Nonrelativistic Coulomb Green's function in parabolic coordinates

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The nonrelativistic Coulomb Green's function $G^{(+)}(\mathbf{r}_1,\mathbf{r}_2,k)$ is evaluated by explicit summation over discrete and continuum eigenstates in parabolic coordinates. This completes the derivation of Meixner, who was able to obtain only the $\mathbf{r}_1 = 0$ and $\mathbf{r}_2 \rightarrow \infty$ limiting forms of the Green's function. Further progress is made possible by an integral representation for a product of two Whittaker functions given by Buchholz. We obtain the closed form for the Coulomb Green's function previously derived by Hostler, via an analogous summation in spherical polar coordinates. The Rutherford scattering limit of the Green's function is also demonstrated, starting with an integral representation in parabolic coordinates.

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1. INTRODUCTION

The nonrelativistic Coulomb Green's function $G(\mathbf{r}_1,\mathbf{r}_2,k)$ $[G(1,2,k)$ for short] is the solution under specified boundary conditions of the equation

$$(k^2 + \nabla_1^2 + 2Z/r_1)G(\mathbf{r}_1,\mathbf{r}_2,k) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{1.1}$$

Atomic units: $\hbar = m = e = 1$, are employed for convenience. Any Green's function can, in principle, be constructed from its spectral representation

$$G(1,2,k) = \sum_n \frac{\psi_n(1)\psi_n^*(2)}{k^2 - \epsilon_n}, \tag{1.2}$$

the summation running over the complete set of discrete and continuum eigenstates. Meixner[1] in 1933 attempted to evaluate the Coulomb Green's function by explicit summation over eigenfunctions in parabolic coordinates. He was able, however, to obtain closed forms only in the special cases $\mathbf{r}_1 = 0$ and $\mathbf{r}_2 \rightarrow \infty$. Hostler[2] first worked out the general closed-form expression for $G(1,2,k)$ by summing over Coulomb eigenfunctions in spherical polar coordinates. A key element in Hostler's derivation was an integral representation for a product of two Whittaker functions given by Buchholz.[3]

We shall demonstrate in this paper that Hostler's result can also be derived by working in parabolic coordinates. We will thus explicitly complete the work of Meixner. In addition, we shall obtain in straightforward fashion the Rutherford scattering limit of the Green's function and also a possible starting point for a compact treatment of the Stark effect.

2. COULOMB EIGENFUNCTIONS IN PARABOLIC COORDINATES

Parabolic coordinates (ξ,η,ϕ) can be defined in terms of spherical polar coordinates (r,θ,ϕ) and Cartesian coordinates (x,y,z) by the relations

$$\xi = r(1+\cos\theta) = r + z,$$
$$\eta = r(1-\cos\theta) = r - z,$$
$$\phi = \phi = \tan^{-1}(y/x). \tag{2.1}$$

Conversely

$$x = (\xi\eta)^{1/2}\cos\phi, \quad y = (\xi\eta)^{1/2}\sin\phi,$$
$$z = \tfrac{1}{2}(\xi - \eta), \quad r = \tfrac{1}{2}(\xi + \eta). \tag{2.2}$$

The volume element is given by

$$d^3\mathbf{r} = \tfrac{1}{4}(\xi + \eta)\, d\xi\, d\eta\, d\phi \quad (0 \leqslant \xi,\eta \leqslant \infty, 0 \leqslant \phi \leqslant 2\pi), \tag{2.3}$$

and the Laplacian operator by

$$\nabla^2 = \frac{4}{\xi+\eta}\left(\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}\eta\frac{\partial}{\partial\eta}\right) + \frac{1}{\xi\eta}\frac{\partial^2}{\partial\phi^2}. \tag{2.4}$$

The Coulomb Schrödinger equation

$$(\epsilon + \nabla^2 + 2Z/r)\psi = 0, \quad \epsilon = 2E = k^2 \tag{2.5}$$

is separable in parabolic coordinates as well as spherical polar coordinates. The factorization

$$\psi(\xi,\eta,\phi) = f_1(\xi)f_2(\eta)e^{im\phi}, \quad m = 0, \pm 1, \pm 2, \cdots, \tag{2.6}$$

leads to the ordinary differential equations[4]

$$\frac{d}{d\xi}\left(\xi\frac{df_1}{d\xi}\right) + \left(Z_1 + \frac{k^2\xi}{4} - \frac{m^2}{4\xi}\right)f_1(\xi) = 0,$$
$$\frac{d}{d\eta}\left(\eta\frac{df_2}{d\eta}\right) + \left(Z_2 + \frac{k^2\eta}{4} - \frac{m^2}{4\eta}\right)f_2(\eta) = 0, \tag{2.7}$$

where

$$Z_1 + Z_2 = Z. \tag{2.8}$$

Either Z_1 or Z_2 labels the one-parameter family of degenerate eigenstates for each value of $\epsilon = k^2$.

