Special Topics on Precision Measurement in Atomic Physics

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LECTURE 1: APPENDIX

• Use of group theory for energy levels:

Before we said that rotational symmetry leads to the l, m quantum numbers, but not necessarily n. However, in certain special cases that can be solved exactly, such as the harmonic oscillator and the hydrogen atom, there is a dynamical symmetry characterized by the Runge-Lenz vector \mathbf{A} defined by

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - mk\mathbf{\hat{r}}$$

corresponding to a Coulomb (or gravitational) potential V(r) = -k/r. A is then an additional dynamical constant of the motion, in addition to energy and angular momentum.



In quantum mechanics, one can then define raising and lowering operators (ladder operators) for the principal quantum number n, just as you can for the magnetic quantum number m in the case of angular momentum, and obtain the Rydberg formula for the energy levels

$$E_n = -\frac{k/a_0}{2n^2}$$

See T.H. Cooke and J.L. Wood, Am. J. Phys. **70**, 945 (2002) https://aapt.scitation.org/doi/pdf/10.1119/1.1491262?class=pdf

Brian Judd in his book Angular Momentum Theory for Diatomic Molecules (Elsevier, 1975) also discusses the Runge-Lenz vector in connection with the four-dimensional group R(4) and the four-dimensional spherical harmonics $Y_{nlm}(\Omega)$. This is the symmetry group of both the rigid rotor and the hydrogen atom.

Judd: Angular Momentum Theory for Diatomic 56 Molecules 3 R(4) in Physical Systems

in $(p^2 + p_0^2)$ and $(p'^2 + p_0^2)$. These are removed by taking

$$\psi(\mathbf{p}) = \frac{4p_0^{5/2}}{(p^2 + p_0^2)^2} \varphi(\Omega), \qquad (3.29)$$

the term $4p_0^{5/2}$ being included in anticipation of normalization requirements for the hydrogen atom. Eq. (3.23) now takes the remarkably simple form,

$$\varphi(\Omega) = \frac{Z}{2\pi^2 a_0 p_0} \int \frac{\exp(-i\mathbf{R} \cdot (\mathbf{p} - \mathbf{p}'))}{4\sin^2 \kappa/2} \varphi(\Omega') \ d\Omega'. \tag{3.30}$$

3.7 THE HYDROGEN ATOM

Equation (3.30) is an example of a Fredholm equation of the second kind [38]. The general method for solving such an equation is to expand both kernel and function in some series of orthonormal polynomials, thereby obtaining a series of equations for the coefficients in the expansion of the function. The natural choice for our polynomials is the four-dimensional spherical harmonics. If we specialize to the hydrogen atom, we can set $\mathbf{R} = 0$, corresponding to a charge Ze at the origin. To expand the kernel $\csc^2 \kappa/2$, we can use Eq. (2.44), getting

$$\varphi(\Omega) = \frac{Z}{a_0 p_0} \sum_{n \, lm} \frac{1}{n} \int Y_{n \, lm}^*(\Omega') Y_{n \, lm}(\Omega) \varphi(\Omega') \, d\Omega'.$$

We now develop $\varphi(\Omega)$ as a series of spherical harmonics:

$$\varphi(\Omega) = \sum_{\lambda \mu} a_{\lambda \mu} Y_{\lambda \mu}(\Omega).$$

The integration over Ω' can be performed at once, and we get

$$\sum_{\boldsymbol{r}\lambda\boldsymbol{\mu}} a_{\boldsymbol{r}\lambda\boldsymbol{\mu}} Y_{\boldsymbol{r}\lambda\boldsymbol{\mu}}(\Omega) = \frac{Z}{a_0 p_0} \sum_{nlm} \frac{1}{n} a_{nlm} Y_{nlm}(\Omega).$$

To obtain equations for the coefficients $a_{r\lambda\mu}$, both sides of this equation are multiplied by $Y_{n'l'm'}^*(\Omega)$ and the integration over Ω is carried out. The resulting secular matrix is diagonal, and for its determinant to vanish we must have

$$1 = Z/a_0 p_0 n$$

for some positive integer n. Thus an acceptable energy is

$$E = -\frac{\hbar^2}{2m} p_0{}^2 = -\frac{\hbar^2 Z^2}{2ma_0{}^2n^2} = -\frac{e^4mZ^2}{2\hbar^2n^2},$$

- WIPM examples of precision measurement:
 - Precision measurement of the weak Einstein equivalence principle in Ming-Sheng Zhan's lab.
 - Fine structure measurement in Li⁺ $2 {}^{3}P$ by Kelin Gau and Hua Guan (in progress).
 - Fine structure measurement in He 2 ${}^{3}P$, 2 ${}^{3}S 2 {}^{3}P$ transition frequency, and m_e/m_p mass ratio from HD by Shui-Ming Hu et al. (USTC, Hefei) with Krzysztof Pachucki. Requires spin-dependent theory up to order $m\alpha^7 = mc^2\alpha^7 = \alpha^5$ a.u.
- Relativistic units:

 $\hbar = c = 1$. Then $e^2/4\pi\epsilon_0 \equiv \alpha$.

• HOMEWORK

- 1. Read Sects. 2.1 and 3.1 of "Variational Methods," (see distributed notes) 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

$$\alpha_x \alpha_y + \alpha_y \alpha_x = 0$$
 and similarly for x, z and y, z
 $\alpha_x \beta + \beta \alpha_x = 0$ and similarly for y and z .

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? Hint: The Pauli spin matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

Show that the matrices anticommute so that $\sigma_x \sigma_y + \sigma_y \sigma_x = 0$ and similarly for xz and yz, in addition to the usual commutation relation $[\sigma_x, \sigma_y] = 2i\sigma_z$.