Physics 827: Homework Set No. 6

Due date: Friday, November 11, 2011, 1:00pm in PRB M2043 (Biao Huang's office)

Total point value of set: 55 points

Problem 1 (10 pts.): Exercise 5.2.1 (Shankar, p. 163)

Problem 2 (20 pts.): Exercise 5.2.2 (Shankar, p. 163). *Hint:* I found it useful to replace the potential $V(x)$ by a suitable Gaussian potential of smaller magnitude in order to put an upper bound on the energy expectation value.

Problem 3 (5 pts.): Exercise 5.3.1 (Shankar, p. 166)

Problem 4 (5 pts.): Exercise 5.3.4 (Shankar, p. 167)

Problem 5 (15 pts.):

(a) (5 pts.) According to Postulate II, the angular momentum operator is defined as $\hat{\vec{L}} = \hat{\vec{X}} \times \hat{\vec{P}}$. Is this operator Hermitean? If not, write down a Hermitean expression for the angular momentum.

(b) (10 pts.) Using Ehrenfest's theorem, derive the equation of motion for the expectation value of angular momentum in an arbitrary state $|\psi\rangle$ for a particle in a 3-dimensional harmonic oscillator potential (with Hamiltonian given by Eq. (4.3.4) in Shankar).

Exercise 5.2.1 (page 163)

The probability amplitude in position space for a particle in the ground state of a box of length L is given by the ground state wavefunction

$$\psi_1(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) & (|x| \le \frac{L}{2}) \\ 0 & (|x| > \frac{L}{2}) \end{cases}$$ (if we put the box symmetrically around $x = 0$).

The ground state for a box of length $2L$ is

$$\phi_1(x) = \begin{cases} \sqrt{\frac{1}{L}} \cos\left(\frac{\pi x}{2L}\right), & |x| \le L \\ 0 & |x| \ge L \end{cases}$$

The probability to find the particle described by $|\psi_1\rangle$ in the state $|\phi_1\rangle$ is

$$P = |\langle \phi_1 | \psi_1 \rangle|^2 = \left(\int_{-L/2}^{L/2} \sqrt{\frac{2}{L^2}} \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{2L}\right) dx \right)^2$$

(the inner product receives contributions only from $-\frac{L}{2} < x < \frac{L}{2}$ where $\psi_1(x) \neq 0$.)

To compute the overlap integral, substitute $\frac{\pi x}{L} = \xi$ ($-\frac{\pi}{2} \le \xi \le \frac{\pi}{2}$, $dx = \frac{L}{\pi} d\xi$):

$$\sqrt{\frac{2}{L^2}} \int_{-L/2}^{L/2} dx \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{2L}\right) = \frac{\sqrt{2}}{\pi} \int_{-\pi/2}^{\pi/2} d\xi \cos(\xi) \cos(\xi/2)$$

$$= \frac{\sqrt{2}}{\pi} \int_{-\pi/2}^{\pi/2} d\xi \, \frac{1}{2} \left(\cos(\xi/2) + \cos(3\xi/2) \right) = \frac{1}{\pi\sqrt{2}} \left[2 \sin(\xi/2) + \frac{2}{3} \sin(3\xi/2) \right]_{-\pi/2}^{\pi/2}$$

$$= \frac{\sqrt{2}}{\pi} \left(2 \cdot \frac{1}{\sqrt{2}} + \frac{1}{3} \cdot 2 \cdot \frac{1}{\sqrt{2}} \right) = \frac{2\sqrt{2}}{\pi} \frac{4}{3\sqrt{2}} = \frac{8}{3\pi}$$

$\left(\sin\frac{\pi}{4} = \sin\left(\frac{3\pi}{4}\right) = \frac{1}{\sqrt{2}} \right)$

$$\Rightarrow \boxed{P = \left(\frac{8}{3\pi}\right)^2} \checkmark$$

Exercise 5.2.2 (page 163)

(a) Show that if $\langle\psi|\psi\rangle = 1$, $\langle\psi|\hat{H}|\psi\rangle \geq E_0$ where E_0 is the lowest energy eigenvalue.

