Physics 741 – Graduate Quantum Mechanics 1

# Solution to Midterm Exam, Fall 2018

Please note that some possibly helpful formulas and integrals appear on the second page. Note also that there is one problem on the second page. Each question is worth 20 points, with points for each part marked separately.

**1. Consider the wave function** $\psi(x) = \begin{cases} \sqrt{12\lambda}\left(e^{-\lambda x} - e^{-2\lambda x}\right) & \text{for } x > 0, \\ 0 & \text{for } x < 0. \end{cases}$

**(a) [16] What are $\langle X \rangle$, $\langle P \rangle$, $\langle X^2 \rangle$, and $\langle P^2 \rangle$ for this state?**

We simply work these out, one at a time:

$$\langle X \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x)\, dx = 12\lambda \int_0^{\infty} x\left(e^{-2\lambda x} - 2e^{-3\lambda x} + e^{-4\lambda x}\right) dx = 12\lambda\left[\frac{1}{(2\lambda)^2} - \frac{2}{(3\lambda)^2} + \frac{1}{(4\lambda)^2}\right]$$

$$= \frac{12\lambda}{\lambda^2}\left(\frac{1}{4} - \frac{2}{9} + \frac{1}{16}\right) = \frac{12}{\lambda}\left(\frac{36 - 32 + 9}{144}\right) = \frac{13}{12\lambda},$$

$$\langle X^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^2 \psi(x)\, dx = 12\lambda \int_0^{\infty} x^2\left(e^{-2\lambda x} - 2e^{-3\lambda x} + e^{-4\lambda x}\right) dx = 12\lambda\left[\frac{2}{(2\lambda)^3} - \frac{2\cdot 2}{(3\lambda)^3} + \frac{2}{(4\lambda)^3}\right]$$

$$= \frac{12\lambda}{\lambda^3}\left(\frac{1}{4} - \frac{4}{27} + \frac{1}{32}\right) = \frac{12}{\lambda^2}\left(\frac{216 - 128 + 27}{864}\right) = \frac{115}{72\lambda^2},$$

$$\langle P \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial}{\partial x} \psi(x)\, dx = i\hbar 12\lambda \int_0^{\infty} \left(e^{-\lambda x} - e^{-2\lambda x}\right)\left(\lambda e^{-\lambda x} - 2\lambda e^{-2\lambda x}\right) dx$$

$$= i\hbar 12\lambda^2 \int_0^{\infty} \left(e^{-2\lambda x} - 3e^{-3\lambda x} + 4e^{-4\lambda x}\right) dx = i\hbar\lambda^2\left[\frac{1}{2\lambda} - \frac{3}{3\lambda} + \frac{2}{4\lambda}\right] = 0,$$

$$\langle P^2 \rangle = (-i\hbar)^2 \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x)\, dx = -12\lambda\hbar^2 \int_0^{\infty} \left(e^{-\lambda x} - e^{-2\lambda x}\right)\left(\lambda^2 e^{-\lambda x} - 4\lambda^2 e^{-2\lambda x}\right) dx$$

$$= -12\lambda^3\hbar^2 \int_0^{\infty} \left(e^{-2\lambda x} - 5e^{-3\lambda x} + 4e^{-4\lambda x}\right) dx = -12\hbar^2\lambda^3\left[\frac{1}{2\lambda} - \frac{5}{3\lambda} + \frac{4}{4\lambda}\right] = \frac{12\hbar^2\lambda^3}{6\lambda} = 2\hbar^2\lambda^2,$$

