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Generalized Sturmian expansions of Coulomb Green's functions and two-photon Gordon formula

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Abstract

A useful representation for the radial part of the Coulomb Green's function is derived in the form of a double series in Laguerre polynomials with *two free (arbitrary) parameters* α *and* α'. An appropriate choice of α and α' leads to a cardinal simplification in calculations of matrix elements involving Green's functions. The results are valid both in the nonrelativistic and in the relativistic case of the second-order Dirac equation. The momentum form of the nonrelativistic Green's function with free parameters is presented and a simple example of a two-photon extension of the well-known Gordon formula is given. © 1998 Published by Elsevier Science B.V.

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Compact expressions for the Coulomb Green's functions (CGF) for hydrogenic systems are useful tools for atomic calculations. A closed expression of the CGF in coordinate space, $G_E(\boldsymbol{r},\boldsymbol{r}')$, was derived first in 1963 [1], in terms of a product of regular and irregular Whittaker functions. The corresponding expression in momentum space and its expansion in terms of four-dimensional spherical harmonics was found by Schwinger [2]. For an analysis of photon–atom interactions in electric-dipole approximation, however, the partial wave expansion of the CGF is most preferable. It has, in the nonrelativistic limit, the form

$$G_E(\boldsymbol{r},\boldsymbol{r}') = \sum_{lm} g_l(E;r,r')Y_{lm}(\hat{\boldsymbol{r}})Y^*_{lm}(\hat{\boldsymbol{r}}'), \tag{1}$$

where $Y_{lm}(\hat{\boldsymbol{r}})$ is a spherical harmonic of unit vector $\hat{\boldsymbol{r}}$. Hostler [3] has given an integral representation for the radial components g_l symmetric in r, r', but the most useful form for multiphoton calculations is the so-called Sturmian expansion of g_l [4], which was generalized also to the relativistic case [5]. In this treatment we have

$$g_\gamma(E;r,r') = \nu \sum_{k=0}^{\infty} \frac{k!\, S_{k\gamma}(2r/\nu)\, S_{k\gamma}(2r'/\nu)}{\Gamma(k+2\gamma+2)(k+\gamma+1-\eta)}, \tag{2}$$

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where $\Gamma(a)$ denotes the Gamma function; $\nu = 1/\sqrt{-2E}$, $\eta = Z\nu$, and the Sturmian function is

$$S_{k\gamma}(2r/\nu) = \frac{2}{\nu}(2r/\nu)^{\gamma}\exp(-r/\nu)\,L_k^{2\gamma+1}(2r/\nu),$$

where L_n^{α} is a generalized Laguerre polynomial: $L_n^{\alpha}(z) \equiv \Gamma(n+\alpha+1)/(n!\,\Gamma(\alpha+1)) \times {}_1F_1[-n;\alpha+1;z]$. For $\gamma = l$ Eq. (2) is valid for the nonrelativistic Coulomb problem, but γ can as well be considered to be noninteger, as for instance for the Fues model potential (Coulomb potential with additional centrifugal potential $\sim r^{-2}$) [6] and also for the radial CGF associated to the second-order Dirac equation with an appropriately modified angular part [5]. Note, that in the latter case the parameters ν, η, γ are $\nu = \alpha/\sqrt{1-\epsilon^2}$, $\epsilon = E/mc^2$, $\alpha = e^2/\hbar c$, $\eta = \epsilon Z\nu$, $\gamma = \sqrt{(j+1/2)^2 - (\alpha Z)^2} + (s-1)/2$, $s = \pm 1$ for $j = l \mp \frac{1}{2}$, j and l are total and orbital momenta of the electron. Sturmian expansions of the radial CGF have been widely used for both nonrelativistic and relativistic analytical calculations. The interested reader is referred, for instance, to the review in Ref. [6] and to recent articles [7]. The use of the CGF is especially convenient in the calculation of multiphoton processes in the perturbative regime and for the analysis of quantum electrodynamical effects in the interaction of hydrogen-like ions with electromagnetic fields. The great interest in hydrogen as a model system is based on the fact that QED matrix elements can be expressed in closed form simplifying quantitative evaluations and permitting analytical estimations of limiting cases. As is well known, real atomic potentials deviate from the idealized point-like Coulomb one. However, for hydrogen-like systems radiative corrections to the central potential or effects of nuclear size can be safely neglected at least for small Z for this class of electromagnetic transitions. Calculations of this type can serve as a reference even in comparison with direct numerical treatments of more complicated, not Coulomb-like systems in order to determine the degree of deviation.