The subtitutions

$$f(x) = x^{-1/2}M(-ikx),$$
$$x = \xi,\eta, \quad z \equiv -ikx, \quad \nu_{1,2} \equiv Z_{1,2}/k, \tag{2.9}$$

bring (2.7) into the form of Whittaker's differential equation

$$M''(z) + \left(-\frac{1}{4} + \frac{i\nu}{z} + \frac{1-m^2}{4z^2}\right)M(z) = 0. \tag{2.10}$$

The solutions to (2.10) regular at $x = 0$ are the Whittaker functions $M^{m/2}_{\pm i\nu}(\mp ikx)$.[5] For $m \geqslant 0$

$$M^{m/2}_{\pm i\nu}(\mp ikx) = (m!)^{-1}(\mp ikx)^{(m+1)/2}e^{\mp ikx/2} \times {}_1F_1((m+1)/2 \pm i\nu; m+1; \pm ikx), \tag{2.11}$$

where ${}_1F_1$ is a confluent hypergeometric function. For $m < 0$, the corresponding Whittaker functions are given through the identity

$$\Gamma((1-m)/2-i\nu)\, M_{i\nu}^{-m/2}(-ikx) = \Gamma((1+m)/2-i\nu)\, M_{i\nu}^{m/2}(-ikx). \quad (2.12)$$

The functions (2.11) with alternative choice of signs are related by

$$M_{-i\nu}^{m/2}(ikx) = e^{i\pi(m+1)/2}\, M_{i\nu}^{m/2}(-ikx), \quad (2.13)$$

which shows incidentally that $e^{i\pi(m+1)/4}M_{i\nu}^{m/2}(-ikx)$ is a real function.

The asymptotic form for M as $x\rightarrow\infty$ is given by[6]:

$$M_{i\nu}^{m/2}(-ikx) \sim e^{-\pi\nu/2}\left[\frac{(kx)^{-i\nu}e^{-ikx/2}}{\Gamma((m+1)/2-i\nu)} + e^{-i\pi(m+1)/2}\frac{(kx)^{i\nu}e^{ikx/2}}{\Gamma((m+1)/2+i\nu)}\right]. \quad (2.14)$$

For positive energy, the wavenumber k is real; to avoid divergences in the wavefunctions (2.9) we must require that

$$|\mathrm{Im}\,\nu| \leqslant \tfrac{1}{2}. \quad (2.15)$$

Positive-energy eigenstates can be specified by the two continuous quantum numbers

$$\nu_1 \equiv Z_1/k \quad \text{and} \quad \nu_2 \equiv Z_2/k. \quad (2.16)$$

Thus, Eq. (2.8) implies

$$k = Z/(\nu_1+\nu_2). \quad (2.17)$$

It is sufficient to assume $k \geqslant 0$ and to choose real values for ν_1 and ν_2. Then both ν_1 and ν_2 can run over the range $(-\infty, +\infty)$ but, by virtue of (2.17), their sum must be nonnegative:

$$\nu_1+\nu_2 \geqslant 0. \quad (2.18)$$

For compactness, we shall continue to write k in the arguments of Whittaker functions, understanding k to be a function of ν_1 and ν_2 via (2.17).

The foregoing considerations lead to the following positive-energy Coulomb eigenfunctions in parabolic coordinates:

$$\psi_{\nu_1\nu_2 m}(\xi,\eta,\phi) = e^{i\pi(m+1)/2}(2\pi)^{-3/2}Z^{-1/2}k e^{\pi(\nu_1+\nu_2)/2} \times |\Gamma((m+1)/2-i\nu_1)|\,|\Gamma((m+1)/2-i\nu_2)|(\xi\eta)^{-1/2} \times M_{i\nu_1}^{m/2}(-ik\xi)\, M_{i\nu_2}^{m/2}(-ik\eta)e^{im\phi}. \quad (2.19)$$

The phase factor $e^{i\pi(m+1)/2}$ is retained for later convenience. These continuum eigenfunctions are orthonormalized according to

$$\int_0^\infty\int_0^\infty\int_0^{2\pi} \psi^*_{\nu_1\nu_2 m}(\xi,\eta,\phi)\psi_{\nu_1'\nu_2' m'}(\xi,\eta,\phi)\tfrac{1}{4}(\xi+\eta)\, d\xi\, d\eta\, d\phi = \delta(\nu_1-\nu_1')\,\delta(\nu_2-\nu_2')\delta_{mm'}. \quad (2.20)$$

Meixner[1] and other authors employed eigenfunctions normalized to $\delta(k-k')\delta(\zeta-\zeta')$, in which ζ corresponds to our variable $(\nu_1-\nu_2)/2$. The more symmetrical normalization scheme we have introduced will facilitate evaluation of the Green's function.

Equation (2.20) can be demonstrated with the help of the following integrals over Whittaker functions:

$$\int_0^\infty M_{i\nu}^{m/2}(-ikx)M_{i\nu}^{m/2}(-ik'x)\, dx = 4\pi e^{-i\pi(m+1)/2}e^{-\pi\nu}\delta(k-k')\Big/\left|\Gamma\left(\frac{m+1}{2}-i\nu\right)\right|^2 \quad (2.21)$$

and

$$\int_0^\infty M_{i\nu}^{m/2}(-ikx)M_{i\nu'}^{m/2}(-ikx)x^{-1}\, dx = 4\pi e^{-i\pi(m+1)/2}e^{-\pi\nu}\delta(\nu-\nu')\Big/\left|\Gamma\left(\frac{m+1}{2}-i\nu\right)\right|^2. \quad (2.22)$$

