UNSW SCHOOL OF PHYSICS

PHYS2111 – Quantum Mechanics

Tutorial 5 SOLUTIONS

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Question 1

(Shankar 1.8.4) An arbitrary $n \times n$ matrix need not have n eigenvectors. Consider as an example

$$\Omega = \begin{pmatrix} 4 & 1 \\ -1 & 2 \end{pmatrix}$$

(a) Show that $\omega_1 = \omega_2 = 3$.

Solving our determinant equation for eigenvalue ω, we have

$$\det \begin{pmatrix} 4-\omega & 1 \\ -1 & 2-\omega \end{pmatrix} = (4-\omega)(2-\omega) + 1 = (\omega-3)^2 = 0$$

which evidently gives a single eigenvector $\omega = 3$.

(b) By feeding in this value show we get only one eigenvector of the form

$$\frac{1}{\sqrt{2|a|^2}} \begin{pmatrix} a \\ -a \end{pmatrix}.$$

We cannot find another linearly independent eigenvector.

With eigenvector $\vec{v} = (a, b)^T$, we can plug $\omega = 3$ into our $(\Omega - \omega I)\vec{v} = 0$ to give

$$\left(\begin{array}{cc|c} 1 & 1 & 0 \\ -1 & -1 & 0 \end{array} \right).$$

Adding the first row to the second row cancels it completely, so we are left only with the first row, which gives

$$a + b = 0.$$

Thus, setting $b = -a$ and normalising, we only get the single eigenvector

$$\frac{1}{\sqrt{2|a|^2}} \begin{pmatrix} a \\ -a \end{pmatrix}$$

as required.

Question 2

Consider the operator

$$\hat{T} = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix}.$$

(a) Is T Hermitian?

Yes!

(b) Find the two eigenvalues of $\hat{T}$, which we label t_1 and t_2, and show that they are real. Find the corresponding eigenvectors $|t_1\rangle$ and $|t_2\rangle$.

I leave it to you to show that

$$\begin{aligned} t_1 = 2: &\quad |t_1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1-i \\ 1 \end{pmatrix} \\ t_2 = -1: &\quad |t_1\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} -1+i \\ 2 \end{pmatrix} \end{aligned}$$

(c) Use the eigenvectors to find the matrix U which diagonalises the matrix $\hat{T}$. That is, find U such that $U^\dagger \hat{T} U = \hat{D}_T$ where $\hat{D}_T$ is a diagonal matrix. What is $\hat{D}_T$?

Stacking together our eigenvectors in a matrix as $\big(|t_1\rangle\, |t_2\rangle\big)$, we get

$$U = \begin{pmatrix} \frac{1}{\sqrt{3}}(1-i) & \frac{1}{\sqrt{6}}(-1+i) \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} \end{pmatrix}.$$

With this ordering of the eigenvectors in U, we have that $D_T = \mathrm{diag}(t_1, t_2)$; that is

$$D = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}.$$

(d) Check that

$$\sum_i t_i \, |t_i\rangle \langle t_i| = \hat{T}.$$

I leave this one to you to go through the algebra and check this!

Question 3

Show that the commutator $\hat{C} = i[\hat{A}, \hat{B}]$ is Hermitian if $\hat{A}$ and $\hat{B}$ are both Hermitian. *Hint:* Remember that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$.

Dropping the hats so I don't have to type them out, let A, B both be Hermitian (that is, $A^\dagger = A, B^\dagger = B$). Now we wish to show that $C \equiv i[A, B]$ is Hermitian. The easiest way to do this is to compute $C^\dagger$ and show we get the same thing back! So, going through the algebra we have

$$\begin{aligned}
C^\dagger &= (i[A,B])^\dagger \\
&= -i([A,B])^\dagger && \text{(conjugating i)} \\
&= -i(AB - BA)^\dagger \\
&= -i((AB)^\dagger - (BA)^\dagger) \\
&= -i(B^\dagger A^\dagger - A^\dagger B^\dagger) && (XY)^\dagger = Y^\dagger X^\dagger \\
&= -i(BA - AB) && \text{(since } A, B \text{ are Hermitian)} \\
&= i(AB - BA) \\
&= i[A,B] \\
&= C
\end{aligned}$$

and so our proof is complete.

Question 4

The Pauli matrices are defined as

$$\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(a) Show that $[\hat{\sigma}_1, \hat{\sigma}_2] = 2i\hat{\sigma}_3$.

I leave it to you to show this!

(b) Use the generalised uncertainty principle

$$\Delta A.\Delta B \geq \left| \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right|$$

to obtain $\Delta\sigma_1 \Delta\sigma_2$ for:

i. the state $|u\rangle$;

ii. the state $|d\rangle$;

iii. the state $\frac{1}{\sqrt{2}}(|u\rangle + |d\rangle)$.

Explain the physical meaning.

