\frac{n'-n_0}{n'+n_0}\right)^{-1}\delta_{n'n''}\,, \quad (123)$$

with $\nu=n_0$. This immediately gives

$$M_l(\rho)_{n'n''}=(n'n'')^{1/2}\sum_{n_1=l+1}^{\infty}U_l(\rho)^T{}_{n'n_1}\frac{n_1(1+\rho)}{n_1+n_0} \times\left(\rho+\frac{n_1-n_0}{n_1+n_0}\right)^{-1}n_1^{-3}(1-\rho^2)^{-3}U_l(\rho)_{n_1n''} \quad (124)$$

and therefore the expression in (96a) becomes, with a little manipulation,

$$[D_{l_0}^{(\pm)}M_{l_0\pm1}(\rho)D_{l_0}^{(\pm)T}]_{n_0n_0} =\sum_{n=l_0+1\pm1}^{\infty}W_{l_0}^{(\pm)}(\rho)_{n_0n}\left[(n+n_0)(1-\rho)\left(\rho+\frac{n-n_0}{n+n_0}\right)\right]^{-1}\times W_{l_0}^{(\pm)}(\rho)^T{}_{nn_0}$$
$$=\sum_{n=l_0+1\pm1}^{\infty}\frac{[W_{l_0}^{(\pm)}(\rho)n_0n]^2}{(n+n_0)(1-\rho)}\times[\rho+(n-n_0)/(n+n_0)]^{-1}\,, \quad (125)$$

where the matrix $W_{l_0}^{(\pm)}(\rho)$ is defined by

$$W_{l_0}^{(\pm)}(\rho)_{n_0n}=\sum_{n'=l_0+1\pm1}^{\infty}(\sqrt{n'})D_{l_0}^{(\pm)}{}_{n_0n'}\times U_{l_0\pm1}(\rho)^T{}_{n'n}/[n(1-\rho^2)]\,. \quad (126)$$

Combining these results, the level shift contribution from (87) is

$$\mathcal{L}'=4n_0^2\left(\frac{l_0+1}{2l_0+1}\sum_{n=l_0+2}^{\infty}\frac{1}{n_0+n}\times\int_0^1\frac{\rho(1+\rho)[W_{l_0}^{(+)}(\rho)_{n_0n}]^2}{\rho+(n-n_0)/(n+n_0)}d\rho+\frac{l_0}{2l_0+1}\sum_{n=l_0}^{\infty}\frac{1}{n_0+n}\times\int_0^1\frac{\rho(1+\rho)[W_{l_0}^{(-)}(\rho)_{n_0n}]^2}{\rho+(n-n_0)/(n+n_0)}d\rho\right). \quad (127)$$

When $n<n_0$ the above integrals have a pole at $\rho=(n_0-n)/(n_0+n)$. In this case we must take the principal value of the integral. In Appendix D it is demonstrated that these poles are merely the dipole transitions. Note that when $n=n_0$, $\rho=0$ is *not* a singularity of the integral although it is in (125).

The functions $W_{l_0}^{(\pm)}(\rho)_{n_0n}$ are easily evaluated in view of (99) and (100); for example,

$$n(1-\rho^2)W_{l_0}^{(-)}(\rho)_{n_0n} =\tfrac{1}{2}n_0^{-1/2}\{[(n_0+l_0)(n_0+l_0-1)]^{1/2}U_{l_0-1}(\rho)_{n,n_0-1} -[(n_0-l_0)(n_0-l_0+1)]^{1/2}U_{l_0-1}(\rho)_{n,n_0+1}\} \quad (128)$$

or

$$W_{l_0}^{(-)}(\rho)_{n_0n}=\frac{(-1)^{(n_0+l_0+1)}(n_0+n)!\rho^{n_0+n-2l_0-1}(1-\rho^2)^{l_0-1}}{2n[n_0(n+l_0-1)!(n-l_0)!(n_0+l_0)!(n_0-l_0-1)!]^{1/2}} \times\left(\frac{(n_0+l_0)(n_0+l_0-1)}{(n_0+n)(n_0+n-1)}F(l_0-n,\, l_0-n_0+1;\, 2-n_0-n;\, 1/\rho^2)-\rho^2F(l_0-n,\, l_0-n_0-1;\, -n-n_0;\, 1/\rho^2)\right). \quad (129a)$$

Using the so-called "contiguous function" relations[11] two or three times, we can write (129a) more symmetrically:

$$\frac{W_{l_0}^{(-)}(\rho)_{n_0n}}{\sqrt{n_0}}=\frac{1}{l_0}\left(\frac{(n^2-l_0^2)^{1/2}}{n}E_{l_0}(n_0,n,\rho)-\frac{(n_0^2-l_0^2)^{1/2}}{n_0}E_{l_0-1}(n_0,n,\rho)\right)$$

and

$$\frac{W_{l_0}{}^{(+)}(\rho)_{n_0n}}{\sqrt{n_0}}=\frac{1}{l_0+1}\left(\frac{[n^2-(l_0+1)^2]^{1/2}}{n}E_{l_0}(n_0,n,\rho)-\frac{[n_0{}^2-(l_0+1)^2]^{1/2}}{n_0}E_{l_0+1}(n_0,n,\rho)\right), \tag{129b}$$

where

$$E_{l_0}(n_0,n,\rho)=\frac{(-1)^{n_0+l_0-1}(1-\rho^2)^{l_0+1}\rho^{n+n_0-2l_0-3}(n+n_0-1)!F(l_0+1-n,\ l_0+1-n_0;\ 1-n_0-n;\ 1/\rho^2)}{2[(n_0+l_0)!(n_0-l_0-1)!(n+l_0)!(n-l_0-1)!]^{1/2}}. \tag{130}$$

By counting powers of ρ, it is easily seen that (130) and hence (129a) define a *polynomial* in ρ. The convergence of the series (127) is proved in Appendix E.