The purpose of this Letter is to derive an expansion $g_\gamma(E;r,r')$,

$$g_\gamma(E;r,r') = \sum_{n,n'=0}^{\infty} g^{\gamma}_{n,n'}(\nu;\alpha,\alpha')\,S_{n\gamma}\left(\frac{2r}{\alpha}\right)S_{n'\gamma}\left(\frac{2r'}{\alpha'}\right), \tag{3}$$

in terms of generalized Sturmian functions with arguments involving, instead of the energy parameter ν, the free parameters α, α'. This independent choice can be made as suitable as possible for each concrete problem. Note, that the idea of introducing a free parameter into the CGF was already exploited successfully in previous calculations. In Ref. [8] a special form of a one-parameter Sturmian expansion of $g_\gamma(E;r,r')$ was suggested and used for the analytical continuation of Sturmian matrix elements into the continuum ($E > 0$ in the nonrelativistic case or $|E| > mc^2$ in the relativistic case). Heller [9] found the one-parameter expansion $g^{\gamma}_{n,n'}(\nu;\alpha,\alpha)$ for the nonrelativistic case when $\gamma = l$, see below Eq. (8), using the alternative technique of three-term recurrence relations for the inversion of the Coulomb Hamiltonian matrix on the square-integrable (L^2-) basis set $S_{kl}(2r/\alpha)$. The high efficiency of this expansion for the analysis of two-photon matrix elements between the same hydrogen-like states was demonstrated in Ref. [10]. We prove here that the most general two-parameter expansion (3) is even more powerful in applications, as it enables the analysis of the matrix elements of the CGF between arbitrary atomic (or Sturmian) states with different energies.

In order to derive $g^{\gamma}_{n,n'}$ in (3) we use first the following formal re-expansion of Sturmian functions in (2),

$$S_{k\gamma}\left(\frac{2r}{\nu}\right) = \sum_{n=0}^{\infty} c_{nk}(\alpha)\,S_{n\gamma}\left(\frac{2r}{\alpha}\right). \tag{4}$$

Using the orthogonality condition for the Laguerre polynomials, the coefficient c_{nk} can be represented as an integral over two of them with different arguments. This is calculated exploiting the well-known generating function [11] for one of the L_n^{α}. After some manipulations we have

$$c_{nk}(\alpha) = (-1)^k\frac{(2\gamma+2)_k}{k!}\left(\frac{4\alpha\nu}{(\alpha+\nu)^2}\right)^{\gamma+1}\left(\frac{\alpha-\nu}{\alpha+\nu}\right)^{n+k}{}_2F_1[-n,-k;2\gamma+2;z].$$

Here and below we use the notations $z = -4\alpha\nu/(\alpha-\nu)^2$, $z' = -4\alpha'\nu/(\alpha'-\nu)^2$, and $(a)_k = \Gamma(a+k)/\Gamma(a)$ denotes Pochhammer's symbol.

Using for the Sturmian function $S_{k\gamma}(2r'/\nu)$ in Eq. (2) the expansion (4) with a free parameter α' and the coefficients $c_{n'k}(\alpha')$ we arrive at the following identity,

$$g^{\gamma}_{n,n'}(\nu;\alpha,\alpha') = f(\alpha,\alpha')\sum_{k=0}^{\infty}\frac{(2\gamma+2)_k\ {}_2F_1[-n,-k;2\gamma+2;z]\ {}_2F_1[-n',-k;2\gamma+2;z']}{k!(k+\gamma+1-\eta)[(1-z)(1-z')]^{k/2}}, \tag{5}$$

where the prefactor f is

$$f(\alpha,\alpha') = \nu\frac{(4\nu\sqrt{\alpha\alpha'})^{2\gamma+2}}{\Gamma(2\gamma+2)}\frac{(\alpha-\nu)^n}{(\alpha+\nu)^{n+2\gamma+2}}\frac{(\alpha'-\nu)^{n'}}{(\alpha'+\nu)^{n'+2\gamma+2}}$$
$$= \frac{\nu}{\Gamma(2\gamma+2)}\left(\frac{zz'}{(1-z)(1-z')}\right)^{\gamma+1}\frac{1}{(1-z)^{n/2}(1-z')^{n'/2}}.$$