Since the generalised uncertainty principle only provides a bound on $\Delta\sigma_1\Delta\sigma_2$, I'll interpret this question as asking us to find that bound (as opposed to finding $\Delta\sigma_1\Delta\sigma_2$ itself. We'll also take $|u\rangle \equiv (1,0)^T$ and $|d\rangle \equiv (0,1)^T$. Then, using the previous question, we see that for these specific operators,

$$\Delta\sigma_1\Delta\sigma_2 \geq |\langle \sigma_3 \rangle| \,.$$

So, for (i) we have

$$\begin{aligned}\Delta\sigma_1\Delta\sigma_2 &\geq \left|\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix}\right| \\ &= \left|\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix}\right| \\ &= 1\end{aligned}$$

while for (ii) we have

$$\begin{aligned}\Delta\sigma_1\Delta\sigma_2 &\geq \left|\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix}\right| \\ &= \left|\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0\\ -1\end{pmatrix}\right| \\ &= 1\end{aligned}$$

and for (iii) we have

$$\begin{aligned}\Delta\sigma_1\Delta\sigma_2 &\geq \left|\begin{pmatrix}1/\sqrt{2} & 1/\sqrt{2}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1/\sqrt{2}\\ 1/\sqrt{2}\end{pmatrix}\right| \\ &= \left|\begin{pmatrix}1/\sqrt{2} & 1/\sqrt{2}\end{pmatrix}\begin{pmatrix}1/\sqrt{2}\\ -1/\sqrt{2}\end{pmatrix}\right| \\ &= 0.\end{aligned}$$

So, to explain the physical interpretation, we see that there is a fundamental limit to how well one can measure σ_1 and σ_2 on the states $|u\rangle, |d\rangle$; they are bound by a reciprocal relationship.

However, for $|\psi\rangle \equiv \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle)$, we have only shown that there may or may not be such a limit (since to reiterate, we have only calculated an upper bound). In fact, while you can show that $|\psi\rangle$ is an eigenvalue of σ_1 (with eigenvalue i) which gives $\Delta\sigma_1 = 0$ for $|\psi\rangle$, you can also show that it is *not* an eigenvalue of σ_2, and indeed that $\Delta\sigma_2 = \sqrt{1-0^2} = 1$. So, while there is no uncertainty in the σ_1 measurement for ψ, there is some fundamental uncertainty to the σ_2 measurement, but the product $\Delta\sigma_1\Delta\sigma_2 = 0 \times 1 = 0$ is still zero.

Question 5

An observable $\hat{A}$ and a particle with a normalised wavefunction $|\psi\rangle$ are represented in some basis by

$$\hat{A} = \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 2\end{pmatrix}, \quad |\psi\rangle = \frac{1}{2}\begin{pmatrix}i\\ 1\\ 1-i\end{pmatrix}.$$

(a) Find the eigenvalues, a_i, and eigenvectors, $|a_i\rangle$, of $\hat{A}$.

I leave it to you to show that the eigenvectors and eigenvalues of A are given by

$$\lambda_1 = 2: \qquad |\lambda_1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\lambda_2 = -1: \qquad |\lambda_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$$

$$\lambda_3 = 1: \qquad |\lambda_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

(b) Find the probability $P_\psi(a_i)$ that a measurement of $\hat{A}$ on the particle gives each of the eigenvalues a_i.

As usual, to calculate probabilities we use

$$P_\lambda = |\langle\lambda|\psi\rangle|^2 .$$

This gives

$$\begin{aligned} P_{\lambda=2} &= \frac{1}{2} \\ P_{\lambda=-1} &= \frac{1}{4} \\ P_{\lambda=1} &= \frac{1}{4}. \end{aligned}$$

(c) Find the expectation value of the measurement, that is

$$\langle A\rangle = \sum_{i=1}^{3} a_i P_\psi(a_i),$$

and check that it is equal to $\langle\psi|\,\hat{A}\,|\psi\rangle$.

From the first formula, we have

$$\langle A\rangle = 2 \times 1/2 - 1 \times 1/4 + 1 \times 1/4 = 1$$

From the second formula, we have

$$\begin{aligned} \langle A\rangle &= \begin{pmatrix} -i/2 & 1/2 & 1/2 + i/2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} i/2 \\ 1/2 \\ 1/2 - i/2 \end{pmatrix} \\ &= \begin{pmatrix} -i/2 & 1/2 & 1/2 + i/2 \end{pmatrix} \begin{pmatrix} 1/2 \\ i/2 \\ 1 - i \end{pmatrix} \\ &= -i/4 + i/4 + 1/2(1+1) \\ &= 1 \end{aligned}$$

which shows that the two formulas are in agreement.

(d) Find the variance of the measurement

$$\sigma_A^2 = (\Delta A)^2 = \sum_{i=1}^{3} P_\psi(a_i)\,(a_i - \langle A \rangle)^2$$

and show that it is equal to $\langle \psi | \hat{A}^2 | \psi \rangle$.