V. NUMERICAL RESULTS

The expressions derived above, after removing the divergent self-energy ΔE_0 of Eq. (69), describe a logarithmically divergent level shift for S states, but are convergent for all others. The energy shifts are traditionally expressed in a cutoff-independent manner in terms of the "average excitation energy" $k_0(n_0,l_0)$ (all expressions are independent of m_0), defined by

$$\frac{\Delta E(n_0,l_0)-\Delta E_0}{\text{Ry}}=\frac{8Z^4}{n_0{}^3}\frac{\alpha^3}{3\pi}\ln\frac{M}{k_0(n_0,l_0)}, \tag{131}$$

where $M=K$, the cutoff in photon energy, when $l_0=0$, and M is arbitrarily set at 1 Ry when $l_0\neq 0$. Even more commonly used is the Bethe logarithm $\ln[k_0(n_0,l_0)/(1\text{ Ry})]$:

$$\ln\frac{k_0(n_0,l_0)}{1\text{ Ry}}=-\frac{3\pi}{\alpha^3}\frac{n_0{}^3}{8Z^4}\frac{\Delta E(n_0,l_0)-\Delta E_0}{1\text{ Ry}}+\left(\ln\frac{K}{1\text{ Ry}}\right)\delta_{l_0,0}. \tag{132}$$

If we insert (67) into (30c) and then into (132) and use the relationship (32) between B and K, we see that the $\ln(K/1\text{ Ry})$ cancels and

$$\ln\frac{k_0(n_0,l_0)}{1\text{ Ry}}=[\ln Z^2-2\ln n_0+2\ln 2+2h(2n_0)-1/2n_0]\delta_{l_0,0}+(\mathcal{L}_{\text{finite}}+\mathcal{L}')/2n_0. \tag{133}$$

The only occurrence of Z in this is the $(\ln Z^2)\delta_{l_0,0}$ which we henceforth drop; the numerical results we get for hydrogen can be extended to all hydrogenic atoms by restoring this term for S states. The term $\mathcal{L}_{\text{finite}}$ comes from the last two terms of (62) and $\mathcal{L}'$ from (127). The function h is defined by (65).

The term $\mathcal{L}_{\text{finite}}$ contains an infinite series which contributes to (133) an amount

$$\Sigma=-\tfrac{1}{2}\sum_{n=l_0+1,n\neq n_0}^{\infty}\times\frac{1}{n}\int_0^1 d\rho\frac{(1-\rho^2)(1+\rho)^2A_{l_0}(n_0,n,\rho)^2}{\rho}. \tag{134}$$

As emphasized in Appendix B, $A_l(n_0,n,\rho)^2$ is a polynomial with rational coefficients (depending upon n, n_0, etc.) and furthermore, for $n\neq n_0$, divisible by ρ. Thus the integral in (134) yields a sum of the form

$$\sum_n\frac{p(n)}{q(n)},$$

where $p(n)$ and $q(n)$ are polynomials in n. Such a series [if convergent, which (134) is[8]], can always be summed *exactly*[12] by resolving into partial fractions

$$\frac{p(n)}{q(n)}=\sum_{k=1}^{m}\left(\frac{a_k}{n+\alpha_k}+\frac{b_k}{(n+\alpha_k)^2}+\frac{c_k}{(n+\alpha_k)^3}+\cdots\right)$$

and applying

$$\sum_{n=1}^{\infty}\frac{p(n)}{q(n)}=\sum_{k=1}^{m}\left(-a_k\psi(1+\alpha_k)+\frac{b_k}{1!}\psi'(1+\alpha_k)-\frac{c_k}{2!}\psi''(1+\alpha_k)+\cdots\right), \tag{135}$$

where[11,12]

$$\psi(z)=\frac{d}{dz}\ln\Gamma(z).$$

In our case it appears to be generally true that the only values ever needed for the polygamma functions are the combinations

$$\psi(\tfrac{3}{2})-\psi(1)=2-2\ln 2 \tag{136}$$

and

$$\psi^{(j)}(1)=(-1)^{j+1}j!\zeta(j), \tag{137}$$

where ζ is the Riemann ζ function.[11]

We next turn to the infinite series term $\mathcal{L}'$. Both series are of the form

$$\sum\frac{1}{n_0+n}\int_0^1\frac{\rho(1+\rho)[W_{l_0}(\rho)_{n_0n}]^2d\rho}{\rho+a(n)}, \tag{138}$$

where $a(n)=(n-n_0)/(n+n_0)$. These series converge like $1/n^3$, i.e., like $\zeta(3)$, as shown in Appendix E. (This is due to the presence of the continuum contribution.) However, if we observe Eqs. (E4) and (E5), we can

[12] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Co., New York, 1953), especially pp. 422 and 423.

break (138) into

$$\sum_n \frac{1}{n_0+n}\int_0^1 d\rho[W_{l_0}(\rho)_{n_0n}]^2 +2n_0\sum_n \frac{1}{(n_0+n)^2}\int_0^1 d\rho\frac{\rho[W_{l_0}(\rho)_{n_0n}]^2}{\rho+a(n)}, \quad (139)$$

where the first series converges like $1/n^3$ and the second like $1/n^4$. The virtue of (139) is that the more slowly convergent series, lacking the $\rho+a(n)$ denominator in the integrand, contains no logarithms and may be summed exactly using (135). This is because the polynomials in W^2 are of degree depending on $\min(n,n_0)$ and so for $n>n_0$ are all of fixed degree. Thus (139) leaves only a $1/n^4$ convergent series to be summed term by term. But we can go further. The reason that we could go from (138) to (139) was the $1+\rho$ factor in the numerator, which we used to cancel the $\rho+a(n)$ in the denominator to leave a more rapidly convergent series to be summed. If we examine Eqs. (E2), we see that W^2 has, for large n, the behavior

$$(1-\rho^2)^{2n_0}=(1-\rho)^{2n_0}(1+\rho)^{2n_0}.$$

The $1-\rho$ factors determine the rate of convergence. The $1+\rho$ factors can be used repeatedly $2n_0$ times, each time resulting in an exactly summable series and a more rapidly nonsummable part. When we exhaust these factors, we will have a series to sum which converges like $2n_0+4$. Actually, the $(1-\rho^2)^{2n_0}$ factor occurs only asymptotically, so that some care is required to extract the $(1+\rho)^{2n_0}$ factor without disturbing the $(1-\rho)^{2n_0}$ part. The details are given in the author's thesis. The first series to be summed will have the general form

$$\sum_n f_{n_0l_0}{}^{(\pm)}(n)\int_0^1 \frac{\rho^{2n-2n_0-1}(1-\rho)^{2n_0}}{\rho+a(n)}d\rho. \quad (140)$$

Therefore the two series for + and − may be combined and only one set of integrals need be computed. The integrals in (140) may be evaluated by combining the integrals

$$I_j(a)=\int_0^1 \frac{\rho^j d\rho}{\rho+a} =\sum_{k=0}^{j-1}\frac{(-a)^k}{j-k}+(-a)^j\ln\left|\frac{1+a}{a}\right|, \quad (141)$$

where the absolute value signs allows us to use the formula even when $a<0(n<n_0)$ and represents the necessary principal value. It is also convenient to use the recurrence formula

$$I_j(a)=1/j-aI_{j-1}(a), \quad (142a)$$

$$I_0(a)=\ln|(1+a)/a|. \quad (142b)$$

Finally, we must discuss truncation of the series (140). We know that for large n the terms are proportional to $1/n^{2n_0+4}$. Thus we can estimate the remainder caused by stopping the series at $n=\bar{n}$ by

$$\text{remainder}\simeq e_{\bar{n}}\zeta_{\bar{n}}(2n_0+4), \quad (143)$$

where

$$e_{\bar{n}}=\bar{n}^{2n_0+4}\times \text{term}\bar{n} \quad (144)$$

and $\zeta_{\bar{n}}(z)$ is the ζ function minus its terms through $1/\bar{n}^z$. Formula (143) gives a method of extrapolation of the truncated series. The error introduced in using (143) as an extrapolation, rather than as a truncation error, is estimated by observing the rate of change of $e_{\bar{n}}$ and of the extrapolated result, as discussed in the author's thesis.

