Special Topics on Precision Measurement in Atomic Physics

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Syllabus (tentative):

1. Basic concepts of atomic structure
2. Overview of theoretical techniques (H.F, C.I., MBPT, Hylleraas)
3. Variational methods for helium and lithium
4. Hylleraas coordinates
5. Mass polarization and finite nuclear mass effects
6. High precision results for nonrelativistic energies: helium
7. High precision results for nonrelativistic energies: lithium
8. Relativistic corrections
9. Quantum electrodynamic effects
10. Angular momentum algebra, 3-j, 6-j and 9-j symbols
11. Applications to states of high angular momentum
12. Applications to radiative transitions
13. Forbidden transitions
14. Two-photon processes
15. Tune-out wavelengths

Favourite text book references:

1. Quantum Mechanics of One- and Two-Electron Atoms, Hans E. Bethe and E.E. Salpeter (Springer, 1957, reprinted as a Dover publication 2008).

2. Angular Momentum in Quantum Mechanics, A.R. Edmonds (Princeton University Press, 1957).

3. Angular Momentum, D.M. Brink and G.R. Satchler (Clarendon Press, Oxford, 1968).

4. Quantum Electrodynamics, A.I. Akhiezer and B.V. Berestetskii (Interscience, New York, 1965).

5. Handbook of Atomic, Molecular and Optical Physics, G.W.F. Drake, edi-

tor (Springer, New York, 2006). A new revised edition is in preparation.

Web pages:

1. http://drake.sharcnet.ca (web:Sharcnet)
2. https://www.dropbox.com/sh/6tazo7lgftbv2od/AADyz0IXBe-xs2Itv7l590vua?dl=0 (web:Dropbox)

1 Basic concepts of atomic structure

MOTIVATION: oldest part of modern physics, so why is atomic physics (or more generally AMO physics) still of interest?

Two basic answers:

1. searches for new physics beyond the Standard Model. New particle accelerators are becoming more and more expensive to build in the search for new particles, and clues about dark matter and dark energy. High precision measurements (and comparisons with high precision theory) can put constraints on possible extensions to the Standard Model.

   Examples are

   - the anomalous magnetic moment $(g-2)$
   - proton size anomaly (depends on both Rydberg constant and proton charge radius r_p)
   - electron electric dipole moment (violation of CPT)
   - cosmological variation of the fundamental constants (especially the fine structure constant α)
   - electron to proton mass ratio m/M from H_2 spectroscopy
   - tests of Lorentz invariance
   - measurements of nuclear charge radius (isotope shift)

2. (ii) applications to plasma physics and astrophysics for both plasma modelling and plasma diagnostics. Spectroscopic observations of line intensi-

ties together with theoretical data determine the temperature and pressure conditions inside the plasma. Especially important for Tokomaks and controlled fusion.

- vast need to radiative transition probabilities (oscillator strengths, Einstein A-coefficients) and collision cross sections. These determine the RATES of processes, as opposed to energy levels.

UNCERTAINTIES In both cases, it is essential to know the uncertainties of associated with theoretical calculations. This has been the usual expectation for experimental data, but not necessarily for theoretical calculations, but the culture is changing. Uncertainty quantification (UQ) has become a hot topic. See Chung et al., J. Phys. D: Appl. Phys. **49**, 363002 (2016). Without uncertainties, it is like using a thermometer that has not been calibrated. To quote Alexander Kramida (NIST), "To publish a number without an uncertainty is a crime against humanity!"

HISTORY

- 1900 Max Planck's explanation of black-body radiation
- 1905 Photoelectric effect: radiation is emitted and absorbed in units of $E = h\nu$, where
  h =Planck's constant and
  ν = frequency of the radiation.
  This is the exact opposite of a classical wave where energy $\propto |\text{amplitude}|^2$, independent of frequency!
- 1911 Rutherford scattering experiment: atom with nucleus.
- 1915 Bohr model of the atom. $E_i - E_f = h\nu$. Theoretical spectroscopy was born.
- 1925 Schroedinger equation - why E_i and E_f?
- 1928 Dirac equation (relativity + QM)
- 1928 Hylleraas coordinates for helium → first nontrivial test of the Schroedinger equation for a system more complicated than hydrogen.