From the first formula, we have

$$\sigma_A^2 = 1/2 \times (2-1)^2 + 1/4 \times (1-(-1))^2 + 1/4 \times (1-1) = 3/2.$$

The second formula has a typo. The variance should be equal to

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2$$

so all that's left to calculate for this is

$$\begin{aligned}
\langle A^2 \rangle = &= \begin{pmatrix} -i/2 & 1/2 & 1/2+i/2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}^2 \begin{pmatrix} i/2 \\ 1/2 \\ 1/2-i/2 \end{pmatrix} \\
&= \begin{pmatrix} -i/2 & 1/2 & 1/2+i/2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} 1/2 \\ i/2 \\ 1-i \end{pmatrix} \\
&= \begin{pmatrix} -i/2 & 1/2 & 1/2+i/2 \end{pmatrix} \begin{pmatrix} i/2 \\ 1/2 \\ 2-2i \end{pmatrix} \\
&= 1/4 + 1/4 + 2 \\
&= 5/2
\end{aligned}$$

which gives

$$\begin{aligned}
\sigma_A^2 &= 5/2 - (1)^2 \\
&= 3/2
\end{aligned}$$

in agreement with the first formula.

Question 6

Consider the Hermitian matrices

$$A = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}, \qquad B = \begin{pmatrix} 6 & -4 & -1 \\ -4 & 6 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

(a) Show that $[A, B] = 0$.

I leave it to you to show this!

(b) Find a common set of eigenvectors of A and B and their respective eigenvalues under A and B.

I leave it to you to show that

$$\det(A - \lambda I) = -\lambda(\lambda - 3)^2$$

which gives (degenerate) eigenvalues $\lambda = 0, 3, 3$, while for B we have that

$$\det(B - \omega I) = -(\omega - 1)(\omega - 4)(\omega - 10)$$

which gives eigenvalues $\omega = 1, 4, 10$. Since B does not have degenerate eigenvalues, let's use that to find our set of eigenvectors. Plugging in our values of ω, I leave it to you to show that the eigenvectors are

$$\begin{aligned}
\omega = 1: &\qquad |\omega = 1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}\\
\omega = 4: &\qquad |\omega = 4\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix}-1\\-1\\2\end{pmatrix}\\
\omega = 10: &\qquad |\omega = 10\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\end{pmatrix}.
\end{aligned}$$

Plugging these into A, I leave it to you to show that

$$\begin{aligned}
A\,|\omega = 1\rangle &= 0 \times |\omega = 1\rangle\\
A\,|\omega = 4\rangle &= 3\,|\omega = 4\rangle\\
A\,|\omega = 10\rangle &= 3\,|\omega = 10\rangle
\end{aligned}$$

so they are also well-defined eigenvectors of A.

(c) Can you find an eigenvector of A that is *not* also an eigenvector of B?

Yes. We can exploit the degeneracy of the $\lambda = 3$ eigenspace to construct an eigenvector of A that is not an eigenvector of B. As an example, consider

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\omega = 4\rangle + |\omega = 10\rangle)$$

which, since $|\omega = 4\rangle$ and $|\omega = 10\rangle$ are in the $\lambda = 3$ eigenspace of A, must itself be in the $\lambda = 3$ eigenspace of A.

However,

$$\begin{aligned}
B\,|\psi\rangle &= \frac{1}{\sqrt{2}}(B\,|\omega = 4\rangle + B\,|\omega = 10\rangle)\\
&= \frac{1}{\sqrt{2}}(4\,|\omega = 4\rangle + 10\,|\omega = 10\rangle)\\
&\neq \text{constant} \times |\psi\rangle
\end{aligned}$$

so $|\psi\rangle$ is an eigenvector of A that is not also an eigenvector of B.

Question 7

The operators $\hat{A}$ and $\hat{B}$ are, in matrix form:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

(a) Show that $\hat{A}$ and $\hat{B}$ do not commute.

I leave it to you to show that

$$[A, B] = AB - BA = \begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 0 \\ -2 & 0 & 0 \end{pmatrix}$$

which is decidedly not zero. Therefore, A and B do not commute.

(b) Find the eigenvalues and eigenvectors of $[\hat{A}, \hat{B}]$.

With the $[A, B]$ calculated in the previous section, I leave it to you to show that the eigenvectors and eigenvalues are

$$\lambda_1 = 2i \qquad |\lambda_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 0 \\ 1 \end{pmatrix}$$

$$\lambda_2 = -2i \qquad |\lambda_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 0 \\ 1 \end{pmatrix}$$

$$\lambda_3 = 0 \qquad |\lambda_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

(c) Are there any kets for which one can simultaneously find a well-defined value of A and B? If so, find them and give their values for A and B.