We now apply these methods to some explicit cases. We begin with the 1S level. By (133) we have

$$\ln\frac{k_0(1S)}{1\,\text{Ry}}=\tfrac{5}{2}+2\ln 2+\tfrac{1}{2}(\mathcal{L}_{\text{finite}}+\mathcal{L}'); \quad (145)$$

$\mathcal{L}_{\text{finite}}$ comes from the last two terms of (64). We use (63)

$$\tfrac{1}{2}\mathcal{L}_{\text{finite}}=-\frac{1}{2}\int_0^1 d\rho\,(1-\rho^2)(2+\rho)+\Sigma=-\frac{19}{24}+\Sigma, \quad (146)$$

where, by (134)

$$\Sigma=-\tfrac{1}{2}\sum_{n=2}^{\infty}\frac{1}{n}\int_0^1 d\rho\,\rho^{2n-3}(1-\rho^2)(1+\rho)^2 =-\tfrac{1}{2}\sum_{j=0}^{\infty}\frac{r(j)}{j+2}, \quad (147)$$

where

$$r(j)=1/(j+1)(j+3)+4/(2j+3)(2j+5). \quad (148)$$

Thus we have two sums to evaluate:

$$\sum_{j=0}^{\infty}\frac{1}{(j+1)(j+2)(j+3)} =\tfrac{1}{2}\sum_{j=0}^{\infty}\left(\frac{1}{j+\frac{1}{2}}-\frac{1}{j+3}\right)\frac{1}{j+2}=\tfrac{1}{4} \quad (149a)$$

and

$$\sum_{j=0}^{\infty}\frac{1}{(j+2)(2j+3)(2j+5)}=\frac{8}{3}-4[\psi(\tfrac{3}{2})-\psi(1)], \quad (149b)$$

the former being a "collapsing" series and the latter by use of (135). Combining results we get

$$\ln\frac{k_0(1S)}{\text{Ry}}=\frac{17}{4}-2\ln 2+\tfrac{1}{2}\mathcal{L}'=2.86370\;56389+\tfrac{1}{2}\mathcal{L}'. \quad (150)$$

The numerical part of (150) is already 96% of the final

TABLE I. Successive approximations to the Bethe logarithm for the 1S state.

n	Term	$e_{\bar{n}}(144)$	Unextrapolated Bethe logarithm	Extrapolated Bethe logarithm
2	0.00910 64204	0.586	2.98329 91174	2.98430
3	0.00066 73039	0.486	2.98296 64213	2.984136
4	0.00011 44907	0.469	2.98408 09120	2.98412 88
5	0.00002 97937	0.465	2.98411 07057	2.98412 848
6	0.00000 99866	0.466	2.98412 06923	2.98412 8494

answer. Now

$$\tfrac{1}{2}\mathfrak{L}'=2\sum_{n=2}^{\infty}\frac{1}{n+1}\int_0^1 d\rho\frac{\rho(1+\rho)[W_0^{(+)}(\rho)_{1n}]^2}{\rho+(n-1)/(n+1)},$$

which converges like $1/n^3$. We can reduce this to a convergence like $1/n^6$ by the techniques mentioned. By (129) and (130),

$$W_0^{(+)}(\rho)_{1n}=\frac{n!}{2[(n-2)!(n+1)!]^{1/2}}\rho^{n-4}(1-\rho^2)\left(\frac{n+1}{n}-\rho^2\right),$$

so that

$$\tfrac{1}{2}\mathfrak{L}'=\tfrac{1}{2}\sum_{n=2}^{\infty}\frac{n-1}{n}\int_0^1\frac{\rho^{2n-3}(1+\rho)(1-\rho^2)^2}{\rho+(n-1)/(n+1)}d\rho,$$

and we see that we have three $1+\rho$ factors in the numerator. When we extract these and perform the sums, we get

$$\tfrac{1}{2}\mathfrak{L}'=13/4-\tfrac{1}{3}\psi'(1)-(38/9)[\psi(\tfrac{3}{2})-\psi(1)]+\Sigma', \quad (151)$$

with

$$\Sigma'=4\sum_{n=2}^{\infty}\frac{n-1}{n(n+1)^3}\int_0^1\frac{\rho^{2n-3}(1-\rho)^2}{\rho+(n-1)/(n+1)}d\rho, \quad (152)$$

which is exactly of the form (140) and converges like $1/n^6$. Inserting (151) into (150), we get

$$\ln\frac{k_0(1S)}{\text{Ry}}=-\frac{17}{18}+\frac{58}{9}\ln 2-\tfrac{1}{3}\psi'(1)+\Sigma'$$

$$=2.97419\ 26970+\Sigma', \quad (153)$$

using $\psi'(1)=\zeta(2)=\frac{1}{6}\pi^2$. We now sum the series Σ' term by term using (141) and (142). The results are summarized in Table I. In the extrapolated Bethe logarithm, use has been made of (143)–(144) and the "remainder" calculated to three figures. On the basis of the figures in the last column and on the variation of $e_{\bar{n}}$, we can state our result

$$\ln[k_0(1S)/1\,\text{Ry}]=2.98412\ 85(3), \quad (154)$$

which is to be compared with the most accurate previously published result of Harriman[13]:

$$\ln[k_0(1S)/1\,\text{Ry}]=2.98414\ 9(3).$$

[13] J. M. Harriman, Phys. Rev. **101**, 594 (1956).

We note that our result differs from this by seven times Harriman's estimated error. In fact, the results in Table I for $n\geq 4$ are all consistent with each other and inconsistent with Harriman's value. Moreover, previous precise calculations[14] for the $2S$ and $2P$ states have shown Harriman's values also in error there. Thus the value given above is very probably correct to within the error stated.

We have similarly calculated the $2S$ and $2P$ Bethe logarithms by these methods. The complete details may be found in the author's thesis. Here we present only the results after the series have been reduced to $1/n^8$ convergence:

$$\ln\frac{k_0(2S)}{1\,\text{Ry}}=2.80917\ 38731+64\sum_{n=3}^{\infty}\frac{(n^2-1)(n-2)^2}{n^3(n+2)^4}\times\int_0^1 d\rho\frac{\rho^{2n-5}(1-\rho)^4}{\rho+(n-2)/(n+2)},$$

$$\ln\frac{k_0(2P)}{1\,\text{Ry}}=-0.03412\ 95488+\frac{16}{3}\sum_{n=3}^{\infty}\frac{(11n^2-12)(n-2)}{n(n+2)^5}\times\int_0^1 d\rho\frac{\rho^{2n-5}(1-\rho)^4}{\rho+(n-2)/(n+2)}.$$

The numerical parts of the two expressions are "exact" (except for possible roundoff) and were obtained using a desk calculator. Note that the integrals in the two series are identical. Also, all the terms are positive.

