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# Polarizabilities and Rydberg States in the Presence of a Debye Potential

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**Abstract:** Polarizabilities and hyperpolarizabilities, $\alpha_1$, $\beta_1$, $\gamma_1$, $\alpha_2$, $\beta_2$, $\gamma_2$, $\alpha_3$, $\beta_3$, $\gamma_3$, $\delta$ and $\varepsilon$ of hydrogenic systems have been calculated in the presence of a Debye–Huckel potential, using pseudostates for the S, P, D and F states. All of these converge very quickly as the number of terms in the pseudostates is increased and are essentially independent of the nonlinear parameters. All the results are in good agreement with the results obtained for hydrogenic systems obtained by Drachman. The effective potential seen by the outer electron is $-\alpha_1/x^4 + (6\beta_1 - \alpha_2)/x^6$ + higher-order terms, where x is the distance from the outer electron to the nucleus. The exchange and electron–electron correlations are unimportant because the outer electron is far away from the nucleus. This implies that the conventional variational calculations are not necessary. The results agree well with the results of Drachman for the screening parameter equal to zero in the Debye–Huckel potential. We can calculate the energies of Rydberg states by using the polarizabilities and hyperpolarizabilities in the presence of Debye potential seen by the outer electron when the atoms are embedded in a plasma. Most calculations are carried out in the absence of the Debye–Huckel potential. However, it is not possible to carry out experiments when there is a complete absence of plasma at a particular electron temperature and density. The present calculations of polarizabilities and hyperpolarizabilities will provide accurate results for Rydberg states when the measurements for such states are carried out.

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## 1. Introduction

Recently, Qi et al. [1] reported a calculation of the dipole polarizability $\alpha_1$ of the hydrogenic systems in the screened Coulomb potential due to the systems being in hot dense plasmas. The screened potential in this case is the Debye–Huckel potential given by Equation (1).

$$V(r) = (-Ze^2/r)\exp(-\mu r), \tag{1}$$

where $1/\mu = (k_BT_e/4\pi e^2 n_e)^{1/2}$ is the Debye screening length, $k_B$ is the Boltzmann constant, $T_e$ and $n_e$ are the plasma electron temperature and density, respectively. There are other calculations of energy and polarizability by Zimmermann [2], Bahar et al. [3], Paul and Ho [4], Fowler [5] and Saha et al. [6]. The expression for polarizabilities is given by Equation (1).

$$S_{i,k} = \Sigma < 0 \mid v_i \mid N> \mid <N \mid v_i \mid 0>/(E_N - E_0)^k, \tag{2}$$

where $v_i = {r_1}^i P_i(\cos\theta_i)$ and the various polarizabilities are given by Equation (2).

$\alpha_i = S_{i,1}$, $\beta_i = S_{i,2}$ and $\gamma_i = S_{i,3}$. $\Psi_N$ are intermediate states of the appropriate angular momentum and $\Sigma$ indicates the sum of all such states.

## 2. Calculations and Results

Qi et al. [1] solved the Schrodinger equation in both the discrete and continuous spectrum of the potential given in Equation (1) by using the symplectic integration scheme. The contribution of the continuum states to the polarizability is particularly important for large $\mu$ when the electron binding energy is small and coupling to the continuum is strong. Saha et al. [6] solved the eigenvalue problem by the variational method using a large Slater-type orbitals basis for the discrete states. The contribution of the continuum states was not considered.

In the present calculation, we used pseudostates [7] for helium and the negative hydrogen ion to calculate polarizabilities and hyperpolarizabilties. In [7], the wave functions were of Hylleraas form because the systems consist of two electrons. Definitive results were obtained for the polarizabilities and hyperpolarizabilties. Now we are dealing with single-electron systems and therefore wave functions consist of one electron only and are very simple.

Pseudostates used in this calculation are given by

$$\Psi_S = \Sigma_{i=0} C_i r^i \exp(-a_s r)\, Y_{00}(\Omega), \tag{3}$$

$$\Psi_P = \Sigma_{i=1} D_i r^i \exp(-a_p r)\, Y_{10}(\Omega), \tag{4}$$

$$\Psi_D = \Sigma_{i=2} E_i r^i \exp(-a_d r)\, Y_{20}(\Omega), \tag{5}$$

$$\Psi_F = \Sigma_{i=3} F_i r^i \exp(-a_f r)\, Y_{30}(\Omega), \tag{6}$$

where $C_i$, $D_i$, $E_i$, and $F_i$, are the eigenvectors. With a few terms and taking the nonlinear parameters equal to 1.0 for hydrogen atoms, we obtained results for $\alpha_i$, $\beta_i$, and $\gamma_i$ which agree very well for $\mu = 0$ with the known results. We varied all the nonlinear parameters in Equations (3)–(6). However, results were not sensitive to the variation of nonlinear parameters. Therefore, we kept it fixed at 1.0. It is certainly possible to use the hydrogenic functions. The use of pseudostates makes calculations very simple and straightforward. This reduces the efforts involved in the computation. We give in Table 1 the presently calculated results for $\alpha_i$ for various values of $\mu$, using 20 terms in the expansion for wave functions (3) and (4). The results are very well converged for shorter expansions as well. We see that the agreement is very good. The present calculation is very easy to carry out compared to that of Qi et al. [1]. They have to calculate each bound state and the wave function corresponding to that state. They also included the continuum of the electron-hydrogenic system. It should be noticed that only those values of $\mu$ can be used to calculate $\alpha_1$ for which the ground state of the hydrogen atom remains bound.

