Tune-out Wavelength for the 1s2s ^{3}S – 1s3p ^{3}P Transition of helium: relativistic effects

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Outline

- Introduction – what is a ”tune-out” wavelength?
- Historical background
- Dipole response theory
- Pseudostate expansions
- Helium wave functions
- Relativistic and QED corrections
- Results and discussion

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 (in collaboration with Ken Baldwin, ANU), and compared with our 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.
- The polarizability in turn is determined by dipole matrix elements, as well as transition energies.

History

- First noted by LeBlanc and Thywissen (PRA **75**, 053612 (2007) in connection with species-specific optical lattices for alkali metals.

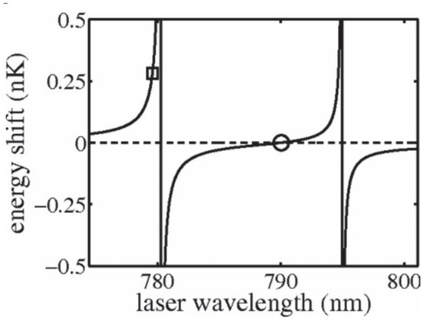


Figure 1

Energy shift as a function of wavelength for ^{87}Rb in the $|F, m_F\rangle = |2, 2\rangle$ state, under linear polarization, for

- Helium $2\,^3S - 3\,^3P$ experiment suggested by Jim Mitroy and Li-Yan Tang, Phys. Rev. A **88**, 052515 (2013).

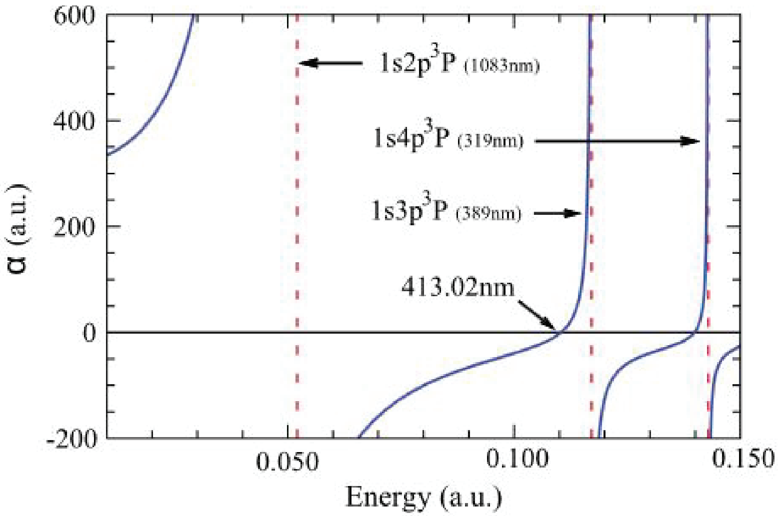
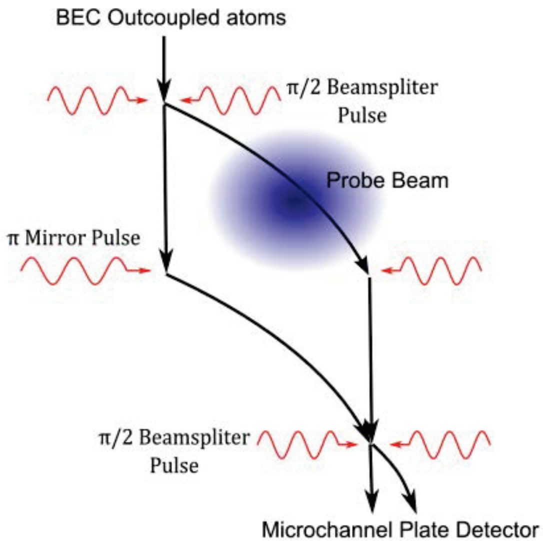


FIG. 1 (color online). Helium polarizability spectrum (solid curves) as a function of energy (a.u.). Triplet transition manifold positions are shown by the dotted vertical lines.