The results, taking terms through $n=7$ and extrapolating with (143) and (144), are given below, together with the electronic computer results of Harriman[13] and of Schwartz and Tiemann[14] for comparison:

$\ln[k_0(2S)/1\,\text{Ry}]=2.81179\ 8(9)$ (Harriman)
$=2.81176\ 9883(28)$ (Schwartz and Tiemann)
$=2.81176\ 98(3)$ (this calc.),

$\ln[k_0(2P)/1\,\text{Ry}]=-0.03001\ 637(1)$ (Harriman)
$-0.03001\ 6697(12)$ (Schwartz and Tiemann)
$-0.03001\ 675(6)$ (this calc.).

Our results are clearly in agreement with those of Schwartz and Tiemann and in disagreement with those of Harriman. Although the former are given more precisely than our values, it should be noted that our numerical results were obtained by one afternoon's effort at an ordinary desk calculator, and could easily be extended in precision electronically. It was not our goal, however, to exceed the precision of Schwartz and Tiemann, but rather to illustrate the effects of the hidden symmetry group on the calcula-

[14] C. Schwartz and J. J. Tiemann, Ann. Phys. (N. Y.) **2**, 178 (1959).

tion and to develop techniques exploiting the $O(4)$ group.

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APPENDIX A: LOWEST TERMS (PHYSICAL SPACE)

The manipulation performed in Sec. III may seem to be obscure from a physical point of view. Here we give an alternative derivation equivalent to the development there but without projecting onto the Fock sphere.

From Eq. (25),

$$\Delta E(n_l l_0 n_0)=\frac{\alpha}{4m^2\pi^2}\sum_{\lambda=1}^{2}\int\frac{(d\mathbf{k})}{k}\langle p_\lambda G p_\lambda\rangle\,, \qquad \text{(A1)}$$

where

$$p_\lambda=\mathbf{p}\cdot\mathbf{e}_\lambda \qquad \text{(A2)}$$

and $\langle\ \rangle$ means the expectation value in the state $n_0l_0m_0$. The Green's-function operator

$$G=(E_{n_0}-k-H)^{-1} \qquad \text{(A3)}$$

[compare (27)] can be rewritten, treating the entire Coulomb interaction as a perturbation,

$$\begin{aligned} H&=H_0+V\,,\\ H_0&=p^2/2m\,,\\ V&=-Z\alpha/r\,, \end{aligned} \qquad \text{(A4)}$$

in terms of the free-electron Green's-function operator

$$G_0=(E_{n_0}-k-H_0)^{-1}. \qquad \text{(A5)}$$

The operators G, G_0 satisfy

$$G=G_0+G_0VG=G_0+GVG_0. \qquad \text{(A6)}$$

Now p_λ commutes with H_0 and so with G_0. Also,

$$G|n_0l_0m_0\rangle=-k^{-1}|n_0l_0m_0\rangle\,, \qquad \text{(A7)}$$

so that

$$\begin{aligned}\langle p_\lambda G p_\lambda\rangle&=\langle p_\lambda(G_0+G_0VG)p_\lambda\rangle\\ &=\langle p_\lambda^2G_0+p_\lambda G_0VGp_\lambda\rangle\\ &=\langle p_\lambda^2G-p_\lambda^2G_0VG\rangle+\langle p_\lambda G_0VGp_\lambda\rangle\\ &\qquad+\langle p_\lambda G_0VGVG_0p_\lambda\rangle. \end{aligned} \qquad \text{(A8)}$$

Applying (A7)

$$\begin{aligned}\langle p_\lambda G p_\lambda\rangle=-k^{-1}\langle p_\lambda^2\rangle+k^{-1}\langle p_\lambda^2G_0V\rangle+\langle p_\lambda G_0VG_0p_\lambda\rangle\\ +\langle p_\lambda G_0VGVG_0p_\lambda\rangle\,, \end{aligned} \qquad \text{(A9)}$$

which separates the terms in powers of V. The first three terms, which depend only on the trivial G_0, correspond to the lowest terms of Sec. III while the last term, involving G, corresponds to the Γ' part of (71).

We may write, correspondingly,

$$\begin{aligned}\Delta E(n_0l_0m_0)=\Delta E^{(0)}(n_0l_0m_0)+\Delta E^{(1)}(n_0l_0m_0)\\ +\Delta E^{(2)}(n_0l_0m_0)\,, \end{aligned} \qquad \text{(A10)}$$

where the first term of (A9) contributes

$$\begin{aligned}\Delta E^{(0)}(n_0l_0m_0)\\ &=-\frac{\alpha}{4m^2\pi^2}\sum_{\alpha=1}^{2}\int\frac{d\mathbf{k}}{k^2}\langle p_\lambda^2\rangle\\ &=-\frac{8\pi}{3}\frac{\alpha}{4m^2\pi^2}\int_0^K dk\left(\int dp\,|\psi_{nlm}(p)|^2p^2\right), \end{aligned} \qquad \text{(A11)}$$

i.e., exactly the renormalization term (69). The last term of (A9) contributes

$$\begin{aligned}\Delta E^{(2)}(n_0l_0m_0)\\ &=+\frac{\alpha}{4m^2\pi}\sum_{\lambda=1}^{2}\int\frac{d\mathbf{k}}{k}\langle p_\lambda G_0VGVG_0p_\lambda\rangle\,, \end{aligned} \qquad \text{(A12)}$$

which, if projected onto the Fock sphere, is easily seen to be the same as the contribution of (71).

The remaining term,

$$\begin{aligned}\Delta E^{(1)}(n_0l_0m_0)=\frac{\alpha}{4m^2\pi^2}\sum_{\lambda=1}^{2}\int\frac{d\mathbf{k}}{k}\\ \times(k^{-1}p_\lambda^2G_0V+p_\lambda G_0VG_0p_\lambda)\,, \end{aligned} \qquad \text{(A13)}$$

constitutes the major portion of the Lamb shift for deep-lying S states [for large n_0 or $l\neq 0$, the contribution from $\Delta E^{(2)}$ is comparable to (A13)]. Since (A13) depends only on known quantities, it can be evaluated by straightforward (but tedious) means. For the $1S$ state, inserting the configuration-space wave function ψ and G_0, we get directly, in terms of the Bethe logarithm (132),

$$\ln\frac{k_0(1S)}{1\,\text{Ry}}=\frac{17}{4}-2\ln 2=2.86370\ 56389\,,$$

exactly as in (150). This differs from the final value (154) by only 4%. For $2S$ the contribution from (A13) is 90% of the total; for $2P$, however, (A13) is almost entirely cancelled by $\Delta E^{(2)}$.