Expand $|\psi\rangle$ in energy eigenstates $|E\rangle$, $\hat{H}|E\rangle = E|E\rangle$:

$$|\psi\rangle = \sum_E \langle E|\psi\rangle |E\rangle \equiv \sum_E a_E |E\rangle$$

$$\Rightarrow \langle\psi|\hat{H}|\psi\rangle = \sum_E \sum_{E'} a_E a_{E'}^* \underbrace{\langle E'|\hat{H}|E\rangle}_{E\,\delta(E,E')}$$

$$= \sum_E |a_E|^2 E \geq \sum_E |a_E|^2 E_0 \quad \text{since } E \geq E_0 \;\forall E.$$

But since $\langle\psi|\psi\rangle = 1 = \sum_E \sum_{E'} a_E a_{E'}^* \underbrace{\langle E'|E\rangle}_{\delta(E,E')} = \sum_E |a_E|^2$

this shows that

$$\langle\psi|\hat{H}|\psi\rangle \geq E_0 \sum_E |a_E|^2 = E_0 \quad \text{(Q.E.D.)}$$

(b) Thm: Every attractive potential in one dimension has at least one bound state.

Proof: Normalize $V(\infty) = 0$ such that $V(x) = -|V(x)| \leq 0$ for all x. Also, we can shift x such that $V(x)$ is minimal at $x = 0$.

Consider the trial wave function

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \qquad \left(\int_{-\infty}^{\infty} |\psi_\alpha(x)|^2 dx = 1\right)$$

which has one adjustable real parameter α.

Calculate

$$E(\alpha) = \langle \psi_\alpha | \hat{H} | \psi_\alpha \rangle = \langle \psi_\alpha | \frac{\hat{p}^2}{2m} - |V(x)| | \psi_\alpha \rangle$$

$$\overset{(x\text{-basis})}{=} \int_{-\infty}^{\infty} dx\, \psi_\alpha^*(x) \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)| \right) \psi_\alpha(x)$$

$$\frac{d\psi_\alpha}{dx} = \left(\frac{\alpha}{\pi}\right)^{1/4} (-\alpha x) e^{-\alpha x^2/2}$$

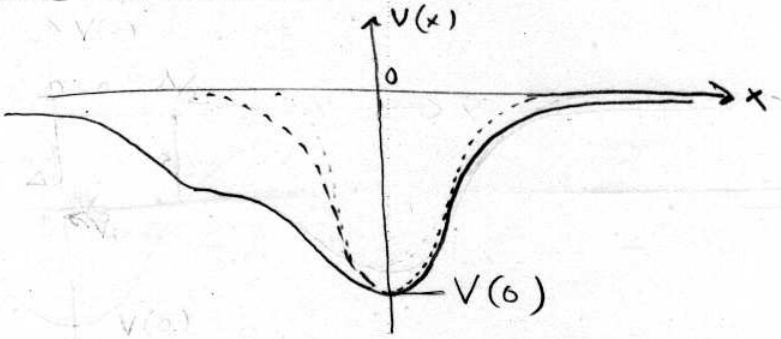
$$\frac{d^2\psi_\alpha}{dx^2} = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(-\alpha e^{-\alpha x^2/2} + \alpha^2 x^2 e^{-\alpha x^2/2} \right)$$

$$\Rightarrow E(\alpha) = \sqrt{\frac{\alpha}{\pi}} \left[-\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} |V(x)| + \alpha \frac{\hbar^2}{2m} \underbrace{\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2}}_{\sqrt{\frac{\pi}{\alpha}}} - \alpha^2 \frac{\hbar^2}{2m} \underbrace{\int_{-\infty}^{\infty} dx\, x^2 e^{-\alpha x^2}}_{\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}} \right]$$

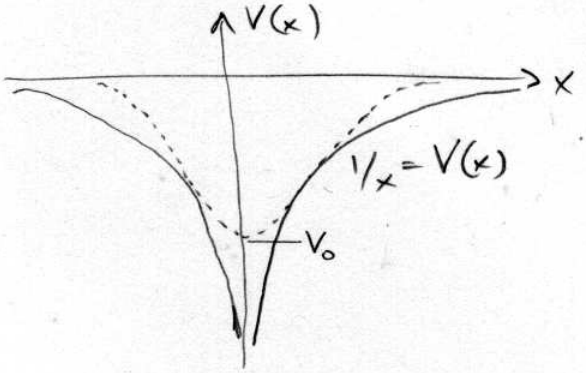
$$= -\sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} |V(x)| + \frac{\alpha \hbar^2}{4m}$$

So the energy $\langle V \rangle_\alpha + \langle T \rangle_\alpha$ is the sum of a negative potential energy term and positive kinetic energy contribution. The kinetic energy decreases linearly with α as $\alpha \to 0$ (i.e. as the wave function spreads out).