Before attacking this question specifically, suppose for arbitrary matrices M, N there existed a state $|\psi\rangle$ which was an eigenvalue for both; that is

$$M |\psi\rangle = m |\psi\rangle$$
$$N |\psi\rangle = n |\psi\rangle .$$

If this were true, then we would have

$$MN |\psi\rangle = mn |\psi\rangle = nm |\psi\rangle = NM |\psi\rangle$$

or, rewritten, that

$$[M, N] |\psi\rangle = 0$$

which means either that $[M, N] = 0$ or $|\psi\rangle$ is a zero eigenvector of the commutator $[M, N]$.

Now, onto our scenario. Clearly, $[A, B] \neq 0$ but we have found a vector $|\lambda_3\rangle$ for which $[A, B]|\lambda_3\rangle = 0$. So, if there's any chance of finding a ket for which A and B both have well-defined eigenvalues, it will be $|\lambda_3\rangle$. I leave it to you to show that

$$A|\lambda_3\rangle = 0|\lambda_3\rangle$$

so it has an eigenvalue of 0 for A, while also

$$B|\lambda_3\rangle = |\lambda_3\rangle$$

so it has an eigenvalue of 1 for B. Thus, from our discussion above, we have that $|\lambda_3\rangle$ is simultaneously an eigenvector of both A and B, and it is also the only such eigenvector (up to a normalization).

Question 8

(Park 4.5) Show that there are no possible solutions for the infinite potential where $E < V < 0$.

The wording of this question is a little enigmatic, so I'm going to assume that it's asking us to prove that there are no $E < 0$ solutions to the infinite potential well defined by

$$V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & \text{elsewhere} \end{cases}.$$

Note that you considered the asymmetric square well in the lectures (ie. only from 0 to a) while I considered the symmetric one; I only realised this after typing up these solutions, but the solution runs in almost the exact same way!

We shall proceed with proof via contradiction. Suppose such a non-zero solution $\psi(x)$ did exist. The goal here will be to essentially show that demanding $E < 0$ will lead to some failure when imposing the boundary condition that $\psi(a) = \psi(-a) = 0$.
So, inside the well, we have that

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi.$$

Then, rearranging, we have

$$\frac{\partial^2}{\partial x^2}\psi = C_E^2\psi$$

where we can define

$$C_E^2 \equiv -\frac{2mE}{\hbar^2}$$

with $C_E^2 > 0$ since $E < 0$. Taking C_E real and positive without loss of generality, this differential equation is clearly solved by the superposition

$$\psi = Ae^{C_E x} + Be^{-C_E x}$$

for some constants A, B to be determined by the boundary conditions. This crucial difference to the $E > 0$ case is that we no longer have the usual periodic complex exponential solutions, since C_E is real.
Now, demanding $\psi(a) = 0$ by continuity of ψ at the boundary of the well, we get

$$Ae^{C_E a} + Be^{-C_E a} = 0$$

and similarly for $\psi(-a) = 0$ we get

$$Ae^{-C_E a} + Be^{C_E a} = 0$$

Subtracting $e^{C_E a}\times$ the second equation from $e^{-C_E a}\times$ the first equation, we get

$$B(e^{2C_E a} - e^{-2C_E a}) = 0$$

which, for $a \neq 0$, implies $B = 0$. In the case $a = 0$, then the well has zero width, and there are no non-zero solutions anyways.

Similarly, subtracting $e^{-C_E a}\times$ the second equation from $e^{C_E a}\times$ the first equation, one can show that $A = 0$. But then going back to our definition for ψ, this gives $\psi = 0$. Since we assumed there was some non-zero solution, we have arrived at a contradiction, and our result is proven.

Question 9

(Zelevinsky 3.2) A particle in the infinitely deep potential box of width a has an initial wave function $\Psi(x, t = 0) = A\sin^3(\pi x/a)$. Find the wave function at arbitrary time $t > 0$. Does the particle return to the initial state at some moment in time T?

Usually, for some stationary state $\Phi(x, t)$ (ie. some eigenstate of the time-independent Hamiltonian), we can (see the lectures) find the time-dependence simply by plugging in $\Phi(x, t) = \Phi(x, 0)e^{-i\frac{E}{\hbar}t}$.

The thing that makes this question a little more challenging is that the given state $\Psi(x, t = 0)$ is **not** an eigenstate of the Hamiltonian, so it doesn't have a well-defined energy and therefore its time dependence is a little more complicated than for stationary states. So, the easiest way to find the time-dependence is to simply rewrite it in terms of the stationary states, given for the infinite potential well (see lectures) by

$$\Phi_n(x, t) = \phi_n(x)e^{i\frac{E_n t}{\hbar}}$$

where we have

$$\phi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$$

and

$$E_n \equiv \frac{\hbar^2\pi^2}{2ma^2}.$$

since they *do* each have that simple complex exponential time dependence.

One way of thinking about this is in terms of a change of basis. Namely, if we find the representation of $\Psi(x, 0)$ in the (stationary) $\phi(x, 0)$ basis – that is, if we can find some c_n such that

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \phi_n(x),$$

then the full time-dependent wave function will simply be

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{-i\frac{E_n}{\hbar}t}.$$

This is why the basis of stationary states is so useful; time-dependence becomes totally trivial in it!

