Contribution of Discrete and Continuum Wave Functions in the Ground State Polarizability of Hydrogen

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ABSTRACT

We analytically derive a discrete radial Green function for a hydrogenic system in terms of associated Leguerre polynomials. We investigate the polarizability of the ground-state hydrogen using the so-called length gauge approximation of electrodynamics. The polarizability is the sum of the polarization matrix elements for the negative and the positive frequency values. We estimate the contribution of discrete wavefunctions to the static ground state polarizability. We found that the contribution of continuum states dominates over that of discrete states to the polarizability by an order of magnitude.

Keywords: Polarizability; Radial Green function; Matrix elements; Discrete and Continuum wave functions.

INTRODUCTION

Electric polarizability of an atom or a molecule is their tendency to have separated positive and negative charge centers, producing an electric dipole [1]. Polarizability is a scalar quantity for an isotropic medium or a spherical system, while it is a tensor for an anisotropic medium or a non-spherical system. The polarizability of an atom can be evaluated quantum electrodynamically with the help of Schrödinger-Coulomb Green function [2,3,4]. Polarizability helps unearth many fundamental quantum phenomena, such as dispersion between two atoms in long-range interaction [5,6,7,8], determining magic wavelength in atomic transitions [9,10,11,12], developing three-dimensional (3D) crystallographic molecular stacking [13]. In addition, polarizability can be a great tool in understanding cold-atom physics, time-keeping using atomic clocks, and the metrology of atomic frequency standards [14]. One can also determine a system's dielectric constant and refractive index using its dipole polarizability [15].

The detailed mathematical derivation is quite involved as it needs to evaluate matrix elements in Schrödinger Coulomb propagator. The reduced discrete Green function is evaluated as the inverse of Hamiltonian minus energy eigenvalue sandwiched between the position operators. The polarization matrix elements for any energy state $|\varphi\rangle$ reads[5]

$$P_\varphi(\omega) = \frac{e^2}{3} \left\langle \varphi \left| \vec{r} \left(\frac{1}{H - E - \hbar\omega} \right) \vec{r} \right| \varphi \right\rangle \tag{1}$$

where e is the electronic charge, $\vec{r}$ is the electron position operator, H is the Schrödinger Hamiltonian, E is the energy of the reference state $|\varphi\rangle$, $\hbar = 1.0545718 \times 10^{-34}$ J s is Planck's eponymous constant, and ω is the angular frequency of the transition. The sum of the polarization matrix elements for the negative and the positive frequency

$\alpha_\varphi(\omega) = P_\varphi(\omega) + P_\varphi(-\omega)$ is the dynamical polarizability for the atom for the state $|\varphi\rangle$. In this work, we evaluate the contribution of the discrete wave functions and the continuous wave functions to the ground-state hydrogen atom polarizability and compare them. This investigation confirms that the continuum contribution is not negligible; instead, it is the dominating one for the hydrogen atom.

We organize the paper as follows. We first determine the discrete radial green function by solving the eigenvalue equation corresponding to the radial wavefunctions of hydrogen. We use the fact that the total wave function can be separated into the radial and angular components, and then the angular components are calculated separately from the radial components. We first perform the Sturmian decomposition of the Schrödinger Green function to evaluate the radial component, and then the radial integrations are carried out. Finally, the summation is carried out over the discrete energy levels. In the next section, we determine the ground state polarizability of hydrogen due to discrete energy levels and compare it with the polarizability due to the continuous part. Finally, we draw a conclusion and present concluding remarks.

DISCRETE RADIAL GREEN FUNCTION

To solve a problem involving partial differential equations, Green function formalism provides a very powerful technique. In what follows, we revisit a derivation of the discrete radial Green function. We begin our derivation with the completeness relation in discrete representation $\langle \vec{r}_1 | \vec{r}_2 \rangle$, which can be written as

$$\langle \vec{r}_1 | \mathbb{1} | \vec{r}_2 \rangle = \sum_{n\ell m} \langle \vec{r}_1 | n\ell m \rangle \langle n\ell m | \vec{r}_2 \rangle$$

$$= \sum_{n\ell m} \psi_{n\ell m}(r_1, \theta_1, \varphi_1) \psi^*_{n\ell m}(r_2, \theta_2, \varphi_2)$$