Equation (2.21) also occurs in the normalization of spherical eigenfunctions. Both (2.21) and (2.22) can be demonstrated from integral representations of Whittaker functions in terms of Bessel functions[7] with use of an integral given by Watson.[8] More simply, by virtue of the fact that the principal contributions to (2.21) and (2.22) come from the asymptotic region $x\rightarrow\infty$, it suffices to approximate the Whittaker functions by their asymptotic forms (2.14). Using (2.16),

$$\delta(\nu_1-\nu_1')\delta(k-k') = (Z_2/k^2)\delta(\nu_1-\nu_1')\delta(\nu_2-\nu_2'),$$
$$\delta(\nu_2-\nu_2')\delta(k-k') = (Z_1/k^2)\delta(\nu_1-\nu_1')\delta(\nu_2-\nu_2'), \quad (2.23)$$

which completes the required normalization.

The negative-energy parabolic eigenfunctions are quite standard.[9] Expressed in terms of Whittaker functions[10]:

$$\psi_{n_1n_2m}(\xi,\eta,\phi) = \frac{Z^{1/2}}{\pi^{1/2}n}\left[\frac{(|m|+n_1)!(|m|+n_2)!}{n_1!n_2!}\right]^{1/2}(\xi\eta)^{-1/2} \times M_{n_1+(|m|+1)/2}^{|m|/2}(Z\xi/n)M_{n_2+(|m|+1)/2}^{|m|/2}(Z\eta/n)e^{im\phi}, \quad (2.24)$$

$$n_1,n_2 = 0,1,2,\cdots;\quad m = 0,\pm 1,\pm 2,\cdots;$$

$$n = n_1+n_2+|m|+1 = 1,2,3,\cdots.$$

We shall also require Whittaker functions of the second kind, $W_{i\nu}^{m/2}(-ikx)$, which represent solutions to (2.10) having the form of outgoing waves. Specifically we note the transformation[11]

$$M_{i\nu}^{m/2}(-ikx) = e^{-\pi\nu}\left[\frac{W_{-i\nu}^{m/2}(ikx)}{\Gamma((m+1)/2-i\nu)} + e^{-i(m+1)\pi/2}\frac{W_{i\nu}^{m/2}(-ikx)}{\Gamma((m+1)/2+i\nu)}\right], \quad (2.25)$$

the identity[12]

$$W_{i\nu}^{-m/2}(-ikx) = W_{i\nu}^{m/2}(ikx), \quad (2.26)$$

and the asymptotic form as $x\rightarrow\infty$ [13]

$$W_{i\nu}^{m/2}(-ikx) \sim (-ikx)^{i\nu}e^{ikx/2}. \quad (2.27)$$

Note that Eq. (2.14) also follows from (2.25) with (2.27).

For values of ν occurring in the discrete spectrum [cf. (2.24)] the two types of Whittaker functions become proportional.[14] Specifically

$$W_{n'+(m+1)/2}^{m/2}(z) = (-)^{n'}(n'+m)!M_{n'+(m+1)/2}^{m/2}(z). \quad (2.28)$$

A key result, both in Hostler's derivation and in the present work, is an integral representation for a product of two Whittaker functions given by Buchholz.[3] With appropriate specialization of the variables, we write

$$\Gamma((m+1)/2-i\nu)M_{i\nu}^{m/2}(-iky)W_{i\nu}^{m/2}(-ikx)$$
$$=(-i)^{m+1}k(xy)^{1/2}\int_0^\infty ds\exp\Big[+\frac{i}{2}k(x+y)\cosh s\Big]$$
$$\times J_m\big(k\sqrt{xy}\sinh s\big)[\coth(s/2)]^{2i\nu},$$
$$\mathrm{Re}((m+1)/2-i\nu)>0,\quad \mathrm{Im}k>0,\quad x>y. \tag{2.29}$$

3. EVALUATION OF THE GREEN'S FUNCTION

The summation (1.2) explicitly written out in terms of discrete and continuum parabolic quantum numbers becomes

$$G(1,2,k)=\sum_{m=-\infty}^{\infty}\Big[\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\Big(k^2+\frac{Z^2}{n^2}\Big)^{-1}\psi_{n_1n_2m}(1)$$
$$\times\psi^*_{n_1n_2m}(2)+\int_{-\infty}^{\infty}d\nu_1\int_{-\infty}^{\infty}d\nu_2\,\theta(\nu_1+\nu_2)$$
$$\times(k^2-\kappa^2)^{-1}\psi_{\nu_1\nu_2m}(1)\psi^*_{\nu_1\nu_2m}(2)\Big]. \tag{3.1}$$

