1. (a) Let $\Psi(x,t) = \psi(x)\phi(t)$ be a separable solution to the time-dependent Schroedinger equation. Discuss the essential mathematical properties of $\Psi(x,t)$.
[*Biar* $\Psi(x,t) = \psi(x)\phi(t)$ *penyelesaian terpisah kepada persamaan Schroedinger tak bersandar masa. Bincangkan ciri-ciri matematik mustahak* $\Psi(x,t)$.]

(8 marks)

(b) At time $t = 0$ a particle is represented by the wavefunction
[*Pada masa* $t = 0$ *fungsi gelombang suatu zarah diwakil oleh*]

$$\Psi(x,0) = \begin{cases} A\frac{x}{a} + A, & \text{if } -a \leq x \leq 0, \\ -A\frac{x}{b} + A, & \text{if } 0 \leq x \leq b, \\ 0, & \text{otherwise,} \end{cases}$$

where A, a and b are constants.
[*di mana* A, a *dan* b *adalah pemalar-pemalar.*]

i. Normalize Ψ (that is, find A in terms of a and b).
[*Normalisasikan* Ψ *(iaitu, dapatkan* A *dalam sebutan-sebutan* a *dan* b*).*]

ii. Sketch $\Psi(x,0)^2$ as a function of x.
[*Lakarkan* $\Psi(x,0)^2$ *sebagai fungsi* x.]

iii. Where is the particle most likely to be found, at $t = 0$?
[*Di manakan zarah paling mungkin dijumpai, pada* $t = 0$?]

iv. What is the probability of finding the particle to the left of $x = 0$?
[*Apakah kebarangkalian menjumpai zarah di sebelah kiri* $x = 0$?]

v. What is the expectation value of x?
[*Apakah nilai jangkaan* x?]

(12 marks)

Solutions
Q1(a)

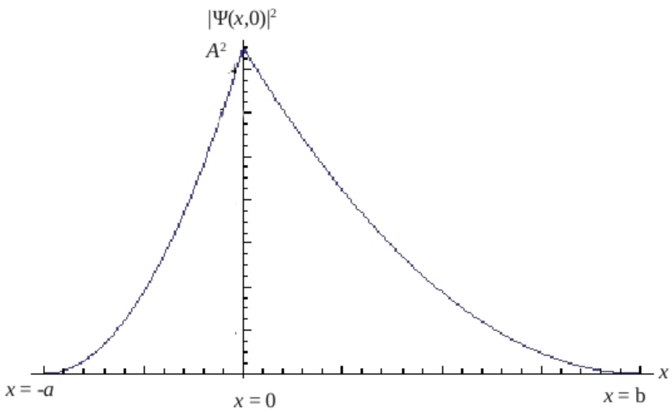
- $\Psi(x,t)$ can be seperated into spatial part, $\psi(x)$, and temporal parts, $\phi(t)$.
- $\psi(x)$ and $\phi(t)$ are independend of each other.
- $\Psi(x,t)$ are orthonomal.
- $\Psi(x,t)$ is time-dependent.
- $\Psi(x,t)$ is a stationary state.
- $\Psi(x,t)$ is generally complex.
- $\Psi(x,t)$ are stationary states.
- $\Psi(x,t)$ is normalised, $\int_{-\infty}^{\infty} \Psi(x,t)^*\Psi(x,t)dx = 1$.

- $\Psi(x,t)$ is square-integrable.
- $\Psi(x,t)$ lives in Hilbert space.
- $|\Psi(x)|$ drops fatster than $1/\sqrt{x}$ as $x \to \pm\infty$.
- $\Psi(x,t)$ is complete, in the sense that the most general solution to TDSE consists of linear combination of invididual solutions $\Psi_n(x,t)$, $\sum_{n=0}^{n=\infty} c_n \Psi_n(x,t)$.
- Normalisation of $\Psi(x,t)$ is time-independent, $\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 0$.
- $\cdots$

