Physics 8.321, Fall 2021

Homework #4

Due **Friday, October 22** by 8:00 PM.

1. [Sakurai and Napolitano Problem 21, Chapter 1 (page 63)]

Evaluate the x-p uncertainty product $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle$ for a one-dimensional particle confined between rigid walls,

$$V = \begin{cases} 0 & \text{for } 0 < x < a, \\ \infty & \text{otherwise} \end{cases}$$

Do this for both the ground and excited states.

Solution:

First, let us derive the energy eigenstates for this potential. Inside the well, that is for $0 < x < a$, the energy eigenvalue equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x) \equiv \frac{\hbar^2 k^2}{2m}\psi(x).$$

In the second equality we defined a parameter $k^2 \equiv 2mE/\hbar^2$ Note that $k \in \mathbb{R}$ since $E > 0$ (For $E \leq 0$ no normalizable solution can be found). This equation is easily solvable, and the general solution is given by

$$\psi(x) = A\sin(kx) + B\cos(kx) \quad \text{for} \quad 0 < x < a,$$

where $A, B \in \mathbb{C}$ are some complex constants we are going to determine below.

Now note that outside the well, $x < 0$ or $x > a$, the wavefunction has to vanish, since the potential, therefore Hamiltonian, is infinite and as a result the energy eigenvalue equation is only satisfied when $\psi = 0$.

We solved the wavefunction for inside and outside of the well, now we need to understand what happens at the boundaries of these two region, at $x = 0, a$. The wavefunction ψ has to be continuos at these points in order to the usual probability interpretation to hold (If it were discontinuous, we would get different probabilities for particle being around $x = 0, a$ by approaching right or left, which doesn't make sense physically).

Therefore at $x = 0$, we must have

$$\psi(0) = B = 0.$$

That gets ridsof the one of the solutions inside the well. Similarly, at $x = a$ we obtain

$$\psi(a) = A\sin(ka) = 0 \implies ka = n\pi \quad \text{where} \quad n = 1, 2, 3, \ldots,$$

which provides us the quantization condition. Note that we don't consider non-positive integers for n, since for $n = 0$ the wavefunction is identically zero everywhere (no particle in the box at all!) and for $n < 0$ we simply get back the wavefunction corresponding to one with $-n$, which implies this case is redundant.

From the quantization condition we can easily read off the energies

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \quad \text{with} \quad n = 1, 2, 3, \ldots,$$

and the corresponding wavefunction would be

$$\psi_n(x) = \begin{cases} A \sin\left(\frac{n\pi x}{a}\right) & \text{for } 0 < x < a, \\ 0 & \text{otherwise} \end{cases}$$

Here subscript on the quantities denotes the n we use for k in the quantization condition.

Finally we need to normalize $\psi(x)$ properly in order to obtain the normalization constant A. Noticing $\psi(x)$ is non-zero only inside the well, we can easily do that as follows:

$$1 = \int_0^a |\psi_n(x)|^2 dx = |A|^2 \int_0^a \sin\left(\frac{n\pi x}{a}\right)^2 dx = \frac{a|A|^2}{2} \implies A = \sqrt{\frac{2}{a}}.$$

Above we choose $A \in \mathbb{R}$ without loss of generality. So the general wavefunction for this particle inside the well where it is nonzero is

$$\psi_n(x) = \langle x|n\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad n = 1, 2, 3, \ldots$$

then it is easy to compute for general n

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, x \psi_n(x)\, dx = \frac{a}{2},$$

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \left(-i\hbar\right) \frac{d\psi_n(x)}{dx} dx = 0,$$

and

$$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\, x^2 \psi_n(x)\, dx = \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2},$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \left(-\hbar^2\right) \frac{d^2\psi_n(x)}{dx^2} dx = \frac{\pi^2 \hbar^2 n^2}{a^2},$$

Now using $\langle(\triangle x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$ and the same for p, we get

$$\boxed{\langle(\triangle x)^2\rangle\langle(\triangle p)^2\rangle = \pi^2 \hbar^2 n^2 \left(\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right) \geq \frac{\hbar^2}{4}.}$$

