Solution scheme to ZCT 205 final examination, academic session 2011/12, School of Physics, USM
Instruction: Answer Five (5) out of Seven (7) questions given. Each question carries 20 marks.

1. (a) i. Explain what is "wave function collapse".

   Solution:
   Various explanation can be accepted. But the answer has to contain essential information relevant to address the question asked in a no-nonsence manner. Answer that beats around the bush will not be considered.
   4 marks

   ii. A system is initially prepared to be in a mixed state $\Psi = a_1\Psi_1 + a_2\Psi_2$, where Ψ_1, Ψ_2 are eigenstates. When a measurement is done on the system, what is the probability to find the measured system in state Ψ_1?

   Solution:

   The probability is $|a|^2$. Just present the answer without the need to derive them.
   2 marks

   iii. If the system is measured to be in state Ψ_1, what is the probability that a subsequent measurement on it results in state Ψ_2?
   Solution:
   The probability is 0. Just present the answer without the need to derive them.
   2 marks

   (b) At $t = 0$, a particle of mass m is in the state

   $$\Psi(x, 0) = Ae^{-amx^2/\hbar},$$

   where A and a are positive real constants.

   i. Find A.

   Solution:

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} |Ae^{-amx^2/\hbar}|^2 dx = 1$$

$$\Rightarrow 2A^2 \int_{0}^{\infty} e^{-2amx^2/\hbar} dx = 1$$

Let $y = x\sqrt{2am/\hbar}$ so that

$$\Rightarrow \frac{2A^2}{\sqrt{2am/\hbar}} \int_{0}^{\infty} e^{-y^2} dy = 1$$

$\int_0^\infty e^{-y^2} dy$ is the error function,

$$\int_{0}^{\infty} e^{-y^2} dy = \lim_{x\to+\infty} \frac{2}{\sqrt{\pi}} \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}.$$

$$\Rightarrow A = \left(\frac{2ma}{\pi\hbar}\right)^{1/4}$$

ii. Calculate the expectation value of x, where x is the position.
Solution:
$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi dx = \int_{-\infty}^{\infty} Ae^{-amx^2/\hbar} x Ae^{-amx^2/\hbar} dx = A^2 \int_{-\infty}^{\infty} e^{-2amx^2/\hbar} x dx.$
This is an integration over an odd function, hence $\langle x \rangle = A^2 \int_{-\infty}^{\infty} e^{-2amx^2/\hbar} x dx = 0$.
Note that it is not necessary to carry out the integration explicitly to obtain the correct answer to this question.
6 marks

iii. Calculate the expectation value of p, where p is the momentum.

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \frac{i}{\hbar} \frac{d}{dx} \Psi dx = \int_{-\infty}^{\infty} Ae^{-amx^2/\hbar} \frac{i}{\hbar} \frac{d}{dx} Ae^{-amx^2/\hbar} dx =$$

$$\frac{i}{\hbar} A^2 \int_{-\infty}^{\infty} e^{-amx^2/\hbar} (-2amx/\hbar) e^{-amx^2/\hbar} dx.$$

This is an integration over an odd function, hence $\langle p \rangle = 0$.
Alternatively, one can use the relation $\langle p \rangle = \frac{d}{dt} \langle x \rangle \frac{1}{m}$ to infer that $\langle p \rangle$ is zero as $\langle x \rangle$ is zero.

Note that it is not necessary to carry out the integration explicitly to obtain the correct answer to this question.
3 marks

(12 marks)

2. (a) i. What are the physical implications if $\hbar = 0$?
Solution
A simple answer is: There will be no quantum effect. (Other reasonably argued answers will also be considered). **(4 marks)**

ii. State Ehrenfest's theorem. Give an example of it.

$$\frac{d\langle p\rangle}{dt} = -\langle\frac{\partial V}{\partial x}\rangle$$

(4 marks)

(b) i. Prove mathematically that if the wave function is normalised at $t = 0$, the normalisation will be guaranteed for all $t > 0$.