Experiment



- Michelson Interferometer
- Sensitive to QED effects

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

[1] B. M. Henson, R. I. Khakimov, R. G. Dall, K. G. H. Baldwin, L.-Y. Tang, and A. G. Truscott, Phys. Rev. Lett. 115, 043004 (2015).
[2] Y.-H. Zhang, L.-Y. Tang, X.-Z. Zhang, and T.-Y. Shi, Phys. Rev. A 93, 052516 (2016).

From standard dipole response theory, the frequency-dependent polarizability is

$$\begin{aligned}\alpha_{\rm d}(\omega) &= 2e^2 \sum_{n\neq 0}^{\infty} \frac{(E_n - E_0)\,\langle\psi_0|\hat{\boldsymbol{\epsilon}}^{\,*}\cdot\mathbf{r}|\psi_n\rangle\langle\psi_n|\hat{\boldsymbol{\epsilon}}\cdot\mathbf{r}|\psi_0\rangle}{(E_n - E_0)^2 - (\hbar\omega)^2} \\ &= \frac{\hbar^2 e^2}{m_{\rm e}} \sum_{n\neq 0}^{\infty} \frac{f_{0,n}}{(E_n - E_0)^2 - (\hbar\omega)^2}\end{aligned}$$

where

$$f_{0,n} = \frac{2m_{\rm e}}{\hbar^2}(E_n - E_0)|\langle\psi_n|\hat{\boldsymbol{\epsilon}}\cdot\mathbf{r}|\psi_0\rangle|^2$$

is the oscillator strength for the $0 \to n$ transition.

Two options:

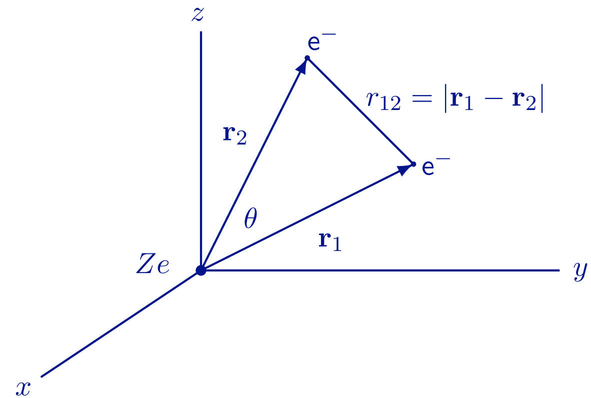
- Use experimental data for the oscillator strengths.
- Introduce a discrete variational basis set to construct a pseudospectrum to represent the intermediate states.

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)

Nonrelativistic Polarization Theory

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 $i + j + k \le \Omega, \quad \Omega = 1,\ 2,\ 3,\ \cdots$.

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.

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 but correlation effects are much more slowly convergent, and finiet nuclear mass effects are difficult to calculate.

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

$$\begin{aligned}\alpha_{\mathrm{D}}(\omega) &= 2e^2 \sum_{n\neq 0} \frac{(E_n - E_0)|\langle 0 \mid z \mid n\rangle|^2}{(E_n - E_0)^2 - (\hbar\omega)^2} \\ &= 0\end{aligned}$$

Relativistic Corrections to the Dynamic Polarizability

Terms of second order in the external electric field and first-order in H_{rel} are

$$\alpha_{\mathsf{D,rel}}(\omega) = \sum_{n,n'\neq 0}\left[\frac{-2(E_{n'}-E_0)\langle 0|H_{\mathsf{rel}}|n\rangle\langle n|z|n'\rangle\langle n'|z|0\rangle}{(E_n-E_0)[(E_{n'}-E_0)^2+\omega^2]} + \frac{\langle 0|z|n'\rangle\langle n'|(\langle H_{\mathsf{rel}}\rangle - H_{\mathsf{rel}})|n\rangle\langle n|z|0\rangle[(E_{n'}-E_0)(E_n-E_0)+\omega^2]}{[(E_n-E_0)^2-\omega^2][(E_{n'}-E_0)^2-\omega^2]}\right]$$

The Breit Interaction and Relativistic Recoil

The Breit interaction $H_{\text{rel}} = B$ comes from lowest-order relativistic corrections (in atomic units)

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

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.