APPENDIX B: A INTEGRALS

In this Appendix we shall evaluate explicitly the $A_l(n,n',\rho)$ integrals introduced in Eq. (43). The integrals surprisingly turn out to be polynomials in ρ. We also derive a generating function for the integrals which is used in Sec. IV. As a byproduct, we obtain some interesting identities for Wigner 6-j coefficients.

Consider the more general integral

$$M(nl,n'l',\rho)=\int_0^\pi \frac{f(\alpha)Z_{nl}(\alpha)Z_{n'l'}(\alpha)\sin^2\alpha\, d\alpha}{1+2\rho\cos\alpha+\rho^2}, \quad \text{(B1)}$$

so that $A_l(n,n',\rho)$ is the special case $f(\alpha)=1, l'=l$. We now use the expansion (18) with $l=0$, $t=-\rho$; the expansion is valid for all complex t inside the unit disk:

$$M(n,l,n'l',\rho)=\sum_{k=0}^{\infty}(-\rho)^k\int_0^\pi f(\alpha)C_k{}^1(\cos\alpha)Z_{nl}(\alpha) \times Z_{n'l'}(\alpha)\sin^2\alpha\, d\alpha. \quad \text{(B2)}$$

Now $C_k{}^1(\cos\alpha)$ is essentially $Z_{k+1,0}(\alpha)$ aside from the normalization factors, so that the product $C_k{}^1(\cos\alpha) \times Z_{nl}(\alpha)$ can be expended in terms of $Z_{n''l}(\alpha)$ by use of the Clebsch-Gordan series for $O(4)$. Because of the local isomorphism between $O(4)$ and $O(3)\otimes O(3)$, the Clebsch-Gordan coefficients can be obtained in terms of ordinary $O(3)$ coefficients. This has been carried out by Biedenharn,[4] with the result for our case being

$$C_k{}^1(\cos\alpha)Z_{nl}(\alpha)=\sum_J (nkl|J)Z_{J+1,l}(\alpha), \quad \text{(B3)}$$

where

$$(nkl|J)=(-1)^{\frac{3}{2}(n+k+J-1)+l}[n(J+1)]^{1/2} \times\begin{Bmatrix} \frac{1}{2}J & \frac{1}{2}(n-1) & \frac{1}{2}k \\ \frac{1}{2}(n-1) & \frac{1}{2}J & l \end{Bmatrix}; \quad \text{(B4)}$$

the latter is the usual Wigner 6-j symbol as defined, say, in Edmonds.[15] The sum in (B4) is over the finitely many values of J permitted by the angular momentum recombination problem implicit in the 6-j symbol. These constraints also guarantee the reality of $(nkl|J)$. Thus we arrive at

$$M(nl,n'l',\rho)=\sum_{k=0}^{\infty}(-\rho)^k\sum_J (nkl|J)\,M(J+1l,n'l',0). \quad \text{(B5)}$$

In the case of A_l we get

$$A_l(n,n',\rho)=\sum_{k=|n'-n|}^{n'+n-2}{}^{*}(-\rho)^k(nkl|n'-1), \quad \text{(B6)}$$

where the limits on k come from the 6-j symbol, and the asterisk on the summation means that k goes between limits *in steps of 2*. Thus we see that $A_l(n,n',\rho)$ is a polynomial containing only even or only odd powers of ρ.

$$A_l(n,n',-\rho)=(-1)^{n-n'}A_l(n,n',\rho). \quad \text{(B7)}$$

For $l=0$, $(nk0|n'-1)=1$ and we have the simple result

$$A_0(n,n',\rho)=\sum_{k=|n-n'|}^{n+n'-2}(-\rho)^k =\frac{(-\rho)^{|n-n'|}-(-\rho)^{n+n'}}{1-\rho^2}, \quad \text{(B8)}$$

and, in particular,

$$A_0(n,n,\rho)=\frac{1-\rho^{2n}}{1-\rho^2}=1+\rho^2+\cdots+\rho^{2n-2}. \quad \text{(B9)}$$

For $l=1$ the coefficients are

$$(nk1|n'-1)=\frac{n^2+n'^2-k^2-2k-2}{[(n^2-1)(n'^2-1)]^{1/2}} \quad \text{(B10)}$$

and no simple form is possible. It will be noted that for $l=1$ the coefficients (B10) involve square roots. These, however, are independent of k so that the coefficients in $A_1(n,n',\rho)^2$ are all rational. This is true for all l as we shall see below, because the square roots come only from the N_{nl} normalization factors.

We now turn to the generating function for A_l. Set

$$I_{nn'}=\int_0^\pi \frac{\sin^{2l+2}\alpha C_{n-l-1}{}^{l+1}(\cos\alpha)C_{n'-l-1}{}^{l+1}(\cos\alpha)d\alpha}{1+2\rho\cos\alpha+\rho^2}, \quad \text{(B11)}$$

so that

$$A_l(n,n',\rho)=N_{nl}N_{n'l}I_{nn'}. \quad \text{(B12)}$$

Let x, y be two complex variables inside the unit disk. Then we have

$$G_l(x,y,\rho)=\sum_{n,n'=l+1}^{\infty}I_{nn'}x^{n-l-1}y^{n'-l-1}=\int_0^\pi \frac{\sin^{2l+2}\alpha d\alpha}{(1+2\rho\cos\alpha+\rho^2)[(1-2x\cos\alpha+x^2)(1-2y\cos\alpha+y^2)]^{l+1}} \quad \text{(B13)}$$

by means of (18). If we look first at $\rho=0$, we have

$$G_l(x,y,0)=\sum_{n,n'=l+1}^{\infty}x^{n-l-1}y^{n'-l-1}\int_0^\pi \sin^{2l+2}\alpha C_{n-l-1}{}^{l+1}(\cos\alpha)C_{n'-l-1}{}^{l+1}(\cos\alpha)d\alpha$$
$$=\sum_{n,n'=l+1}^{\infty}x^{n-l-1}y^{n'-l-1}\frac{\delta_{nn'}}{N_{nl}{}^2}$$
$$=\frac{(2l+1)!K_l}{l+1}g_l(xy), \quad \text{(B14)}$$

[15] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, N. J., 1957).

