

Week 10 Worksheet

Fine Structure and Variational Principle

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March 17, 2024

Exercise 1. Broken Symmetries. In classical mechanics, $\frac{1}{r}$ potentials have an additional conserved quantity that is rarely covered in introductory courses. This quantity is called the **Runge-Lenz vector**, and it is given by

$$\mathbf{F} = \mathbf{p} \times \mathbf{L} - \frac{\gamma}{r} \mathbf{r},$$

where γ is the constant associated to the potential $V(r) = -\gamma/r$, e.g. $\gamma = e/4\pi\epsilon_0$ or $\gamma = MG$.

- a) If we replace all the classical dynamical variables in the above expression by quantum operators, explain why the result is ambiguous.
- b) It turns out¹ that the correct quantum mechanical version of \mathbf{F} is

$$\mathbf{F} = \frac{1}{2m} (\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{\gamma}{r} \mathbf{r}.$$

It can be shown in a lengthy computation that $[H, \mathbf{F}] = \mathbf{0}$, where H is the hydrogen atom hamiltonian (please try this at home), so \mathbf{F} is a symmetry of the hydrogen atom. In fact, \mathbf{F} is responsible for the “accidental” degeneracy in ℓ . Show that $[\mathbf{F}, \mathbf{L} \cdot \mathbf{S}]$ is not zero, so that fine structure breaks this symmetry. This explains why the degeneracy in ℓ disappears once we consider fine structure effects.

- c) Show that $[\mathbf{F}, p^4] \neq \mathbf{0}$ either, so this explains why the relativistic correction lifts the degeneracy in ℓ .

Exercise 2. Prove the variational principle,

$$E_{\text{gs}} \leq \langle \psi | H | \psi \rangle.$$

Exercise 3. Use the variational principle to get an approximation for the ground state energy in the **Yukawa potential**

$$V(r) = e^{-\alpha r} \frac{e^2}{r},$$

¹The way you would prove this is by matching Poisson bracket relations with \mathbf{F} in classical mechanics to corresponding ones in quantum mechanics (upgrading the Poisson brackets to commutators). This would then allow you to determine the right combination of $\mathbf{p} \times \mathbf{L}$ and $\mathbf{L} \times \mathbf{p}$ to take.

using the trial function

$$\psi(r) = \sqrt{\frac{b^3}{\pi}} e^{-br}.$$

Show that when $\alpha = 0$, the trial function saturates the bound; why? Comment on the accuracy of the bound you obtain as α increases.