

# Special Topics on Precision Measurement in Atomic Physics: Lecture 5

## Mass Polarization and Finite Nuclear Mass Effects

Instructor: Gordon W.F. Drake, University of Windsor

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In previous lectures the nucleus was assumed to be infinitely heavy, thereby providing an inertial frame of reference. The next level of approximation is to take into account the finite mass  $M$  of the nucleus relative to the much smaller electron mass  $m_e$ . The nucleus then moves in the centre-of-mass frame, and its motion must be included in the overall dynamics of the full three-body problem. This introduces an additional term into the Hamiltonian called *mass polarization*, and produces what is called the *specific isotope shift*, in addition to an overall rescaling of all the energies, called the *normal isotope shift*.

The Hamiltonian in an inertial frame as shown in Fig. 1 is

$$H = -\frac{\hbar^2}{2M}\nabla_{\mathbf{X}}^2 - \frac{\hbar^2}{2m}\nabla_{\mathbf{x}_1}^2 - \frac{\hbar^2}{2m}\nabla_{\mathbf{x}_2}^2 - \frac{Ze^2}{|\mathbf{X} - \mathbf{x}_1|} - \frac{Ze^2}{|\mathbf{X} - \mathbf{x}_2|} + \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|} \quad (1)$$

with coordinate  $\mathbf{X}$  for the nucleus and  $\mathbf{x}_1$  and  $\mathbf{x}_2$  for the two electrons. In the absence of external fields, the motion of the centre-of-mass is then an ignorable coordinate that can be eliminated by transforming to centre-of-mass plus relative coordinates  $\mathbf{R}$ ,  $\mathbf{r}_1$ ,  $\mathbf{r}_2$  according to

$$\begin{aligned} \mathbf{R} &= \frac{M\mathbf{X} + m\mathbf{x}_1 + m\mathbf{x}_2}{M + 2m} \\ \mathbf{r}_1 &= \mathbf{X} - \mathbf{x}_1 \\ \mathbf{r}_2 &= \mathbf{X} - \mathbf{x}_2 \end{aligned} \quad (2)$$

The transformed Hamiltonian is then

$$H = -\frac{\hbar^2}{2\mu}\nabla_{r_1}^2 - \frac{\hbar^2}{2\mu}\nabla_{r_2}^2 - \frac{\hbar^2}{M}\nabla_{r_1} \cdot \nabla_{r_2} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (3)$$

where  $\mu = \frac{m_e M}{m_e + M}$  is the electron reduced mass. It is then convenient to

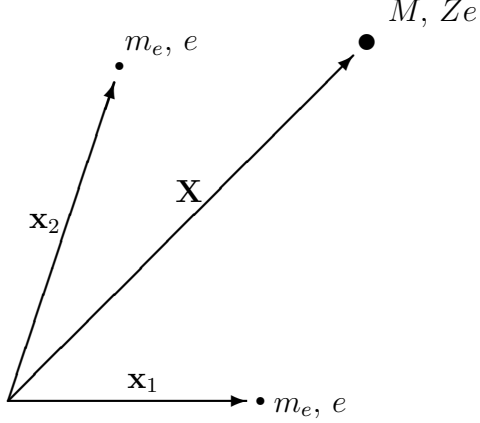


Figure 1: Inertial coordinate system for the full three-body problem of a helium nucleus of mass  $M$  and two electrons of mass  $m_e$ .

express distances and energies in mass-scaled atomic units according to

$$\boldsymbol{\rho} = \mathbf{r}/a_\mu \quad (4)$$

$$\mathcal{E} = E/(e^2/a_\mu) \quad (5)$$

where  $a_\mu = \frac{\hbar^2}{\mu e^2}$  is the reduced mass Bohr radius, and  $\frac{e^2}{a_\mu} = 2R_\mu = 2\frac{\mu}{m_e}R_\infty = 2\left(1 - \frac{\mu}{M}\right)R_\infty$  is the reduced-mass unit of energy. The Schrödinger equation is then (in these mass-scaled atomic units)

$$\left\{ -\frac{1}{2}\nabla_{\rho_1}^2 - \frac{1}{2}\nabla_{\rho_2}^2 - \frac{\mu}{M}\nabla_{\rho_1} \cdot \nabla_{\rho_2} - \frac{Z}{\rho_1} - \frac{Z}{\rho_2} + \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|} \right\} \Psi = \mathcal{E}\Psi \quad (6)$$

In this form, it is formally identical to the Schrödinger equation with the infinite mass Hamiltonian except for the additional mass-polarization term

$$H_{\text{MP}} = -\frac{\mu}{M}\nabla_{\rho_1} \cdot \nabla_{\rho_2} \quad (7)$$

If the ratio  $\mu/M$  is small, then  $H_{\text{MP}}$  can be treated by perturbation theory with the perturbation expansions

$$\Psi = \Psi_0 + \frac{\mu}{M}\Psi_1 + \left(\frac{\mu}{M}\right)^2\Psi_2 + \dots \quad (8)$$

$$\mathcal{E} = \mathcal{E}_0 + \frac{\mu}{M}\mathcal{E}_1 + \left(\frac{\mu}{M}\right)^2\mathcal{E}_2 + \dots \quad (9)$$