The Heaviside function

$$\theta(x)\equiv\begin{cases}1, & \text{for } x\geqslant 0,\\ 0, & \text{for } x<0.\end{cases} \tag{3.2}$$

has been introduced to take account of the condition (2.18). The wavenumber in the eigenfunctions has been redesignated κ, to reserve k for the Green's function. Putting in the eigenfunctions (2.19) and (2.24), we obtain

$$G(1,2,k)=\sum_{m=-\infty}^{\infty}\frac{e^{im(\phi_1-\phi_2)}}{(\xi_1\xi_2\eta_1\eta_2)^{1/2}}$$
$$\times\Big\{\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\Big(k^2+\frac{Z^2}{n^2}\Big)^{-1}\frac{Z}{\pi n^2}\frac{(|m|+n_1)!(|m|+n_2)!}{n_1!n_2!}$$
$$\times M^{|m|/2}_{n_1+(|m|+1)/2}(Z\xi_1/n)M^{|m|/2}_{n_1+(|m|+1)/2}(Z\xi_2/n)$$
$$\times M^{|m|/2}_{n_2+(|m|+1)/2}(Z\eta_1/n)M^{|m|/2}_{n_2+(|m|+1)/2}(Z\eta_2/n)$$
$$+e^{i\pi(m+1)}\frac{Z}{8\pi^3k^2}\int_{-\infty}^{\infty}d\nu_1\int_{-\infty}^{\infty}d\nu_2\theta(\nu_1+\nu_2)$$
$$\times[(\nu_1+\nu_2)^2-Z^2/k^2]^{-1}e^{\pi(\nu_1+\nu_2)}$$
$$\times\Big|\Gamma\Big(\frac{m+1}{2}-i\nu_1\Big)\Big|^2\Big|\Gamma\Big(\frac{m+1}{2}-i\nu_2\Big)\Big|^2$$
$$\times M^{m/2}_{i\nu_1}(-i\kappa\xi_1)M^{m/2}_{i\nu_1}(-i\kappa\xi_2)$$
$$\times M^{m/2}_{i\nu_2}(-i\kappa\eta_1)M^{m/2}_{i\nu_2}(-i\kappa\eta_2)\Big\}. \tag{3.3}$$

The M function of the argument $\xi_>$ (the greater of ξ_1,ξ_2) can be transformed to a sum of W functions using (2.25). We find

$$e^{i\pi(m+1)/2}e^{\pi\nu_1}\Big|\Gamma\Big(\frac{m+1}{2}-i\nu_1\Big)\Big|^2$$
$$\times M^{m/2}_{i\nu_1}(-i\kappa\xi_1)M^{m/2}_{i\nu_1}(-i\kappa\xi_2)$$
$$=\Gamma\Big(\frac{m+1}{2}+i\nu_1\Big)M^{m/2}_{-i\nu_1}(i\kappa\xi_<)W^{m/2}_{-i\nu_1}(i\kappa\xi_>)$$
$$+\Gamma\Big(\frac{m+1}{2}-i\nu_1\Big)M^{m/2}_{i\nu_1}(-i\kappa\xi_<)W^{m/2}_{i\nu_1}(-i\kappa\xi_>). \tag{3.4}$$

We have made use of (2.13) to get $M^{m/2}_{-i\nu_1}$ to multiply $W^{m/2}_{-i\nu_1}$. Now the first term ΓMW in (3.4) can be transformed into the second by the substitutions

$$\nu_1\to-\nu_1,\quad \nu_2\to-\nu_2. \tag{3.5}$$

By applying this in the continuum integral and noting the identity

$$\theta(\nu_1+\nu_2)+\theta(-\nu_1-\nu_2)=1, \tag{3.6}$$

the Heaviside function is eliminated.

The functions of η_1 and η_2 are transformed in an analogous way. Under the double integration, the two terms ΓMW make equal contributions. The continuum part of the Green's function thus reduces to the compact form

$$\frac{Z}{4\pi^3k^2}\int_{-\infty}^{\infty}d\nu_1\int_{-\infty}^{\infty}d\nu_2\,[(\nu_1+\nu_2)^2-Z^2/k^2]^{-1}$$
$$\times\Gamma\Big(\frac{m+1}{2}-i\nu_1\Big)M^{m/2}_{i\nu_1}(-i\kappa\xi_<)W^{m/2}_{i\nu_1}(-i\kappa\xi_>)$$
$$\times\Gamma\Big(\frac{m+1}{2}-i\nu_2\Big)M^{m/2}_{i\nu_2}(-i\kappa\eta_<)W^{m/2}_{i\nu_2}(-i\kappa\eta_>). \tag{3.7}$$

The integrals in (3.7) can be most readily evaluated by interpreting them as contour integrals in the complex planes of ν_1 and ν_2. The integrand is an analytic function of each variable in its lower half-plane with the exception of a set of simple poles. One should verify this, in particular, for $\nu_2=0$ and $\nu_1\to0$ with $\mathrm{Im}\nu_1<0$. This corresponds to $\kappa=Z/\nu_1\to\infty$ with $\mathrm{Im}\kappa>0$. From (2.23) and (2.27) we find the relevant asymptotic dependence

$$\Gamma((m+1)/2-i\nu)M^{m/2}_{i\nu}(-i\kappa x_<)W^{m/2}_{i\nu}(-i\kappa x_>)$$
$$\sim e^{i\kappa(x_>-x_<)/2}, \tag{3.8}$$

which approaches zero as $|\kappa|\to\infty$ with $\mathrm{Im}\kappa>0$. By virtue of (2.12) and (2.26), m in the functions ΓMW can be replaced by $|m|$. This will make more explicit the poles of the integrand.