Using the differential form for one of the hypergeometric polynomials in (5), here with parameter $-n$ [12] (Chapter 2, Section 2.8, Eq. (17)) and the trivial identity,

$$(k+\gamma+1-\eta)^{-1} = \int_0^1 \mathrm{d}t\, t^{k+\gamma-\eta},$$

to simplify the denominator, the series (5) is summed using the generating function [12] (Chapter 2, Section 2.5.1) for hypergeometric polynomials ${}_2F_1[-n',-k;2\gamma+2;z']$.

After some manipulations we obtain

$$g^{\gamma}_{n,n'}(\nu;\alpha,\alpha') = f(\alpha,\alpha')\frac{\mathrm{d}^n}{\mathrm{d}z^n}\{\varphi_n(z)I_{n'}(z)\}\Big|_{z_0=z},$$

where

$$\varphi_n(z) = [z(1-z_0)]^n\left(\frac{z}{z_0}\right)^{2\gamma+1}\left(\frac{1-z_0}{1-z}\right)^{\gamma+1+\eta},$$
$$I_{n'}(z) = \int_0^{(1-z_0)/(1-z)}\mathrm{d}t\frac{t^{\gamma-\eta}(1-yt)^{n'}}{(1-y't)^{n'+2\gamma+2}}, \qquad y = \sqrt{\frac{1-z'}{1-z_0}}, \qquad y' = \frac{1}{\sqrt{(1-z')(1-z_0)}}. \tag{6}$$

The differentiation of $\varphi_n(z)$ yields again a hypergeometric polynomial

$$\frac{\mathrm{d}^{n-p}}{\mathrm{d}z^{n-p}}\varphi_n(z)\Big|_{z_0=z} = \frac{(2\gamma+2)_n}{(2\gamma+2)_p}[z(1-z)]^p\ {}_2F_1[-n+p,\gamma+1-\eta+p;2\gamma+2+p;z].$$

The integral $I_{n'}(z)$ at $z_0 = z$ is the Appell function F_1 [12] (Chapter 5, Section 5.8, Eq. (5))

$$I_{n'} \equiv I_{n'}(z)|_{z_0=z} = \frac{1}{\gamma+1-\eta}F_1[\gamma+1-\eta;-n',n'+2\gamma+2;\gamma+2-\eta;y,y']. \tag{7}$$

As is evident from Eq. (6) at $\alpha = \alpha'$ all the derivatives of $I_{n'}(z)$ with respect to the variable z, up to order n', vanish at $z_0 = z$. For this reason we suppose below, that $n = n_< = \min\{n,n'\}$ and $n' = n_> = \max\{n,n'\}$. If $n' < n$, then in all formulas below for $g^{\gamma}_{n,n'}(\nu;\alpha,\alpha')$ the substitution $(n,\alpha) \rightleftharpoons (n',\alpha')$ should be made.

At $\alpha = \alpha'$ we have $y = 1$ and the Appell function in $I_{n'}$ reduces to a Gauss function ${}_2F_1$. Thus the final result in this case has the form

$$g^{\gamma}_{n,n'}(\nu;\alpha,\alpha) = \frac{\nu}{\Gamma(2\gamma+2)} \frac{{}_2F_1[-n,\gamma+1-\eta;2\gamma+2;z]}{(1-z)^{n/2}} \times \left(\frac{\sqrt{1-z}}{-z}\right)^{n'} \frac{n'!\,{}_2F_1[n'+1,n'+2\gamma+2;n'+\gamma+2-\eta;1/z]}{(\gamma+1-\eta)_{n'+1}} . \tag{8}$$

For integer $\gamma = l$ this result coincides with the result of Ref. [9] (see also Ref. [10]), in which it was derived by a technique based on the three-term recurrence relations.