The potential energy $\langle V \rangle_\alpha$ decreases monotonically with increasing $|V(x)|$. So we can put an upper bound on the potential energy by replacing the potential by a Gaussian around $x=0$ that "fits inside the potential":



If $V(0)$ is infinite, we can still fit a finite Gaussian inside the potential such as follows:



in this case $V_0 \neq V(0)$, $|V_0| < |V(0)|$

We thus have

$$E(\alpha) \leq -\sqrt{\frac{\alpha}{\pi}}\,|V_0| \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} e^{-x^2/\Delta^2} + \frac{\alpha \hbar^2}{4m}$$

where Δ is the width of the Gaussian potential and $|V_0|$ is its depth. Doing the Gaussian integral gives

$$E(\alpha) \leq -\sqrt{\frac{\alpha}{\pi}}\,|V_0| \sqrt{\frac{\pi}{\alpha + 1/\Delta^2}} + \frac{\alpha \hbar^2}{4m} = -|V_0| \sqrt{\frac{\alpha}{\alpha + 1/\Delta^2}} + \frac{\alpha \hbar^2}{4m}$$

For $\alpha \to 0$ the right hand side becomes negative since the positive kinetic energy approaches zero faster than the negative potential energy.

Since from part (a) $E_0 \leq E(\alpha)$ irrespective of the value for α and from part (b) $E(\alpha) < 0$ for sufficiently large α, we know that $E_0 < 0$. So the lowest energy eigenstate is bound ($E_0 < V(\infty)$), hence the potential has at least one bound state. (Q.E.D.)

Exercise 5.3.1 (page 166)

$$\hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}(\hat{x}) \quad \text{where} \quad V(x) = V_r - iV_i \qquad (V_r, V_i \text{ real constants}).$$
$$= \frac{\hat{P}^2}{2m} + (V_r - iV_i)\hat{I}$$
$$\hat{H}^+ = \left(\frac{\hat{P}^2}{2m}\right)^+ + \hat{V}^+ = \frac{\hat{P}^2}{2m} + V_r\hat{I} + iV_i\hat{I} \neq \hat{H}$$

$\hat{H}$ is <u>not</u> Hermitean.

In this case

$$P(t) = \langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\hat{U}^+(t)\,\hat{U}(t)|\psi(0)\rangle$$
$$= \langle\psi(0)|\left(e^{-i\hat{H}t/\hbar}\right)^+ e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$$
$$= \langle\psi(0)|\, e^{i\hat{H}^+t/\hbar}\, e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle$$
$$= \langle\psi(0)|\, e^{i(iV_i)\hat{I}t/\hbar - i(-iV_i)\hat{I}t/\hbar}|\psi(0)\rangle \qquad \left(\text{since } \hat{P}^2 \text{ commutes with } \hat{I} \text{ and with itself}\right)$$
$$= e^{-2V_it/\hbar}\langle\psi(0)|\psi(0)\rangle = e^{-\frac{2}{\hbar}V_it}P(0)$$

$\Rightarrow$ $P(t)$ decreases exponentially with time.

Exercise 5.3.4 (page 167)

Consider $\psi(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$.

Compute

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

$$= \frac{\hbar}{2mi}\left[\left(A^* e^{-ipx} + B^* e^{ipx/\hbar}\right)\frac{ip}{\hbar}\left(Ae^{ipx/\hbar} - Be^{-ipx/\hbar}\right)\right.$$
$$\left. - \left(Ae^{+ipx/\hbar} + Be^{-ipx/\hbar}\right)\frac{ip}{\hbar}\left(-A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar}\right)\right]$$

$$= \frac{p}{2m}\left[\left(|A|^2 - A^*Be^{-2ipx/\hbar} + B^*Ae^{2ipx/\hbar} - |B|^2\right)\right.$$
$$\left. - \left(-|A|^2 + AB^* e^{2ipx/\hbar} - BA^* e^{-2ipx/\hbar} + |B|^2\right)\right]$$

$$= \frac{p}{m}\left(|A|^2 - |B|^2\right) \quad \checkmark$$

Problem 5

(a) Angular momentum: $\hat{\vec{L}} = \hat{\vec{X}} \times \hat{\vec{P}} = \left(\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z, \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x\right)$

Since $\hat{X}, \hat{Y}, \hat{Z}, \hat{P}_x, \hat{P}_y, \hat{P}_z$ are all Hermitean and $\hat{X}$ commutes with $\hat{P}_y, \hat{P}_z$, $\hat{Y}$ commutes with $\hat{P}_x, \hat{P}_z$, and $\hat{Z}$ commutes with $\hat{P}_x, \hat{P}_y$, all 3 components of $\hat{\vec{L}}$ are Hermitean.