by recognizing that the integral is the orthonormalization integral for Z_{nl}, and by use of (19). In (B14) we have set

$$g_l(xy)=\sum_{m=0}^{\infty}(xy)^m\binom{m+2l+1}{m}\frac{l+1}{m+l+1}$$
$$=F(2l+2,\,l+1;\,l+2;\,xy)\,, \tag{B15}$$

where we have identified the series as an ordinary ${}_2F_1$ hypergeometric function. Using the identities[11]

$$F(a,b;c;z)=(1-z)^{c-a-b}F(c-a,\,c-b;\,c;\,z)$$
$$=(1-z)^{-a}F\left(a,\,c-b;\,c;\,\frac{z}{(z-1)}\right), \tag{B16}$$

we get

$$G_l(x,y,0)=\frac{(2l+1)!K_l}{l+1}\frac{1}{(1-xy)^{2l+1}}\times F(-l,\,1;\,l+2;\,xy)\,, \tag{B17a}$$

$$G_l(x,y,0)=\frac{(2l+1)!K_l}{l+1}\frac{1}{(1-xy)^{l+1}}\times F\left(-l,\,l+1;\,l+2;\,\frac{xy}{xy-1}\right). \tag{B17b}$$

Because of the negative integer $-l$ in (B17) the hypergeometric series terminate, i.e., are *polynomials*.

To see how $G_l(x,y,\rho)$ is obtained from $G_l(x,y,0)$, we put $e^{i\alpha}=z$ and change (B13) to a contour integral:

$$G_l(x,y,\rho)=\frac{(-1)^{l+1}}{2^{2l+3}i}\oint\frac{(1-z^2)^{2l+2}dz}{(1+\rho z)(\rho+z)[(1-xz)(z-x)(1-yz)(z-y)]^{l+1}}\,, \tag{B18}$$

where the integral is around the unit circle. The integrand has a simple pole at $z=-\rho$ and poles of order $l+1$ at $z=x$, y all inside the circle, plus similar reciprocal poles outside. In (B18) we change variables by

$$u=\frac{z+\rho}{1+\rho z}\,,\qquad z=\frac{u-\rho}{1-u\rho}\,, \tag{B19}$$

which maps the disk conformally onto itself with the pole at $z=-\rho$ going over to a pole at $u=0$ (and $z=-1/\rho$ to $u=\infty$). Then (B18) becomes

$$G_l(x,y,\rho)=\frac{(-1)^{l+1}}{2^{2l+3}i}(1-\rho^2)^{2l+1}\times\oint\frac{du(1-u^2)^{2l+2}}{u\{[(1+x\rho)-u(\rho+x)][(1+x\rho)u-(x+\rho)][(1+y\rho)-u(\rho+y)][(1+y\rho)u-(y+\rho)]\}^{l+1}}\,, \tag{B20}$$

$$G_l(x,y,\rho)=\frac{(1-\rho^2)^{2l+1}}{[(1+x\rho)(1+y\rho)]^{2l+2}}G_l\left(\frac{x+\rho}{1+x\rho},\,\frac{y+\rho}{1+y\rho},\,0\right)$$

Thus we get finally [inserting K_l from (19b)] from (B17)

$$G_l(x,y,\rho)=\frac{\pi}{2^{2l+1}}\binom{2l+1}{l}\frac{F(-l,\,1;\,l+2;\,(x+\rho)(y+\rho)/(1+x\rho)(1+y\rho))}{(1-xy)^{2l+1}(1+x\rho)(1+y\rho)}\,, \tag{B21a}$$

$$G_l(x,y,\rho)=\frac{\pi}{2^{2l+1}}\binom{2l+1}{l}\frac{(1-\rho^2)^lF(-l,\,l+1;\,l+2;\,-(x+\rho)(y+\rho)/(1-\rho^2)(1-xy))}{[(1+x\rho)(1+y\rho)(1-xy)]^{l+1}}\,. \tag{B21b}$$

This, coupled with (B12) and (B13), gives a generating function for A_l. It is obvious from (B12) and (B21) that the coefficients $(nkl|n'-1)$ in the polynomial $A_l(n,n',\rho)$ are rational multiples of $N_{nl}N_{n'l}$. Therefore $A_l(n,n',\rho)^2$ is a polynomial with rational coefficients. *This is very important because it allows one to perform many sums in Sec. V exactly.*

It is worth remarking that (B21) and (B12) provide a three-variable generating function for a class of **6-j coefficients through (B6) and (B4).**

We can also use (B21) to prove some interesting identities. For an illustration, set $\rho=1$ in (B21a). The hypergeometric function at 1 can be evaluated and is, in our case, $(l+1)/(2l+1)$. From this we deduce

$$\int_0^{\pi}\frac{C_m^{l+1}(\cos\alpha)C_n^{l+1}(\cos\alpha)\sin^2\alpha\,d\alpha}{1+\cos\alpha}=\frac{\pi}{2^{2l}}\frac{(2l)!}{(l!)^2}(-1)^{n+m}\binom{\min(n,m)+2l+1}{2l+1}\,, \tag{B22}$$

which appears to be a new identity for Gegenbauer functions. As its counterpart (B23) can be expressed in terms of $A_l(n,n',1)$ as

$$A_l(n,n',1)=\frac{n_<}{2l+1}(-1)^{n+n'}\times\left(\frac{(n_<^2-1^2)(n_<^2-2^2)\cdots(n_<^2-l^2)}{(n_>^2-1^2)(n_>^2-2^2)\cdots(n_>^2-l^2)}\right)^{1/2} \tag{B23}$$

(where the square root is one if $l=0$), with $n_<=\min(n,n')$, $n_>=\max(n,n')$. That is,

$$\sum_{k=|n-n'|}^{n+n'-2}{}^{*}(-1)^{\frac{1}{2}(k-n-n')+l}\begin{Bmatrix}\frac{1}{2}(n'-\frac{1}{2}) & \frac{1}{2}(n-1) & \frac{1}{2}k\\ \frac{1}{2}(n-1) & \frac{1}{2}(n'-1) & l\end{Bmatrix}=\frac{-1}{2l+1}\left(\frac{(n_<+l)(n_<+l-1)\cdots(n_<-l)}{(n_>+l)(n_>+l-1)\cdots(n_>-l)}\right)^{1/2} \tag{B24}$$

and, for $n=n'$, $A_l(n,n,1)=n/(2l+1)$, so that

$$\sum_{k=0}^{n-1}(-1)^{k-n+l-1}\begin{Bmatrix}\frac{1}{2}(n-1) & \frac{1}{2}(n-1) & k\\ \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & l\end{Bmatrix}=\frac{1}{2l+1}. \tag{B25}$$