Solution

Suppose the wavefunction is normalised at $t = 0$,

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1.$$

At later time t, the probability density is $|\Psi(x,t)|^2$. In order to prove that above statement, we need to show that $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx$ is a constant in time, so that it always equals to the constant value since $t = 0$, which is 1. To prove that $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx$ is constant in time, you need to show

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 0$$

Some steps leading to this proof:

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 0$$

6 marks

ii. Prove that $\langle p\rangle$, which is defined via $\langle p\rangle = m\frac{d}{dt}\langle x\rangle$ is given by

$$\langle p\rangle = \int \Psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi.$$

Solution

Using integration-by-parts and applying the boundary condition that the wave function vanishes at infinity, (limits of the the integration will be suppressed for the sake of brevity)

$$\begin{aligned}\frac{d}{dt}\langle x\rangle &= \int x\frac{\partial}{\partial t}|\Psi|^2 dx = \cdots = \frac{-i\hbar}{2m}\int\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx = \cdots \\ &= \frac{1}{m}\int \Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right)dx \equiv \frac{\langle p\rangle}{m}.\end{aligned}$$

(6 marks)

3. (a) i. Explain what are stationary states.

Solution
Stationary states are states with definite energy. Their probability densities and expectation values are time-independent. If a system comprised of only one stationary state, it is certainly to get energy of that state when a measurement is made.
4 marks

ii. In solving QM problems, you are given a (time-independent) potential $V(x)$ and the starting wave function $\Psi(x,0)$. Your task is to find the wave function, $\Psi(x,t)$, for any subsequent time t by solving the (time-dependent) Schroedinger equation. Describe qualitatively your step-by-step strategy to obtain the solution $\Psi(x,t)$.

Solution

A. First solve the time-independent Schroedinger equations for the complete set of stationary states, $\{\psi_1(x), \psi_2(x), \cdots\}$, each with its own associated energy $\{E_1, E_2, \cdots\}$.

B. Find the general solution at $t = 0$, i.e., $\Psi(x,0) = \sum_{n=0}^{\infty} c_n \psi_n(x)$ by finding the coefficients c_n that fit the initial and boundary conditions.

C. Once all the c_n are found, the general time-dependent solution is obtained as

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar} = \sum_{n=0}^{\infty} c_n \Psi_n(x,t)$$

4 marks

(b) i. The time-independent Schroedinger equation yields an infinite collection of solutions $\{\psi_1(x),\, \psi_2(x), \cdots\}$, where

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1 t/\hbar}, \Psi_2(x,t) = \psi_2(x)e^{-iE_2 t/\hbar}, \cdots$$

with each $\Psi_n(x,t)$ is associated with the energy E_n. Show that the linear combination of solutions,

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-itE_n/\hbar}$$

is itself a solution.

Solution

TISE says

$$H\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t} \tag{1}$$

Look that the LHS of Eq (1):

$$H\Psi(x,t) = \sum_{n=0}^{\infty} c_n H\psi_n(x) e^{-itE_n/\hbar}. \tag{2}$$

Also, TDSE says

$$H\psi_n(x) = E_n \psi(x).$$

Slot the TDSE into Eq. (2), we have

$$H\Psi(x,t) = \sum_{n=0}^{\infty} c_n H\psi_n(x) e^{-itE_n/\hbar} = \sum_{n=0}^{\infty} c_n E_n \psi_n(x) e^{-itE_n/\hbar} \tag{3}$$

Now look at the RHS of Eq (1):

$$\begin{aligned}
i\hbar\frac{\partial\Psi(x,t)}{\partial t} &= i\hbar\frac{\partial}{\partial t}\sum_{n=0}^{\infty} c_n\psi_n(x)e^{-itE_n/\hbar} \\
&= i\hbar\sum_{n=0}^{\infty} c_n\left(\frac{\partial\psi_n(x)}{\partial t}e^{-itE_n/\hbar} + \psi_n(x)\frac{\partial e^{-itE_n/\hbar}}{\partial t}\right) \\
&= i\hbar\sum_{n=0}^{\infty} c_n\psi_n(x)(-iE_n/\hbar)e^{-itE_n/\hbar} \\
&= \sum_{n=0}^{\infty} c_nE_n\psi_n(x)e^{-itE_n/\hbar} \qquad (4)
\end{aligned}$$