**(b)[4] Find the uncertainties $\Delta x$ and $\Delta p$, and show they satisfy the uncertainty relation.**

$$\Delta x = \sqrt{\langle X^2 \rangle - \langle X \rangle^2} = \sqrt{\frac{115}{72\lambda^2} - \left(\frac{13}{12\lambda}\right)^2} = \frac{1}{\lambda}\sqrt{\frac{230 - 169}{144}} = \frac{\sqrt{61}}{12\lambda},$$

$$\Delta p = \sqrt{\langle P^2 \rangle - \langle P \rangle^2} = \sqrt{2\hbar^2\lambda^2 - 0^2} = \hbar\lambda\sqrt{2},$$

$$(\Delta x)(\Delta p) = \tfrac{\sqrt{122}}{12}\hbar \approx 0.9204\hbar \geq \tfrac{1}{2}\hbar.$$

2. **A particle of mass *m* lies in the infinite square well with allowed region $0 < x < a$. The wave function at *t* = 0 in this region is**
$\Psi(x,0) = \psi(x) = \left(2/\sqrt{3a}\right)\sin(5\pi x/a)\left[1 + i\cos(2\pi x/a)\right]$.

**(a) [7] Write this state in the form $|\psi\rangle = \sum_n c_n |\phi_n\rangle$, where $|\phi_n\rangle$ are the energy eigenstates. Some helpful formulas are provided on the next page.**

The normalized eigenstates and energies are given in the helpful equations. To find the coefficients $c_n$, we simply use the equations

$$c_n = \langle \phi_n | \psi \rangle = \left(2/\sqrt{3a}\right)\sqrt{2/a}\int_0^a \sin(n\pi x/a)\left\{\sin(5\pi x/a)\left[1 + i\cos(2\pi x/a)\right]\right\}$$
$$= \frac{2\sqrt{2}}{a\sqrt{3}}\left\{\frac{1}{2}a\delta_{n5} + \frac{1}{4}ia\left(\delta_{n+2,5} + \delta_{2+5,n} - \delta_{n+5,2}\right)\right\} = \sqrt{\frac{2}{3}}\delta_{n5} + \frac{i}{\sqrt{6}}\left(\delta_{n3} + \delta_{n7} - \delta_{n,-3}\right).$$

The only positive values of *n* for which this doesn't vanish are 3, 5, and 7, so we have $c_5 = \sqrt{\frac{2}{3}}$ and $c_3 = c_7 = \frac{i}{\sqrt{6}}$, all other $c_i$'s vanish. We therefore write the initial state as

$$|\psi\rangle = \tfrac{i}{\sqrt{6}}|\phi_3\rangle + \sqrt{\tfrac{2}{3}}|\phi_5\rangle + \tfrac{i}{\sqrt{6}}|\phi_7\rangle$$

**(b) [7] Check the normalization in both the coordinate and eigenstate basis.**

In the coordinate basis, this is

$$1 \stackrel{?}{=} \int_{-\infty}^{\infty}\psi^*(x)\psi(x)\,dx = \tfrac{4}{3a}\int_0^a \left\{\sin(5\pi x/a)\left[1 - i\cos(2\pi x/a)\right]\right\}\left\{\sin(5\pi x/a)\left[1 + i\cos(2\pi x/a)\right]\right\}dx$$
$$= \frac{4}{3a}\int_0^a \left\{\sin^2(5\pi x/a) + \sin^2(5\pi x/a)\cos^2(2\pi x/a)\right\}dx = \frac{4}{3a}\left\{\frac{1}{2}a\delta_{55} + \frac{1}{4}a - \frac{1}{8}a\delta_{53}\right\} = \frac{4}{3a}\cdot\frac{3}{4}a = 1.$$

In the eigenstate basis, this is far simpler:

$$1 \stackrel{?}{=} \sum_n |c_n|^2 = |c_3|^2 + |c_5|^2 + |c_7|^2 = \tfrac{1}{6} + \tfrac{2}{3} + \tfrac{1}{6} = 1.$$

