Week 10 Worksheet
Fine Structure and Variational Principle

Jacob Erlikhman

March 20, 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. $\gamma = e/4\pi\varepsilon_0$ 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 out[1] that the correct quantum mechanical version of $\mathbf{F}$ is

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

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: We can write $\mathbf{p} \times \mathbf{L}$ using the triple product identity classically. If we try to do this in quantum mechanics, we will end up with an expression that's ambiguous, but only up to factors of $i\hbar$.

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,

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

[1]The 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

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