So, how do we find these c_n? I'm going to start by showing you the long way of doing this, which will work in general – and then I'll comment on the shorter way of doing it, which gives you the same thing much faster in this specific example.

Long way first. You may recall (and if you do not, then try and prove it!) that the stationary states ϕ_n form an **orthonormal basis**. As such, to find our c_n, let's first rewrite things in terms of the usual bra and ket notation; we have that

$$|\Psi(x, 0)\rangle = \sum_{n=1}^{\infty} c_n |\phi_n\rangle .$$

Now, let's take one $\langle\phi_j|$ for some j and apply it to both sides on the left; this gives

$$\begin{aligned}
\langle\phi_j|\Psi(x, 0)\rangle &= \langle\phi_j| \sum_{n=1}^{\infty} c_n |\phi_n\rangle \\
&= \sum_{n=1} c_n \langle\phi_j|\phi_n\rangle \\
&= \sum_{n=1} c_n \delta_{jn} \qquad \text{(by orthonormality of the } \phi\text{s)} \\
&= c_j.
\end{aligned}$$

So, to find our c_n, we just have to take inner products! This is great. Recalling the definition of inner products for a function space (ie. $\langle a|b\rangle = \int dx a^*(x) b(x)$) we have

$$c_n = \langle\phi_n|\Psi(x = 0)\rangle = A\sqrt{\frac{2}{a}} \int_0^a \sin^3 \frac{\pi x}{a} \sin \frac{n\pi x}{a} dx.$$

This is not an obvious integral to evaluate, but we can make it a lot simpler using some tricks. First of all, let's use the triple angle formula

$$\sin 3\theta = 3 \sin\theta - 4 \sin^3 \theta$$

to write

$$c_n = \frac{A}{4}\sqrt{\frac{2}{a}}\int_0^a [3\sin\frac{\pi x}{a} - \sin\frac{3\pi x}{a}]\sin\frac{n\pi x}{a}dx.$$

Now, to evaluate these integrals, let's recall one fact we used to get this expression for our c_n in the first place; namely, that ϕ_j are orthonormal! That means that

$$\langle\phi_n|\phi_m\rangle = \frac{2}{a}\int_0^a \sin\frac{n\pi x}{a}\sin\frac{m\pi x}{a}dx = \delta_{nm}$$

or, rearranging, that

$$\int_0^a \sin\frac{n\pi x}{a}\sin\frac{m\pi x}{a}dx = \frac{a}{2}\delta_{nm}.$$

With this, we can go back to our expression for c_n and immediately write

$$c_n = \frac{A}{4}\sqrt{\frac{a}{2}}[3\delta_{n1} - \delta_{n3}]$$

or, more illuminatingly, that

$$c_n = \begin{cases} 3\frac{A}{4}\sqrt{\frac{a}{2}} & \text{when } n = 1 \\ -\frac{A}{4}\sqrt{\frac{a}{2}} & \text{when } n = 3 \\ 0 & \text{otherwise.} \end{cases}$$

Written in terms of our basis functions explicitly, then, we have that

$$\begin{aligned}\Psi(x, t = 0) &= \frac{A}{4}\sqrt{\frac{a}{2}}[3\phi_1 - \phi_3] \\ &= \frac{A}{4}[3\sin\frac{\pi x}{a} - \sin\frac{3\pi x}{a}].\end{aligned}$$

Reading this, you may have now guessed the short way of doing all this. Namely, we could have just used the triple angle trick from the beginning to immediately write the $\sin^3$ term in terms of the triple and single angle sin functions, and then simply "read off" the c_n that way. Usually when you get powers of trig functions, that's the most efficient way of approaching these sorts of questions. But I wanted to show you the more general way of doing this, which will work even when you don't start out with a trig function.

Anyways, looking back at the comments I made at the start of this answer, one can now immediately write down the full time-dependent wave function as

$$\Psi(x, t) = \frac{A}{4}[3\sin\frac{\pi x}{a}e^{-i\frac{E_1}{\hbar}t} - \sin\frac{3\pi x}{a}e^{-i\frac{E_3}{\hbar}t}]$$

where the energies are as defined above.

Finally, we want to answer this question of: does it ever return to the same state? To do this, let's factor out an overall phase of $e^{-i\frac{E_1}{\hbar}t}$ such that

$$\Psi(x, t) = e^{-i\frac{E_1}{\hbar}t}\frac{A}{4}[3\sin\frac{\pi x}{a} - \sin\frac{3\pi x}{a}e^{-i\frac{(E_3 - E_1)}{\hbar}t}].$$

Recalling that **overall** complex phases don't matter when it comes to defining a quantum state (note my emphasis on *overall* here - *relative* phases absolutely do matter), requiring that $\Psi(x,T) = \Psi(x,0)$ (up to a complex phase) evidently amounts to demanding that

$$e^{-i\frac{(E_3-E_1)}{\hbar}T} = 1.$$

If we write $1 = e^{-2\pi ik}$ for integer k, then evidently for

$$T = \frac{2\pi\hbar k}{E_3 - E_1}$$

our state will return to the original one!