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

$$+ 1 \leftrightarrow 2$$

QED Corrections

Include the additional "Lamb shift" type perturbations

$$
\begin{aligned}
C_1 &= \frac{8\alpha^3}{3}\left(\frac{19}{30} - 2\ln\alpha - \ln k_0\right)[\delta(r_1) + \delta(r_2)] \\
C_2 &= \alpha^3\left(\frac{164}{15} + \frac{14}{3}\ln\alpha\right)\delta(r_{12}) \\
C_3 &= -\frac{7\alpha^3}{6\pi}\left(\frac{1}{r_{12}^3}\right)_{\text{PV}}
\end{aligned}
$$

in the same way as the relativistic corrections, where $\ln k_0$ is the Bethe logarithm (approximate by the field-free value).

Results

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.	–0.000 080 359 7(3)	–0.000 080 358(27)[a]
Total[c]	1.383 729 626 7(3)	

[a] Sapirstein and Pachucki [3].

[b] Puchalski et al. [4].

[c] Does not include relativistic recoil.

Contributions to the static dipole polarizability for the ^{4}He $1s2s\ ^3S$ state.

Contribution	Present work (a_0^3)	Relativistic CI[a] (a_0^3)
Nonrelativistic	315.631 472 3765(2)	315.631 5(2)
	315.631 468(12)[b]	
Finite Mass with Mass Scaling	0.188 877 5703(3)	0.188 9(3)
Relativistic $(m=1)$	–0.095 967 12(3)	–0.095 6(3)
Rel. (Finite Mass)$(m=1)$	0.000 010 70(3)	
Stone term $\tilde{\Delta}_2$	–0.000 075 659 571(1)	
Total $(m=1)$	315.724 296 422(11)	315.724 8(4)

[a] Y.-H. Zhang, L.-Y. Tang, X.-Z. Zhang, and T.-Y. Shi, Phys. Rev. A **93**, 052516 (2016).

[b] Z.-C. Yan and J. F. Babb, Phys. Rev. A **58**, 1247 (1998).

Contributions to the tune-out wavelength for the ^{4}He $1s2s\ ^3S$ state.

Contribution	Present work (nm)	Relativistic CI (nm)
Nonrel. (inf. mass)	413.038 304 399(3)	413.038 28(3)
Nonrel. (finite mass)	0.100 917 093(7)	0.100 91(5)
Breit terms	–0.055 307 35(11)	
Spin-dependent (M=1)	0.001 955 58(16)	
Stone term $\tilde{\Delta}_2$	–0.000 044 47(17)	
Total $(M=1)$	413.085 825 25(12)	413.085 9(4)

Tune-out wavelength for the ^{4}He $1s2s\ ^3S$ state: Summary

Contribution	Tune-out Wavelength (nm)
Nonrelativistic + relativistic theory	413.085 825 25(12)
QED (estimate)	0.009 1(10)
Total $(m=1)$	413.094 9(10)
Experiment	413.093 8(9$_{\text{stat}}$)(20$_{\text{sys}}$)

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.
- Relativistic recoil corrections and the Stone term of order $\alpha^2\mu/M$ a.u. have been calculated for the first time and shown to be important relative to the QED corrections to be studied.
- Ultimately, the best precision will be obtained by combining the nonrelativistic Hylleraas approach for the electron correlation part with the relativistic CI approach for the higher-order relativistic corrections.
- 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

[1] B. M. Henson, R. I. Khakimov, R. G. Dall, K. G. H. Baldwin, L.-Y. Tang, and A. G. Truscott, Phys. Rev. Lett. 115, 043004 (2015).

[2] Y.-H. Zhang, L.-Y. Tang, X.-Z. Zhang, and T.-Y. Shi, Phys. Rev. A 93, 052516 (2016).

[3] J. Sapirstein and K. Pachucki, Phys. Rev. A **63**, 012504, (2000).

[4] M. Puchalski, K. Piszczatowski, J. Komasa, B. Jeziorski, and K. Szalewicz, Phys. Rev. A **93**, 032515 (2016).