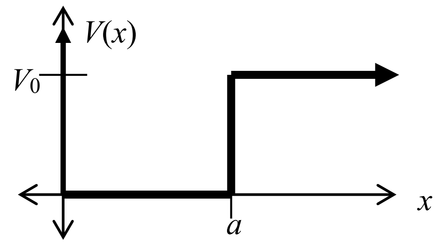
Physics 741 – Graduate Quantum Mechanics 1

Solutions to Midterm Exam, Fall 2022

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. A particle of mass *m* lies in a potential *V*(*x*), where

$$V(x)=\begin{cases}\infty & x<0\\ 0 & 0<x<a\\ V_0 & x>a\end{cases}$$



This potential is sketched at right. We will attempt to find bound states, $0 < E < V_0$.

(a) [7] For the region $0 < x < a$, write the most general solution of Schrödinger's time independent equation, and relate any parameters to the energy *E*, applying appropriate boundary conditions at $x = 0$.

Schrödinger's equation in this region is just

$$E\psi=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}.$$

Because the energy is positive, we need to find functions that have a second derivative that is equal to minus itself. The possible solutions look like $\sin(kx)$ and $\cos(kx)$. Since we need the function to vanish at the origin, we reject $\cos(kx)$. Substituting $\sin(kx)$ into Schrödinger's equation, we find the energy and the general solution to the equation:

$$\psi_I = A\sin(kx),\quad E=\frac{\hbar^2k^2}{2m}.$$

(b) [7] Repeat for the region $x > a$, applying appropriate boundary conditions at $x = \infty$.

In this region, Schrödinger's equation is now

$$E\psi=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V_0\psi,\quad \text{or}\quad (V_0-E)\psi=\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}.$$

Since $V_0 > E$, the solutions to this equation now look like $e^{\pm\beta x}$. But we don't want the wave function to blow up at infinity. Substituting $e^{-\beta x}$ into Schrödinger's equation, we find

$$\psi_{II}=Be^{-\beta x},\quad V_0-E=\frac{\hbar^2\beta^2}{2m}.$$

(c) [6] What boundary conditions can you at $x = a$? Take the ratio (or substitute) these equations to find a relation between the parameters found in parts (a) and (b), cancelling any normalization factors. You do not need to solve these equations.

Because the potential is finite at $x = a$, the wave function and its first derivative must both be continuous, so $\psi_I(a) = \psi_{II}(a)$ and $\psi_I'(a) = \psi_{II}'(a)$. Substituting our explicit forms, this becomes

$$A\sin(ka) = Ce^{-\beta a} \quad \text{and} \quad Ak\cos(ka) = -C\beta e^{-\beta a}.$$

If we substitute the first equation into the second, we find $Ak\cos(ka) = -A\sin(ka)e^{-\beta a}$, or

$$k\cot(ka) = -\beta.$$

It is not hard to see that $k^2 + \beta^2 = 2mV_0/\hbar^2$, so if we want we can rewrite this entirely a function of k, but you then have to solve the equation numerically.

2. A quantum mechanical system is two dimensional, and in a choice of basis, the Hamiltonian is $H = \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -2 \end{pmatrix}$ and $B = b\begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix}$. At $t = 0$, it is in the state $|\Psi(t=0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

(a) [7] For the operator B, find the eigenvalues and normalized eigenvectors.

Ignoring the factor of b, we can find the eigenvalues of the remaining matrix by solving the characteristic equation

$$0 = \det\begin{pmatrix} 4-\lambda & 2 \\ 2 & 1-\lambda \end{pmatrix} = (4-\lambda)(1-\lambda) - 2\cdot 2 = 4 - \lambda - 4\lambda + \lambda^2 - 4 = \lambda^2 - 5\lambda = \lambda(\lambda - 5).$$

The eigenvalues for this matrix are therefore 0 and 5, or restoring the factor of b, 0 and $5b$.

