Polarizability and tune-out wavelength for the helium 1s2s ^{3}S state

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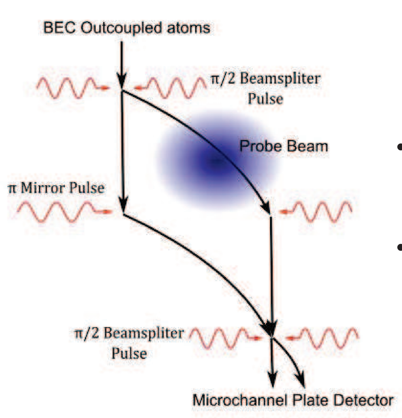
Motivation

- Find new ways to detect and test quantum electrodynamic (QED) effects in atoms, other than energy differences (Lamb shift).
- So-called "tune-out" wavelengths can be measured to very high precision, and compared with theory.
- the tune-out wavelength is determined primarily by the frequency-dependent polarizability. It is the wavelength (or equivalent frequency) where the frequency-dependent polarizability vanishes.

Experiment



- Michelson Interferometer
- Sensitive to QED effects

4

in collaboration with Ken Baldwin [1] (experiment, Australian National University), and Li-Yan Tang [2] (relativistic theory, Wuhan Institute of Physics and Mathematics).

Polarizability Theory

Static Field Case

Interaction potential with an external electric field of strength F in the z-direction is $V = -eFz$. The second-order interaction energy is $\Delta E^{(2)} = -\alpha_D^1 F^2$ where

$$\alpha_D = 2e^2 \sum_n \frac{|\langle \psi_0 \mid z \mid \psi_n \rangle|^2}{E_n - E_0}$$

summed over all intermediate states n, where α_D is the dipole polarizability and $H_0\psi_n = E_n\psi_n$ is the unperturbed eigenvalue problem.

Oscillating Field Case

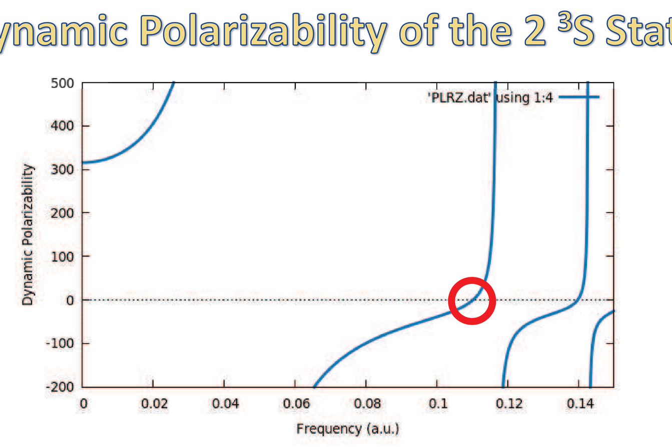
If the electric field is oscillating with frequency ω, the frequency-dependent (or dynamic) polarizability is

$$\alpha_D(\omega) = 2e^2 \sum_n \frac{(E_n - E_0)|\langle \psi_0 \mid z \mid \psi_n \rangle|^2}{(E_n - E_0)^2 - (\hbar\omega)^2}$$

The Tuneout Wavelength

The tuneout wavelengths correspond to the frequencies where $\boldsymbol{\alpha(\omega) = 0}$.

Dynamic Polarizability of the 2 ^{3}S State



Nonrelativistic tune-out wavelength with mass polarization

$\lambda = 413.082\,574\,821\,912(73)$ nm

9

Resonances correspond to the $1s2s\,^3S - 1s2p\,^3P$, $1s2s\,^3S - 1s3p\,^3P$, $1s2s\,^3S - 1s4p\,^3P$, $\cdots$ transition frequencies.

TABLE 1. Contributions to the static dipole polarizability and their orders of magnitude (in units of a_0^3, where a_0 is the Bohr radius).

