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Relativistic and QED corrections to the polarizability of helium

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Relativistic and leading QED corrections to the static electric dipole polarizability of helium are calculated. The resulting theoretical uncertainty is estimated to be under 2 ppm.

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The molar polarizability of a gas A_ϵ is related to the static electric dipole polarizability of the constituents of the gas α_0, the Avagadro constant N_{A}, and the permittivity of the vacuum ϵ_0 through

$$A_\epsilon = \frac{N_A \alpha_0}{3\epsilon_0}. \tag{1}$$

As N_A is known quite precisely [0.089 parts per million (ppm) relative uncertainty] [1], an accurate theoretical determination of α_0 allows a determination of the molar polarizability to that same accuracy. Experimental measurements of A_ϵ can then be used to either determine the Boltzmann constant k [2] or equivalently, establish pressure [3] or temperature [4] standards.

The most promising gas to use for this purpose is helium because of the relative simplicity of its wave function. However, to be useful for high accuracy work, not only must a nonrelativistic calculation be done, but in addition both relativistic and quantum electrodynamic corrections must be considered. While the nonrelativistic calculations have already been performed [5–7], there are discrepant results in the literature for the relativistic corrections [8,9], and no QED results have been presented for helium, although they have for heliumlike lithium [9]. It is the purpose of this paper to present a high accuracy determination of the relativistic corrections along with a calculation of the dominant QED term. The neglected QED is estimated to enter at under the 2 ppm level. As the uncertainty of k is presently 1.7 ppm, this is adequate until the experimental uncertainty described in Refs. [2, 3, and 4] is decreased by about an order of magnitude.

The static electric dipole polarizability of helium is denoted $\alpha_0(^4\mathrm{He})$. We will present results in terms of the related quantity

$$\alpha_0^*(^4\mathrm{He}) = \frac{\alpha_0(^4\mathrm{He})}{4\pi a_0^3(1+m_e/m_\alpha)^3}. \tag{2}$$

The Bohr radius a_0 and the electron to the α particle mass ratio m_e/m_α are known with negligible uncertainty. In the following we will refer to $\alpha_0^*(^4\mathrm{He})$ as α_{NR} and α_{MP} for the nonrelativistic case without and with mass polarization, respectively, and corrections to the polarizability as $\delta\alpha$.

We first treat the nonrelativistic problem without mass polarization, and evaluate

$$\alpha_{\mathrm{NR}} = \frac{2}{3}\left\langle 0 \left| (\boldsymbol{r}_1+\boldsymbol{r}_2)\frac{1}{H-E_0}(\boldsymbol{r}_1+\boldsymbol{r}_2) \right| 0 \right\rangle. \tag{3}$$

Here $|0\rangle$ represents the ground state of helium with energy E_0 and H is the nonrelativistic Hamiltonian. To carry out the numerical evaluation of α and corrections to it we follow the approach of Korobov [10] and use a basis set of the form

$$\phi(r_1,r_2,r_{12}) = \sum_{i=1}^{N} v_i[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} + (1\leftrightarrow 2)] \tag{4}$$

for the ground state and

$$\boldsymbol{\phi}(r_1,r_2,r_{12}) = \sum_{i=1}^{N} v_i[\boldsymbol{r}_1 e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} + (1\leftrightarrow 2)] \tag{5}$$

for singlet P states, with $\alpha_i, \beta_i, \gamma_i$ chosen in a random fashion between certain minimum and maximum values, as described in more detail by Korobov [10]. This basis set has the advantage that matrix elements for all operators can be easily derived in a compact form, though all numerics have to be treated in quadruple precision. By a careful choice of the range of the parameters high accuracy energies and wave functions can be obtained without the need for extrapolation; for example, with the largest basis set we use here, $N=900$, the ground-state energy is

$$E_0 = -2.903\,724\,377\,034\,119(1), \tag{6}$$

in agreement with the still far more accurate result of Korobov in [10]. The nonrelativistic polarizability, given by Eq. (3), was calculated by inverting the nonrelativistic Hamiltonian in the basis set of Eq. (5), with lengths of $N=100$, 300, 600, and 900; the results are tabulated in Table I. From the pattern of convergence shown there we assign an uncertainty of no more than 1 in the last digit of

$$\alpha_{\mathrm{NR}} = 1.383\,192\,174\,455(1). \tag{7}$$

This is in agreement with, though considerably more accurate than, the previous determinations given in Refs. [5, 6, and 7].

TABLE I. Helium static electric dipole polarizability: relativistic corrections in units of 10^{-6}.

Basis-set size	NR limit	H_{MP}	Orbit-orbit	$\delta(r_1)$	$\delta(r_{12})$	p^4
$N=100$	1.383 192 016 915	48.850	−23.229	862.179	65.941	−983.007
$N=300$	1.383 192 173 884	48.862	−23.234	864.754	66.053	−988.043
$N=600$	1.383 192 174 454	48.862	−23.234	864.664	66.070	−987.845
$N=900$	1.383 192 174 455	48.862	−23.234	864.678	66.071	−987.873

We next consider the effect of mass polarization, described by

$$H_{\mathrm{MP}}=\frac{\mu}{m_\alpha}\boldsymbol{p}_1\cdot\boldsymbol{p}_2. \tag{8}$$

