

Week 10 Worksheet

Fine Structure and Variational Principle

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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

$$\mathbf{F} = \frac{1}{m} \mathbf{p} \times \mathbf{L} - \frac{\gamma}{r} \mathbf{r},$$

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.

Hints: When we upgrade $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ to a quantum operator, note that $\mathbf{L} = -\mathbf{p} \times \mathbf{r}$ as operators. Why? Does $\mathbf{p} \times \mathbf{L} = -\mathbf{L} \times \mathbf{p}$ as operators?

- 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 (note(!) that $[\mathbf{L} \cdot \mathbf{S}, L^2] = 0$). This explains why the degeneracy in ℓ disappears once we consider fine structure effects.

Hint: Rather than working with each of the terms in \mathbf{F} , try to first show that the commutator with the last term is nonzero. Then, make an argument for why that commutator cannot cancel with the one arising from the first two terms.

- 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,

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

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.

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

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

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. Note that

$$\nabla^2 f(r) = \frac{1}{r^2} \partial_r (r^2 \partial_r f(r)).$$

Hint: You won't get a closed form solution for b when $\alpha \neq 0$, but you can still give a physical explanation of what's going on as α increases.