Due Oct. 22, Tuesday

Problem 1 (30 points) As a very crude model of a molecule, we consider a double delta function potential:

$$V(x) = -\alpha\left[\delta(x+a) + \delta(x-a)\right]$$

where $\alpha > 0$. We will approach this problem perturbatively, assuming that $2a$ is large enough so that the problem can be viewed as two almost separate potential wells. For one well, the solution for a bound state can be found from Eq. T2.129 ("T" means textbook). Consider two states

$$\begin{aligned} |R\rangle &\doteq \psi(x-a) \\ |L\rangle &\doteq \psi(x+a) \end{aligned}$$

where $\psi(x)$ is as given in Eq. T2.129.

Note: This problem is simple at its core, but it can lead to complex calculations, if a "perturbation" mars the clarity of thinking. As a general rule, in my homework (or for problems in any reasonable book), too complicated calculations are frowned upon, so please stop and think/ask if calculations seem to become too complicated. On the other hand, if you can calmly see through this problem, and can confidently reason through this problem by being able to check orders of perturbation without much fuss, you can be called an expert in the perturbation theory—have someone pat you on the back. In sum, this is a fairly advanced simple problem—you might want to do it after finishing other problems.

(a) Calculate $\langle R|L\rangle$ as a function of m (mass), α and a. How does it behave in the limit of large a? Provide a qualitative justification of that behavior. We will use $\langle R|L\rangle$ as the smallness parameter of this problem, from now on.

(b) Note that $|R\rangle$ and $|L\rangle$ are not orthogonal. However, it is possible to find two real numbers A (≈ 1) and η with $|\eta| \ll 1$ (assuming large a) such that

$$\begin{aligned} |R'\rangle &= A\left(|R\rangle + \eta\,|L\rangle\right) \\ |L'\rangle &= A\left(|L\rangle + \eta\,|R\rangle\right) \end{aligned}$$

are orthonormal. Find A and η, up to leading order of the smallness parameter defined in (a).

(c) Find the Hamiltonian matrix representation for the two state basis, $|R'\rangle$ and $|L'\rangle$, to the leading order of smallness. Then, obtain eigenvalues to the leading order of smallness and corresponding eigenstates. [Hint: $\hat{H} = \hat{H}_L - \alpha\delta(\hat{x}-a) = \hat{H}_R - \alpha\delta(\hat{x}+a)$, where $\hat{H}_R|R\rangle = E|R\rangle$ (E as given in Eq. T2.129) and $\hat{H}_L|L\rangle = E|L\rangle$.]

(d) For the Hamiltonian obtained in the previous step, identify the unperturbed Hamiltonian. Would you call the degeneracy of the unperturbed Hamiltonian an "accidental degeneracy"? Justify your answer. [Hint: in one dimension, the only possible spatial symmetries are translation and parity.]

Problem 2 (20 points) Let us consider the p orbital problem that we discussed in Section 6.4.

(a) In Eq. 6.26, we found how to express $|l=1, m_z\rangle$'s in terms of $|l=1, m_x\rangle$'s. Find similar expressions (three equations) for expanding $|l=1, m_x\rangle$'s in terms of $|l=1, m_z\rangle$'s.

(b) Find similar expressions (three equations) for expanding $|l=1, m_z\rangle$'s in terms of $|l=1, m_y\rangle$'s.

(c) Find $\hat{\mathcal{R}}_x\left(\frac{\pi}{2}\right)|p_x\rangle$, $\hat{\mathcal{R}}_y\left(\frac{\pi}{2}\right)|p_x\rangle$, and $\hat{\mathcal{R}}_z\left(\frac{\pi}{2}\right)|p_x\rangle$. Explain why your answers are reasonable.

Problem 3 (20 points) Prove the following commutator algebra, where $\hat{\vec{L}}$ is the orbital angular momentum operator. Each of j, k, l can take the value of 1, 2, or 3 corresponding to x, y, or z, respectively (e.g., $\hat{x}_1 \equiv \hat{x}$, $\hat{x}_2 \equiv \hat{y}$, and $\hat{x}_3 \equiv \hat{z}$), and ϵ_{ijk} is the Levi-Civita symbol. $\vec{A}^2 \equiv \vec{A}\cdot\vec{A}$.