We use $m_e/m_\alpha=0.000\,137\,093\,356\,11(29)$ from [1]: the mass factors in the above follow from scaling $\vec{p}_i\to\mu\vec{p}_i$ in the original term $\vec{p}_1\cdot\vec{p}_2/m_\alpha$ and working in reduced mass units. If this is included in the nonrelativistic Hamiltonian, we find

$$\alpha_{\mathrm{MP}}=1.383\,241\,008\,958(1), \tag{9}$$

in good agreement with Bhatia and Drachman's 1.383 241 014. Alternatively, one can treat mass polarization perturbatively. As shown in Table I, the answer rapidly converges to

$$\delta\alpha_{\mathrm{MP}}=0.000\,048\,862. \tag{10}$$

The small difference between α_{MP}, which is valid to all orders in m_e/m_α, and $\alpha_{\mathrm{NR}}+\delta\alpha_{\mathrm{MP}}$, which is valid only to first order in the mass ratio, is consistent with the neglect of second-order terms. The general formula we use for the perturbation due to an operator δH is

$$\delta\alpha=2\times\frac{2}{3}\left\langle\delta H\frac{1}{(E_0-H)'}(\boldsymbol{r}_1+\boldsymbol{r}_2)\frac{1}{H-E_0}(\boldsymbol{r}_1+\boldsymbol{r}_2)\right\rangle+\frac{2}{3}\left\langle(\boldsymbol{r}_1+\boldsymbol{r}_2)\frac{1}{H-E_0}(\langle\delta H\rangle-\delta H)\frac{1}{H-E_0}(\boldsymbol{r}_1+\boldsymbol{r}_2)\right\rangle. \tag{11}$$

The operators needed for the calculation of relativistic corrections to the ground state of helium are given by

$$H_{\mathrm{REL}}=-\frac{1}{8m^3}(p_1^4+p_2^4)+\frac{\pi\alpha}{m^2}\delta^3(r_{12})+\frac{Z\alpha\pi}{2m^2}[\delta^3(r_1)+\delta(r_2)]-\frac{\alpha}{2m^2}p_1^i\left(\frac{\delta_{ij}}{r_{12}}+\frac{r_{12}^ir_{12}^j}{r_{12}^3}\right)p_2^j. \tag{12}$$

We refer to the four terms of the above equation as p_1^4, $\delta(r_{12})$, $\delta(r_1)$, and orbit-orbit, respectively, and present their individual contributions in Table I. It is noticeable that the more singular operators have relatively slow convergence, though the uncertainty is well under the ppm level. The net result,

$$\alpha_{\mathrm{REL}}=-0.000\,080\,358(27), \tag{13}$$

is one of our main results. It is in fair agreement with [9], which quotes $-0.000\,080\,013$, but is somewhat discrepant with a relativistic configuration interaction calculation [8], which quotes $-0.000\,076\,5$.

We finally include QED effects. The formula for the Lamb shift in ground-state helium is given by

$$E_{\mathrm{QED}}=\left[\frac{164}{15}+\frac{14}{3}\ln\alpha\right]\frac{\alpha^2}{m^2}\langle\delta^3(r_{12})\rangle-\frac{14}{3}m\alpha^5\left\langle\frac{1}{4\pi}P\left(\frac{1}{(m\alpha r_{12})^3}\right)\right\rangle+\left[\frac{19}{30}+\ln(\alpha^{-2})-\ln k_0\right]\frac{4Z\alpha^2}{3m^2}\langle\delta^3(r_1)+\delta^3(r_2)\rangle. \tag{14}$$

Here P is defined through

$$\left\langle\phi\left|P\left(\frac{1}{r^3}\right)\right|\psi\right\rangle=\lim_{a\to0}\int d^3r\,\phi^*(\boldsymbol{r})\psi(\boldsymbol{r})\left[\frac{1}{r^3}\Theta(r-a)+4\pi\delta^3(r)(\gamma+\ln a)\right], \tag{15}$$

and the two-electron Bethe logarithm $\ln k_0$ has recently been accurately evaluated for the ground state [11] as

$$\ln k_0(1^1S_0)=-4.370\,160\,2. \tag{16}$$

If it were correct to write $E_{\mathrm{QED}}=\langle\delta H_{\mathrm{QED}}\rangle$, the calculation of QED corrections would simply involve using δH_{QED} in Eq. (11). The only new term is the distribution P, as the δ function operators have already been treated in the relativistic calculation. We find

$$\delta\alpha_{\mathrm{QED}}=0.000\,030\,474(1). \tag{17}$$

However, this treatment is only an approximation, because the Bethe logarithm does not arise from an operator proportional to $\delta^3(r_1)+\delta^3(r_2)$, but instead is defined by

$$\ln k_0=\frac{1}{D}\left\langle(\boldsymbol{p}_1+\boldsymbol{p}_2)(H-E)\ln\left[\frac{2(H-E)}{\alpha^2m}\right](\boldsymbol{p}_1+\boldsymbol{p}_2)\right\rangle, \tag{18}$$

$$D=2\pi\alpha Z\langle\delta^3(r_1)+\delta^3(r_2)\rangle. \tag{19}$$

An exact treatment will require evaluating the second-order correction to Eq. (18) due to a static electric field. We estimate the uncertainty to be of order of 10% of the total $\ln k_0$ contribution, which leads to a 2 ppm uncertainty in the final result. We have checked that corrections to the equation we use for the effect of QED, Eq. (14), enter in higher order in the fine-structure constant α. It is an amusing, but presumably accidental fact, that the mass polarization, relativistic, and QED corrections calculated here cancel out almost completely in the final result, which is

$$\alpha = 1.383\,191(2). \tag{20}$$

As mentioned in the Introduction, this means that the molar polarizability of helium is now theoretically determined with an uncertainty under 2 ppm, which will, when combined with expected experimental advances, allow the determination of the Boltzman constant and pressure and temperature standards with very high accuracy.

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