At $\alpha \neq \alpha'$ the derivatives of $I_{n'}(z)$, are calculated using the generating function for Appell functions F_1 [13]. Hence, the final result may be written as follows,

$$g^{\gamma}_{n,n'}(\nu;\alpha,\alpha') = f(\alpha,\alpha') \sum_{p=0}^{n} C_p^n (-z)^p \frac{{}_2F_1[-n+p,\gamma+1-\eta+p;2\gamma+2+p;z]}{(2\gamma+2)_p} \Phi_p(y,y') . \tag{9}$$

Here C_p^n is the binomial coefficient, $\Phi_0(y,y') = I_{n'}$ (see Eq. (7)),

$$y = \sqrt{(1-z')/(1-z)}, \qquad y' = 1/\sqrt{(1-z)(1-z')},$$

$$\Phi_{p>0}(y,y') = -\frac{(\gamma+2+\eta-p)_{p-1}(y-1)^{n'}}{(y'-1)^{n'+2\gamma+2}} \times F_1[-(p-1);-n',n'+2\gamma+2;\gamma+2+\eta-p;1/(1-y),1/(1-y')] .$$

It is noted that the Appell function in $\Phi_{p>0}$ is a finite polynomial in both arguments. Therefore, Eq. (9) contains two essentially different groups of terms: The term with $p = 0$ involves the linear combination of $(n'+1)$ non-terminating hypergeometric functions, see Eq. (7). The terms with $p > 0$ reduce to products of hypergeometric polynomials of one variable, in the ${}_2F_1$ function, and of two variables, in the F_1 function. At $\alpha = \alpha'$, Eq. (9) reduces to Eq. (8). Based on Eq. (9), a detailed study of two-photon transitions between the highly excited states of hydrogen-like atoms including numerical analysis and analytical calculations for limiting cases will be published elsewhere. Here we proceed to the derivation of a closed analytical two-photon Gordon formula [14].

The closed expression of the CGF in momentum-space representation for the nonrelativistic hydrogen atom has also a simple form. Using Eq. (3) for $g_l(E;r,r')$ and calculating the integrals of products between Laguerre polynomials $L_n^{\alpha}(x)$ and spherical Bessel functions $j_l(pr)$, originating from the Fourier transform, together with the use of the generating functions for $L_n^{\alpha}(x)$ and for Gegenbauer polynomials $C_k^{\beta}(\cos\varphi)$, we find

$$G_E(\boldsymbol{p},\boldsymbol{p}') = \sum_{lm} \sum_{k,k'=l+1}^{\infty} G^l_{k,k'}(\nu;\alpha,\alpha') Y_{klm}(\xi) Y^*_{k'lm}(\xi') . \tag{10}$$

Here $Y_{klm}(\xi)$ are four-dimensional spherical harmonics [2] orthonormalized on the 4-sphere, the so-called "Fock's sphere" $S^3 \in \mathcal{R}^4$, with unit 4-radius $\xi = \{\cos\varphi,\ \sin\varphi\ \hat{\boldsymbol{p}}\}$, and $\cos\varphi = (1-\alpha^2\boldsymbol{p}^2)/(1+\alpha^2\boldsymbol{p}^2)$. The kernel $G^l_{k,k'}$ is

$$G^l_{k,k'}(\nu;\alpha,\alpha') = (-1)^{k+k'} \sqrt{\frac{k(k-l-1)!}{(k+l)!}} \left(\frac{4\alpha\alpha'}{(1+\alpha^2\boldsymbol{p}^2)(1+\alpha'^2\boldsymbol{p}'^2)}\right)^2 g^l_{k-l-1,k'-l-1}(\nu;\alpha,\alpha') ,$$

with $g^l(\nu;\alpha,\alpha')$ determined by (8) or (9). At $\alpha = \alpha' = \nu$, Eq. (10) reduces to the well-known Schwinger's form of $G_E(\boldsymbol{p},\boldsymbol{p}')$ [2], which is evidently a momentum-space analog of the standard Sturmian expansion (1), (2).