The eigenstates can be found by putting in an arbitrary vector and demanding that the matrix times the vector is the vector times the appropriate eigenvalue, so our equations are:

$$\begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 5\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 5\alpha \\ 5\beta \end{pmatrix}.$$

We then expand these out, in each case getting two equations:

$$\begin{Bmatrix} 4\alpha + 2\beta = 0 \\ 2\alpha + \beta = 0 \end{Bmatrix} \quad \text{or} \quad \begin{Bmatrix} 4\alpha + 2\beta = 5\alpha \\ 2\alpha + \beta = 5\beta \end{Bmatrix},$$

$$\beta = -2\alpha \quad \text{or} \quad \alpha = 2\beta.$$

As usual, in each case we get redundant equations. Our eigenvectors are now

$$|0\rangle = \begin{pmatrix} \alpha \\ -2\alpha \end{pmatrix} \quad \text{or} \quad |5b\rangle = \begin{pmatrix} 2\beta \\ \beta \end{pmatrix}.$$

We still have to normalize these, which is achieved by demanding $4\alpha^2 + \alpha^2 = 1 = \beta^2 + 4\beta^2 = 1$. So we find $\alpha = \beta = 1/\sqrt{5}$, but to normalization, and we have

$$|0\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ -2 \end{pmatrix} \quad \text{and} \quad |5b\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 1 \end{pmatrix}.$$

(b) [4] At time *t* = 0, the system is measured using the operator *B*. What is the probability that the result comes out the more positive eigenvalue? Assuming it does, what is the state immediately after the measurement?

The probability of getting the positive eigenvalue $5b$ is given by

$$P(5b) = |\langle 5b|\Psi\rangle|^2 = \left|\frac{1}{\sqrt{5}}(2 \quad 1)\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right|^2 = \left(\frac{2}{\sqrt{5}}\right)^2 = \frac{4}{5} = 80\%.$$

Afterwards the state will be an eigenstate of B with eigenvalue $5b$, so it is in the state $|5b\rangle$.

(c) [5] After the measurement described in part (b), what is the state vector at general time *t*? What is it at the specific time *t* = *π*/*ω*?

The Hamiltonian is diagonal, so each of the two components will simply acquire a phase of $e^{-iEt/\hbar}$, which works out to $e^{-i\omega t}$ on the top component, and $e^{2i\omega t}$ on the lower component. So we would have the state evolve from

$$\Psi(t=0) = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 1 \end{pmatrix} \quad \to \quad \Psi(t) = \frac{1}{\sqrt{5}}\begin{pmatrix} 2e^{-i\omega t} \\ e^{2i\omega t} \end{pmatrix}.$$

At $\omega t = \pi$, $e^{-i\pi} = -1$ and $e^{i2\pi} = 1$, so

$$\Psi(t = \pi/\omega) = \frac{1}{\sqrt{5}}\begin{pmatrix} -2 \\ 1 \end{pmatrix}.$$

(d) [4] At this time, *B* is measured again. What is the probability *this time* that the result will be the more positive eigenvalue?

We use the same formula as before, namely

$$P(5b) = |\langle 5b|\Psi\rangle|^2 = \left|\frac{1}{\sqrt{5}}(-2 \quad 1)\frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 1 \end{pmatrix}\right|^2 = \left|\frac{1}{5}(-4+1)\right|^2 = \left(\frac{3}{5}\right)^2 = \frac{9}{25} = 36\%.$$

3. **A particle of mass *m* lies in the potential** $V(x,y,z)=\alpha\left(x^4+y^4+z^4\right)+\beta\left(x^2z-y^2z\right)+\gamma xyz$**. Consider the rotation operator that rotates by 90° around the *z*-axis and then flips *z*, so that** $\mathcal{R}(x,y,z)=(y,-x,-z)$**, *i.e.*** $x'=y$, $y'=-x$, $z'=-z$ **.**

   (a) **[6] Show that this is a symmetry operation; that is, *V* is unchanged by this transformation.**

We simply substitute and start calculating:

$$\begin{aligned}V(x',y',z)&=\alpha\left(x'^4+y'^4+z'^4\right)+\beta\left(x'^2z'-y'^2z'\right)+\gamma x'y'z'\\&=\alpha\left(y^4+(-x)^4+(-z)^4\right)+\beta\left(y^2(-z)-(-x)^2z\right)+\gamma y(-x)(-z)\\&=\alpha\left(x^4+y^4+z^4\right)+\beta\left(x^2z-y^2z\right)+\gamma xyz=V(x,y,z).\end{aligned}$$