2. [Sakurai and Napolitano Problem 22, Chapter 1 (page 63)]

Estimate the rough order of magnitude of the length of time that an ice pick can be balanced on its point if the only limitation is that set by the Heisenberg uncertainty principle. Assume that the point is sharp and that the point and the surface on which it rests are hard. You may make approximations that do not alter the general order of magnitude of the result. Assume reasonable values for the dimensions and weight of the ice pick. Obtain an approximate numerical result and express it *in seconds*

Solution:

Let's start with intuitive reasoning:

a. The angle with respect to the vertical line, θ, grows exponentially (i.e. it is unstable): $\theta = \theta_0 e^{\lambda t}$, where θ_0 is the initial angle, $\lambda = \sqrt{\frac{g}{R}}$, g is the gravitational acceleration constant, R is the distance from center of mass of the ice pick to the ground along the ice pick. The behavior of θ can be obtained from $\ddot{\theta} = \lambda^2 \theta$, which is the small θ approximation for the full equation of motion shown at the end of this problem.

b. Let's assume there is a critical angle θ_c which defines the balance, that is for $\theta > \theta_c$ the ice pick falls down (you have to give θ_c a reasonable value at the end). Note that we can relate θ_0 and θ_c as $\theta_c = \theta_0 e^{\lambda t_c}$, so $t_c = \frac{1}{\lambda} \ln \frac{\theta_c}{\theta_0}$.

c. Initially $x_0 \sim R\theta_0$ and $p_0 = m(R\dot{\theta}) \sim mR\lambda\theta_0$, for which x_0, p_0 are initial position and momentum.

d. Now the uncertainty relation comes in: $x_0 p_0 \sim \frac{\hbar}{2}$, and we finally get

$$t_c \sim \frac{1}{\lambda} \ln \left(\frac{\theta_c}{\sqrt{\frac{\hbar}{2mR^2\lambda}}} \right).$$

e. Now put in numerics: $g = 9.8\,\mathrm{m/sec^2}$, $\hbar = 1.055 \times 10^{-34}$ J s, $R = 0.2\,\mathrm{m}$, $m = 0.1$ kg, and $\theta_c = 5°$ (the latter three are quite arbitrary. However, an estimate of the weight to be 0.5 kg is probably *too* much of an overestimate, these handy tools usually are lightweight! – Although this overestimate wouldn't change the numerical result, since m is suppressed by Log) and get $t_c \sim 5.03$ sec.

f. The expression for θ_0 can be obtained more accurately if you solve

$$\theta = c_1 e^{\lambda t} + c_2 e^{-\lambda t},$$

which is obtained from solving the equation of motion $mR^2 d^2\theta/dt^2 = mgR\sin\theta$ at small angle.

3. Let $H = \frac{p^2}{2m} + V(x)$ be the Hamiltonian for a one-dimensional quantum system with discrete eigenstates $H|a\rangle = E_a|a\rangle$. Show the following results:

(a) $\sum_{a'} |\langle a|x|a'\rangle|^2(E_{a'} - E_a) = \frac{\hbar^2}{2m}$.

(b) $\langle a|p|a'\rangle = \frac{im}{\hbar}(E_a - E_{a'})\langle a|x|a'\rangle$
and hence $\sum_{a'} |\langle a|x|a'\rangle|^2(E_{a'} - E_a)^2 = \frac{\hbar^2}{m^2}\langle a|p^2|a\rangle$.

(c) Generalize to 3 dimensions and show the quantum virial theorem
$\langle a|\frac{p^2}{2m}|a\rangle = \frac{1}{2}\langle a|\mathbf{x} \cdot \nabla V(\mathbf{x})|a\rangle$.

