

Due Oct. 23, Tuesday

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

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

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.

- (a) Calculate  $\langle R|L\rangle$  as a function of  $m$  (mass),  $\alpha$  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  $A$  ( $\approx 1$ ) and  $\eta$  with  $|\eta| \ll 1$  (assuming large  $a$ ) such that

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

are orthonormal. Find  $A$  and  $\eta$ , 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  $\hat{L}$  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  $\epsilon_{ijk}$  is the Levi-Civita symbol.  $\vec{A}^2 \equiv \vec{A} \cdot \vec{A}$ .

- (a)  $[\hat{L}_j, \hat{p}_k] = i\hbar \sum_l \epsilon_{jkl} \hat{p}_l$
- (b)  $[\hat{L}_j, \hat{x}_k] = i\hbar \sum_l \epsilon_{jkl} \hat{x}_l$
- (c)  $[\hat{L}_j, \hat{p}^2] = 0$
- (d)  $[\hat{L}_j, \hat{r}^2] = 0$

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

**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  $k \rightarrow k + 2\pi j/a$  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

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

show that

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

where  $\frac{d}{d\hat{x}}$  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
- $V(\hat{r}) \propto \hat{r}^n$
- , where
- $\hat{r}$
- is the magnitude of
- $\hat{r}$
- , 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,
- $V(\hat{r}) = \frac{1}{2}k\hat{r}^2$
- , and (iii) Hydrogen-like atom problem defined by Eq. 6.12.