(a) $\left[\hat{L}_j, \hat{p}_k\right] = i\hbar \sum_l \epsilon_{jkl}\hat{p}_l$

(b) $\left[\hat{L}_j, \hat{x}_k\right] = i\hbar \sum_l \epsilon_{jkl}\hat{x}_l$

(c) $\left[\hat{L}_j, \hat{\vec{p}}^2\right] = 0$

(d) $\left[\hat{L}_j, \hat{\vec{r}}^2\right] = 0$

Hint: use the canonical commutator $[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{j,k}$ and the definition $\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$.

Problem 4 (20 points) (Bloch's theorem, crystal momentum) Suppose that the Hamiltonian in one dimension is given by

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{V} && T \text{ is kinetic energy} \\ \hat{V} &\doteq V(x) && \\ V(x+a) &= V(x) && a \text{ is a fixed length scale} \end{aligned}$$

(a) Show that the Hamiltonian is invariant under translation by na, where n is an arbitrary integer.

(b) Write down the most general form of eigenfunction of the unitary operator that corresponds to this discrete translation symmetry ("lattice translation symmetry").

(c) Show that an eigenfunction of this Hamiltonian can be written as

$$\psi(x) = \exp(ikx)u(x)$$

where $u(x+a) = u(x)$. Note that $k \to k + 2\pi j/a$ where j is an arbitrary integer, does not change the nature of this solution. I.e., k and $k + 2\pi j/a$ are completely equivalent. The quantity $\hbar k$ is so-called "crystal momentum," a conserved quantity associated with the discrete lattice translation symmetry of a crystal, as opposed to the continuous translational symmetry of free space.

Problem 5 (30 points) Virial theorem, QM version.

(a) Consider the following Hamiltonian in one spatial dimension

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

where $\hat{T}$ is the kinetic energy, and $\hat{V}$ is the potential energy. Let us consider the so-called "virial," $\hat{x}\,\hat{p}$. Show that for any state $|\Psi(t)\rangle$, we have

$$\frac{d}{dt}\langle \hat{x}\,\hat{p}\rangle = \left\langle \frac{\hat{p}^2}{m} \right\rangle - \left\langle \hat{x}\frac{d}{d\hat{x}}V(\hat{x}) \right\rangle$$

where $\langle \hat{O} \rangle \equiv \langle \Psi(t) | \hat{O} | \Psi(t) \rangle$. [Hint: use the general "equation of motion"

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

which was proved as part of the solution for HW 1.3.]

(b) Continuing the previous part, for a stationary state, and a power law potential energy $V(\hat{x}) \propto \hat{x}^n$, show that

$$\langle \hat{T} \rangle = \frac{n}{2}\langle \hat{V} \rangle$$

(c) For the Hamiltonian in arbitrary spatial dimensions

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}})$$

show that

$$\frac{d}{dt}\left\langle \hat{\vec{x}} \cdot \hat{\vec{p}} \right\rangle = \left\langle \frac{\hat{\vec{p}}^2}{m} \right\rangle - \left\langle \hat{\vec{x}} \cdot \frac{d}{d\hat{\vec{x}}}V(\hat{\vec{r}}) \right\rangle$$

where $\frac{d}{d\hat{\vec{x}}}$ means the gradient operation, and $\vec{A}^2 \equiv \vec{A} \cdot \vec{A}$.

(d) Continuing the previous part, show that, for a stationary state and $V(\hat{\vec{r}}) \propto \hat{r}^n$, where $\hat{r}$ is the magnitude of $\hat{\vec{r}}$, the same result of (b)

$$\langle \hat{T} \rangle = \frac{n}{2}\langle \hat{V} \rangle$$

applies in this general case, as well.

(e) Find the relation between $\langle \hat{T} \rangle$ and $\langle \hat{V} \rangle$ for a stationary state for (i) one dimensional simple Harmonic oscillator, (ii) three dimensional simple Harmonic oscillator, $V(\hat{\vec{r}}) = \frac{1}{2}k\hat{r}^2$, and (iii) Hydrogen-like atom problem defined by Eq. 6.12.