(b) $\frac{d}{dt}\langle \hat{\vec{L}} \rangle = -\frac{i}{\hbar}\langle [\hat{\vec{L}}, \hat{H}] \rangle$ Ehrenfest theorem

So we must compute $[\hat{\vec{L}}, \hat{H}]$.

Start with $[\hat{L}_x, \hat{\vec{P}}\cdot\hat{\vec{P}}] = [\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y, \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2]$

$$= \hat{Y}\underbrace{[\hat{P}_z, \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2]}_{0} + [\hat{Y}, \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2]\hat{P}_z$$

$$- \hat{Z}\underbrace{[\hat{P}_y, \hat{\vec{P}}^2]}_{0} - [\hat{Z}, \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2]\hat{P}_y$$

$$= \left(\underbrace{[\hat{Y}, \hat{P}_y]}_{i\hbar\hat{I}}\hat{P}_y + \hat{P}_y\underbrace{[\hat{Y}, \hat{P}_y]}_{i\hbar\hat{I}}\right)\hat{P}_z - \left(\underbrace{[\hat{Z}, \hat{P}_z]}_{i\hbar\hat{I}}\hat{P}_z + \hat{P}_z\underbrace{[\hat{Z}, \hat{P}_z]}_{i\hbar\hat{I}}\right)\hat{P}_y$$

$$= 2i\hbar\left(\hat{P}_y\hat{P}_z - \hat{P}_z\hat{P}_y\right) = 0$$

By inspection it is obvious that we will similarly find

$$[\hat{L}_y, \hat{\vec{P}}\cdot\hat{\vec{P}}] = [\hat{L}_z, \hat{\vec{P}}\cdot\hat{\vec{P}}] = 0$$

i.e. the angular momentum operator commutes with the kinetic energy operator.

Next we compute

$$\left[\hat{L}_x, \hat{\vec{X}}\cdot\hat{\vec{X}}\right] = \left[\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y, \hat{X}^2+\hat{Y}^2+\hat{Z}^2\right]$$

$$= \hat{Y}\left[\hat{P}_z, \hat{X}^2+\hat{Y}^2+\hat{Z}^2\right] + \underbrace{\left[\hat{Y}, \hat{X}^2+\hat{Y}^2+\hat{Z}^2\right]}\hat{P}_z$$

$$- \hat{Z}\left[\hat{P}_y, \hat{X}^2+\hat{Y}^2+\hat{Z}^2\right] - \underbrace{\left[\hat{Z}, \hat{X}^2+\hat{Y}^2+\hat{Z}^2\right]}_{0}\hat{P}_y$$

$$= -\hat{Y}\left[\hat{Z}^2, \hat{P}_z\right] + \hat{Z}\left[\hat{Y}^2, \hat{P}_y\right]$$

$$= -\hat{Y}\left(\hat{Z}\underbrace{\left[\hat{Z}, \hat{P}_z\right]}_{i\hbar\hat{I}} + \underbrace{\left[\hat{Z}, \hat{P}_z\right]}_{i\hbar\hat{I}}\hat{Z}\right) + \hat{Z}\left(\hat{Y}\underbrace{\left[\hat{Y}, \hat{P}_y\right]}_{i\hbar\hat{I}} + \underbrace{\left[\hat{Y}, \hat{P}_y\right]}_{i\hbar\hat{I}}\hat{Y}\right)$$

$$= 2i\hbar\left(-\hat{Y}\hat{Z} + \hat{Z}\hat{Y}\right) = 0$$

Similarly $\left[\hat{L}_y, \hat{\vec{X}}^2\right] = \left[\hat{L}_z, \hat{\vec{X}}^2\right] = 0$, i.e. all components of $\hat{\vec{L}}$ also commute with the potential energy operator.

In summary, $\left[\hat{\vec{L}}, \hat{H}\right] = 0$, hence

$$\boxed{\frac{d}{dt}\left\langle\hat{\vec{L}}\right\rangle = 0}$$

i.e. the expectation value of the angular momentum operator in <u>any</u> state is time independent

$\longrightarrow$ angular momentum conservation.