We note also the asymptotic behavior as $\nu_1\to\infty$ with ν_2 fixed. As $k\to0$[15]

$$\Gamma((m+1)/2-i\nu)M^{m/2}_{i\nu}(-iky)W^{m/2}_{i\nu}(-ikx)\sim k. \tag{3.9}$$

Thus each factor $\Gamma MW\sim\nu_1^{-1}$. Including the energy denominator ($\sim\nu_1^{-2}$), the entire integrand behaves as ν_1^{-4} when $|\nu_1|\to\infty$.

Evidently, the ν_1 integral can be evaluated by application of the residue theorem after the contour is closed from below with a semicircle at infinity. As $|\nu_1|\to\infty$, the contribution from the semicircle approaches zero as a result of the asymptotic behavior discussed above. The singular points in the integrand arise from the factors $\Gamma((|m|+1)/2-i\nu_1)$ and $[(\nu_1+\nu_2)^2-Z^2/k^2]^{-1}$. The gamma function has poles at the points

$$\nu_1=-i((|m|+1)/2+n_1),\quad n_1=0,1,2,\cdots, \tag{3.10}$$

with the corresponding residues $i(-)^{n_1}/n_1!$. The energy denominator has a pole in the lower half-plane at $\kappa = k + i\delta$ or

$$\nu_1 = -\nu_2 + Z/k - i\delta', \tag{3.11}$$

with residue $k/2Z$. $\mathrm{Im}k > 0$ is taken, such that the resulting Green's function will correspond to $G^{(+)}(1,2,k)$.

The ν_1 integral thereby reduces to $(-2\pi i)$ times the sum of the residues in the lower half-plane. The continuum integral (3.7) can thereby be expressed as a sum of two contributions: (3.12) plus (3.13). From the poles of the gamma function [cf. (3.10)]:

$$-2\pi i \frac{Z}{4\pi^3 k^2} \sum_{n_1=0}^{\infty} \frac{i(-)^{n_1}}{n_1!} \times \int_{-\infty}^{\infty} d\nu_2 \left[(\nu_1' + \nu_2)^2 - \frac{Z^2}{k^2}\right]^{-1} \times M_{i\nu_1'}^{|m|/2}(-i\kappa'\xi_<) W_{i\nu_1'}^{|m|/2}(-i\kappa'\xi_>) \Gamma\left(\frac{|m|+1}{2} - i\nu_2\right) \times M_{i\nu_2}^{|m|/2}(-i\kappa'\eta_<) W_{i\nu_2}^{|m|/2}(-i\kappa'\eta_>), \tag{3.12}$$

$$\nu_1' \equiv -i\left(\frac{|m|+1}{2} + n_1\right), \quad \kappa' \equiv Z/(\nu_1' + \nu_2).$$

From the energy factor [cf. (3.11)]:

$$-2\pi i \frac{Z}{4\pi^3 k^2} \frac{k}{2Z} \int_{-\infty}^{\infty} d\nu_2 \Gamma\left(\frac{|m|+1}{2} - i\nu + i\nu_2\right) \times M_{i\nu - i\nu_2}^{|m|/2}(-ik\xi_<) W_{i\nu - i\nu_2}^{|m|/2}(-ik\xi_<) \times \Gamma\left(\frac{|m|+1}{2} - i\nu_2\right) M_{i\nu_2}^{|m|/2}(-ik\eta_<) \times W_{i\nu_2}^{|m|/2}(-ik\eta_>) \quad (\nu \equiv Z/k). \tag{3.13}$$

The second integration in (3.12) can be carried out in an exactly analogous way. The ν_2 contour, again closed by an infinite semicircle in the lower half-plane, encloses only the poles of $\Gamma((|m|+1)/2 - i\nu_2)$, at the points

$$\nu_2 = -i((|m|+1)/2 + n_2), \quad n_2 = 0,1,2,\cdots. \tag{3.14}$$

Thus, in Eq. (3.12),

$$\nu' = -i(n_1 + n_2 + |m| + 1) \equiv -in, \quad n = 1,2,3,\cdots,$$
$$\kappa' = Z/\nu' = iZ/n, \tag{3.15}$$

and (3.12) becomes

$$(-2\pi i)^2 \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \frac{i^2(-)^{n_1+n_2}}{n_1! n_2!} \frac{Z}{4\pi^3 k^2} \left(-n^2 - \frac{Z^2}{k^2}\right)^{-1} \times M_{n_1+(|m|+1)/2}^{|m|/2}(Z\xi_</n) W_{n_1+(|m|+1)/2}^{|m|/2}(Z\xi_>/n) \times M_{n_2+(|m|+1)/2}^{|m|/2}(Z\eta_</n) W_{n_2+(|m|+1)/2}^{|m|/2}(Z\eta_>/n). \tag{3.16}$$

