

Reduced Coulomb Green's Function for Bound-State Calculations

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The known closed form expression for the coordinate space Coulomb Green's function is specialized for applications involving perturbations of the ground state of the hydrogen atom by removing the ground-state pole term and evaluating the finite part at the pole. The resulting closed form expression is simpler than the full Green's function and may be quite useful.

I. INTRODUCTION

The function

$$G^n(\vec{r}_2, \vec{r}_1) = -\frac{\hbar^2}{2m} \sum_{k \neq n} \sum_l \frac{\varphi_{kl}(\vec{r}_2) \varphi_{kl}^*(\vec{r}_1)}{E_k - E_n} \quad (1.1)$$

plays an essential role in the Rayleigh-Schrödinger bound-state perturbation theory for a quantum-mechanical particle moving in a potential field $V(\vec{r})$. Here the E_k denote the distinct energy eigenvalues of the unperturbed Hamiltonian,

$$H_0 = -(\hbar^2/2m)\nabla^2 + V(\vec{r}), \quad (1.2)$$

including continuum eigenvalues if they occur.¹ The $\varphi_{kl}(\vec{r})$ are the corresponding eigenfunctions of H_0 , l being a degeneracy quantum number. The energy E_n is one of the bound state eigenvalues of H_0 .

The function $G^n(\vec{r}_2, \vec{r}_1)$ enters in the calculation of the first-order corrections to the bound-state wave functions belonging to the eigenvalues E_n , and also in the second-order corrections to the energies of these states when the Hamiltonian H_0 is modified by the addition of a perturbation term. For example, if the ground state, $\varphi_1(\vec{r})$ say, of H_0 is nondegenerate, and if the perturbation is simply caused by a small additional potential $U(\vec{r})$, then the (unnormalized) perturbed ground-state wave function is given correct to first order by²

$$\begin{aligned} \psi_1(\vec{r}_2) &= \varphi_1(\vec{r}_2) \\ &+ (2m/\hbar^2) \int d^3r_1 G^1(\vec{r}_2, \vec{r}_1) U(\vec{r}_1) \varphi_1(\vec{r}_1), \end{aligned} \quad (1.3)$$

and the increase in the ground-state energy is given correct to second order by

$$\begin{aligned} \Delta E_1 &= \int d^3r_1 \varphi_1(\vec{r}_1) U(\vec{r}_1) \varphi_1(\vec{r}_1) \\ &+ (2m/\hbar^2) \int d^3r_2 \int d^3r_1 \varphi_1^*(\vec{r}_2) \\ &\times U(\vec{r}_2) G^1(\vec{r}_2, \vec{r}_1) U(\vec{r}_1) \varphi_1(\vec{r}_1). \end{aligned} \quad (1.4)$$

The function $G^n(\vec{r}_2, \vec{r}_1)$ is related to the Green's function,

$$G(\vec{r}_2, \vec{r}_1; E) = -\frac{\hbar^2}{2m} \sum_k \sum_l \frac{\varphi_{kl}(\vec{r}_2) \varphi_{kl}^*(\vec{r}_1)}{E_k - E}, \quad (1.5)$$

of the Hamiltonian H_0 , in that $G^n(\vec{r}_2, \vec{r}_1)$ is obtained from $G(\vec{r}_2, \vec{r}_1; E)$ by removing the n th pole term,

$$-\frac{\hbar^2}{2m} \sum_l \frac{\varphi_{nl}(\vec{r}_2) \varphi_{nl}^*(\vec{r}_1)}{E_n - E},$$

and evaluating the other terms at $E = E_n$. We shall refer to $G^n(\vec{r}_2, \vec{r}_1)$ as the "reduced n th state Green's function" and (when necessary to avoid ambiguity) to $G(\vec{r}_2, \vec{r}_1; E)$ as the "full Green's function."