Solution:

(a) Observe:

$$\begin{aligned}
I &\equiv \sum_{a'} |\langle a|x|a'\rangle|^2(E_{a'} - E_a) \\
&= \sum_{a'} \langle a|x|a'\rangle\langle a'|x|a\rangle(E_{a'} - E_a) \\
&= \left(\sum_{a'} \langle a|xE_{a'}|a'\rangle\langle a'|x|a\rangle\right) - \langle a|x^2|a\rangle E_a \\
&= \langle a|xHx|a\rangle - \langle a|x^2|a\rangle E_a.
\end{aligned}$$

Above $E_{a'}|a'\rangle = H|a'\rangle$ and $\sum_{a'} |a'\rangle\langle a'| = \mathbb{1}$ are used. There are two possible places we can put E_a: before and after x^2, and we get

$$\begin{aligned}
I = I_1 &\equiv \langle a|xHx - Hx^2|a\rangle = \langle a|[x, H]x|a\rangle \\
= I_2 &\equiv \langle a|xHx - x^2H|a\rangle = -\langle a|x[H, x]|a\rangle.
\end{aligned}$$

Then using commutation relations we get

$$\begin{aligned}
I &= \frac{1}{2}(I_1 + I_2) \\
&= \frac{1}{2}\langle a|\,[\,[x, H], x]\,|a\rangle \\
&= \frac{1}{2}\langle a|[\frac{i\hbar p}{m}, x]|a\rangle \\
&= \frac{1}{2}\langle a|\frac{\hbar^2}{m}|a\rangle \\
&= \frac{\hbar^2}{2m}.
\end{aligned}$$

(b) Observe:

$$\begin{aligned}
(E_a - E_{a'})\langle a|x|a'\rangle &= \langle a|Hx - xH|a'\rangle \\
&= -\langle a|[x, H]|a'\rangle \\
&= \frac{\hbar}{im}\langle a|p|a'\rangle.
\end{aligned}$$

Using this fact, we can easily show the second part

$$\begin{aligned}
\frac{\hbar^2}{m^2}\langle a|p^2|a\rangle &= \frac{\hbar^2}{m^2}\sum_{a'}\langle a|p|a'\rangle\langle a'|p|a\rangle \\
&= \sum_{a'} i(E_a - E_{a'})\langle a|x|a'\rangle i(E_{a'} - E_a)\langle a'|x|a\rangle \\
&= \sum_{a'}(E_a - E_{a'})^2|\langle a|x|a'\rangle|^2.
\end{aligned}$$

In the last line we used $\langle a|x|a'\rangle^* = \langle a'|x|a\rangle$.

(c) Using $[\mathbf{p}, H] = \frac{\hbar}{i}\nabla V(x)$ and the 3D versions of the expression in part (b) above

$$\begin{aligned}
I &\equiv \frac{1}{2}\langle a|\mathbf{x}\cdot\nabla V|a\rangle \\
&= \frac{1}{2}\frac{i}{\hbar}\langle a|\mathbf{x}\cdot[\mathbf{p}, H]|a\rangle \\
&= \frac{1}{2}\frac{i}{\hbar}\langle a|\mathbf{x}\cdot\mathbf{p}H - \mathbf{x}\cdot(H\mathbf{p})|a\rangle \\
&= \frac{1}{2}\frac{i}{\hbar}\left(\sum_{a'}\langle a|\mathbf{x}|a'\rangle\cdot\langle a'|\mathbf{p}|a\rangle E_a - \langle a|\mathbf{x}|a'\rangle\cdot\langle a'|\mathbf{p}|a\rangle E_{a'}\right) \\
&= \frac{1}{2}\frac{i}{\hbar}\sum_{a'}\langle a|\mathbf{x}|a'\rangle\cdot\langle a'|\mathbf{p}|a\rangle(E_a - E_{a'}) \\
&= \frac{1}{2}\frac{i}{\hbar}\sum_{a'}\langle a'|\mathbf{p}|a\rangle\cdot\frac{\hbar}{im}\langle a|\mathbf{p}|a'\rangle \\
&= \langle a|\frac{\mathbf{p}^2}{2m}|a\rangle
\end{aligned}$$

Note that here the (quantum) average is taken with respect to the state, while in classical mechanics the average is taken with respect to time (say, for one period T).