- 1929 Slater determinant for antisymmetric wave functions
- 1929 Breit interaction for relativistic electron-electron interaction

By 1930, the ground work was laid for theoretical atomic physics.

ROLE OF SYMMETRY

- **Noether's Theorem** (1918): to every symmetry property of a physical system there is a corresponding conservation law.
- For example, from Hamilton's equations of motion,

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i} \\ \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \text{and so } p_i &= \text{const. if } \quad \frac{\partial H}{\partial q_i} = 0. \end{aligned}$$

- In QM, only those things that are conserved can be quantized.
- Group Theory provides the QM labels (quantum numbers) to label the stages of a quantum system.

  > To every N-fold degenerate eigenvalue of the Schroedinger equation, there corresponds an N-dimensional irreducible representation of the symmetry group that commutes with the Hamiltonian H. The group labels are the quantum numbers. For example, n, l, m for hydrogen

  For further discussion about group theory, see *Pages 1-4 Spectroscopy 1a* and *Pages 5-10 Spectroscopy 1b* in web:Sharcnet Lecture Notes.

SCHROEDINGER EQUATION FOR HYDROGEN ATOM

- $H = T + V$ (ordinary conservative systems)

- Substitute $p \to \frac{\hbar}{i}\nabla$ to form a wave equation

$$H\Psi = E\Psi$$

with

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

in SI units, with ϵ_0 = vacuum permittivity.

- Solutions are of the form

$$\begin{aligned} \Psi &= R_{nl}(r)Y_l^M(\theta,\phi) \\ &= \text{(radial function)} \times \text{(angular function)} \end{aligned}$$

DIRAC EQUATION

- Obtain by linearizing the relativistic energy-momentum connection

$$E^2 = c^2p^2 + m^2c^4$$

to obtain the corresponding wave equation (see Homework problem 2)

$$\left[c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V(r)\right]\Psi = E\Psi$$

- Amazingly successful. Predicted the g-factor of 2 for the electron, and the existence of antimatter from the negative energy solutions.

ATOMIC UNITS

- Solve equations in atomic units with $e = \hbar = m_e = 1$. The Bohr radius is then

$$a_0 = \frac{\hbar^2}{me^2} = 5.291\,772\,109\,03(80) \times 10^{-11} \text{ m}$$

and the atomic unit of energy is

$$\begin{aligned} E_h &= \frac{e^2}{a_0} \\ &\mathit{or}\ \frac{e^2}{4\pi\epsilon_0 a_0} \text{ in SI units} \\ &= 2.194\,746\,313\,6320(43) \times 10^7 \text{m}^{-1} \\ &= 6.579\,683\,920\,502(13) \times 10^{15} \text{ Hz} \end{aligned}$$

(see https://physics.nist.gov/cuu/Constants/index.html).

- Can we also set $c = 1$?
  The fine structure constant is

$$\alpha = \frac{e^2}{\hbar c} = 137.035\,999\,084(21)$$

HOMEWORK

1. Read Sects. 2.1 and 3.1 of "Variational Methods," (see web:Dropbox) and complete the derivation of the Schroedinger equation (102) from the Hamilton-Jacobi equation (100). (Hint: compare with (30) and (31) as an example.)

2. Complete the derivation of the Dirac equation by writing

$$E = c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc$$

Square both sides and compare with

$$E^2 = c^2 p^2 + m^c c^4$$

to obtain the anticommutation relations

$$\begin{aligned} \alpha_x\alpha_y + \alpha_y\alpha_x &= 0 \text{ and similarly for } x, z \text{ and } y, z \\ \alpha_x\beta + \beta\alpha_x &= 0 \text{ and similarly for } y \text{ and } z. \end{aligned}$$

What is the simplest matrix representation for the α's and β, and why is a 2×2 representation in terms of Pauli spin matrices not possible, even thought the Pauli spin matrices also anticommute?