Quantum Mechanics 115C: Homework 4

Spring 2023
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4.1 Virial theorem in one and three dimensions

In class, we used the virial theorem to avoid calculating a few integrals. In general, the virial theorem is an extremely helpful tool for simplifying problems, especially those with r^n potentials.

(a) Using the relation

$$\frac{d}{dt}\langle \hat{Q} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}] \rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle,$$

where $\hat{Q}$ is an observable, show that:

$$\frac{d}{dt}\langle xp \rangle = 2\langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle.$$

(b) Show that for a stationary state, the left side of the equation is zero so that:

$$2\langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle$$

(c) Apply the virial theorem to the one-dimensional harmonic oscillator and show that

$$\langle T \rangle = \langle V \rangle = E_n/2$$

(d) Prove the three-dimensional generalization of the virial theorem:

$$2\langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle$$

(e) Apply the three-dimensional virial theorem to the hydrogen atom to show that:

$$\langle T \rangle = -E_n \qquad \text{and} \qquad \langle V \rangle = 2E_n.$$

4.2 Spin-1/2 particle in a magnetic field

Consider a spin-1/2 particle in a magnetic field environment.[1] In this problem, there are two sources of magnetic fields, one with the field pointed in the z-direction and one with the field pointed in the x-direction. The Hamiltonian is:

$$H = -\gamma \mathbf{B} \cdot \hat{\mathbf{S}} = -\gamma(B_x \hat{S}_x + B_z \hat{S}_z) \tag{1}$$

(a) Using the Pauli spin matrices or otherwise, solve for the exact energy eigenvalues of this Hamiltonian.

[1] Later in this class, you'll see why problems of this form are so relevant to quantum optics and information.

(b) Use a trial wavefunction of the form:

$$\psi_{trial} = \cos(\phi/2)\begin{pmatrix}1\\0\end{pmatrix} + \sin(\phi/2)\begin{pmatrix}0\\1\end{pmatrix} \tag{2}$$

to obtain an upper bound the ground state energy. Note that this trial wavefunction is automatically normalized with this choice of variational parameter, so you can just go ahead and use it.

(c) How close to the exact ground state did you get? Why is this the case? Is there a degree of freedom that we have not taken into consideration in this trial function?

4.3 Variational principle for the first excited state of the infinite square well

In this problem, we will look at the variational principle not for the ground state, but for the first excited state. Using the variational principle for the first excited state will work if you exploit certain *symmetries* of the problem.

(a) (Same as Griffiths 7.4) Prove the following corollary to the variational principle: If $\langle\psi_{trial}|\psi_{gs}\rangle = 0$, then $\bar{H} = \langle\psi_{trial}| H |\psi_{trial}\rangle \geq E_{fe}$, where E_{fe} is the energy of the first excited state.

(b) Consider the following trial wavefunction for the first excited state of the infinite square well:

$$\langle x|\psi_{trial}\rangle = \psi_{trial}(x) = Nx(a/2 - x)(a - x) \tag{3}$$

Sketch the wavefunction over the region of the square well (i.e. from 0 to a.) Don't worry about normalization for this part; the magnitudes don't have to be correct, just the rough overall shape. (Optional: If you would like, plot $\psi_{trial}(x)$ and $\psi_{fe}(x)$ for the infinite square well problem in a software package like Python or Mathematica and compare the two functions. But only do this after you've already sketched the function!)

(c) The infinite square well problem exhibits parity symmetry about the point $x = a/2$. Because the wavefunctions of the infinite square well problem must be parity eigenstates, the ground state is parity even while the first excited state is parity odd. This means that $\psi_n(x < a/2) = \psi_n(x > a/2)$ for $n = 1, 3, 5\ldots$, while $\psi_n(x < a/2) = -\psi_n(x < a/2)$ for $n = 2, 4, 6\ldots$, where $n = 1$ denotes the ground state.

Verify that the trial wavefunction, $\psi_{trial}(x)$ chosen above is parity odd. Also, verfiy that it is orthogonal to $\psi_0(x) = N'\sin(\pi x/a)$. [2]

(d) Verify also that the trial wavefunction above, $\psi_{trial}(x)$, is orthogonal to our ground state trial wavefunction from class, $\psi(x) = N''x(a - x)$.

(e) Normalize $\psi_{trial}(x)$.

(f) Calculate $\bar{H} = \langle\psi_{trial}| H |\psi_{trial}\rangle$ and check to see if the energy is greater than that of the first excited state of the infinite square well. What is the discrepancy between $\bar{H}$ and E_{fe}, the energy

[2] Here, Griffiths would quote Peter Lorre and say "Do it ze *kveek* vay, Johnny!". I highly suspect that this is a reference to the film *Casablanca*. If any of you knows (or figures out) where this comes from, please let me know.

of the first excited state? Would you say that this was a “good” trial wavefunction? (Optional: see if you can find a better trial wavefunction.)