$$= \sum_{n\ell m} R_{n\ell}(r_1) R_{n\ell}(r_2) Y_{\ell m}(\theta_1, \varphi_1) Y^*_{\ell m}(\theta_2, \varphi_2)$$

$$= \sum_{n\ell m} \frac{(n-\ell-1)!}{2n(n+\ell)!} \left(\frac{2}{na_0}\right)^3 \exp\left(-\frac{r_1+r_2}{na_0}\right) \left(\frac{2r_1}{na_0}\right)^\ell \left(\frac{2r_2}{na_0}\right)^\ell L^{2\ell+1}_{n-\ell-1}\left(\frac{2r_1}{na_0}\right) L^{2\ell+1}_{n-\ell-1}\left(\frac{2r_2}{na_0}\right) \quad (2)$$

where $\langle \vec{r} | n\ell m \rangle = \psi_{n\ell m}(r, \theta, \varphi)$ is the complete eigenfunction for Schrödinger-Coulomb Hamiltonian; n, ℓ, m are the principal, orbital, and magnetic quantum numbers; and a_0 is the Bohr radius. We have used an ansatz which states that the total eigenfunctions can be expressed as the product of a radial part and an angular part as

$$\psi_{n\ell m}(r, \theta, \varphi) = R_{n\ell}(r) Y_{\ell m}(\theta, \varphi) \quad (3)$$

where the radial wave function $R_{n\ell}(r)$ is given by [16]

$$R_{n\ell}(r) = \left[\frac{(n-\ell-1)!}{(n+\ell)!}\right]^{1/2} \frac{2^{\ell+1}}{n^2} \frac{1}{a_0^{3/2}} \left(\frac{r}{na_0}\right)^\ell \exp\left(-\frac{r}{na_0}\right) L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na_0}\right) \quad (4)$$

and the angular part $Y_{\ell m}(\theta, \varphi)$ is the usual spherical harmonics given by

$$Y_{\ell m}(\theta, \varphi) = \left[\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}\right]^{1/2} P^m_\ell(\cos(\theta)) e^{im\varphi} \quad (5)$$

Here, $L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na_0}\right)$ and $P^m_\ell(\cos(\theta))$ are respectively the associated Laguerre and the associated Legendre polynomials. Figure 1Radial functions for $n = 1$ i.e., $R_{1s}(r)$ and $n = 2$ i.e., $R_{2s}(r)$ and $R_{2p}(r)$figure.1 shows radial functions for $n = 1$, and 2 as an example.
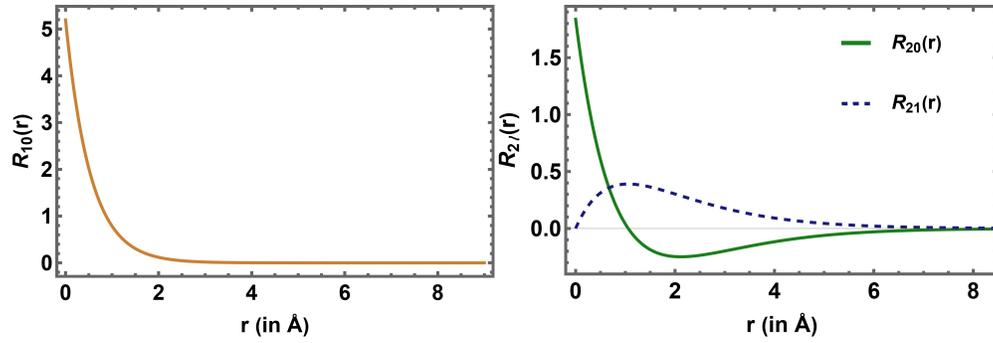
FIGURE 1. Radial functions for $n = 1$ i.e., $R_{1s}(r)$ and $n = 2$ i.e., $R_{2s}(r)$ and $R_{2p}(r)$.