**Table 1.** Comparison of the presently calculated results for $\alpha_i$ for hydrogen atom for various values of $\mu$, using 20 terms in the wave functions.

| **M** | **Present** | **Qi et al. [1]** |
|---|---|---|
| 0.00 | 4.500 | 4.500 |
| 0.01 | 4.50220 | **A** |
| 0.02 | 4.50868 | 4.50820 |
| 0.025 | 4.51346 | **4.51299** |
| 0.050 | 4.55220 | 4.55176 |
| 0.0625 | 4.58049 | 4.58003 |
| 0.10 | 4.69978 | 4.69933 |
| 0.20 | 5.27637 | 5.27661 |

**A**: No results are given for this value of $\mu$ by the authors.

In Table 2, we give $\beta_1$, $\gamma_1$, $\alpha_2$, $\beta_2$, $\gamma_2$, $\alpha_3$, $\beta_3$, $\gamma_3$, $\varepsilon$ and $\delta$ for a few values of $\mu$. The third-order polarizability $\delta$ has the following form [8]:

$$\delta = \Sigma_{N,M} <0 \mid v_i \mid N><N \mid v_j \mid M><M \mid <M \mid v_k \mid 0>/(E_N - E_0)(E_M - E_0), \tag{7}$$

**Table 2.** Polarizabilities and hyperpolarizabilities for hydrogen atoms for various values of μ.

| | **μ = 0.0** | **0.02** | **0.025** | **0.05** | **0.0625** | **0.10** | **0.20** |
|---|---|---|---|---|---|---|---|
| $\beta_1$ | 5.3750 | 5.3917 | 5.4009 | 5.4751 | 5.5305 | 5.7636 | 6.9384 |
| $\gamma_1$ | 6.6458 | 6.6750 | 6.6911 | 6.8219 | 6.9182 | 7.3313 | 9.5128 |
| $\alpha_2$ | 15.000 | 15.0540 | 15.0838 | 15.3246 | 15.5008 | 16.2498 | 20.0479 |
| $\beta_2$ | 13.3750 | 13.4453 | 13.4840 | 13.7977 | 14.0284 | 15.0195 | 20.3300 |
| $\gamma_2$ | 12.4948 | 12.5829 | 12.6315 | 13.0262 | 13.3179 | 14.5872 | 21.8128 |
| $\alpha_3$ | 131.2500 | 131.989 | 132.396 | 135.6875 | 138.1049 | 148.490 | 204.341 |
| $\beta_3$ | 102.031 | 102.817 | 103.249 | 106.758 | 109.349 | 120.632 | 185.434 |
| $\gamma_3$ | 83.2044 | 84.0320 | 84.4974 | 88.1980 | 90.9547 | 103.142 | 178.390 |
| E | 59.2125 | 59.7110 | 59.9307 | 61.7172 | 63.0371 | 68.7756 | 101.226 |
| Δ | 106.500 | 107.036 | 107.331 | 109.724 | 111.484 | 119.044 | 159.391 |

The values that (ijk) can take are all the permutations of [1,2].

The fourth-order hyperpolarizability only involving dipole terms has the following form [8]:

$$\varepsilon = \Sigma_{N,M,P} <0 \mid v_1 \mid N><N \mid v_1 \mid M><M \mid v_1 \mid P \mid 0>/(E_N - E_0)(E_M - E_0)(E_P - E_0) \tag{8}$$

In Equations (7) and (8), potentials $v_1$, $v_2$, and $v_3$ are given reference [8] and are not repeated here. The notation $|0>$, $|N>$, $|M>$. and $|P>$ represent wave functions for the angular momenta *S, P, D,* and *F* given in Equations (3)–(6) to be appropriately used to obtain nonzero matrix elements in Equations (7) and (8).

Similarly, by taking the nonlinear parameters equal to 2.0, we obtain results which agree with those obtained by Drachman [7] for μ = 0, using the Dalgarno and Lewis method [9]. The present results are given in Table 3. It can be seen that the polarizabilities and hyperpolarizabilities increase as μ increases. Since the ground state of the He ion is very tightly bound compared to that of the hydrogen atom, it is possible to have much larger values of μ.