The zero-order problem is the Schrödinger equation for infinite nuclear mass

$$\left\{ -\frac{1}{2}\nabla_{\rho_1}^2 - \frac{1}{2}\nabla_{\rho_2}^2 - \frac{Z}{\rho_1} - \frac{Z}{\rho_2} + \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|} \right\} \Psi_0 = \mathcal{E}_0 \Psi_0 \quad (10)$$

The so-called “normal” isotope shift corresponds to a uniform shift of all the energies by the common scale factor

$$\Delta E_{\text{normal}} = -\frac{\mu}{M} \left( \frac{\mu}{m} \right) \mathcal{E}_0 \quad 2R_\infty \quad (11)$$

correct to all orders in  $\mu/M$ . On the other hand, the first-order “specific” isotope shift due to  $H_{\text{MP}}$  is different for every state. In first-order, it is given by the expectation value

$$\Delta E_{\text{specific}}^{(1)} = \frac{\mu}{M} \left( \frac{\mu}{m} \right) \mathcal{E}_1 \quad 2R_\infty \quad (12)$$

with  $\mathcal{E}_1 = -\langle \Psi_0 | \nabla_{\rho_1} \cdot \nabla_{\rho_2} | \Psi_0 \rangle$ , and the second-order specific isotope shift is

$$\Delta E_{\text{specific}}^{(2)} = \left( \frac{\mu}{M} \right)^2 \left( \frac{\mu}{m} \right) \mathcal{E}_2 \quad 2R_\infty \quad (13)$$

with  $\mathcal{E}_2 = -\langle \Psi_0 | \nabla_{\rho_1} \cdot \nabla_{\rho_2} | \Psi_1 \rangle$  and  $\Psi_1$  satisfies the first-order perturbation equation

$$(H_0 - \mathcal{E}_0) | \Psi_1 \rangle - \nabla_{\rho_1} \cdot \nabla_{\rho_2} | \Psi_0 \rangle = \mathcal{E}_1 | \Psi_0 \rangle \quad (14)$$

The advantages of organizing the problem in this way are two-fold. First, it provides a clear separation between the trivially calculated normal isotope shift due to the mass-scaling of the energies, and the specific isotope shift due to the mass polarization term. Second, once the coefficients  $\mathcal{E}_0$ ,  $\mathcal{E}_1$  and  $\mathcal{E}_2$  are evaluated, the energy for any isotope  $M$  of helium can be accurately calculated according to

$$E_M = \frac{\mu}{m_e} \left[ \mathcal{E}_0 + \frac{\mu}{M} \mathcal{E}_1 + \left( \frac{\mu}{M} \right)^2 \mathcal{E}_2 + O(\mu/M)^3 \right] \quad (15)$$

Since  $\mu/M \sim 1.370\,745\,620 \times 10^{-4}$  for  ${}^4\text{He}$ , the next term is of order  $(\mu/M)^3 \sim 10^{-12}$ , and so is negligible for most purposes. If higher accuracy is needed, then the mass polarization term can be included explicitly in the nonrelativistic Hamiltonian and the total energy calculated directly for a specific

isotope. As an example, the coefficients for the ground state of helium are

$$\begin{aligned}\mathcal{E}_0 &= -2.903\,724\,377\,044\,1195 \\ \mathcal{E}_1 &= 0.159\,069\,475\,085\,84 \\ \mathcal{E}_2 &= -0.470\,391\,870(1)\end{aligned}$$

Note that since  $\nabla_{\rho_1} \cdot \nabla_{\rho_2}$  has the same angular properties as  $\rho_1 \cdot \rho_2$ , the operator is like the product of two dipole operators. For product type wave functions of the form

$$\psi = \psi_{1s}(\mathbf{r}_1)\psi_{nl}(\mathbf{r}_2) \pm \text{exchange} \quad (16)$$

(such as the Hartree-Fock approximation) the matrix element vanishes for all but the exchange term for  $P$ -states. The following table illustrates the point for the  $n = 2$  states of helium.  $\mathcal{E}_1$  is an order of magnitude bigger for the  $P$ -states than for the  $S$ -states. In contrast, the values of  $\mathcal{E}_2$  are similar in magnitude.

First- and second-order mass polarization coefficients  
 $\mathcal{E}_1 = -\langle \Psi_0 | \nabla_{\rho_1} \cdot \nabla_{\rho_2} | \Psi_0 \rangle$  and  $\mathcal{E}_2$  for the  $n = 2$  states of  
helium (in a.u.)

State	$\mathcal{E}_1$	$\mathcal{E}_2$
$2^1S$	0.009 503 864 419 29(1)	-0.135 276 865 15(4)
$2^3S$	0.007 442 130 706 02(0)	-0.057 495 846 2(19)
$2^1P$	0.046 044 524 928 44(8)	-0.168 271 322 5(5)
$2^3P$	-0.064 572 425 026 89(2)	-0.204 959 898 4(12)

Because of the special importance of the  $\nabla_1 \cdot \nabla_2$  term for  $P$ -states, we include  $p(1)s(2)$ -type terms in the basis set; i.e. the angular momenta are interchanged while keeping the nonlinear parameters the same.

Similar results for all states of helium up to  $n = 10$  and  $L = 7$  are given in G.W.F. Drake and Z.-C. Yan, Phys. Rev. A **46**, 2378 (1992), and in Chapter 11 of the Springer Atomic, Molecular and Optical Physics Handbook.