One can express the Green function in terms of position operators, Hamiltonian and energy eigenvalues as[17,18,19]

$$G^{\text{dis}}(\vec{r}_1, \vec{r}_2, E) = \langle \vec{r}_1 | \frac{\mathbb{1}}{H - E} | \vec{r}_2 \rangle \tag{6}$$

which can be expanded with the help of the spectral decomposition of unity as

$$= \sum_{n\ell m} \langle \vec{r}_1 | n\ell m \rangle \frac{1}{H - E} \langle n\ell m | \vec{r}_2 \rangle$$

$$= \sum_{n\ell m} \frac{\psi_{n\ell m}(r_1, \theta_1, \varphi_1) \psi_{n\ell m}^*(r_2, \theta_2, \varphi_2)}{E_n - E}$$

$$= \sum_{n\ell m} \frac{1}{E_n - E} \frac{(n - \ell - 1)!}{2n(n + \ell)!} \left(\frac{2}{na_0} \right)^3 \exp\left(-\frac{r_1 + r_2}{na_0} \right) \left(\frac{2r_1}{na_0} \right)^\ell \left(\frac{2r_2}{na_0} \right)^\ell$$

$$\times L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_1}{na_0} \right) L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_2}{na_0} \right) Y_{\ell m}(\theta_1, \varphi_1) Y_{\ell m}^*(\theta_2, \varphi_2) \tag{7}$$

Here, E_n is the energy eigenvalues corresponding to the eigenvalue equation

$$HR_{n\ell}(r) = \left(-\frac{\hbar^2}{2m_e} \vec{\nabla}^2 - \frac{\alpha\hbar c}{r} \right) R_{n\ell}(r) = E_n R_{n\ell}(r) \tag{8}$$

Let us rewrite $R_{n\ell}(r)$ as

$$R_{n\ell}(r) = C_{n\ell} \, r^\ell \exp\left(-\frac{r}{na_0} \right) \mathbb{L} \tag{9}$$

where

$$C_{n\ell} = \left[\frac{(n - \ell - 1)!}{(n + \ell)!} \right]^{1/2} \frac{2^{\ell+1}}{n^2} \frac{1}{a_0^{3/2}} \left(\frac{1}{na_0} \right)^\ell \tag{10}$$

is a constant independent of r and $\mathbb{L} = L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0} \right)$.

With the aid of Eqs. (8equation.0.8) and (9equation.0.9), one can write the eigenvalue equation as

$$HR_{n\ell}(r) = \left(-\frac{\hbar^2}{2m_e}\vec{\nabla}^2 - \frac{\alpha\hbar c}{r}\right)C_{n\ell}\, r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= \left[-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2}\right) - \frac{\alpha\hbar c}{r}\right]C_{n\ell}\, r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= -\frac{\hbar^2}{2m_e}C_{n\ell}\frac{\partial}{\partial r}\left[\ell r^{\ell-1}\exp\left(-\frac{r}{na_0}\right)\mathbb{L} - \frac{r^\ell}{na_0}\exp\left(-\frac{r}{na_0}\right)\mathbb{L} + r^\ell\exp\left(-\frac{r}{na_0}\right)\frac{\partial}{\partial r}\mathbb{L}\right]$$
$$- \frac{\hbar^2}{2m_e}C_{n\ell}\frac{2}{r}\left[\ell r^{\ell-1}\exp\left(-\frac{r}{na_0}\right)\mathbb{L} - \frac{1}{na_0}r^\ell\exp\left(-\frac{r}{na_0}\right)\mathbb{L} + r^\ell\exp\left(-\frac{r}{na_0}\right)\frac{\partial}{\partial r}\mathbb{L}\right]$$
$$- \frac{\hbar^2}{2m_e}C_{n\ell}\left[-\frac{\ell(\ell+1)}{r^2} + \frac{2m_e\alpha c}{\hbar r}\right]r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= -\frac{\hbar^2}{2m_e}C_{n\ell}\left[\frac{\ell(\ell-1)}{r^2}\mathbb{L} - \frac{\ell}{na_0 r}\mathbb{L} + \frac{\ell}{r}\frac{\partial}{\partial r}\mathbb{L} - \frac{\ell}{na_0 r}\mathbb{L} + \frac{1}{(na_0)^2}\mathbb{L} - \frac{1}{na_0}\frac{\partial}{\partial r}\mathbb{L}\right.$$
$$\left. + \frac{\ell}{r}\frac{\partial}{\partial r}\mathbb{L} - \frac{1}{na_0}\frac{\partial}{\partial r}\mathbb{L} + \frac{\partial^2}{\partial r^2}\mathbb{L}\right]r^\ell\exp\left(-\frac{r}{na_0}\right) - \frac{\hbar^2}{2m_e}C_{n\ell}\frac{2}{r}\left[\frac{\ell}{r}\mathbb{L} - \frac{1}{na_0}\mathbb{L} + \frac{\partial}{\partial r}\mathbb{L}\right]$$
$$\times r^\ell\exp\left(-\frac{r}{na_0}\right) - \frac{\hbar^2}{2m_e}C_{n\ell}\left[-\frac{\ell(\ell+1)}{r^2} + \frac{2m_e\alpha c}{\hbar r}\right]r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= -\frac{\hbar^2}{2m_e}C_{n\ell}\, r^{\ell-1}\exp\left(-\frac{r}{na_0}\right)\left\{r\frac{\partial^2}{\partial r^2}\mathbb{L} + \left(2\ell+2 - \frac{2r}{na_0}\right)\frac{\partial}{\partial r}\mathbb{L} + (n-\ell-1)\mathbb{L}\right\}$$
$$- \frac{\hbar^2}{2m_e}C_{n\ell}\left[-\frac{2\ell}{na_0 r} - \frac{2}{na_0 r} + \frac{1}{(na_0)^2} + \frac{2m_e\alpha c}{\hbar r} - \frac{2n}{na_0 r} + \frac{2\ell}{na_0 r} + \frac{2}{na_0 r}\right]$$
$$\times r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L} \tag{11}$$