Recently, Hameka² has derived a relatively simple closed form expression for the S-wave component of the reduced ground-state Coulomb Green's function. We will here derive the more general result

$$\begin{aligned} G^1(\vec{r}_2, \vec{r}_1) &= -\frac{e^{-|\vec{r}_2 - \vec{r}_1|/a_1}}{4\pi|\vec{r}_2 - \vec{r}_1|} \\ &+ \frac{e^{-\frac{1}{2}(u+v)}}{2\pi a_1} [-g(v) + \ln(u) + \frac{1}{2}(u+v) - \frac{5}{2} + \gamma], \end{aligned} \quad (1.6)$$

$$u = (r_2 + r_1 + |\vec{r}_2 - \vec{r}_1|)a_1^{-1},$$

$$v = (r_2 + r_1 - |\vec{r}_2 - \vec{r}_1|)a_1^{-1},$$

expressing the complete reduced ground-state Coulomb Green's function, including all partial-wave contributions, in closed form. Here a_1 is the first Bohr radius, $a_1 = 4\pi\hbar^2/mZe^2$, γ is the Euler-Mascheroni constant, and $g(v)$ is the function defined by

$$g(v) = \int_0^v dt \frac{e^t - 1}{t} = -ve^v \int_0^1 dt e^{-tv} \ln(1-t). \quad (1.7)$$

It is quite remarkable that the expression (1.6) is apparently not more complicated than the S-wave part calculated by Hameka, the difference between the two expressions amounting almost to the mere replacement of Hameka's variables $2r_>(a_1)^{-1}$ and $2r_<(a_1)^{-1}$ by the well-known Coulomb variables u and v , respectively. The expression (1.6) is simpler than the full Coulomb Green's function³ and may prove to be quite useful for applications.

II. REDUCED GROUND-STATE COULOMB GREEN'S FUNCTION IN CLOSED FORM

1. Uniqueness

The function $G^1(\vec{r}_2, \vec{r}_1)$ satisfies the differential equation,

$$\begin{aligned} & (\nabla_2^2 + 2/a_1 r_2 - 1/a_1^2)G^1(\vec{r}_2, \vec{r}_1) \\ & = \delta^3(\vec{r}_2 - \vec{r}_1) - \varphi_{100}(\vec{r}_2)\varphi_{100}^*(\vec{r}_1), \end{aligned} \quad (2.1)$$

together with suitable regularity conditions at the origin and at infinity. Here

$$\varphi_{100}(\vec{r}) = \pi^{-\frac{1}{2}}(a_1)^{-\frac{3}{2}}e^{-r/a_1}$$

is the ground-state Coulomb wave function. If $F(\vec{r}_2, \vec{r}_1)$ and $G(\vec{r}_2, \vec{r}_1)$ are two solutions of the differential equation and the boundary conditions, one can deduce the identity,

$$\begin{aligned} F(1, 3) - \varphi_{100}(1) \int d^3 r_2 \varphi_{100}^*(2) F(2, 3) \\ = G(3, 1) - \varphi_{100}(3) \int d^3 r_2 \varphi_{100}^*(2) G(2, 1), \end{aligned}$$

by applying Green's theorem in the familiar way. Setting $G=F$, we learn that the expressions occurring on either side of this identity are symmetric in their free arguments, \vec{r}_1 and \vec{r}_3 . Thus the identity can be rewritten in the form

$$\begin{aligned} F(3, 1) - \varphi_{100}(3) \int d^3 r_2 \varphi_{100}^*(2) F(2, 1) \\ = G(3, 1) - \varphi_{100}(3) \int d^3 r_2 \varphi_{100}^*(2) G(2, 1). \end{aligned} \quad (2.2)$$

2. Derivation of $G^1(\vec{r}_2, \vec{r}_1)$

We begin with the following expression⁴ for the Coulomb Green's function

$$G(\vec{r}_2, \vec{r}_1; E) = -\frac{\Gamma(1-i\nu)}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} W_{i\nu; \frac{1}{2}}(u/i\nu) & \mathfrak{M}_{i\nu; \frac{1}{2}}(v/i\nu) \\ \dot{W}_{i\nu; \frac{1}{2}}(u/i\nu) & \mathfrak{M}_{i\nu; \frac{1}{2}}(v/i\nu) \end{vmatrix}, \quad (2.3)$$

$$\nu = (ka_1)^{-1}, \quad k = (2mE)^{1/2}/\hbar, \quad 0 < \text{arc}(k) < \pi.$$

The variables u , v , and a_1 are as defined in Eq. (1.6). The functions W and \mathfrak{M} are Whittaker functions as defined in Buchholz.⁵ The expression (2.3) is an analytic function of E on the complex plane cut along the positive real axis $0 \leq E < +\infty$ (the continuous spectrum of the Coulomb Hamiltonian) with the exception of the poles of the gamma function factor $\Gamma(1-i\nu)$. These occur for $i\nu = n = 1, 2, 3, \dots$ corresponding to E values of $-mc^2 Z^2 \alpha^2 / 2n^2$, $\alpha = e^2 / 4\pi\hbar c$, the bound-state energy levels of the system.