   (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?**

Logically, if you are rotating around *z* four times by 90°, that would end up as no rotation. If you are simultaneously flipping the *z*-direction, doing it four times also result in no flip, so the answer to this question is four operations equals the identity operator. You can also demonstrate this by performing the rotation operator four times, each time switching the first two arguments and then placing a minus sign on the second and third operators:

$$\mathcal{R}^4(x,y,z)=\mathcal{R}^3(y,-x,-z)=\mathcal{R}^2(-x,-y,z)=\mathcal{R}(-y,x,-z)=(x,y,z).$$

   (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?**

The kinetic term is invariant under any rotation, and we have already demonstrated that the potential is also invariant under this transformation. Hence this rotation commutes with the Hamiltonian, and therefore the states can be simultaneously diagonalized. Hence we can choose our eigenstates of the Hamiltonian to also be eigenstates of $R(\mathcal{R})$, so we have

$$H|\lambda,n\rangle=E_n|\lambda,n\rangle,\quad R(\mathcal{R})|\lambda,n\rangle=\lambda|\lambda,n\rangle.$$

Interestingly, if you repeat the operation four times, you get one, so $R(\mathcal{R})^4=R(\mathcal{R}^4)=R(1)=1$. It follows that

$$|\lambda,n\rangle=R(\mathcal{R})^4|\lambda,n\rangle=\lambda^4|\lambda,n\rangle.$$

It follows that $\lambda^4=1$. The eigenvalues of this are $e^{2\pi ij/4}=e^{\pi ij/2}$, where j = 0, 1, 2, 3, so the values are $e^0=1$, $e^{\pi i/2}=i$, $e^{\pi i}=-1$, and $e^{3\pi i/2}=i$, or in summary, $\lambda=\pm1$ or $\lambda=\pm i$.

4. A particle is in the ground state of the infinite square well at time *t* = 0.

(a) [10] Calculate the expectation values $\langle X\rangle$, $\langle X^2\rangle$, $\langle P\rangle$ and $\langle P^2\rangle$ for this state.

This is straightforward, though many of the integrals are a little messy. We start with the wave function, which for the ground state is $\psi_1(x)=\sqrt{2/a}\sin(\pi x/a)$. We therefore have

$$\langle X\rangle = \int \psi^*(x)\,x\psi(x)\,dx = \frac{2}{a}\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)dx = \frac{2}{a}\cdot\frac{a^2}{4}=\frac{a}{2},$$

$$\langle X^2\rangle = \int \psi^*(x)\,x^2\psi(x)\,dx = \frac{2}{a}\int_0^a x^2\sin^2\left(\frac{\pi x}{a}\right)dx = \frac{2}{a}\left(\frac{1}{6}-\frac{1}{4\pi^2}\right)a^3 = \left(\frac{1}{3}-\frac{1}{2\pi^2}\right)a^2,$$

$$\langle P\rangle = -i\hbar\int \psi^*(x)\frac{d}{dx}\psi(x)\,dx = -\frac{2i\hbar}{a}\int \sin\left(\frac{\pi x}{a}\right)\frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right)dx = 0,$$

$$\langle P^2\rangle = (-i\hbar)^2\int \psi^*(x)\frac{d^2}{dx^2}\psi(x)\,dx = -\frac{2\hbar^2}{a}\int \sin\left(\frac{\pi x}{a}\right)\left(\frac{\pi}{a}\right)^2\left[-\sin\left(\frac{\pi x}{a}\right)\right]dx = \frac{2\pi^2\hbar^2}{a^3}\cdot\frac{a}{2}=\frac{\pi^2\hbar^2}{a^2}.$$

(b) [5] Find the uncertainties Δx and Δp, and check the uncertainty relation.