**(c) [6] Write the wave function $\Psi(x,t)$ at all times.**

The general formula for the state vector is $|\Psi(t)\rangle = \sum_n c_n |\phi_n\rangle e^{-iE_n t/\hbar}$. Substituting in the explict form for our states and energies, we have

$$\Psi(x,t) = \frac{2}{\sqrt{3a}}\sin\left(\frac{5\pi x}{a}\right)\exp\left(-\frac{25\pi^2\hbar i t}{2ma^2}\right)$$
$$+ \frac{i}{\sqrt{3a}}\left[\sin\left(\frac{3\pi x}{a}\right)\exp\left(-\frac{9\pi^2\hbar i t}{2ma^2}\right) + \sin\left(\frac{7\pi x}{a}\right)\exp\left(-\frac{49\pi^2\hbar i t}{2ma^2}\right)\right].$$

**3. A particle of mass *m* lies in the potential $V(x,y,z)=\alpha\left(x^2+y^2+z^2\right)^2+\gamma\left(x^2y+y^2z+z^2x\right)$. Consider the rotation operator that rotates the three coordinates among each other, so that $\mathcal{R}(x,y,z)=(y,z,x)$, *i.e.* $x'=y$, $y'=z$, $z'=x$.**

**(a) [6] Show that this is a symmetry operation; that is, *V* is unchanged by this transformation. You may assume that the kinetic term in the Hamiltonian is also unchanged.**

We simply check if $V(x',y',z')=V(x,y,z)$:

$$V(x',y',z')=V(y,z,x)=\alpha\left(y^2+z^2+x^2\right)^2+\gamma\left(y^2z+z^2x+x^2y\right)=V(x,y,z).$$

That was easy!

**(b) [7] Argue that if this symmetry operation were performed a particular number of times, the resulting symmetry operation would correspond with the identity operation. How many times?**

If we perform the symmetry operation three times, we would have

$$\mathcal{R}\left(\mathcal{R}\left(\mathcal{R}(x,y,z)\right)\right)=\mathcal{R}\left(\mathcal{R}(y,z,x)\right)=\mathcal{R}(z,x,y)=(x,y,z)$$

Hence the rotation cubed is $\mathcal{R}^3=1$, the identity rotation, and hence if $R(\mathcal{R})$ is the corresponding operator, we would have $\left[R(\mathcal{R})\right]^3=R(\mathcal{R})R(\mathcal{R})R(\mathcal{R})=R\left(\mathcal{R}^3\right)=R(1)=1$.

**(c) [7] Argue that eigenstates of the Hamiltonian can be chosen to also be eigenstates of this symmetry operation. What are the possible eigenvalues of these states under the symmetry operation?**

Since the rotation leaves the potential unchanged, this means the corresponding operator commutes with the potential, and since we are allowed to assume the same thing about the kinetic term, $R(\mathcal{R})$ commutes with the Hamiltonian. Hence we can diagonalize these simultaenously, and our eigenstates of the Hamiltonian will look like $|\lambda,n\rangle$, with eigenvalue $E_n$ under the Hamiltonian, and eigenvalue $\lambda$ under $R(\mathcal{R})$. Because rotating it three times brings it back to itself, we must have

$$|\lambda,n\rangle=R(1)|\lambda,n\rangle=R\left(\mathcal{R}^3\right)|\lambda,n\rangle=\left[R(\mathcal{R})\right]^3|\lambda,n\rangle=\lambda^3|\lambda,n\rangle.$$

We therefore have $\lambda^3=1$, an equation with solutions $\lambda=e^{2\pi ij/3}$ for $j$ = 0, 1, and 2. Working these out in each case, the solutions are $\lambda=1$ and $\lambda=-\frac{1}{2}\pm\frac{\sqrt{3}}{2}i$.