If we multiply the expression (1.5) through by the factor $(E - E_1)$, where E_1 is the ground-state energy, and differentiate with respect to E we eliminate the ground-state term. Substituting $E = E_1$ in the resulting expression - which is now finite at $E = E_1$ - and comparing with Eq. (1.1), we find the following formula for the reduced ground-state Green's function

$$G^1(\vec{r}_2, \vec{r}_1) = \frac{\partial}{\partial E} \left[(E - E_1) G(\vec{r}_2, \vec{r}_1; E) \right] \Big|_{E=E_1} \quad (2.4)$$

The differentiation here is more conveniently carried out in terms of the variable

$$z = 1 - i\nu, \quad (2.5)$$

rather than the energy. The variable z assumes the value $z = 0$ for $E = E_1$. Substituting Eq. (2.3) into

We have here a partial uniqueness theorem for the reduced Green's function: The reduced Green's function is determined uniquely by the differential equation and the boundary conditions except as regards its component (in the sense of Hilbert space) along the state $\varphi_{100}(\vec{r})$. It has been verified by direct substitution that the expression on the right-hand side of Eq. (1.6) actually satisfies the differential equation, Eq. (2.1), of the reduced Coulomb Green's function. Since this expression also satisfies the appropriate boundary conditions, it must indeed be equal to $G^1(\vec{r}_2, \vec{r}_1)$ except possibly for the coefficient of the term

$$(2\pi a_1)^{-1} e^{-(r_2 + r_1)/a_1} = \frac{1}{2} a_1^{-2} \varphi_{100}(\vec{r}_2) \varphi_{100}^*(\vec{r}_1).$$

The coefficient of this term is checked by the calculation presented in Sec. II, Sub. 3 in which the S-wave part of Eq. (1.6) is projected out and found to agree with Hamerka's result for this special case. [Since the term

$$(2\pi a_1)^{-1} \exp[-(r_2 + r_1)/a_1]$$

in Eq. (1.6) contains no angular dependence, it will remain unaltered except for a numerical factor in projecting out the S-wave part. Any error in the coefficient of this term in Eq. (1.6) will imply an identical error in the coefficient of the corresponding term $2(a_1)^{-1} \exp(-x)$ in Eq. (2.24) for the S-wave part.]

Eq. (2.4) and expressing everything in terms of z , we find⁶

$$G^1(\vec{r}_2, \vec{r}_1) = \frac{\partial}{\partial z} \left[\frac{1}{2}(2-z)(1-z)^{-2} \Gamma(1+z) F(\vec{r}_2, \vec{r}_1; z) \right] \Big|_{z=0}, \quad (2.6)$$

$$F(\vec{r}_2, \vec{r}_1; z) = -\frac{1}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} W_{1-z; \frac{1}{2}}(u/(1-z)) & \mathfrak{M}_{1-z; \frac{1}{2}}(v/(1-z)) \\ \dot{W}_{1-z; \frac{1}{2}}(u/(1-z)) & \dot{\mathfrak{M}}_{1-z; \frac{1}{2}}(v/(1-z)) \end{vmatrix}. \quad (2.7)$$

All functions in Eq. (2.6) are analytic at $z=0$. Consequently, the evaluation of the expression (2.6) for the reduced Green's function involves no limiting processes, but only differentiation and substitution of $z=0$. In evaluating the right-hand side of Eq. (2.6), it was found convenient to work with F in its determinantal form. The various terms generated by the differentiation can be evaluated with the help of formulas from the following list:

$$\dot{\Gamma}(1) = -\gamma; \quad (2.8)$$

$$\mathfrak{M}_{1; \frac{1}{2}}(v) = ve^{-\frac{1}{2}v}, \quad W_{1; \frac{1}{2}}(u) = ue^{-\frac{1}{2}u}; \quad (2.9)$$

$$\frac{\partial}{\partial z} \mathfrak{M}_{1-z; \frac{1}{2}}(v) \Big|_{z=0} = e^{-\frac{1}{2}v} [v - (e^v - 1) + vg(v)]; \quad (2.10)$$

$$\frac{\partial}{\partial z} W_{1-z; \frac{1}{2}}(u) \Big|_{z=0} = [1 - u \ln(u)] e^{-\frac{1}{2}u}. \quad (2.11)$$