Using the fact that $\mathbb{L} \equiv L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$ satisfies the associated Laguerre differential equation:

$$r\frac{\partial^2}{\partial r^2}\mathbb{L} + \left(2\ell+2 - \frac{2r}{na_0}\right)\frac{\partial}{\partial r}\mathbb{L} + (n-\ell-1)\mathbb{L} = 0 \tag{12}$$

Eq. (11) can be written as:

$$HR_{n\ell}(r) = -\frac{\hbar^2}{2m_e}\left[\frac{1}{(na_0)^2} + \frac{2m_e\alpha c}{\hbar r} - \frac{2}{a_0 r}\right]C_{n\ell}\, r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= \left[-\frac{\hbar^2}{2m_e n^2 a_0^2} - \frac{\hbar\alpha c}{r} + \frac{\hbar^2}{m_e a_0 r}\right]C_{n\ell}\, r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L}$$

$$= -\frac{\alpha^2 m_e c^2}{2n^2}C_{n\ell}\, r^\ell \exp\left(-\frac{r}{na_0}\right)\mathbb{L} = -\frac{\alpha^2 m_e c^2}{2n^2}R_{n\ell}(r) \tag{13}$$

Here, we have used $a_0 = \hbar/(\alpha m_e c)$, where $\hbar = 1.0545718 \times 10^{-34}$ J s is Plank's eponymous constant, $\alpha = 1/137.035999$ is the fine structure constant, m_e is the mass of an electron, and c is the speed of light in a vacuum. From Eq. (13equation.0.13), the eigenvalues E_n can be written as

$$E_n = -\frac{\alpha^2 m_e c^2}{2n^2} \tag{14}$$

If we define a new quantum number k such that $k = n - \ell - 1$, the associated Laguerre polynomials $L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$ becomes $L_k^{2\ell+1}\left(\frac{2r}{(k+\ell+1)a_0}\right)$ and the energy eigenvalues, in this condition, can be written as

$$E_{k\ell} = -\frac{\alpha^2 m_e c^2}{2\left(k+\ell+1\right)^2} \tag{15}$$

The energy difference $E_n - E$ in Eq. (6equation.0.6) is thus given by

$$E_n - E = -\frac{\alpha^2 m_e c^2}{2n^2} - \left(-\frac{\alpha^2 m_e c^2}{2\nu^2}\right) = \frac{\alpha^2 m_e c^2}{2}\left(\frac{1}{\nu^2} - \frac{1}{n^2}\right) = \frac{\hbar^2}{2m_e a_0^2}\left(\frac{n^2 - \nu^2}{n^2\nu^2}\right) \tag{16}$$

where ν is the principal quantun number associated with the energy E. Substituting the value of the energy difference $E_n - E$ from Eq. (16equation.0.16) to Eq. (6equation.0.6), we get