Application of (2.28) shows now that (3.16) exactly cancels the sum over the discrete spectrum in (3.3). The Green's function is thus reduced to the contribution containing (3.13). Writing λ in place of ν_2 and reintroducing m in place of $|m|$:

$$G^{(+)}(1,2,k) = \frac{1}{4\pi^2 ik} \sum_{m=-\infty}^{\infty} \frac{e^{im(\phi_1 - \phi_2)}}{(\xi_<\xi_>\eta_<\eta_>)^{1/2}} \times \int_{-\infty}^{\infty} d\lambda \left[\Gamma\left(\frac{m+1}{2} - i\nu + i\lambda\right) M_{i\nu - i\lambda}^{m/2}(-ik\xi_<) W_{i\nu - i\lambda}^{m/2}(-ik\xi_>)\right] \times \left[\Gamma\left(\frac{m+1}{2} - i\lambda\right) M_{i\lambda}^{m/2}(-ik\eta_<) W_{i\lambda}^{m/2}(-ik\eta_>)\right]. \tag{3.17}$$

This can also be expressed in the form

$$G^{(+)}(1,2,k) = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} e^{im(\phi_1 - \phi_2)} \left(-\frac{1}{2\pi i}\right) \int_{-\infty}^{\infty} dZ_2\, g_m^{(+)}(\xi,\xi',Z - Z_2) g_m^{(+)}(\eta,\eta',Z_2), \tag{3.18}$$

in which

$$g_m^{(+)}(x,x',Z_{1,2}) = (ikx)^{-1/2}(ikx')^{-1/2} \Gamma\left(\frac{m+1}{2} - i\nu_{1,2}\right) M_{i\nu_{1,2}}^{m/2}(-ikx_<) W_{i\nu_{1,2}}^{m/2}(-ikx_>) \quad (Z_{1,2} = k\nu_{1,2}). \tag{3.19}$$

The convolution integral in (3.17) or (3.18) is standard for Green's functions of separable operators. In the present case, a contour can be closed by an infinite semicircle in the lower half-plane such as to enclose the poles of $\Gamma((m+1)/2 - i\lambda)$ but exclude those of $\Gamma((m+1)/2 - i\nu + i\lambda)$. Equation (3.19) represents the Green's function for the differential equation (2.7) obtained after separation of variables, viz.,

$$\left(Z_{1,2} + \frac{\partial}{\partial x} x \frac{\partial}{\partial x} + \frac{k^2 x}{4} - \frac{m^2}{4x}\right) g_m^{(+)}(x,x',Z_{1,2}) = \delta(x - x'). \tag{3.20}$$

Note that $Z_{1,2}$ rather than E now plays the role of eigenvalue. This formulation of the separated Schrödinger equation is convenient for treatment of the Stark effect.[16] Reduced Green's functions derived from (3.19) can provide an elegant alternative for computation of Stark-effect perturbation energies.

Returning now to Eq. (3.17), Buchholz's integral representation (2.29) can be applied to each factor ΓMW giving, after some rearrangement:

$$G^{(+)}(1,2,k) = \frac{ik}{4\pi^2} \int_{-\infty}^{\infty} d\lambda \int_0^{\infty} ds \int_0^{\infty} dt\, e^{-ik/2(\xi_1 + \xi_2)\cosh s} e^{-ik/2(\eta_1 + \eta_2)\cosh t} [\coth(s/2)]^{2i\nu - 2i\lambda} [\coth(t/2)]^{2i\lambda} \times \sum_{m=-\infty}^{\infty} e^{im(\phi_1 - \phi_2)} J_m(k(\xi_1\xi_2)^{1/2} \sinh s) J_m(-k(\eta_1\eta_2)^{1/2} \sinh t). \tag{3.21}$$

We have now been able to revert to the original parabolic coordinates $\xi_1,\eta_1,\xi_2,\eta_2$. In the sum over Bessel functions we have noted that $J_{-m}(z) = J_m(-z) = (-)^m J_m(z)$. The integral over λ gives a delta function:

$$\int_{-\infty}^{\infty} d\lambda\, [\coth(s/2)]^{-2i\lambda} [\coth(t/2)]^{2i\lambda}$$
$$= \pi\delta(\ln\coth(t/2) - \ln\coth(s/2))$$
$$= \pi \sinh s\, \delta(t-s). \qquad (3.22)$$

The integral over t is thus immediate. The sum is in the form of Graf's addition theorem[17]:

$$J_0(r) = \sum_{m=-\infty}^{\infty} J_m(p) J_m(q) e^{im\phi},$$
$$r = (p^2 + q^2 - 2pq\cos\phi)^{1/2}, \qquad (3.23)$$

where we identify

$$p = k(\xi_1\xi_2)^{1/2}\sinh s,$$
$$q = -k(\eta_1\eta_2)^{1/2}\sinh s, \quad \phi = \phi_1 - \phi_2,$$
$$r = k[\xi_1\xi_2 + \eta_1\eta_2 + 2(\xi_1\xi_2\eta_1\eta_2)^{1/2}\cos(\phi_1-\phi_2)]^{1/2}\sinh s. \qquad (3.24)$$

The Green's function thus reduces to

$$G^{(+)}(1,2,k) = \frac{ik}{4\pi}\int_0^\infty ds\,\sinh s\, e^{ikv\cosh s}$$
$$\times J_0(ku\sinh s)[\coth(s/2)]^{2iv}, \qquad (3.25)$$

where [cf. (2.1)]

$$v \equiv \tfrac{1}{2}(\xi_1 + \xi_2 + \eta_1 + \eta_2) = r_1 + r_2 = \tfrac{1}{2}(x+y),$$
$$u \equiv [\xi_1\xi_2 + \eta_1\eta_2 + 2(\xi_1\xi_2\eta_1\eta_2)^{1/2}\cos(\phi_1-\phi_2)]^{1/2}$$
$$= (2\mathbf{r}_1\cdot\mathbf{r}_2 + 2r_1r_2)^{1/2} = (xy)^{1/2}, \qquad (3.26)$$

in terms of the variables

$$x \equiv r_1 + r_2 + r_{12}, \quad y \equiv r_1 + r_2 - r_{12}. \qquad (3.27)$$