Equation (2.8) can be found in Whittaker and Watson⁷ and Eqs. (2.9) can be found in Buchholz.⁸ The function $g(v)$ in Eq. (2.10) has been defined before [cf. Eq. (1.7)]. Equation (2.10) can be derived by expressing the Whittaker function in terms of the confluent hypergeometric function using the formula⁹

$$\mathfrak{M}_{k; \frac{1}{2}\mu}(v) = v^{\frac{1}{2}(1+\mu)} e^{\mp \frac{1}{2}v} {}_1F_1\left(\frac{1}{2}(1+\mu) \mp k; 1+\mu; \pm v\right) / \Gamma(1+\mu) \quad (2.12)$$

(with the upper sign), writing out the power series expansion of the confluent hypergeometric function and differentiating term by term. This derivation would not be essentially different from the derivation given by Hameka² in his discussion of the S -wave part of the reduced Green's function and is not repeated here.¹⁰ However, the derivation of Eq. (2.11) does not seem to be available in the literature so we outline this derivation in the Appendix. Other expressions occurring in the evaluation of Eq. (2.6) and not contained in the above list of formulas can be evaluated by differentiation with respect to u or v of the formulas already in that list. We list here for reference the principal intermediate steps in the calculation.

$$-\frac{1}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} W_{1; \frac{1}{2}}(u) & \mathfrak{M}_{1; \frac{1}{2}}(v) \\ \dot{W}_{1; \frac{1}{2}}(u) & \dot{\mathfrak{M}}_{1; \frac{1}{2}}(v) \end{vmatrix} = \frac{-2}{4\pi a_1} e^{-\frac{1}{2}(u+v)}, \quad (2.13)$$

$$-\frac{1}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} u\dot{W}_{1; \frac{1}{2}}(u) & v\dot{\mathfrak{M}}_{1; \frac{1}{2}}(v) \\ \dot{W}_{1; \frac{1}{2}}(u) & \dot{\mathfrak{M}}_{1; \frac{1}{2}}(v) \end{vmatrix} = -\frac{(2-u)(2-v)}{8\pi a_1} e^{-\frac{1}{2}(u+v)}, \quad (2.14)$$

$$-\frac{1}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} W_{1; \frac{1}{2}}(u) & \mathfrak{M}_{1; \frac{1}{2}}(v) \\ u\dot{W}_{1; \frac{1}{2}}(u) & v\dot{\mathfrak{M}}_{1; \frac{1}{2}}(v) \end{vmatrix} = \frac{uv}{8\pi a_1} e^{-\frac{1}{2}(u+v)}, \quad (2.15)$$

$$-\frac{1}{4\pi|\vec{r}_2 - \vec{r}_1|} \det \begin{vmatrix} \frac{\partial}{\partial z} W_{1-z; \frac{1}{2}}(u) & \frac{\partial}{\partial z} \mathfrak{M}_{1-z; \frac{1}{2}}(v) \\ \dot{W}_{1; \frac{1}{2}}(u) & \dot{\mathfrak{M}}_{1; \frac{1}{2}}(v) \end{vmatrix} \Big|_{z=0}$$

$$= - [2e^{-\frac{1}{2}(u+v)} / 4\pi a_1(u-v)] \{ (1 - \frac{1}{2}v)[1 - u \ln(u)] - (1 - \frac{1}{2}u)[v - e^v + 1 + vg(v)] \}, \quad (2.16)$$

$$- \frac{1}{4\pi |\vec{r}_2 - \vec{r}_1|} \det \left| \begin{array}{cc} W_{1; \frac{1}{2}}(u) & \mathfrak{M}_{1; \frac{1}{2}}(v) \\ \frac{\partial}{\partial z} W_{1-z; \frac{1}{2}}(u) & \frac{\partial}{\partial z} \mathfrak{M}_{1-z; \frac{1}{2}}(v) \end{array} \right| \Big|_{z=0}$$

$$= - [2e^{-\frac{1}{2}(u+v)} / 4\pi a_1(u-v)] \{ u(1 - \frac{1}{2}v)[1 + g(v)] + \frac{1}{2}ue^v - \frac{3}{2}u + \frac{3}{2}v + v(1 - \frac{1}{2}u) \ln(u) \}. \quad (2.17)$$

When the results (2.13) through (2.17) are combined with the proper factors, as required by Eq. (2.6), the closed form expression (1.6) of the reduced ground-state Coulomb Green's function emerges.