We have

$$\Delta x = \sqrt{\langle X^2\rangle - \langle X\rangle^2} = \sqrt{\left(\frac{1}{3}-\frac{1}{2\pi^2}\right)a^2 - \frac{1}{4}a^2} = a\sqrt{\frac{1}{12}-\frac{1}{2\pi^2}},$$

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

$$(\Delta x)(\Delta p) = a\sqrt{\frac{1}{12}-\frac{1}{2\pi^2}}\,\frac{\pi\hbar}{a} = \hbar\sqrt{\frac{\pi^2}{12}-\frac{1}{2}} = 0.568\hbar.$$

The uncertainty relation says the final expression must exceed $\hbar/2$, which it does.

(c) [5] Suppose that *before* we did the measurement, we allowed the system to evolve under the influence of the Hamiltonian until an arbitrary time *t*. How would this change the answers to parts (a) and (b)?

Because it is in an eigenstate of the Hamiltonian, the wave function will simply get multiplied by $e^{-iEt/\hbar}$. This phase change simply factors out of every factor of ψ, and it will then cancel with the factor of $e^{+iEt/\hbar}$ appearing in ψ^*. Therefore the answer to every part of the question will be unchanged.

5. **A particle of mass *m* lies in the harmonic oscillator potential $V = \frac{1}{2}m\omega^2 x^2$. At *t* = 0, the wave function is given by $\Psi(x,t=0) = Nx^2 e^{-\alpha x^2/2}$, where $\alpha = m\omega/\hbar$.**
   (a) [4] What is the normalization constant *N*? Some possibly helpful integrals are given below.

We find the normalization of the state by demanding that

$$1 = \int \Psi^* \Psi dx = N^2 \int x^4 e^{-\alpha x^2} dx = N^2 \alpha^{-5/2} \Gamma\left(\tfrac{5}{2}\right) = \frac{3}{4} N^2 \sqrt{\frac{\pi}{\alpha^5}}.$$

Solving for *N*, we have

$$N = \sqrt{\frac{4}{3}\sqrt{\frac{\alpha^5}{\pi}}} = \frac{2\alpha}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/4.},$$

so that the wave function at $t = 0$ is

$$\Psi(x,t=0) = \left(\frac{\alpha}{\pi}\right)^{1/4.} \frac{2}{\sqrt{3}} \alpha x^2 e^{-\alpha x^2/2}.$$

   (b) [6] Write this wave function in the form $|\Psi(t=0)\rangle = \sum_n c_n |\phi_n\rangle$, where $|\phi_n\rangle$'s are the eigenstates of the Hamiltonian. The explicit forms for the first three are given below. Check that the state vector is normalized in the new basis of the $|\phi_n\rangle$'s.

We need to combine the ϕ's in such a way to make the constant terms cancel, but keep the quadratic term. It is pretty obvious that

$$\phi_0(x) + \sqrt{2}\phi_2(x) = (\alpha/\pi)^{1/4} 2\alpha x^2 e^{-\alpha x^2/2}.$$

Comparison with $\Psi(x,0)$ then tells us that
The wave function at $t = 0$ is therefore

$$\Psi(x,0) = \frac{1}{\sqrt{3}}\phi_0(x) + \sqrt{\frac{2}{3}}\phi_2(x),$$

or to put it more succinctly, $|\Psi(0)\rangle = \frac{1}{\sqrt{3}}|\phi_0\rangle + \sqrt{\frac{2}{3}}|\phi_2\rangle$. Hence we have $c_0 = \frac{1}{\sqrt{3}}$ and $c_2 = \sqrt{\frac{2}{3}}$, with all the other c_n's vanishing. It is obvious that $\sum_n |c_n|^2 = c_0^2 + c_2^2 = 1$, so it is normalized in this new basis.

(c) [5] Write the state vector $|\Psi(t)\rangle$ at all times.

The energy of the n'th state of the harmonic oscillator is $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$, and each of the eigenstates is then multiplied by a factor of $\exp\left(-iE_n t/\hbar\right) = \exp\left[-i\omega t\left(n+\frac{1}{2}\right)\right]$, so we have

$$|\Psi(t)\rangle = \tfrac{1}{\sqrt{3}}|\phi_0\rangle e^{-i\omega t/2} + \sqrt{\tfrac{2}{3}}|\phi_2\rangle e^{-5i\omega t/2}.$$

(d) [5] Find the probability density that the particle is at the origin $x = 0$ at all times. Simplify as much as possible.