$$G^{\text{dis}}(\vec{r}_1, \vec{r}_2, \nu) = \frac{2m_e}{\hbar^2}\sum_{n\ell m}\frac{a_0^2 n^2 \nu^2}{n^2 - \nu^2}\frac{(n-\ell-1)!}{2n(n+\ell)!}\left(\frac{2}{na_0}\right)^3\exp\left(-\frac{r_1+r_2}{na_0}\right)\left(\frac{2r_1}{na_0}\right)^\ell$$

$$\times \left(\frac{2r_2}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_1}{na_0}\right)L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_2}{na_0}\right)Y_{\ell m}(\theta_1, \varphi_1)Y_{\ell m}^*(\theta_2, \varphi_2)$$

$$= \frac{4m_e}{\hbar^2}\sum_{n\ell m}\frac{\nu^2}{n^2 - \nu^2}\frac{(n-\ell-1)!}{n(n+\ell)!}\left(\frac{2}{na_0}\right)^{2\ell+1}\exp\left(-\frac{r_1+r_2}{na_0}\right)(r_1 r_2)^\ell$$

$$\times L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_1}{na_0}\right)L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_2}{na_0}\right)Y_{\ell m}(\theta_1, \varphi_1)Y_{\ell m}^*(\theta_2, \varphi_2) \tag{17}$$

The total discrete Green function can be expressed in terms of the discrete radial Green function $g_\ell^{\text{dis}}(r_1, r_2, \nu)$ as[17]

$$G^{\text{dis}}(\vec{r}_1, \vec{r}_2, \nu) = \sum_{n\ell m} g_\ell^{\text{dis}}(r_1, r_2, \nu)Y_{\ell m}(\theta_1, \varphi_1)Y_{\ell m}^*(\theta_2, \varphi_2) \tag{18}$$

Comparing Eq.[18] with Eq.[17], we get the discrete radial Green function $g_\ell^{\text{dis}}(r_1, r_2, \nu)$ as

$$g_\ell^{\text{dis}}(r_1, r_2, \nu) = \frac{4m_e}{\hbar^2}\sum_{n=0}^{\infty}\frac{\nu^2}{n^2 - \nu^2}\frac{(n-\ell-1)!}{n(n+\ell)!}\left(\frac{2}{na_0}\right)^{2\ell+1}\exp\left(-\frac{r_1+r_2}{na_0}\right)(r_1 r_2)^\ell$$

$$\times L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_1}{na_0}\right)L_{n-\ell-1}^{2\ell+1}\left(\frac{2r_2}{na_0}\right) \tag{19}$$

The (ℓ=1)-component of the discrete radial Green function $g_{\ell=1}^{\text{dis}}(r_1, r_2, \nu)$ reads

$$g_{\ell=1}^{\text{dis}}(r_1, r_2, \nu) = \frac{4m_e}{\hbar^2}\sum_{n=2}^{\infty}\frac{\nu^2}{(n^2 - \nu^2)n^2(n^2-1)}\left(\frac{2}{na_0}\right)^3\exp\left(-\frac{r_1+r_2}{na_0}\right)(r_1 r_2)$$

$$\times L_{n-2}^3\left(\frac{2r_1}{na_0}\right)L_{n-2}^3\left(\frac{2r_2}{na_0}\right) \tag{20}$$

Note that the sum over n starts from 2 not from zero as $L_{-2}^3(x) = 0 = L_{-1}^3(x)$

DISCRETE GROUND STATE POLARIZABILITY

The ground state static polarizability due to discrete energy levels is given by[5,17]

$$
\alpha_{1S}^{\text{dis}}(\omega = 0) = 2P_{1S}^{\text{dis}}(\omega = 0) = 2\frac{e^2}{3}\left\langle 1S\left|r_1\,\frac{1}{H-E}\,r_2\right|1S\right\rangle
$$

$$
= \frac{2\,e^2}{3}\int_0^\infty r_1^2\,\mathrm{d}r_1\int_0^\infty r_2^2\,\mathrm{d}r_2\,R_{10}(r_1)\,r_1\,g_{\ell=1}^{\text{dis}}(r_1,r_2,\nu)\,R_{10}(r_2)\,r_2
$$

$$
= \frac{32 m_e\,e^2}{3\hbar^2 a_0^3}\int_0^\infty r_1^4\,\mathrm{d}r_1\int_0^\infty r_2^4\,\mathrm{d}r_2\,\exp\left(-\frac{r_1+r_2}{a_0}\right)\sum_{n=2}^\infty \frac{1}{n^2\,(n^2-1)^2}
$$

$$
\times\left(\frac{2}{na_0}\right)^3\exp\left(-\frac{r_1+r_2}{na_0}\right)L_{n-2}^3\left(\frac{2r_1}{na_0}\right)L_{n-2}^3\left(\frac{2r_2}{na_0}\right) \tag{21}
$$