These are identities of the Racah-Elliot type,

APPENDIX C: GENERATING FUNCTIONS FOR MATRICES

Let A_{nm}, B_{nm} be matrices, n, $m=0, 1, 2, \cdots$. We define generating functions for A_{nm} and B_{nm}:

$$A(x,y)=\sum_{n,m=0}^{\infty}A_{nm}x^ny^m,\qquad B(x,y)=\sum_{n,m=0}^{\infty}B_{nm}x^ny^m, \tag{C1}$$

where x, y are complex variables. We assume the series were well behaved for all x,y in the unit disk $|x|\leq 1$, $|y|\leq 1$. Consider the contour integral

$$C(x,z)=\frac{1}{2\pi i}\oint_{|y|=1}\frac{dy}{y}A\left(x,\frac{1}{y}\right)B(y,z) \tag{C2}$$

(on the circle $|y|=1$, $y^*=1/y$). If we insert (C1), we get

$$C(x,z)=\sum_{n,m,n',m'=0}^{\infty}A_{nm}B_{n'm'}x^nz^{m'}\times\frac{1}{2\pi i}\oint\frac{dy}{y}y^{-m}y^{n'}. \tag{C3}$$

The latter integral is just $2\pi i\delta_{n'm}$, so that $C(x)$ yields

$$C(x,z)=\sum_{nm'=0}^{\infty}\left[\sum_{m=0}^{\infty}A_{nm}B_{mm'}\right]x^nz^{m'}. \tag{C4}$$

Therefore $C(x,z)$ is the generating function for the product matrix AB. Thus (C2) is the formula for multiplying matrices with their generating functions.

Similarly, for a matrix times a vector and the scalar product of two vectors,

$$Av \text{ generated by } \frac{1}{2\pi i}\oint_{|y|=1}A\left(x,\frac{1}{y}\right)v(y)\frac{dy}{y}, \tag{C5}$$

$$u\cdot v=\frac{1}{2\pi i}\oint_{|y|=1}u\left(\frac{1}{y}\right)v(y)\frac{dy}{y}. \tag{C6}$$

APPENDIX D: DIPOLE TRANSITION AND GORDON'S FORMULA

The pole in the integrands of (127) occur at $(n_0>n)$

$$\rho_{n_0n}=(n_0-n)/(n_0+n). \tag{D1}$$

Using (32) and (35) this corresponds to a photon energy

$$k_{n_0n}=\frac{\rho_{n_0n}^2}{m}\beta_{n_0n}=\tfrac{1}{2}(Z\alpha)^2m\left(\frac{1}{n^2}-\frac{1}{n_0^2}\right), \tag{D2}$$

which is just the energy difference $E_{n_0}-E_n$ corresponding to a transition. Referring to (25), we see that the residue at this pole (the imaginary part of the level shift) is

$$\text{Im}\Delta E(n_0l_0m_0)=-\tfrac{2}{3}\alpha\sum_n k_{n_0n}|\mathbf{v}_{n_0n}|^2. \tag{D3}$$

Now

$$\mathbf{v}_{n_0n}=k_{n_0n}\mathbf{r}_{n_0n}, \tag{D4}$$

by taking matrix elements of

$$-i[\mathbf{r},H]=\mathbf{p}/m=\mathbf{v}, \tag{D5}$$

and so

$$\text{Im}\Delta E(n_0l_0m_0)=-\tfrac{2}{3}\alpha\sum_n k_{n_0n}^3|\mathbf{r}_{n_0n}|^2. \tag{D6}$$

In the notation of Bethe and Salpeter[10] we can identify

$$\text{Im}\Delta E(n_0l_0\to nl_0-1)=-\tfrac{2}{3}\alpha k_{n_0n}^3|R_{n_0l_0}^{nl_0-1}|^2\times l_0/(2l_0+1), \tag{D7}$$

$$\text{Im}\Delta E(n_0l_0\to nl_0+1)=-\tfrac{2}{3}\alpha k_{n_0n}^3|R_{n_0l_0}^{nl_0+1}|^2\times(l_0+1)/(2l_0+1), \tag{D8}$$

where we have separated the individual dipole transitions.

Using (127) and (30) we correspondingly pick out

$$\mathrm{Im}\Delta E(n_0l_0\to nl_0-1)=-\frac{2}{3}\frac{Z^4\alpha^5 m}{n_0^4}\frac{l_0}{l_0+1}4n_0^2\frac{2n_0(n_0-n)}{(n_0+n)^3}\times[W_{l_0}^{(-)}(\rho_{n_0n})_{n_0n}]^2 \quad \text{(D9a)}$$

and

$$\mathrm{Im}\Delta E(n_0l_0\to nl_0+1)=-\frac{2}{3}\frac{Z^4\alpha^5 m}{n_0^4}\frac{l_0+1}{2l_0+1}4n_0^2\frac{2n_0(n_0-n)}{(n_0+n)^3}\times[W_{l_0}^{(+)}(\rho_{n_0n})_{n_0n}]^2, \quad \text{(D9b)}$$

and so

$$|R_{n_0l_0}{}^{nl_0\pm1}|=\frac{8}{Z\alpha m}\frac{1}{n_0^{1/2}(n_0-n)}\left(\frac{nn_0}{n+n_0}\right)^3\times|W_{l_0}^{(\pm)}(\rho_{n_0n})_{n_0n}|. \quad \text{(D10)}$$

The dimensional quantity $1/Z\alpha m$ is the atomic radius a_0; the absolute value signs in (D10) arise because we have only equations relating the squares of R and W. We thus arrive at, via (129) and (130),

$$R_{n_0l_0}{}^{nl_0-1}=\pm\frac{a_0(n+n_0-1)!(4nn_0)^{l_0+3}(n_0-n)^{n+n_0-2l_0-4}}{16l_0[(n_0+l_0)!(n_0-l_0-1)!(n+l_0-1)!(n-l_0)!]^{1/2}(n+n_0)^{n+n_0}}$$
$$\times\left[\left(\frac{n-l_0}{n}\right)\left(\frac{4nn_0}{(n+n_0)^2}\right)F\left(l_0+1-n_0,l_0+1-n;1-n-n_0;\left(\frac{n+n_0}{n_0-n}\right)^2\right)\right.$$
$$\left.+\left(\frac{n_0+l_0}{n_0}\right)\left(\frac{n_0-n}{n_0+n}\right)^2F\left(l_0-n_0,l_0-n;1-n-n_0;\left(\frac{n_0+n}{n_0-n}\right)^2\right)\right]. \quad \text{(D11)}$$

This is essentially Gordon's formula[11,16] through not in the same form as published there. (D11) can be converted to Gordon's form via the identity

$$F(l_0-n,l_0-n_0;1-n-n_0;z)=\frac{(n_0+l_0+1)!(n+l_0-1)!}{(2l_0-1)!(n+n_0-1)!}\times F(l_0-n_0,l_0-n;2l_0;1-z), \quad \text{(D12)}$$

which can be proved by equating coefficients of powers of z, and the continguous functions relations.[11]