Comparing Eq. (4) with Eq. (3), we proved that indeed $\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-itE_n/\hbar}$ is a solution to the TISE. **(8 marks)**

ii. Suppose a particle starts out in a linear combination of stationary states:

$$\Psi(x,0) = c_1\psi_1(x) + c_2\psi_2(x),$$

where c_1, c_2 are constants. What is the wave function $\Psi(x,t)$ at subsequent times?
Solution The wave function at subsequent time is obatained by simply tagging the exponential factor to each time-independent solutions,

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}.$$

(4 marks)

4. (a) i. Consider a particle in an infinite square well. Explain the mathematical origin that give rise to the quantisation of the energies.
Solution
The quantisation of energy in an infinite square well arises due to the boundary conditions that demand $\Psi(x=0) = \Psi(x=a) = 0$.
(**4 marks**)

ii. Explain why a particle in an infinite square well can not have zero energy, $E = 0$.
Solution
This is because $E = 0$ implies that the particle is totally at

rest, and hence violate the Uncertainty principle $\Delta x \Delta p_x \geq \hbar/2$.
Frist optional answer: $E = 0$ implies the solution to the TISE is trivial. This is uncaapetable because it is not normalisable and violate the Born's probabilistic interpretation of to the wave function.

Second optional answer: In TISE, $\frac{\partial^2}{\partial x^2}\Psi(x) \propto [V(x) - E]\Psi(x)$. As a result, in order for the wavefunction to be normalised, it is necessary that $E > V_{\text{min}}$. For infinite quantum well, $V_{\text{min}} = 0$. Hence, it follows that $E > 0 \Rightarrow E \neq 0$.

(**4 marks**)

(b) The infinite square well is given by

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

i. Sketch the graph for $V(x)$.

Solution (**2 marks**)

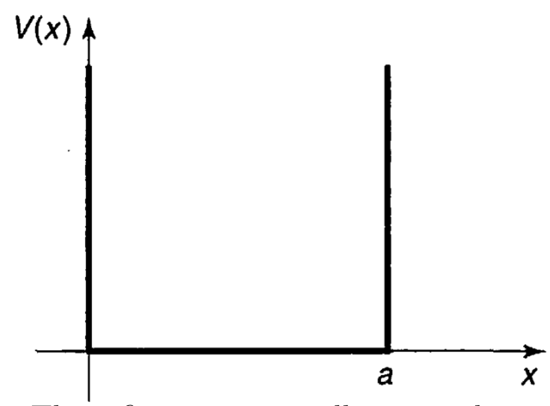

Figure 1: The infinite square well potential

ii. Write down the Schroedinger equation for particle in the infinite square well.

Solution

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

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \text{ where } k \equiv \frac{\sqrt{2mE}}{\hbar}; k^2 \geq 0$$

(2 marks)

iii. What is the boundary conditions for the wave function in the infinite square well?

Solution
$\Psi(x = 0) = \Psi(x = a) = 0$
(2 marks)

iv. What is the most general solution to the Schroedinger equation for particle in the infinite square well?
Solution
The most general solution for

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

is

$$\Psi(x) = A\sin(kx) + B\cos(kx)$$

(2 marks)

v. Based on your answers to 4(b)iii, 4(b)iv, show that the allowed energies of E are given by
Solution

Impose BC $\Psi(x = 0) = 0$ into

$$\Psi(x) = A\sin(kx) + B\cos(kx)$$

gives

$$\Psi(0) = B\cos(k\dot{0}) = 0$$

Implying $B = 0$.
Impose BC $\Psi(x = a) = 0$ into

$$\Psi(a) = A\sin(ka) = 0$$

gives

$$k = k_n = \frac{n\pi}{a}, n = \pm1, \pm2, \cdots .$$

Since $k \equiv \frac{\sqrt{2mE}}{\hbar}, \Rightarrow E_n = n^2\frac{\pi^2\hbar^2}{2ma^2}$.
(4 marks)