Here, we have used the value of $g_{\ell=1}^{\text{dis}}(r_1,r_2,\nu)$ from Eq. (20equation.0.20) with $\nu=1$ and substituted the radial part of the ground state wave function of hydrogen, i.e., $R_{10}(r) = 2/\sqrt{a_0^3}\mathrm{e}^{-r/a_0}$. One can substitute the other excited state's radial functions and evaluate the excited state's static polarizability in a similar fashion.

Let us use dimensionless variables ρ defined as $\rho_i = 2r_i/(na_0)$ and make substitutions in Eq. (21equation.0.21) to get

$$
\alpha_{1S}^{\text{dis}}(\omega=0) = \frac{32 m_e\,e^2}{3\,\hbar^2 a_0^3}\sum_{n=2}^\infty \frac{1}{n^2\,(n^2-1)^2}\left(\frac{na_0}{2}\right)^7\int_0^\infty \rho_1^4\,\mathrm{d}\rho_1\int_0^\infty \rho_2^4\,\mathrm{d}\rho_2
$$

$$
\times\exp\left(-\frac{\rho_1 n+\rho_2 n}{2}\right)\exp\left(-\frac{\rho_1+\rho_2}{2}\right)L_{n-2}^3\left(\rho_1\right)L_{n-2}^3\left(\rho_2\right)
$$

$$
= \frac{a_0^4\,m_e\,e^2}{12\hbar^2}\sum_{n=2}^\infty \frac{n^5}{(n^2-1)^2}\int_0^\infty \rho_1^4\,\exp\left(-\frac{(1+n)\rho_1}{2}\right)L_{n-2}^3\left(\rho_1\right)\mathrm{d}\rho_1
$$

$$
\times\int_0^\infty \rho_2^4\,\exp\left(-\frac{(1+n)\rho_2}{2}\right)L_{n-2}^3\left(\rho_2\right)\mathrm{d}\rho_2 \tag{22}
$$

Interestingly, the ρ_1-integral is identical to the ρ_2-integral. Hence, one can write Eq. (22equation.0.22) as

$$
\alpha_{1S}^{\text{dis}}(\omega=0) = \frac{e^2\,a_0^2}{12\,E_h}\sum_{n=2}^\infty \frac{n^5}{(n^2-1)^2}\left[\int_0^\infty u^4\,\mathrm{e}^{-(1+n)u/2}L_{n-2}^3\left(u\right)\mathrm{d}u\right]^2 \tag{23}
$$

Here, we have also used $\alpha = \hbar/(a_0 m_e c)$, and $E_h = \alpha^2 m_e c^2$, where α and E_h are respectively the fine-structure constant and the Hartree energy. We can evaluate the u-integral in Eq. (23equation.0.23) using the standard integral identity [20]

$$
\int_0^\infty \mathrm{d}\rho\,\mathrm{e}^{s\rho}\,\rho^\gamma L_n^\mu(\rho) = \frac{\Gamma(\gamma+1)\Gamma(n+\mu+1)}{n!\Gamma(\mu+1)}(-s)^{-(\gamma+1)}{}_2F_1\left(-n,\gamma+1;\mu+1;-\frac{1}{s}\right) \tag{24}
$$

which yields

$$\int_0^\infty u^4 \, e^{-(1+n)u/2} L_{n-2}^3 (u) \, du = \frac{\Gamma(5)\Gamma(n+2)}{(n-2)!\Gamma(4)} \left(\frac{2}{1+n}\right)^5 \, {}_2F_1\left(2-n,5;4;\frac{2}{1+n}\right) \tag{25}$$