Alternatively, it can be proved by computing the commutator $[H, \mathbf{x}\cdot\mathbf{p}]$ and using the fact that $\langle[H, \mathbf{x}\cdot\mathbf{p}]\rangle = 0$ for stationary states.

4. A particle of mass m is in a 1D potential $V(x) = v\delta(x-a) + v\delta(x+a)$ where $v < 0$.

(a) Find the wave function for a bound state with even parity ($\psi(x) = \psi(-x)$).

(b) Find an expression for the energy for even parity states, and determine how many such states exist.

(c) Solve for the even parity bound state energy when $\frac{ma|v|}{\hbar^2} \ll 1$.

(d) Repeat parts (a) and (b) for odd parity ($\psi(x) = -\psi(-x)$). For what values of v are there bound states?

(e) Find the even and odd parity state binding energies for $\frac{ma|v|}{\hbar^2} \gg 1$, and explain physically why these energies move closer together as $a \to \infty$

Solution:

Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi + (v\delta(x-a) + v\delta(x+a))\varphi = E\varphi$$

Integrate from $a^- = a - \epsilon$ to $a^+ = a + \epsilon$:

$$-\frac{\hbar^2}{2m}\varphi'(x)|_{a^-}^{a^+} + v\varphi(a) = 0$$

where it is 0 as $a^+ - a^- \to 0$ because the $\varphi(x)$ is smooth and finite: $\varphi(a^-) = \varphi(a^+)$. Solve this and we get the wave function $\varphi(x) \sim e^{-k|x-a|}$ The same expression holds at $x = -a$, the wave function is $\varphi(x) \sim e^{-k|x+a|}$, where from Schrödinger equation, $E = -\frac{\hbar^2 k^2}{2m}$.

(a) In the region $-a \le x \le a$, in order to form the even state, we need equal (symmetric) contribution from the bound states:

$$\varphi(x) \sim e^{-k(-(x-a))} + e^{-k(x+a)} = 2e^{-ka}\cosh kx$$

So the wave function for all region is

$$\varphi(x) = \begin{cases} A\,e^{-k(x-a)} & \text{if } x \ge a; \\ 2Be^{-ka}\cosh kx & \text{if } -a \le x \le a; \\ A\,e^{k(x+a)} & \text{if } x \le -a. \end{cases}$$

Here A, B are complex constants independent of a, k. By imposing the condition $\varphi(a^-) = \varphi(a^+)$, we get $A = B(1 + e^{-2ka})$. Therefore,

$$\varphi(x) = \begin{cases} B(1+e^{-2ka})\,e^{-k(x-a)} & \text{if } x \ge a; \\ 2B\cosh kx & \text{if } -a \le x \le a; \\ B(1+e^{-2ka})\,e^{k(x+a)} & \text{if } x \le -a. \end{cases}$$

b. From Schrödinger equation at any $x \neq \pm a$, we get $E = -\frac{\hbar^2 k^2}{2m} < 0$. Substitute the wave function obtained in part (a) into the integrated Schrödinger equation, we get

$$k = \frac{m|v|}{\hbar^2}(1 + e^{-2ka})$$

Multiply by a on both sides to make it dimensionless:

$$ka = \frac{m|v|a}{\hbar^2}(1 + e^{-2ka}) \equiv s(1 + e^{-2ka})$$

It is apparent from this expression that for any s, i.e., any combination of v and a, there is always one and only one solution for ka. A typical graphic for these two curves look like