To complete the derivation, we make use of the identity

$$J_0(ku\sinh s) = \frac{1}{ku\sinh s}\frac{\partial}{\partial u} uJ_1(ku\sinh s), \qquad (3.28)$$

in conjunction with the integral representation (2.29) with $m = 1$. We obtain thereby

$$G^{(+)}(1,2,k) = \frac{1}{4\pi iku}\frac{\partial}{\partial u}\Gamma(1-iv)M^{1/2}_{iv}(-iky)$$
$$\times W^{1/2}_{iv}(-ikx). \qquad (3.29)$$

Noting, finally, that [cf. (3.26), (3.27)]

$$\frac{1}{u}\frac{\partial}{\partial u} = -\frac{2}{x-y}\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)$$
$$= -\frac{1}{r_{12}}\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right), \qquad (3.30)$$

we obtain Hostler's expression for the Coulomb Green's function [2]

$$G^{(+)}(1,2,k) = -\frac{1}{4\pi ikr_{12}}\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\Gamma(1-iv)$$
$$\times M^{1/2}_{iv}(-iky)W^{1/2}_{iv}(-ikx). \qquad (3.31)$$

The Green's function (3.31) applies to both attractive and repulsive Coulomb interactions. Most generally one can redefine

$$v \equiv -ZZ'/k, \qquad (3.32)$$

in which Z and Z' are the charges (in atomic units) of the interacting particles. For an electron interacting with a nucleus, the problem we have considered explicitly, $Z' = -1$.

4. RUTHERFORD SCATTERING LIMIT

The continuum eigenfunction (2.19) with quantum numbers $m = 0$, $\nu_1 = -i/2$, $\nu_2 = \nu + i/2$ ($\nu = -ZZ'/k$) represents scattering of an incident plane wave by a nucleus (Rutherford scattering). With use of (2.11) we obtain[18]:

$$\psi_R^{\rm RUTH}(\mathbf{r}) = e^{ik\xi/2}e^{-ik\eta/2}\,{}_1F_1(i\nu;1;ik\eta)$$
$$= e^{ikz}\,{}_1F_1(i\nu;1;ik\eta) \qquad (4.1)$$

normalized such that $\psi(0) = 1$. It is of interest to obtain this Rutherford scattering limit in an alternative way, by reduction of the Coulomb Green's function. $G^{(+)}(\mathbf{R},\mathbf{r},k)$ can be interpreted as the amplitude at point $\mathbf{r}$ for scattering of a spherical wave originating at $\mathbf{R}$ by the nucleus at $\mathbf{r} = 0$. As $\mathbf{R}$ is moved to infinity along the negative z axis, the spherical wave approaches modified plane-wave behavior in the vicinity of the origin. The Rutherford scattering wave function (4.1) can thereby be represented as a limiting form of the Green's function as follows:

$$\psi_k^{\rm RUTH}(\mathbf{r}) = \lim_{R\to\infty}\frac{G^{(+)}(\mathbf{R},\mathbf{r},k)}{G^{(+)}(\mathbf{R},0,k)}. \qquad (4.2)$$

The denominator $G^{(+)}(\mathbf{R},0,k)$ is obtained readily from (3.31) with $x = 2R$, $y = 0$. From the limiting forms of $M^{1/2}_{i\nu}(-iky)$ and its derivative[15] we obtain

$$G^{(+)}(\mathbf{R},0,k) = -\frac{1}{4\pi R}\Gamma(1-i\nu)W^{1/2}_{i\nu}(-2ikR). \qquad (4.3)$$

To evaluate the limiting form of $G^{(+)}(\mathbf{R},\mathbf{r},k)$ we make use of the integral formula (3.17) with the following specialization of the parabolic coordinates:

$$\xi_< = \xi_1 = r_1 + z_1 = R - R = \epsilon \to 0,$$
$$\eta_> = \eta_1 = r_1 - z_1 = 2R \to \infty,$$
$$\xi_> = \xi_2 = \xi, \quad \eta_< = \eta_2 = \eta. \qquad (4.4)$$

For the factor in (3.17) containing $\xi_< = \epsilon$[15]:

$$\lim_{\epsilon\to 0}\epsilon^{-1/2}M^{m/2}_{i\nu-i\nu_2}(-ik\epsilon) = (-ik)^{1/2}\delta_{m,0}, \qquad (4.5)$$

which eliminates all but the $m = 0$ term of the summation. With use of (4.3)–(4.5), the wavefunction (4.2) reduces to

$$\psi_k^{\rm RUTH}(\mathbf{r}) = \lim_{R\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda\,\frac{\Gamma(\tfrac{1}{2} - i\nu + i\lambda)\Gamma(\tfrac{1}{2} - i\lambda)}{\Gamma(1-i\nu)}$$
$$\times\frac{M^0_{i\lambda}(-ik\eta)}{(-ik\eta)^{1/2}}\frac{W^0_{i\nu-i\lambda}(-ik\xi)}{(-ik\xi)^{1/2}}$$
$$\times\left[(-2ikR)^{1/2}\frac{W^0_{i\lambda}(-2ikR)}{W^0_{i\nu}(-2ikR)}\right]. \qquad (4.6)$$