3. Projection of the S-Wave Component

The partial-wave components $G_l^1(r_2, r_1)$, $l=0, 1, 2, \dots$, of the reduced ground-state Green's function, may be defined by the equation

$$G^1(\vec{r}_2, \vec{r}_1) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\cos\theta) G_l^1(r_2, r_1), \quad (2.18)$$

where θ is the angle between the vectors \vec{r}_2 and \vec{r}_1 . On projecting out the S-wave component, we find

$$G_0^1(r_2, r_1) = 2\pi \int_{-1}^{+1} d(\cos\theta) G^1(\vec{r}_2, \vec{r}_1). \quad (2.19)$$

We now substitute from Eq. (1.6) into Eq. (2.19) and carry out the integration explicitly. This will provide us with a result for direct comparison with Hameka's work. It is convenient to introduce the new variables

$$x = \frac{1}{2}(u+v) = (r_2 + r_1)(a_1)^{-1}, \quad (2.20)$$

$$y = \frac{1}{2}(u-v) = |\vec{r}_2 - \vec{r}_1| (a_1)^{-1},$$

and to integrate on y instead of on $\cos\theta$. We have

$$G_0^1(r_2, r_1) = 2\pi \int_z^x y dy (a_1^2 / r_2 r_1) G^1(\vec{r}_2, \vec{r}_1), \quad (2.21)$$

$$z = |r_2 - r_1| (a_1)^{-1}.$$

Some of the integrations are elementary, and we obtain

$$G_0^1(r_2, r_1) = (a_1/2r_2r_1)(e^{-x} - e^{-z})$$

$$+ (a_1/2r_2r_1)(x^2 - z^2)(x - \frac{5}{2} + \gamma)e^{-x}$$

$$+ (a_1/2r_2r_1)e^{-x} \int_z^x d(y^2) [-g(x-y) + \ln(x+y)]. \quad (2.22)$$

The functions $g(x-y)$ and $\ln(x+y)$ can be eliminated from the integrand by integration by parts.

$$G_0^1(r_2, r_1) = (a_1/2r_2r_1)(e^{-x} - e^{-z})$$

$$+ (a_1/2r_2r_1)(x^2 - z^2)(x - \frac{5}{2} + \gamma)e^{-x}$$

$$+ (a_1/2r_2r_1)e^{-x} [x^2 \ln(2x)$$

$$+ z^2 g(x-z) - z^2 \ln(x+z)$$

$$- \int_0^{x-z} (d\xi/\xi)(\xi-x)^2 (e^\xi - 1)$$

$$- \int_{x+z}^{2x} (d\xi/\xi)(\xi-x)^2]. \quad (2.23)$$

To obtain Eq. (2.23) we have used the facts that $g(0)=0$, and $g'(v) = (e^v - 1)/v$. Also, the integration variables in the two integrals occurring in Eq. (2.23) have been changed from y to $\xi = x-y$ and $\xi = x+y$, respectively. These two integrals are elementary, except for a term

$$-x^2 \int_0^{x-z} (d\xi/\xi)(e^\xi - 1) = -x^2 g(x-z).$$

The final result of integrating and combining similar terms is

$$G_0^1(r_2, r_1) = (2/a_1)e^{-x} [-f(x-z)$$

$$+ \ln(x+z) - (x+z)^{-1} + x - \frac{5}{2} + \gamma], \quad (2.24)$$

$$f(v) = \int_0^v (d\xi/\xi^2)(e^\xi - 1 - \xi).$$

This is seen to agree with Eqs. (97) of the erratum to Hameka's article. [In order to convert to Hameka's notation, it will be necessary to use the relations $x+z = 2r_>(a_1)^{-1}$ and $x-z = 2r_<(a_1)^{-1}$.]