As a conclusion, Eqs. (3), (9) for the radial CGF are convenient in different applications, since the energy dependence of each term in series (3) is separated from the radial variables r, r'. Each integration on r, r' can be performed while putting α, α' as it is suitable for each concrete problem. In particular, in calculating two-photon matrix elements, α and α' can be set as the principal quantum numbers of the initial and final states divided by Z for transitions between physical atomic states. They can also be chosen to be equal to the parameters ν', ν'' of other CGF in the calculation of higher-order multiphoton amplitudes.

One important application of the above results is the closed-form calculation of two-photon dipole matrix elements between hydrogen-like states $|n_0, l_0\rangle$ and $|n, l = l_0, l_0 \pm 2\rangle$ with arbitrary n_0, l_0, n. This result is a two-photon generalization of the well-known Gordon formula for the hydrogenic radial dipole matrix elements [14]. As an example, we present here this result for the simplest case of transitions between $1s$ or $2s$ states ($n_0 = 1, 2$) and ns states with $n \geqslant 2$ (the velocity gauge is used for the photon–atom interaction and we put $Z = 1$ for simplicity),

$$\langle ns|\boldsymbol{e}'\cdot\nabla_{r'}G_E(\boldsymbol{r}',\boldsymbol{r})\boldsymbol{e}\cdot\nabla_r|n_0 s\rangle = (\boldsymbol{e}\cdot\boldsymbol{e}')\sqrt{\frac{n_0}{n}}\left[T_{n_0,n}(\nu) - \delta_{n_0,2}\frac{64n^3\nu^2}{3(\nu^2-4)(n^2-4)^2}\left(\frac{n-2}{n+2}\right)^n\right],$$

where $\boldsymbol{e}$ and $\boldsymbol{e}'$ are unit polarization vectors of the photons involved in the process,

$$T_{n_0,n}(\nu) = (n+1)(n+2)g^1_{0,n-1}(\nu;n_0,n) - (n-1)(n-2)g^1_{0,n-3}(\nu;n_0,n)\,.$$

For the case $g^1_{0,n'}$ considered here we have the compact form (cf. (9))

$$g^1_{0,n'} = \frac{\nu}{6(2-\nu)}\left(\frac{16n_0n\nu^2}{(n_0+\nu)^2(n+\nu)^2}\right)^2\left(\frac{n-\nu}{n+\nu}\right)^{n'}F_1[2-\nu;-n',n'+4;3-\nu;y,y']\,,$$

where

$$y = \frac{(n_0-\nu)(n+\nu)}{(n_0+\nu)(n-\nu)}, \qquad y' = \frac{(n_0-\nu)(n-\nu)}{(n_0+\nu)(n+\nu)}.$$

Note, that for the transitions from the ground state ($n_0 = 1$) our result coincides with the results obtained by other methods [15].

Two-photon Gordon formulas for an arbitrary n_0 and l_0 have a similar structure, but they involve four different $g^{l'}_{k,k'}(n_0/Z, n/Z)$ terms with $k, k' \neq 0$. In contrast to the one-photon Gordon formula [14], which involves only a combination of two hypergeometric polynomials, the two-photon generalizations have therefore a more complicated structure: They contain a linear combination of algebraic terms and hypergeometric functions. To summarize, our results provide a simple and tractable method to derive general closed-form expressions for two-photon transition amplitudes between *arbitrary excited atomic states*. Such expression should be useful for the analysis of different problems in two-photon spectroscopy of hydrogen-like states. By substituting $n \to i/p$ the results can be also analytically continued to the case of two-photon bound-free transitions in the continuum with energy $E' = p^2/2$. Finally, let us mention that the two-parameter expansion (9) for the CGF will be convenient for the extension of existing results on multiphoton transitions from the ground state of hydrogen-like atoms, e.g. such as recent three photon calculations [16], to the case of highly-excited initial states $|n_0, l_0\rangle$.

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