From the asymptotic form of the W functions [cf. (2.27)], the bracket in (4.6) can be reduced to

$$(-2ikR)^{1/2-i\nu+i\lambda}. \qquad (4.7)$$

Note that (4.7) approaches zero as $R \to \infty$ for $\text{Im}\lambda > 0$. Thus the integral (4.6) can be evaluated by closing a contour with a semicircle in the upper half of the complex λ plane. The integrand, specifically $\Gamma(\frac{1}{2} - i\nu + i\lambda)$, possesses poles in the upper half-plane at the points where

$$\tfrac{1}{2} - i\nu + i\lambda = -n, \quad n = 0,1,2,\cdots. \tag{4.8}$$

However, the limit of the factor (4.7) as $R \to \infty$ will approach zero unless $n = 0$. Thus (4.6) reduces to $2\pi i$ times the residue at $\lambda = \nu + i/2$ ($i\lambda = i\nu + \frac{1}{2}$), viz,

$$\psi_k^{\text{RUTH}}(\mathbf{r}) = \frac{M^0_{i\nu-1/2}(-ik\eta)}{(-ik\eta)^{1/2}} \frac{W^0_{1/2}(-ik\xi)}{(-ik\xi)^{1/2}}. \tag{4.9}$$

Now[19]

$$W^0_{1/2}(-ik\xi) = (-ik\xi)^{1/2} e^{ik\xi/2}, \tag{4.10}$$

while [cf. (2.11)]

$$M^0_{i\nu-1/2}(-ik\eta) = (-ik\eta)^{1/2} e^{-ik\eta/2}\,{}_1F_1(i\nu;1;ik\eta), \tag{4.11}$$

which results in the Rutherford eigenfunction (4.1).

The Rutherford scattering cross section follows from the asymptotic form (2.14):

$$\begin{aligned}\psi_k^{\text{RUTH}}(\mathbf{r}) &= e^{ik\xi/2} \frac{M^0_{i\nu-1/2}(-ik\eta)}{(-ik\eta)^{1/2}} \\ &\sim e^{-\pi\nu/2} e^{ik\xi/2} \left[\frac{(k\eta)^{-i\nu}}{\Gamma(1-i\nu)} e^{-ik\eta/2} - i \frac{(k\eta)^{i\nu-1}}{\Gamma(i\nu)} e^{ik\eta/2} \right] \\ &= \frac{e^{-\pi\nu/2}}{\Gamma(1-i\nu)} \left[e^{ikz - i\nu \log[k(r-z)]} - \frac{i}{k} \frac{\Gamma(1-i\nu)}{\Gamma(i\nu)} \frac{e^{ikr + i\nu\log[k(r-z)]}}{(r-z)} \right].\end{aligned} \tag{4.12}$$

This corresponds to a scattering amplitude

$$f(\theta) = \frac{-i\Gamma(1-i\nu)}{k\Gamma(i\nu)(1-\cos\theta)}, \tag{4.13}$$

which leads to the famous Rutherford formula

$$\sigma(\theta) = |f(\theta)|^2 = \frac{\nu^2}{k^2(1-\cos\theta)^2} = \frac{Z^2Z'^2e^4}{16E^2} \csc^4 \frac{\theta}{2}. \tag{4.14}$$

[1] J. Meixner, Math. Z. **36**, 677 (1933).
[2] L. Hostler, J. Math. Phys. **5**, 591 (1964).
[3] H. Buchholz, *The Confluent Hypergeometric Function* (Springer, New York, 1969), p. 86, Eq. (5c).
[4] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic, New York, 1957), p. 27.
[5] Ref. 3, pp. 11 *ff*. We follow throughout the notation of Buchholz except that we write, for compactness, $M_\kappa^{\mu/2}(z)$ in place of $\mathscr{M}_{\kappa,\mu/2}(z)$ and $W_\kappa^{\mu/2}(z)$ in place of $W_{\kappa,\mu/2}(z)$.
[6] Ref. 3, p. 91, Eq. (3).
[7] Ref. 3, p. 82, Eq. (1).
[8] G.N. Watson, *Theory of Bessel Functions*, 2nd. ed. (Cambridge U.P., Cambridge, 1966), p. 395, Eq. (1).
[9] Ref. 4, p. 29.
[10] Ref. 3, p. 214, Eq. (1a).
[11] Ref. 3, p. 19, Eq. (20a).
[12] Ref. 3, p. 19, Eq. (19).
[13] Ref. 3, p. 90, Eq. (1b).
[14] Ref. 3, p. 214, Eq. (1c).
[15] Ref. 3, p. 28.
[16] Ref. 4, p. 229 *ff*.
[17] Ref. 8, p. 359, Eq. (1).
[18] Ref. 4, p. 30.
[19] Ref. 3, p. 207.