APPENDIX

The derivation of Eq. (2.11) will be outlined here briefly. We begin with the formulas¹¹

$$W_{1-z; \frac{1}{2}}(u) = [\Gamma(-1+z)]^{-1} [\mathfrak{M}_{1-z; \frac{1}{2}}(u) \ln(u) + H_{1-z; \frac{1}{2}}(u)], \quad (A1)$$

$$H_{1-z; \frac{1}{2}}(u) = \frac{ue^{-\frac{1}{2}u}}{\Gamma(z)} \left(\sum_{\lambda=0}^{\infty} \frac{\Gamma(z+\lambda)}{(1+\lambda)!} [\psi(z+\lambda) - \psi(1+\lambda) - \psi(2+\lambda)] \frac{u^\lambda}{\lambda!} + \Gamma(-1+z)u^{-1} \right). \tag{A2}$$

The function ψ is the logarithmic derivative of the gamma function,

$$\psi(z) = (\partial/\partial z) \ln \Gamma(z). \tag{A3}$$

Inside the parentheses in Eq. (A2) are two factors $\Gamma(z)$ (occurring in the sum for $\lambda=0$) and $\Gamma(-1+z)$ which are singular at $z=0$. These are canceled by the factors $[\Gamma(z)]^{-1}$ in front of the parentheses in Eq. (A2) and $[\Gamma(-1+z)]^{-1}$ in front of the bracket in Eq. (A1). For this reason it is convenient to write these terms separately. Also, it was found helpful to exhibit the zeros of the factors $[\Gamma(z)]^{-1}$ and $[\Gamma(-1+z)]^{-1}$ by rewriting them in the form $z[\Gamma(1+z)]^{-1}$ and $z(-1+z)[\Gamma(1+z)]^{-1}$, respectively.⁶ In this way the following formula was obtained:

$$\begin{aligned} \frac{\partial}{\partial z} \left(\frac{H_{1-z; \frac{1}{2}}(u)}{\Gamma(-1+z)} \right) &= -\frac{\Gamma'(1+z)}{[\Gamma(1+z)]^2} ue^{-\frac{1}{2}u} \{(-1+z)z\psi(z) + z(1-z)[\psi(1) + \psi(2)] + z/u\} \\ &\quad + [ue^{-\frac{1}{2}u}/\Gamma(1+z)] \{z\psi(z) + (-1+z)(d/dz)[z\psi(z)] + (1-2z)[\psi(1) + \psi(2)] + 1/u\} \\ &\quad + \frac{\partial}{\partial z} \left\{ \frac{z^2(-1+z)ue^{-\frac{1}{2}u}}{[\Gamma(1+z)]^2} \sum_{\lambda=1}^{\infty} \frac{\Gamma(\lambda+z)}{(1+\lambda)!} [\psi(z+\lambda) - \psi(1+\lambda) - \psi(2+\lambda)] \frac{u^\lambda}{\lambda!} \right\}. \end{aligned} \tag{A4}$$

The last term here, involving the sum over λ , clearly vanishes at $z=0$ because it is the derivative of z^2 times a function analytic at $z=0$. It remains to substitute $z=0$ in the other terms. For this purpose the relation $\Gamma'(1) = -\gamma$ is required.⁷ Also, the values of the functions $z\psi(z)$ and $(\partial/\partial z)[z\psi(z)]$ at $z=0$ are required. These can be derived from the identity,¹²

$$\psi(1-z) - \psi(z) = \pi \operatorname{ctn}(\pi z). \tag{A5}$$

Multiplying (A5) through by z and taking the limit as z approaches zero, we find $[z\psi(z)]|_{z=0} = -1$. If we multiply through by z , differentiate first, and then take the limit as z approaches zero, we find $(\partial/\partial z)[z \times \psi(z)]|_{z=0} = -\gamma$. The result of evaluating (A4) at $z=0$ can then be simplified by using the relation $\psi(2) = 1 - \gamma$, which follows from differentiating both sides of the equation $\Gamma(2+z) = (1+z)\Gamma(1+z)$. This result is simply

$$\frac{\partial}{\partial z} \left[\frac{H_{1-z; \frac{1}{2}}(u)}{\Gamma(-1+z)} \right] \Big|_{z=0} = e^{-\frac{1}{2}u}. \tag{A6}$$

To complete the derivation of Eq. (2.11) we must add to the expression (A6) the derivative with respect to z evaluated at $z=0$ of the first term,

$$\ln(u) \mathfrak{M}_{1-z; \frac{1}{2}}(u)/\Gamma(-1+z) = z(-1+z) \ln(u) \mathfrak{M}_{1-z; \frac{1}{2}}(u)/\Gamma(1+z),$$

in Eq. (A1). Owing to the zero of the factor z here, the derivative of the expression in parentheses does not contribute. Thus

$$\frac{\partial}{\partial z} \left[\frac{\mathfrak{M}_{1-z; \frac{1}{2}}(u)}{\Gamma(-1+z)} \ln(u) \right] \Big|_{z=0} = -\mathfrak{M}_{1; \frac{1}{2}}(u) \ln(u).$$