APPENDIX E: CONVERGENCE OF SERIES

To prove the convergence of (127), we use the asymptotic relation (as $n\to\infty$)

$$F(l_0+1-n,l_0+1-n_0;1-n-n_0;x)\sim F(l_0+1-n_0,-n_0;-n_0;x)=(1-x)^{n_0-l_0-1}, \quad \text{(E1)}$$

from which

$$W_{l_0}^{(-)}(\rho)_{n_0n}\sim\frac{-(n+n_0-1)!\rho^{n-n_0-1}(1-\rho^2)^{n_0}}{2[n_0(n_0+l_0)!(n_0-l_0-1)!(n+l_0-1)!(n-l_0)!]^{1/2}} \quad \text{(E2a)}$$

and

$$W_{\rho_0}^{(+)}(\rho)_{n_0n}\sim\frac{+(n+n_0-1)!\rho^{n-n_0+1}(1-\rho^2)^{n_0}}{2[n_0(n_0+l_0)!(n_0-l_0-1)!(n+l_0+1)!(n-l_0-2)!]^{1/2}}. \quad \text{(E2b)}$$

[16] W. Gordon, Ann. Physik. (5) 2, 1031 (1929).

Now the integrals (127),

$$I_n^{\pm}=\int_0^1 d\rho\,\rho(1+\rho)\left(\rho+\frac{n-n_0}{n+n_0}\right)^{-1}[W_l^{\pm}(\rho)_{n_0n}]^2, \quad \text{(E3)}$$

can be written using the observation

$$1+\rho=\left(\rho+\frac{n-n_0}{n+n_0}\right)+\frac{2n_0}{n+n_0} \quad \text{(E4)}$$

as

$$I_n^{\pm}=J_n^{\pm}+\frac{2n_0}{n+n_0}K_n^{\pm}, \quad \text{(E5)}$$

where

$$J_n^{\pm}=\int_0^1 d\rho\,\rho[W_{\rho_0}^{(\pm)}(\rho)_{n_0n}]^2, \quad \text{(E6a)}$$

$$K_n^{\pm}=\int_0^1 d\rho\,\rho\left(\rho+\frac{n-n_0}{n+n_0}\right)^{-1}[W_{l_0}^{\pm}(\rho)_{n_0n}]^2. \quad \text{(E6b)}$$

Comparing (E6b) and (E3) we see that, since $1+\rho\geq1$, we have $K_n^{\pm}<I_n^{\pm}$, and so

$$I_n^{\pm}<J_n^{\pm}+\frac{2n_0}{n+n_0}I_n^{\pm},$$

that is,

$$I_n^{\pm}<\frac{n+n_0}{n-n_0}J_n^{\pm}. \quad \text{(E7)}$$

Thus the series (127) will converge if

$$\sum_{n>n_0} \frac{J_n^{\pm}}{n-n_0} < \infty . \qquad \text{(E8)}$$

But the integrals $J_n^{\pm}$, lacking the denominator, are much more tractable than the I_n. In fact, for n large, we deduce from (E2) that the $J_n^{\pm}$ reduce to

$$\int_0^1 \rho^{2n-2n_0-1}(1-\rho^2)^{2n_0} d\rho = \frac{(n-n_0-1)!(2n_0)!}{2(n+n_0)!} \qquad \text{(E9)}$$

apart from outside factorials. Application of Stirling's formula then shows that the series in (E8) converges like $1/n^3$.

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Many-Level Formula for Scattering from Extremely Strong Square Potentials*

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A version of the many-level formula for scattering is introduced, considering the potential strength as the fundamental variable. It is applied to extremely strong square potentials. Under such circumstances, we must deal with a sum over a large number of nonresonant terms. The mathematical technique developed here will be directly applicable in the discussion of a singular potential scattering. Furthermore, McVoy, Heller, and Bolsterli have pointed out that a deep square well and a high barrier produce similar scattering amplitudes, in spite of the difference in sign. This intriguing effect is analyzed in the light of the many-level formula. We can understand it clearly in terms of the dominance of the orthogonality effect. It refers to such an effect as is a consequence of the fact that the wave function is orthogonal to any normalizable function introduced within the range of the square potential, which occurs if the potential strength tends to infinity. In the case of attraction, the depth of the square well must be outside the "width of a resonance" in order that this effect may dominate. We may define the relative probability of encountering a resonance with the ratio of the width of a resonance to the distance between two adjacent resonances. It tends to zero as the depth increases without limit.

1. INTRODUCTION

If there is no strong singularity or long-range tail, any interaction (generalized potential) can be expanded in a series whose individual term is in separable form and associated with a particular form factor. An individual form factor is defined as an eigenfunction of the kernel of the partial-wave Lippmann-Schwinger equation, and is labeled by the number of nodes, i.e., "the radial quantum number." Taking into account multiple scattering effects, the T matrix will be given in the form of a sum over contributions from such form factors. This form of the T matrix bears a similarity to the many-level formula (Breit-Wigner formula)[1] in that the poles and the residues of the T matrix are clearly indicated, though the potential strength is used as the variable instead of the energy. Therefore, an extended use of such terms as "levels" and "widths" in referring to contributions from individual form factors is naturally suggested. The "many-level" formula enables us to understand perfectly the analytic property of the T matrix as a function of potential strength. The proofs for these statements can be carried out with the use of what we call the approach through the finite-rank approximations, namely, by approximating a given generalized potential with a converging sum of separable potentials. This method was originally developed by Weinberg[2] in a different form, and its merit was emphatically demonstrated by Coester.[3] The present author analyzed its mathematical aspects from the physicist's point of view and gave a rigorous proof.[4] It is the purpose of this paper to study extremely strong square potentials in order to shed light on scattering from a singular potential. The method developed here

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[1] An approach similar in form to the present one was developed earlier and independently by H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958), **19**, 287 (1962); further references are given there. Duke and Wigner applied Wigner's R-matrix theory to the potential scattering from a square well; C. B. Duke and E. P. Wigner, Rev. Mod. Phys. **36**, 584 (1964). The Wigner R matrix is essentially equal to the tangent of the phase shift, as measured relative to the phase shift of a hard-core scattering (where the radius of the hard core is equal to the radius of the internal region). A summation over the number of nodes, which we call the "radial quantum number," was employed in their paper as in the present paper; however, since it requires a substantial amount of work to compare the two results, we do not attempt it in the present paper.

[2] S. Weinberg, Phys. Rev. **131**, 440 (1963); **130**, 776 (1963); M. Scadron and S. Weinberg, *ibid.* **133**, B1589 (1964); S. Weinberg, J. Math. Phys. **5**, 743 (1964); M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. **135**, B202 (1964).

[3] F. Coester, Phys. Rev. **133**, B1516 (1964).

[4] S. Tani, Ann. Phys. (N. Y.) **37**, 411; **37**, 451 (1966); these papers will be referred to as I in the following.