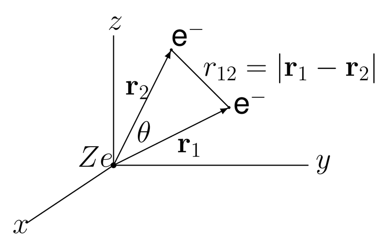
Magnitude	Physical origin
unity	nonrelativistic Schrödinger equation
$\mu/M \simeq 10^(-4)$	mass pol. operator $-(\mu/M)\nabla_1 \cdot \nabla_2$
$\alpha^2 \simeq 10^{-4}$	Breit interaction
$\alpha^2\mu/M \simeq 10^{-7}$	Relativistic recoil + Stone term
$\alpha^3 \simeq 10^{-6}$	QED terms (not yet calculated)

Two Theoretical Aproaches

1. **Present work – nonrelativistic:** Begin with the nonrelativistic Schrödinger equation, and include relativistic effects of relative $O(Z\alpha^2)$ by perturbation theory, where $\alpha \simeq 1/137.03599976$ is the fine structure constant.
   Advantage: Hylleraas coordinates allow accurate calculation of electron correlation effects.
2. **Zhang et al. [2] – relativistic:** Begin with the relativistic Dirac equation, including the electron-electron interaction, and treat electron correlation by means of configuration interaction.
   Advantage: Automatically includes higher-order one-electron relativistic corrections, but correlation effects are more slowly convergent.

Calculations

Wave Functions



The Hamiltonian in atomic units is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \frac{\mu}{M}\nabla_1 \cdot \nabla_2$$

where the last term is the mass polarization term, and μ is the electron reduced mass. Expand

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i,j,k} a_{ijk}\, r_1^i r_2^j r_{12}^k\, e^{-\alpha r_1 - \beta r_2}\, \mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \pm \mathbf{1} \leftrightarrow \mathbf{2}$$

(Hylleraas, 1929), with $i + j + k \le \Omega$, $\ \Omega = 1,\ 2,\ 3,\ \cdots$.

Pseudospectral Representation of Intermediate P-states

Replace the summation over the complete set of intermediate P-states (including an integration over the continuum) by a discrete summation over the set of N pseudostates obtained by diagonalizing the Hamiltonian in an N-dimensional basis set of P-states.

TABLE 2. Convergence study for the nonrelativistic tune-out wavelength λ. N is the number of terms in the basis set.

N	λ (nm)	Difference (nm)
140	413.082 328 731 87	
190	413.082 581 514 32	0.000 252 782 45
246	413.082 578 777 26	–0.000 002 737 06
315	413.082 575 775 67	–0.000 003 001 59
393	413.082 574 808 89	–0.000 000 966 78
485	413.082 574 887 63	0.000 000 078 74
587	413.082 574 836 65	–0.000 000 050 98
705	413.082 574 825 76	–0.000 000 010 89
843	413.082 574 823 05	–0.000 000 002 71
981	413.082 574 822 39	–0.000 000 000 66
1140	413.082 574 822 16	–0.000 000 000 23
1319	413.082 574 821 98	–0.000 000 000 18
1906	413.082 574 821 91	–0.000 000 000 07

The Breit Interaction and Relativistic Recoil

The Breit interaction B comes from lowest-order relativistic corrections (in atomic units)

$$B = \alpha^2 \sum_{i=1}^{2} \left[-\frac{1}{8}\nabla_i^4 + \frac{\pi Z}{2}\delta(\mathbf{r}_i) \right] + \cdots$$

The "Stone" term (after A.P. Stone) of order $\alpha^2\mu/M$ comes from transforming the Breit interaction to c.m. plus relative coordinates.

$$\tilde{\Delta}_2 = \frac{Z\alpha^2}{2}\frac{\mu}{M}\left\{ \frac{1}{r_1}(\nabla_1 + \nabla_2)\cdot\nabla_1 + \frac{1}{r_1^3}\mathbf{r}_1 \cdot [\mathbf{r}_1 \cdot (\nabla_1 + \nabla_2)]\nabla_1 \right\}$$
$$+\, 1 \leftrightarrow 2$$

Lowest order QED corrections come from the Lamb shift operator

$$\delta H_{\rm QED} = \frac{4Z\alpha^3}{3}\left[\frac{19}{30} - \ln(Z\alpha)^2 - \ln k_0\right]\left[\delta^3(\mathbf{r}_1) + \delta^3(\mathbf{r}_2)\right] - \frac{14\alpha^3}{3}Q$$

where $Q = (4\pi r_{12}^3)^{-1}_{PV}$ and $\ln k_0$ is the Bethe logarithm.