Substituting in our explicit forms for the wave functions, we have

$$\begin{aligned}\Psi(x,t) &= \left(\frac{\alpha}{\pi}\right)^{1/4}\frac{1}{\sqrt{3}}e^{-\alpha x^2/2}e^{-i\omega t/2} + \left(\frac{\alpha}{\pi}\right)^{1/4}\sqrt{\frac{2}{3}}\frac{1}{\sqrt{2}}\left(\alpha x^2-1\right)e^{-\alpha x^2/2}e^{-5i\omega t/2} \\ &= \frac{1}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2}\left(2\alpha x^2 e^{-5i\omega t/2} + e^{-i\omega t/2} - e^{-5i\omega t/2}\right).\end{aligned}$$

Evaluating this at $x = 0$, we have

$$\Psi(x,0) = \frac{1}{\sqrt{3}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(e^{-i\omega t/2} - e^{-5i\omega t/2}\right).$$

The probability density at $x = 0$ is then

$$\begin{aligned}\rho(x,0) = \Psi(x,0)^*\Psi(x,0) &= \frac{1}{3}\sqrt{\frac{a}{\pi}}\left(e^{i\omega t/2} - e^{5i\omega t/2}\right)\left(e^{-i\omega t/2} - e^{-5i\omega t/2}\right) \\ &= \frac{1}{3}\sqrt{\frac{\alpha}{\pi}}\left(1 - e^{-2i\omega t} - e^{2i\omega t} + 1\right) = \frac{2}{3}\sqrt{\frac{\alpha}{\pi}}\left[1-\cos(2\omega t)\right].\end{aligned}$$

Infinite Square well: mass m, region $0 < x < a$: $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n x}{a}\right)$, $\quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$.

Harmonic Oscillator Wave Functions:

$$\phi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}, \quad \phi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\, x e^{-\alpha x^2/2}, \quad \phi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} \left(2\alpha x^2 - 1\right) e^{-\alpha x^2/2}.$$

Possibly Helpful Integrals: n is assumed to be a positive integer, and A is positive

$$\int_{-\infty}^{\infty} x^n e^{-Ax^2} dx = \begin{cases} \Gamma\left(\frac{n+1}{2}\right) A^{-(n+1)/2} & n \text{ even,} \\ 0 & n \text{ odd.} \end{cases}$$

$$\Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma\left(\tfrac{3}{2}\right) = \tfrac{1}{2}\sqrt{\pi}, \quad \Gamma\left(\tfrac{5}{2}\right) = \tfrac{3}{4}\sqrt{\pi}, \quad \Gamma\left(\tfrac{7}{2}\right) = \tfrac{15}{8}\sqrt{\pi}, \quad \Gamma\left(\tfrac{9}{2}\right) = \tfrac{105}{16}\sqrt{\pi}, \quad \Gamma\left(\tfrac{11}{2}\right) = \tfrac{945}{32}\sqrt{\pi}.$$

$$\int_0^a \sin^2\left(\frac{\pi n x}{a}\right) dx = \int_0^a \cos^2\left(\frac{\pi n x}{a}\right) dx = \frac{a}{2}, \quad \int_0^a \sin\left(\frac{\pi n x}{a}\right) \cos\left(\frac{\pi n x}{a}\right) dx = 0,$$

$$\int_0^a x \sin^2\left(\frac{\pi n x}{a}\right) dx = \int_0^a x \cos^2\left(\frac{\pi n x}{a}\right) dx = \frac{a^2}{4}, \quad \int_0^a x \sin\left(\frac{\pi n x}{a}\right) \cos\left(\frac{\pi n x}{a}\right) dx = -\frac{a^2}{4\pi n},$$

$$\int_0^a x^2 \sin^2\left(\frac{\pi n x}{a}\right) dx = \left(\frac{1}{6} - \frac{1}{4\pi^2 n^2}\right) a^3, \quad \int_0^a x^2 \cos^2\left(\frac{\pi n x}{a}\right) dx = \left(\frac{1}{6} + \frac{1}{4\pi^2 n^2}\right) a^3.$$