Question 10

(Zelevinsky 3.3) A particle is initially in the ground state of an infinite potential box where the box limits are $x = 0$ and $x = a$. At $t = 0$ the right wall is instantaneously moved from $x = a$ to $x = b > a$. What is the probability thfor the particle to turn out at $t > 0$ in an excited state of the new box. Specifically discuss the case of $b = 2a$

We know from the lectures that for $t < 0$, the (spatial part of the) ground state of the infinite square well is given by

$$\psi_1(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}$$

while the full wavefunction is given by

$$\Psi(x,t) = \psi_1(x)e^{-i\frac{E_1 t}{\hbar}}$$

where

$$E_1 \equiv \frac{\hbar^2\pi^2}{2ma^2}.$$

Now, for $t \geq 0$, the potential instantaneously shifts. As such, we can essentially treat the $t < 0$ and $t \geq 0$ as disconnected, time-independent patches (since for all times $t \neq 0$, the potential is static), whereby the $t < 0$ solution becomes the "initial state" for the $t \geq 0$ potential. Since the potential changes instantaneously, we can reasonably assume that the wavefunction itelf does not significantly change at $t = 0$, and only begins to change afterwards.

The plan, then, is simply to find the transition probability of Ψ into Ψ'_n, the n'th eigenstate of the $t \geq 0$ potential. These new eigenstates are given by

$$\Psi'_n(x,t) = \psi'_n(x)e^{i\frac{E'_n t}{\hbar}}$$

where we have

$$\psi'_n(x) = \sqrt{\frac{2}{b}}\sin\frac{n\pi x}{b}$$

and

$$E'_n \equiv \frac{\hbar^2\pi^2}{2mb^2}.$$

As usual, then, the probability for Ψ to be measured as some excited state Ψ'_n of the shifted potential is given by

$$P_n = \left|\left\langle \Psi'_n | \Psi \right\rangle\right|^2$$

where **(ignoring the temporal phases, since they cancel out in the absolute magnitude squared)** we have

$$\left\langle \Psi'_n | \Psi \right\rangle = \frac{2}{\sqrt{ab}} \int_0^a \sin\frac{\pi x}{a} \sin\frac{n\pi x}{b} dx$$

where we only integrate between 0, and $-a$ since Ψ is zero outside that region. Doing some lengthy computations involving the product-to-sum formulas (I suggest you plug this into some integral calculator for the full working), one can show that the full result is

$$\left\langle \Psi'_n | \psi \right\rangle = \frac{2b\sqrt{ab}\sin\left(\frac{\pi a n}{b}\right)}{\pi\left(b-an\right)\left(b+an\right)}$$

Before plugging back into our probability formula, let's look at a simpler case to get something nice and numerical. Specifically for $b = 2a$ and $n = 1$ (ie. the well doubles in size, and we're looking at the transition from the old ground state to the new ground state), this simplifies to

$$\left\langle \Psi'_n | \psi \right\rangle = \frac{4\sqrt{2}}{3\pi}$$

which gives a transition probability of

$$P_1 = \frac{32}{9\pi^2} \approx 36\%$$

Curiously, that means that there's about a 64% chance that the old ground state is measured as something other than the new ground state (ie. some excited state)!

Question 11

(Zelevinsky 3.5) A particle is placed in a potential well of finite depth U_0. The width a of the well is fixed in such a way that the particle has only one bound state with binding energy $\epsilon = U_0/2$. Calculate the probabilities of finding the particle in classically allowed and classically forbidden regions.

Here, we'll extensively make use of the lecture on the Square Well Potential, so read up on that if you're confused! We're given here that $E = U_0/2$, which should simplify the simultaneous equations describing the different coefficients in each regime. First, we have

$$k^2 = \frac{2mE}{\hbar^2} = \frac{mU_0}{\hbar^2}$$

while

$$\beta^2 = \frac{(U_0 - E)2m}{\hbar^2} = \frac{U_0 m}{\hbar^2} = k^2.$$

We take $\beta, k > 0$ both. Then, with k, β now solved for, we can solve Equations (36) $-$ (39) of the lecture notes; namely (after some simplifying using the fact that $\beta = k$, and redefining $A' \equiv e^{\beta a} A$ and $B' \equiv e^{\beta a} B$) we have

$$\begin{aligned} 2A' \sin ka &= (C - D) \\ 2A' \cos ka &= (D - C) \\ 2B' \cos ka &= (C + D) \\ 2B' \sin ka &= (C + D). \end{aligned}$$

Adding together the first two, and subtracting the second two, we get

$$\begin{aligned} A'(\sin ka - \cos ka) &= 0 \\ B'(\sin ka + \cos ka) &= 0. \end{aligned}$$

while adding the first and last, and the second and third give

$$\begin{aligned} C &= (A' + B') \sin ka \\ D &= (A' + B') \cos ka \end{aligned}$$

There are some (slightly overlapping) cases to consider, essentially depending on the size of the well a and the energy depth U_0.