**4. A particle is in the state** $|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}$**, when the operator** $B = b\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}$ **is measured.**

**What are the possible outcomes, and what would be the corresponding probabilities? For each of these possible outcomes, what would be the state vector after measurrement?**

The first step is to find the eigenvalues and eigenvectors of *B*. We first note that *B* is block diagonal, and therefore we can immediately identify one of the eigenvalues as *b*, which corresponds to an eigenvector with just 1 in the third position The remaining two eigenvectors and eigenvalues require that we diagonalize the first two rows an colums of the matrix, which if you remove the factor of *b* just requires that we find the eigenvalues and eigenvectors of $\begin{pmatrix}0&1\\1&0\end{pmatrix}$. We do this by solving the characteristic equation, which is

$$0 = \det\begin{pmatrix}-\lambda & 1\\ 1 & -\lambda\end{pmatrix} = \lambda^2 - 1 = (\lambda-1)(\lambda+1), \quad \lambda = \pm 1.$$

It is not hard to find and normalize the corredponding eigenvectors, which work out to be $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\\pm 1\end{pmatrix}$. When you put back in the factor of *b*, expand these back to all three components, and add in the eigenstate we found trivially, we find the three eigenstates:

$$|b,1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad |-b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix}, \quad |b,2\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}.$$

The only possible outcomes of the measurement are the eigevnalues $\pm b$. We note that two of the states have the same eigenvalue.

Now we start calculating probabilities and finding the state afterwards. For *b*, we find

$$P(b) = |\langle b,1|\psi\rangle|^2 + |\langle b,2|\psi\rangle|^2 = \left|\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\0\\\frac{1}{\sqrt{2}}\end{pmatrix}\right|^2 + \left|\begin{pmatrix}0&0&1\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\0\\\frac{1}{\sqrt{2}}\end{pmatrix}\right|^2 = \left(\tfrac{1}{2}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2 = \tfrac{3}{4}.$$

The state vector afterwards is

$$|\psi^+\rangle = \frac{1}{\sqrt{P(+b)}}\left(|b,1\rangle\langle b,1|\psi\rangle + |b,2\rangle\langle b,2|\psi\rangle\right) = \sqrt{\tfrac{4}{3}}\left(\tfrac{1}{2}|b,1\rangle + \tfrac{1}{\sqrt{2}}|b,2\rangle\right) = \tfrac{1}{\sqrt{3}}\begin{pmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\\0\end{pmatrix} + \sqrt{\tfrac{2}{3}}\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{6}}\\\frac{1}{\sqrt{6}}\\\sqrt{\frac{2}{3}}\end{pmatrix}.$$

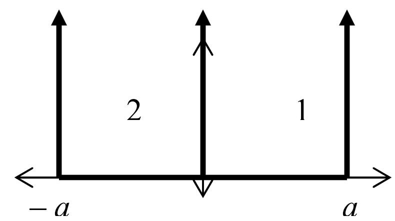
For outcome –*b*, we have

$$P(-b) = \left|\langle -b|\psi\rangle\right|^2 = \left|\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}\right|^2 = \left(\tfrac{1}{2}\right)^2 = \tfrac{1}{4}, \quad |\psi^+\rangle = \frac{1}{\sqrt{\frac{1}{4}}}|-b\rangle\langle -b|\psi\rangle = 2|-b\rangle\tfrac{1}{2} = |-b\rangle .$$

Of course, because there was only one eigenstate with this eigenvalue, the final state was inevitable.

**5. A particle of mass *m* is in an infinite square well with a spike in the middle, with potential**

$$V(x) = \begin{cases} \infty & \text{if } |x| > a, \\ \lambda\delta(x) & \text{if } |x| < a. \end{cases}$$




**This potential is sketched at right. In region 1, the solution to Schrödinger's equation is $\psi_1 = \sin(ka - kx)$ with energy $E = \hbar^2 k^2 / 2ma^2$ .**

**(a) [7] Argue based on symmetry that there are "even" and "odd" solutions. For the odd solutions, argue that $\psi(0) = 0$ . Find all possible values for *k* in this case. For the even solutions, show in region 2 that $\psi_2(x) = \sin(ka + kx)$ .**

The potential is symmetric, $V(-x) = V(x)$. As argued in class, under this assumption we expect our eigenstates to also be eigenstates of parity, with eigenvalue $\pm 1$, and therefore $\psi(-x) = \pm\psi(x)$, which we call the even (+) and odd (–) states.