Results

TABLE 3. Nonrelativistic, relativistic, and finite-mass contributions to the static dipole polarizability for the ^{4}He $1s2s\ ^3S$ state, including relativistic recoil of order $\alpha^2\mu/M$.

Terms included	$\alpha_D\ (a_0^3)$	Zhang [2]
Nonrelativistic	315.820 349 9468(2)	315.820 4(2)
NR + Rel. $(M = 0)$	315.716 003(2)	315.716 05(1)
NR + Rel. $(M = \pm 1)$	315.724 297(2)	315.724 38(1)
α^3 QED	0.006 885 12	0.006 895 171
α^4 QED	0.000 119 876 [a]	0.000 119 876
$\alpha^3\,\delta\ln(k_0)$ [b]	0.000 07(1) [a]	0.000 07(1)
Nuclear size	0.000 004 58 [a]	0.000 004 58
Total $(M = 0)$	315.723 08(1)	315.723 14(4)
Total $(M = \pm 1)$	315.731 38(1)	315.731 47(4)

[a] From Zhang et al. [2] and private communication.
[b] Additional field correction to the Bethe logarithm (estimate).

TABLE 4. Nonrelativistic, relativistic, QED, and finite-mass contributions to the static dipole polarizability for the ^{4}He $1s^2\ ^1S$ state.

Terms included	$\alpha_D\ (a_0^3)$	Other
NR infinite mass	1.383 241 008 9569(7)	1.383 241 008 958(1) [a]
NR finite mass	1.383 809 986 4008(7)	1.383 809 986 408(1) [b]
Rel. Breit corr. [c]	–0.000 080 359 7(3)	–0.000 080 358(27) [a]
α^3 QED	0.000 030 473 78(8)	0.000 030 474(1)

[a] Sapirstein and Pachucki [3].
[b] Puchalski et al. [4].
[c] For comparison, does not include relativistic recoil.

TABLE 5. Nonrelativistic, relativistic, and finite-mass contributions to the tuneout wavelength for the ^{4}He $1s2s\ ^3S$ state, including relativistic recoil of order $\alpha^2\mu/M$.

Terms included	λ_t (nm)	Zhang [2]
Nonrelativistic	413.038 304 39(4)	413.820 4(2)
NR + Rel. $(M = 0)$	413.079 958(2)	413.080 00(1)
NR + Rel. $(M = \pm 1)$	413.085 828(2)	413.085 89(1)
α^3 QED	0.004 1531	0.004 145 555(2)
α^4 QED	0.000 072 077 [a]	0.000 072 077
$\alpha^3\,\delta\ln(k_0)$	0.000 04(1) [a]	0.000 04(1)
Nuclear size	0.000 002 75 [a]	0.000 002 75
Total $(M = 0)$	413.084 23(1)	413.084 26(4)
Total $(M = \pm 1)$	315.090 10(1)	413.090 15(4)

[a] From Zhang et al. [2] and private communication.

Conclusions

- Very high precision has been obtained for the lowest-order nonrelativistic tune-out wavelength, including mass polarization and relativistic corrections.
- Good agreement has been obtained with the less accurate calculations of Zhang et al. [2] obtained by the relativistic CI method, except for the QED corection of $O(\alpha^3)$, where there appears to be a significant discrepancy (see Tables 3 and 5). As a check, we obtain good agreement with the corresponding QED correction to the polarizability [3,4] for the $1s^2\ ^1S$ state, as shown in Table 4.
- The results provide a firm foundation for the interpretation of high precision measurements of the tune-out wavelength currently in progress at ANU .

Acknowledgments

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References

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