CASE 1: $\sin ka = \cos ka = 0$
It's clear enough from the four equations we've written out that in this scenario $A' = B' = C = D = 0$ and there is no wavefunction. However, this solution can never actually occur, since $\sin ka = 0 \implies \cos ka \neq 0$ (and vice versa).

CASE 2: $\sin ka = \cos ka \neq 0$
From this, we get that A' is free and $B = 0$. Thus $C = A' \sin ka$ and $D = A' \cos ka = A' \sin ka = C$. With this, we can write our wavefunction as (restoring A, B in terms of A', B')

$$\psi(x) = \begin{cases} (Ae^{ka} \sin ka) e^{kx} & x < -a \\ A \sin kx & -a \leq x \leq a \\ (Ae^{ka} \sin ka) e^{-kx} & x > a. \end{cases}$$

All that's left to do before we can find the probability is to calculate A! And to do that, we need one final condition: namely, the normalization of the overall wavefunction. So, demanding wavefunction normalization and taking A real, we have

$$\begin{aligned}
1 &= A^2[e^{2ka}\sin^2 ka(\int_{-\infty}^{-a} e^{2kx}dx + \int_a^{\infty} e^{-2kx}dx) + \int_{-a}^{a}\sin^2 kx dx] \\
&= A^2[e^{2ka}\sin^2 ka(2e^{-2ka}) + a - \frac{\sin 2ka}{2k}] \\
&= A^2[\sin^2 ka + a - \frac{\sin 2ka}{2k}]
\end{aligned}$$

such that

$$A = \frac{1}{\sqrt{\sin^2 ka + a - \frac{\sin 2ka}{2k}}}.$$

With that, we can immediately get the classically allowed (ie. $-a \le x \le a$, inside the well) and classically forbidden (ie. $x < -a$, $x > a$, inside the barrier) regions by integrating $\psi^*\psi$ inside those regions. Doing so, we get

$$\begin{aligned}
P_{\text{classically allowed}} &= \frac{(a - \frac{\sin 2ka}{2k})}{\sin^2 ka + a - \frac{\sin 2ka}{2k}} \\
P_{\text{classically forbidden}} &= \frac{\sin^2 ka}{\sin^2 ka + a - \frac{\sin 2ka}{2k}}.
\end{aligned}$$

CASE 3: $\sin ka = -\cos ka \neq 0$
Similarly, from this we get that $A' = 0$, while B' is free and $C = -D = B'\cos ka$. With this, we can write our wavefunction as (restoring A, B in terms of A', B')
Repeating essentially the same steps as in Case 2, one gets

$$\begin{aligned}
P_{\text{classically allowed}} &= \frac{(a + \frac{\sin 2ka}{2k})}{\cos^2 ka + a + \frac{\sin 2ka}{2k}} \\
P_{\text{classically forbidden}} &= \frac{\cos^2 ka}{\cos^2 ka + a + \frac{\sin 2ka}{2k}}.
\end{aligned}$$

CASE 4: $\sin ka \neq \cos ka$ and $\sin ka \neq -\cos ka$
Evidently then, the only solution is again $A' = B' = C = D = 0$, so there is no wavefunction.

Question 12

(past exam) Consider a particle confined inside a three-dimensional potential 'box' with side lengths a, b and c, as shown in Fig. 1.

(a) Starting with the three-dimensional Schrödinger Equation in cartesian coordinates and assuming a separable variable solution, derive an expression for the wave functions and the corresponding energies.

The basic idea here is to rewrite this 3D problem in terms of 3 $1D$ problems. Let us proceed.

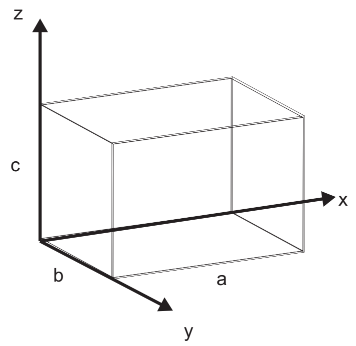

Figure 1:

First of all, since our potential is time-independent, we can factor out the time-dependence using the usual separation of variables. Then, the $3D$ (time-independent) Schrödinger equation in Cartesian coordinates can be written as

$$-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_z^2)\psi + V\psi = E\psi$$

where we use the conventional notation that $\partial_x^2 \equiv \frac{\partial^2}{\partial x^2}$, and so on for y and z. Inside the well in particular, we have that $V = 0$; outside the well, we take that $\psi = 0$ everywhere.