5. (a) i. State the (spatial) region which is considered "forbidden" for an one-dimensional classical harmonic oscillator as far as energy is concerned.
[*Nyatakan rantau (dalam ruang kedudukan) yang merupakan rantau terlarang bagi pengayun harmonik klasik satu dimensi, di mana hanya pertimbangan tenaga diambil kira.*]

ii. List the essential differences between a classical and a quantum harmonic oscillator (QHO) (list them in a table comprised of two columns for easy comparison).
[*Senaraikan perbezaan-perbezaan mustahak di antara pengayun harmonik klasik dan pengayun harmonik kuantum (untuk memudahkan perbandingan, senaraikan perbezaan-perbezaan dalam bentuk jadual mengandungi dua lajur.)*]

(8 marks)

(b) Consider the time-independent Schroedinger equation (TISE) for a 1D quantum harmonic oscillator expressed in the form
[*Pertimbangkan persamaan Schroedinger tak tersandar-masa untuk pengayun harmonik satu dimensi dalam bentuk*]

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi, \tag{5}$$

where [*di mana*]

$$\xi = x\sqrt{\frac{m\omega}{\hbar}},$$
$$K \equiv \frac{2E}{\hbar\omega}.$$

ω a constant characterising the angular frequency and m the mass of the oscillator.

[*ω pemalar yang mencirikan frekuensi sudut, dan m jisim pengayun.*]

i. Assume the solution can be expressed in terms of $\psi(\xi) = h(\xi)e^{-\xi^2/2}$, show that the TISE can be cast into the form

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0.$$

ii. The solution for the equation in 5(b)i can be obtained via a power series method by assuming the solution as a series in the form of
[*Penyelesaian kepada persamaan dalam 5(b)i boleh diperolehi melalui kaedah siri kuasa dalam bentuk*]

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j.$$

Show that the coefficients a_j obey
[*Tunjukkan bahawa koefisien-koefisien* a_j *mematuhi*]

$$\sum_{j=0}^{\infty} \left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right] \xi^j = 0$$

for all powers of j. [*untuk semua kuasa* j.]

(12 marks)

6. (a) i. Consider two functions $f(x), g(x)$, both belong to Hilbert space. Define the inner product of them.
Solution
$\langle f|g\rangle = \int_{-\infty}^{\infty} f(x)^* g(x) dx$
(4 marks)

ii. Explain what it means by the statement "a set of functions is **complete**".

Solution

A set of functions $\{\psi_n(x)\}$ is complete if any other functions $f(x)$ can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

(4 marks)

(b) The Schroedinger equation says

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi,$$

where H is the Hamiltonian.

Show that

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle,$$

where $\hat{Q}$ is the Hermitian operator representing a generic observable.

Solution

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle = \langle\frac{\partial\Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle\Psi|\frac{\partial\hat{Q}}{\partial t}\Psi\rangle + \langle\Psi|\hat{Q}\frac{\partial\Psi}{\partial t}\rangle.$$

Combine it with the Shroedinger equation

$$\frac{\partial\Psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\Psi,$$

$$\begin{aligned}
\frac{d}{dt}\langle Q\rangle &= \langle\frac{1}{i\hbar}\hat{H}\Psi|\hat{Q}\Psi\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle \\
&= -\frac{1}{i\hbar}\langle\Psi|\hat{H}\hat{Q}\Psi\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle \\
&= +\frac{1}{i\hbar}\left(\langle\Psi|\hat{Q}\hat{H}\Psi\rangle - \langle\Psi|\hat{H}\hat{Q}\Psi\rangle\right) + \langle\frac{\partial\hat{Q}}{\partial t}\rangle \\
&= +\frac{1}{i\hbar}\langle\Psi|\left(\hat{Q}\hat{H} - \hat{H}\hat{Q}\right)\Psi\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle \\
&= \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle \qquad (6)
\end{aligned}$$