**Table 3.** Polarizabilities and hyperpolarizabilities for the helium ion for various values of μ.

| | **μ = 0.0** | **0.02** | **0.025** | **0.05** | **0.0625** | **0.10** | **0.20** |
|---|---|---|---|---|---|---|---|
| $\alpha_1$ | 0.28125 | 0.28139 | 0.28146 | 0.28209 | 0.28255 | 0.28451 | 0.29374 |
| $\beta_1$ | 0.08394 | 0.08406 | 0.08409 | 0.08439 | 0.08461 | 0.08556 | 0.09006 |
| $\gamma_1$ | 0.02596 | 0.02599 | 0.02601 | 0.02614 | 0.02623 | 0.02665 | 0.02864 |
| $\alpha_2$ | 0.23438 | 0.23459 | 0.02347 | 0.23568 | 0.23640 | 0.23945 | 0.25390 |
| $\beta_2$ | 0.05225 | 0.05232 | 0.05235 | 0.05267 | 0.05291 | 0.05389 | 0.58670 |
| $\gamma_2$ | 0.01220 | 0.01222 | 0.01224 | 0.01234 | 0.01241 | 0.01272 | 0.14245 |
| $\alpha_3$ | 0.51269 | 0.51343 | 0.51384 | 0.51717 | 0.51962 | 0.53003 | 0.58004 |
| $\beta_3$ | 0.09964 | 0.09984 | 0.09994 | 0.10083 | 0.10148 | 0.10426 | 0.11780 |
| $\gamma_3$ | 0.02031 | 0.02037 | 0.02039 | 0.02063 | 0.02080 | 0.02153 | 0.02518 |
| ε | 0.05792 | 0.05802 | 0.05808 | 0.05853 | 0.05886 | 0.06027 | 0.06716 |
| δ | 0.41602 | 0.41655 | 0.41684 | 0.41926 | 0.42104 | 0.42861 | 0.46501 |

## 3. Rydberg States of He

The long-range potential, in terms of polarizabilities, seen by the outer electron is given by

$$U(x) = -\alpha_1/x^4 + (6\beta_1 - \alpha_2)/x^6 + (\delta + 16\gamma/5)/x^7 + (-\alpha_3 + 15\beta_2 - \varepsilon - \alpha_1\beta_1 - 72\gamma_1\,[1 + L(L+1)/10])/x^8, \quad (9)$$

where x is the distance of the outer electron from the nucleus. In Table 4, we give the expectation value of U(x) in MHz for the wave function of the outer electron in N = 10 and L = 7 and 8 states and compare the present results for μ = 0.0 with those obtained by Drachman [10] without the second-order corrections. We see that the agreement is very good even when very simple wave functions are used.

**Table 4.** Comparison of the presently calculated Rydberg states with the results of Drachman.

| N | L | Present (MHz) | Drachman [6] (MHz) |
|---|---|---|---|
| 10 | 7 | −48.60605124 | −48.60604738 |
| 10 | 8 | −24.17853458 | −24.17853458 |

The expectation values of $1/x^n$ for n = 4, 5, 6, 7, 8, 9 and 10 were calculated for μ = 0.0 and therefore cannot be used when the helium atoms are embedded in the plasma.

## 4. Transition Rates

Transition rates are given by

$$A(np \to 1s) = 8.032 \times 10^9 \frac{(E_{np} - E_{1s})^3}{9} \int_0^\infty R_{np}(r) r^3 R_{1s}(r) dr \quad (10)$$

In the above equation, $R_{np}(r)$ and $R_{1s}(r)$ are the hydrogen functions for $np$ and $1s$ states. In Table 5, we show how the transition rates from 4p, 3p and 2p states to the 1s state in hydrogen atoms change with the screening parameter. It can be seen that all the rates decrease with the increase in the screening parameter μ. Using the exact wave functions, we find the transition rates for 2p, 3p and 4p states to 1s state equal to 0.626, 0.167 and 0.0682 in units of $10^9$ $s^{-1}$ when there is no screening and exact hydrogenic functions are used. The last one is not in agreement with the one obtained from pseudostates while the first two are in good agreement with those obtained using pseudostates.

**Table 5.** Transition rates in sec $^{(-1)}$ 4p, 3p and 2p states of hydrogen atoms to the 1s state. The rates have been multiplied by $10^{(-9)}$.

| μ | A (2p→1s) | A (3p→1s) | A (4p→1s) |
|---|---|---|---|
| 0.000 | 0.624293 | 0.166670 | 0.071760 |
| 0.020 | 0.618343 | 0.160013 | 0.066440 |
| 0.025 | 0.615137 | 0.156613 | 0.064150 |
| 0.050 | 0.590180 | 0.131877 | 0.053783 |
| 0.0625 | 0.572693 | 0.115647 | 0.051620 |
| 0.1000 | 0.503290 | 0.061607 | 0.058523 |
| 0.2000 | 0.215653 | 0.034923 | 0.070210 |

## 5. Conclusions

We showed that by using pseudostates, it is possible to obtain good results for polarizabilities and hyperpolarizabilties for hydrogenic systems, energies of Rydberg states in the helium atoms and transition rates in hydrogen atoms. The present results obtained using pseudostates for μ = 0 agree with those obtained using elaborate wave functions. Since there is always the presence of a plasma at a particular electron temperature and density, the present results will be useful for comparison with observations. A detailed account of development of the field and possible applications is given in reference [10]. Using the perturbation theory, wave functions, polarizabilities and hyperpolarizabilities given here, the energies of various Rydberg states of any quantum numbers can easily be calculated in the Debye potential.

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