Assuming a separable variable solution amounts to assuming that

$$\psi(x, y, z) = \psi_x(x)\psi_y(y)\psi_z(z)$$

where $\psi_x(x), \psi_y(y), \psi_z(z)$ are independent, single-variable wavefunctions in each of the three spatial dimensions. Plugging this into the Schrödinger equation above, we have

$$-\frac{\hbar^2}{2m}[(\partial_x^2\psi_x)\psi_y\psi_z + \psi_x(\partial_y^2\psi_y)\psi_z + \psi_x\psi_y(\partial_z^2\psi_z)] = E\psi_x\psi_y\psi_z$$

where we have set $V = 0$ inside the well. Now, assuming that $\psi \neq 0$ (in which case the Schrodinger equation holds trivially), we can divide both sides by $\psi = \psi_x\psi_y\psi_z$, which gives

$$-\frac{\hbar^2}{2m}[\frac{\partial_x^2\psi_x}{\psi_x} + \frac{\partial_y^2\psi_y}{\psi_y} + \frac{\partial_z^2\psi_z}{\psi_z}] = E.$$

Now, let's differentiate both sides of this equation with respect to - say - x. The second and third derivative terms are independent of x, and E is a constant, so this gives

$$\partial_x[-\frac{\hbar^2}{2m}\frac{\partial_x^2\psi_x}{\psi_x}] = 0.$$

So, integrating both sides (and noting that it is only a function of x, so there can be no y, z dependence), we must have that

$$-\frac{\hbar^2}{2m}\frac{\partial_x^2\psi_x}{\psi_x} = E_x$$

for some constant E_x. That is, rearranging slightly, we have shown that

$$-\frac{\hbar^2}{2m}\partial_x^2\psi_x = E_x\psi_x$$

that is, that ψ_x itself satisfies a 1D schrodinger equation, for some 1D energy E_x!

Of course, we can do the same thing for y, z, which gives

$$-\frac{\hbar^2}{2m}\partial_y^2\psi_y = E_y\psi_y$$
$$-\frac{\hbar^2}{2m}\partial_z^2\psi_z = E_z\psi_x$$

for energies E_y, E_z. Comparing this to our original Schrödinger equation, then, we have

$$E = E_x + E_y + E_z$$

which intuitively makes sense: in the separable case, the total energy is comprised of the sum of each of the separate wavefunctions!

Finally, in each of these 1D cases, we're just solving the infinite square well problem, which has been done in the lectures. We have, for positive integers n_x, n_y, n_z, the following 1D eigenfunctions and eigenergies:

$$\psi_x^{n_x} = \sqrt{\frac{2}{a}}\sin\frac{n_x\pi x}{a} \qquad E_x^{n_x} = \frac{\hbar^2\pi^2 n_x^2}{2ma^2}$$
$$\psi_y^{n_y} = \sqrt{\frac{2}{b}}\sin\frac{n_y\pi y}{b} \qquad E_y^{n_y} = \frac{\hbar^2\pi^2 n_y^2}{2mb^2}$$
$$\psi_z^{n_z} = \sqrt{\frac{2}{c}}\sin\frac{n_z\pi z}{c} \qquad E_z^{n_z} = \frac{\hbar^2\pi^2 n_z^2}{2mc^2}$$

which combine to the full 3D solution as

$$\Psi^{n_x,n_y,n_z} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}}\sqrt{\frac{2}{c}}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{b}\sin\frac{n_z\pi z}{c}$$

and full energy

$$E^{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}]$$

(b) Determine an expression for the normalisation constant for the wave function.

I leave it to you to check that the wavefunction written in the previous section is normalised. Keep in mind that you now have to do a 3D integral

$$1 = \int_0^a dx \int_0^b dy \int_0^c dz\psi^*\psi$$

but since our wavefunction is separable as $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$, this simplifies to 3 1D integrals as

$$1 = \int_0^a dx \psi_x^*(x)\psi_x(x) \int_0^b dy \psi_y^*(y)\psi_y(y) \int_0^c dz \psi_z^*(z)\psi_z(z)$$

(c) Calculate the probability that the particle will be found on the interval $a/2 \leq x \leq 3a/4$ if the particle is in the ground state.

As usual, all we have to do is integrate the wavefunction over this region. That is,

$$P = \int_{a/2}^{3a/4} dx \psi_x^*(x)\psi_x(x) \int_0^b dy \psi_y^*(y)\psi_y(y) \int_0^c dz \psi_z^*(z)\psi_z(z)$$

where the second and third integrals evaluate to 1 since the separated y, z wavefunctions are normalised over the region, giving

$$\begin{aligned} P &= \int_{a/2}^{3a/4} dx \psi_x^*(x)\psi_x(x) \\ &= \frac{2}{a} \int_{a/2}^{3a/4} \sin^2(\frac{\pi x}{a}) \end{aligned}$$

where we have plugged in the specific ground state wavefunction. Using the usual tricks, you can show that this integral evaluates to

$$P = \frac{\pi + 2}{4\pi} \approx 41\%.$$