For odd solutions, we have $\psi(-x) = -\psi(x)$, which at zero gives $\psi(0) = 0$. Hence we have $\sin(ka) = 0$, which has solutions whenever $ka = \pi n$, so $k = \pi n / a$. For even solutions, region 2 is just the reflection of region 1, so $\psi_2(x) = \psi_1(-x) = \sin(ka + kx)$.

**(b) [7] Integrate Schrödinger's equation from $-\varepsilon$ to $+\varepsilon$ across the origin, in the limit $\varepsilon \to 0^+$ to find a formula for the discontinuity in the derivative.**

We start with Schrödinger's equation with the potential and integrate it over this small region:

$$\int_{-\varepsilon}^{\varepsilon} E\psi(x)\,dx = \int_{-\varepsilon}^{\varepsilon} \left\{ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \lambda\delta(x)\psi \right\} dx = -\frac{\hbar^2}{2m}\left[\psi'(\varepsilon) - \psi'(-\varepsilon)\right] + \lambda\psi(0),$$

where we used the fundemental theorem of calculus to simplify the first term. In the limit $\varepsilon \to 0^+$, the left side will vanish, and this formula becomes simply

$$\tfrac{1}{2}\hbar^2\left[\psi_1'(0) - \psi_2'(0)\right] = m\lambda\psi(0).$$

**(c) [6] For the even solutions, use this to find a formula for $k\cot(ka)$.**

Using our explicit formula in the two regions, this simply says

$$\tfrac{1}{2}\hbar^2\left[-k\cos(ka-0)-k\cos(ka+0)\right]=m\lambda\sin(ka)\,,$$

$$-\hbar^2 k\cos(ka)=m\lambda\sin(ka)\,,$$

$$k\cot(ka)=-\frac{m\lambda}{\hbar^2}\,.$$

**Possibly Helpful Formulas:**

| |
|---|
| Infinite Square Well |
| mass *m*, region $0<x<a$ |
| $\psi_n(x)=\sqrt{2/a}\sin(\pi nx/a)$ |
| $E_n=\dfrac{n^2\pi^2\hbar^2}{2ma^2}$ |

**Possibly Helpful Integrals:** *n*, *p* and *q* are assumed to be positive integers

$$\int_0^\infty x^n e^{-\alpha x}dx=\frac{n!}{\alpha^{n+1}}\,,\qquad \int_0^a \sin\left(\frac{\pi nx}{a}\right)dx=\begin{cases}\frac{2a}{\pi n} & \text{if } n \text{ odd,}\\ 0 & \text{if } n \text{ even.}\end{cases}\qquad \int_0^a \sin\left(\frac{\pi nx}{a}\right)\sin\left(\frac{\pi px}{a}\right)dx=\tfrac{1}{2}a\delta_{np}\,,$$

$$\int_0^a \sin\left(\frac{\pi nx}{a}\right)\cos\left(\frac{\pi px}{a}\right)dx=\begin{cases}\frac{2an}{\pi(n^2-p^2)} & \text{if } n+p \text{ odd,}\\ 0 & \text{if } n+p \text{ even.}\end{cases}$$

$$\int_0^a \sin\left(\frac{\pi nx}{a}\right)\sin\left(\frac{\pi px}{a}\right)\cos\left(\frac{\pi qx}{a}\right)dx=\tfrac{1}{4}a\left(\delta_{n,p+q}+\delta_{p,n+q}-\delta_{q,n+p}\right),$$

$$\int_0^a \sin^2\left(\frac{\pi nx}{a}\right)\cos^2\left(\frac{\pi px}{a}\right)dx=a\left(\tfrac{1}{4}-\tfrac{1}{8}\delta_{np}\right)\qquad \int_0^a \cos\left(\frac{\pi nx}{a}\right)\sin^2\left(\frac{\pi px}{a}\right)dx=\tfrac{1}{4}a\delta_{n,2p}\,.$$