Using Eq. (2.9) this becomes

$$\frac{\partial}{\partial z} \left[\frac{\mathfrak{M}_{1-z; \frac{1}{2}}(u)}{\Gamma(-1+z)} \right] \Big|_{z=0} = -ue^{-\frac{1}{2}u} \ln(u). \tag{A7}$$

Equation (2.11) now follows when Eqs. (A6) and (A7) are added.

¹Quantization in a large sphere would be required to give the sum in Eq. (1.1) a meaning for the continuum states.

²H. F. Hameka, *J. Chem. Phys.* **47**, 2728 (1967); and erratum in *J. Chem. Phys.* **48**, 4810 (1968).

³See Eq. (2.3) of this article.

⁴L. Hostler, *J. Math. Phys.* **5**, 591 (1964).

⁵Herbert Buchholz, *Die Konfluente Hypergeometrische Funktion* (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1953).

⁶Here the formula $z\Gamma(z) = \Gamma(1+z)$ is required. See Whittaker and Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England,

1927), 4th ed., p. 237.

⁷Ref. 6, p. 236.

⁸Ref. 5, Eqs. (1a) and (2), p. 208.

⁹Ref. 5, Eq. (7), p. 12.

¹⁰However, Hameka expresses his result in terms of the function $f(v)$ defined in Sec. II, Sub. 3, Eq. (2.24), instead of the function $g(v)$. As one can show by integrating by parts, these two functions are related as follows:

$$v^{-1}(e^v - 1) + f(v) = 1 + g(v).$$

¹¹Ref. 5, Eq. (25a), p. 22, and Eq. (24a), p. 21.

¹²Ref. 6, p. 240.

Spin Orientation of Photoelectrons Ejected by Circularly Polarized Light*

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Photoelectrons emitted by Cs vapor exposed to circularly polarized light with $2750 \lesssim \lambda \lesssim 3150$ Å should have spin orientation $\gtrsim 85\%$ parallel to the light's angular momentum. Measurements of this orientation along the spectrum may be represented by a parameter x defined theoretically in terms of a Hilbert transform of the spectrum of unperturbed dipole matrix elements weighted by the effect of spin-orbit interaction. The theory of this parameter is adapted from Fermi's interpretation of doublet intensity ratios and from Seaton's related interpretation of photoabsorption minima. Semiquantitative estimates are drawn from experimental data on photoabsorption.

I. INTRODUCTION

Considerable efforts have been devoted recently to the production of spin-oriented electrons by collision with atoms and molecules,¹ utilizing the spin-orbit interaction, and by photoeffect on spin-oriented atoms.² The experimental study of these processes can provide information on the dynamics of electrons in atomic systems. The possibility of providing intense sources of spin-oriented electrons for high-energy accelerators has lent particular interest to these efforts.

This paper points out that, owing to a combination of known circumstances, irradiation of Cs vapor by a broad spectral band of circularly polarized light must yield photoelectrons with nearly complete spin orientation. This spectral band extends from the proximity of the photoelectric threshold (say, from ~ 3150) to ~ 2750 Å. The effect results from the influence of the (weak) spin-orbit coupling on the light absorption in the continuum adjoining the principal series, an influence that has been studied long ago by Fermi³ for the

discrete spectrum and by Seaton⁴ for the continuum. Operationally, the phenomenon considered here differs from that observed in Ref. 2 through replacement of the preorientation of target atoms by the prepolarization of the incident light beam; light polarization can be efficient in the range of quartz optics. This phenomenon should occur in all alkali vapors and perhaps in other materials; Cs merely seems to afford the most convenient opportunity for observations.

A criterion for selecting circumstances that favor the production of spin-oriented electrons has been emphasized by Kessler.⁵ Orientation by elastic scattering occurs when the scattering amplitude approaches zero. The approach to zero magnifies the relative difference between the amplitudes for alternative mutual orientations of spin and orbit, a difference that otherwise tends to escape attention. Indeed, these two scattering amplitudes have *small values of opposite sign* over a limited range of scattering angles near their points of zero, thus enabling their interference to *suppress* one of the spin orientations in the labor-