(8 marks)

ii. Prove that the eigenvalues of a hermitian operator $\hat{Q}$ is real.
Solution
The eigenvalue equation for an operator Q is

$$\hat{Q}f = qf.$$

Since Q is a Hermitian operator,

$$\langle f|\hat{Q}f\rangle = \langle\hat{Q}f|f\rangle.$$

It then follows that

$$q\langle f|f\rangle = q^*\langle f|f\rangle.$$

So, $q = q^*$, and hence q is real. QED

(4 marks)

7. (a) i. The allowed energies of a hydrogen atom are given by $E_n = -E_0/n^2$, where $n = 1, 2, 3, \cdots$, $E_0 = 13.6$eV the ground state energy. Explain qualitatively what will happen to the solutions of the time-independent Schroedinger equation if the constant E, as appear in the TISE, is not equal to any of the discretised values $-E_0/n^2$.

ii. Usually the Schroedinger equation for a hydrogen atom is solved in spherical coordinates using separation of variable method to split the solution into a radial part and an angular part. In principle one can also solve the Schroedinger equation for hydrogen atom in Cartesian coordinate system by splitting the solution into x-,y- and z- parts instead. Explain why is the latter approach less convenient than the former.
[*Biasanya persamaan Schroedinger bagi atom hidrogen diselesaikan dalam koordinat-koordinat sfera dan memakai kaedah pemisahan pembolehubah untuk membelahkan penyelesaian kepada bahagian jejarian dan bahagian sudutan. Secara prinsipnya kita juga boleh menyelesaikan persamaan Schroedinger bagi atom hidrogen dalam sistem koordinat Carte dengan membelahkan penyelesaian kepada bahagian-bahagian $x-$, $y-$ dan $z-$. Terangkan mengapa pendekatan yang terkemudian tidak semudah berbanding dengan pendekatan yang terdahulu.*]

(8 marks)

(b) Consider the 3D hydrogen atom which potential is defined by the Coulombic form
[*Pertimbangkan atom hidrogen dalam tiga dimensi yang mana keupayaannya ditakrifkan dalam bentuk Coulomb*]

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0 r}.$$

Using separation of variable method and by splitting the solution $\psi(\mathbf{r})$ in spherical coordinates into the separable form $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ (and by denoting the separation of variable constant as $\ell(\ell + 1)$),
[*Dengan kaedah pemisahan pembolehubah serta membelahkan penyelesaian* $\psi(\mathbf{r})$ *dalam koordinat-koordinat sfera kepada bentuk terpisah* $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ *(dan menwakili pemalar pemisahan pembolehubah sebagai* $\ell(\ell + 1)$*),*]

i. shows that the radial function $R(r)$ obeys the equation
[*tunjukkan bahawa fungsi jejarian* $R(r)$ *mematuhi persamaan*
]

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(\mathbf{r}) - E\right] = \ell(\ell+1).$$

ii. Shows that the angular parts obey the equation
[*Tunjukkan bahawa bahagian sudutan mematuhi persamaan*]

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right)\right] = -\ell(\ell+1).$$

(12 marks)

Appendix

- Integration by parts:

$$\int_a^b f(x)g'(x)dx = f(x)g(x)\Big|_a^b - \int_a^b g(x)f'(x)dx.$$

- Time-dependent Schroedinger equation in 1D:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t).$$

- Time-independent Schroedinger equation in 1D:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x) = E\psi(x).$$

- Time-independent Schroedinger equation in 3D:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

- In spherical coordinates the Laplacian ∇^2 takes the form

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right).$$

- Error function is defined as $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du$. In the limit $x \to \pm\infty$, $\mathrm{erf}(x) \to \pm 1$.

- Expectation value for an observation $\hat{Q}$ is defined as

$$\langle Q\rangle = \int \Psi^*\hat{Q}\Psi dx.$$