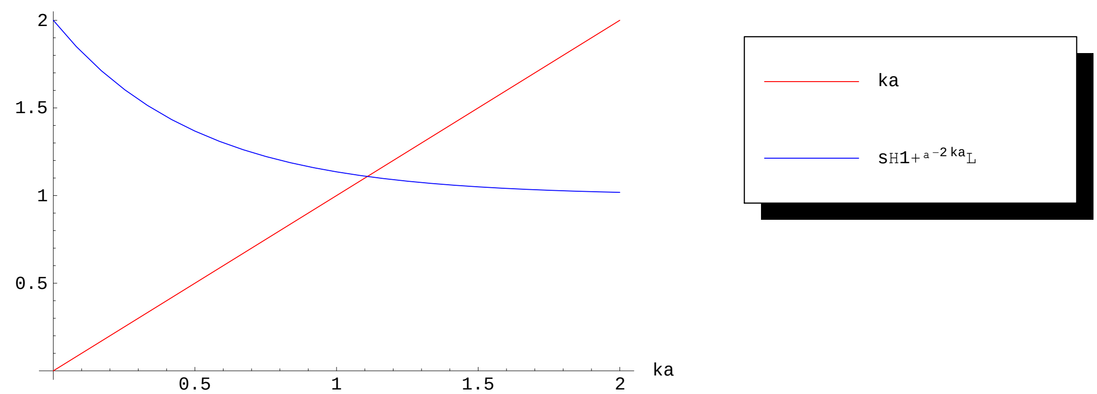

Figure 1: $ka = s(1 + e^{-2ka})$

Therefore, there is only one bound state. The energy is

$$\boxed{E = -\frac{\hbar^2 k^2}{2m} = -\frac{m}{2\hbar^2}\left(v^2(1 + e^{-2ka})^2\right)}$$

This is very reasonable: since for one delta potential, for any strength of $v < 0$, there is always one and only one bound state. Here we form the even parity state from bound states of two delta potentials, it's obvious that there's still only one bound state.

(c) When $s \ll 1 \Rightarrow ka \ll 1$. So

$$ka = s(1 + e^{-2ka}) \sim s(1 + 1 - 2ka) \Rightarrow ka = \frac{2s}{2s+1},$$

So

$$E = -\frac{\hbar^2 k^2}{2m} = -\left(\frac{\hbar^2}{2ma^2}\right)\left(\frac{2s}{2s+1}\right)^2,$$

You can expand further according to $\left(\frac{2s}{2s+1}\right)^2 \sim 4s^2(1-2s)^2$ and get

$$\boxed{E = -\frac{2mv^2}{\hbar^2}(1 - 2\frac{m|v|a}{\hbar^2})^2.}$$

.

(d) Follow the steps in the previous parts, we get

$$\varphi(x) = \begin{cases} A\,e^{-k(x-a)} & \text{if } x \geq a; \\ 2Be^{-ka}\sinh kx & \text{if } -a \leq x \leq a; \\ -A\,e^{k(x+a)} & \text{if } x \leq -a. \end{cases}$$

and $A = B(1 - e^{-2ka})$. Substitute into the integrated Schrödinger equation, we get

$$ka = \frac{m|v|a}{\hbar^2}(1 - e^{-2ka}) \equiv s(1 - e^{-2ka}).$$

This kind of analysis happens frequently so let's look at it more carefully. We'd like to know for what s, the equation $x = s(1 - e^{-2x})$ has solution. Graphically, we plot two curves, $y = x$, and $y = s(1 - e^{-2x})$ for a range of s and see if there's intersection(s). You then will find that, as long as $y = s(1 - e^{-2x})$ has slope > 1 at $x = 0$, then there's one and only one intersection at $x > 0$. The slope is $2s$, so the condition is

$$\boxed{2s > 1 \Rightarrow s > 1/2 \Rightarrow \frac{m|v|a}{\hbar^2} > 1/2.}$$

There is one bound state when the condition is satisfied, otherwise there is no bound state.

(e) For even and odd parity solutions, we have

$$ka = \frac{m|v|a}{\hbar^2}(1 \pm e^{-2ka}) \equiv s(1 \pm e^{-2ka})$$

When $s \gg 1$, $ka \sim s$, and $E = -\frac{\hbar^2}{2m}\frac{s^2}{a^2}$, which is the energy for one delta potential. This is also reasonable: $a \to \infty$ means the two potentials are far away from each other and become separated. The existence of another potential hardly interferes the energy of one potential, so both even and odd parity energies reduce to the unique bound state energy of single Dirac delta potential.