Substituting the value of the integral in Eq. (23equation.0.23) and simplifying the expression using standard integral identity [20]

$$_2F_1\left(-k,a+1;a;z\right) = (1-z)^k \frac{(z-1)a+kz}{a(z-1)} \tag{26}$$

we get

$$\alpha_{1S}^{\text{dis}}(\omega=0) = \frac{e^2 a_0^2}{E_h} \sum_{n=2}^\infty \frac{1024}{3} \frac{n^9}{(n-1)^6 (n+1)^8} \left(\frac{n-1}{n+1}\right)^{2n} \tag{27}$$

which yields

$$\alpha_{1S}^{\text{dis}}(\omega=0) = 0.362\,240\,952 \frac{e^2 a_0^2}{E_h} \tag{28}$$

The total ground state dynamical polarizability of a hydrogen atom is the sum of polarization matrix elements $P_{1s}(\pm\omega)$

$$\alpha_{1S}(\omega) = \sum_{\pm} P_{1s}(\pm\omega) \tag{29}$$

where $P_{1s}(\omega)$ is given as[11,21]

$$P_{1S}(\omega) \equiv P_{1S}(t) = \frac{e^2 a_0^2}{E_h} \left[\frac{2t^2(-3+3t+12t^2-12t^3-19t^4+19t^5+26t^6+38t^7)}{3(-1+t)^5 (1+t)^4} \right.$$
$$\left. - \frac{256t^9}{3(-1+t)^5(1+t)^5} \, {}_2F_1\left(1,-t;1-t;\left(\frac{1-t}{1+t}\right)^2\right) \right] \tag{30}$$

where $t = (1+2\hbar\omega/E_h)^{-1/2}$ is a dimensionless energy parameter. One obtains the total ground state static polarizability $\alpha_{1S}(\omega=0)$ of a hydrogen atom expanding the series for $\alpha_{1S}(\omega)$ and substituting $\omega = 0$ or $t = 1$ and convinces that it comes out to be

$$\alpha_{1S}(\omega=0) = \frac{9}{2} \frac{e^2 a_0^2}{E_h} \tag{31}$$
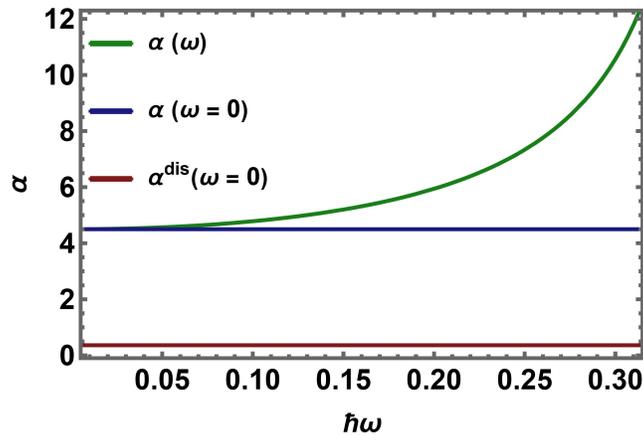
FIGURE 2. Comparison of different contributions to the polarizability of the ground state hydrogen. Polarizabilities are plotted as a function of energy $\hbar\omega$. The static polarizabilities are constant with frequency while the dynamical polarizability $\alpha(\omega)$ does vary with the frequency.

For illustrative purposes, the comparison of dynamical polarizability, static polarizability, and the discrete wavefunction contribution to the polarizability on the ground state hydrogen atom are presented in Fig. 2Comparison of different contributions to the polarizability of the ground state hydrogen. Polarizabilities are plotted as a function of energy $\hbar\omega$. The static polarizabilities are constant with frequency while the dynamical polarizability $\alpha(\omega)$ does vary with the frequencyfigure.2. The comparison shows that the major contribution in the ground state, static polarizability comes from the continuum wave functions.

CONCLUSION

Starting from the completeness relation, we derived the total discrete Green function and the radial discrete Green function in terms of the associated Laguerre polynomial. We obtained an analytical expression for the polarizability of the ground-state hydrogen atom. The polarizability can be expressed as the sum of the polarization matrix elements calculated using position operators for frequency's positive and negative values. The static value of polarizability is obtained from the dynamic polarizability as a special case of $\omega = 0$ or $t = 1$. We carried out the numerical value for the discrete ground state polarizability and found that the contribution of the discrete wavefunctions is smaller by an order of magnitude compared to the continuum states, revealing that the continuous wave functions dominate the ground state static polarizability. This is consistent with the result presented in Ref. [22] for the Stark shift for the ground state of hydrogen.

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