Q1(bi)
Normalising $\Psi(x,0)$:

$$
\begin{aligned}
1 &= \int_{-\infty}^{\infty} \Psi(x,t)^* \Psi(x,t) dx = \int_{-a}^{0} (A + Ax/a)^2 dx + \int_{0}^{b} (A - Ax/a)^2 dx \\
&= A^2 \int_{0}^{b} (1 + (x/a)^2 + 2x/a) dx + A^2 \int_{0}^{b} (1 + (x/a)^2 - 2x/a) dx \\
&= A^2 (a+b)/3 \\
\Rightarrow A &= \pm\sqrt{\frac{3}{a+b}}
\end{aligned}
$$

Q1(bii)



Q1(biii)
The particle is most likely to be found at the location where the probability density is highest, i.e., at $x = 0$.

Q1(biv)
$p(-a \le x \le 0) = \int_{x=-a}^{x=0} |\Psi(x,t)|^2 dx = \int_{x=-a}^{x=0} (A + Ax/a)^2 dx = \cdots = \frac{a}{a+b}$.

Q1(bv)
$\langle x \rangle = \int_{x=-a}^{x=0} x(A + Ax/a)^2 dx + \int_{x=0}^{x=b} (A - Ax/a)^2 dx = \cdots = \frac{(b-a)}{4}$

2. (a) i. Explain in your own words what is meant by a 'stationary state'.
[*Terangkan dalam ayat-ayat anda sendiri apa yang dimaksudkan oleh 'keadaan*

pegun'.]

ii. Explain, in your own words, why must a wavefunction be normalised?
[*Terangkan dalam ayat-ayat anda sendiri kenapa fungsi gelombang mesti dinormalisasikan.*]

(8 marks)

(b) i. Is a linear combination of two stationary states with distinct energies, $E_1 \neq E_2$,
[*Adakah kombinasi linear dua keadaan pegun yang mempunyai tenaga-tenaga yang berlainan, $E_1 \neq E_2$,*]

$$\Psi(x) = a_1\psi_1(x) + a_2\psi_2(x)$$

a solution to the **time-independent** Schroedinger equation? Prove your answer mathematically.
[*penyelesaian kepada persamaan Schroedinger* **tak bersandar masa**? *Buktikan jawapan anda secara matematik.*]

ii. Suppose a particle starts out in a linear combination of stationary states:
[*Katakan suatu zarah bermula sebagai kombinasi linear keadaan-keadaan pegun*]

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

where c_1, c_2 are constants. What is the wave function $\Psi(x, t)$ at subsequent times?
[*di mana c_1, c_2 adalah pemalar-pemalar. Apakah fungsi gelombang $\Psi(x, t)$ pada masa yang seterusnya?*]

(12 marks)

Solutions

Q2(a)i

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.

Q2(a)ii

A wavefunction must be normalised so that the total probability to find the particle in space equals to one, so that the quantum mechanical formulation is mathematically consistent with the Born interpretation of wavefunction.

Q2(b)i

NO, $\Psi(x) = a_1\psi_1(x) + a_2\psi_2(x)$ is NOT a solution to the time-independent Schroedinger equation. If it were, then the statement

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[a_1\psi(x)_1 + a_2\psi_2(x)\right] + V(x)\left[a_1\psi(x)_1 + a_2\psi_2(x)\right] = \text{ constant } \times\left[a_1\psi(x)_1 + a_2\psi_2(x)\right]$$

is true. We shall prove that this this not the case.

Substitute $\Psi(x) = a_1\psi_1(x) + a_2\psi_2(x)$ into TISE $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$.
LHS:

$$
\begin{aligned}
& -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[a_1\psi(x)_1 + a_2\psi_2(x)\right] + V(x)\left[a_1\psi(x)_1 + a_2\psi_2(x)\right] \\
= \;& a_1\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_1(x) + V(x)\psi_1(x)\right] + a_2\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x) + V(x)\psi_2(x)\right] \\
= \;& a_1E_1\psi_1(x) + a_2E_2\psi_2(x) \text{ (since } \psi_1(x), \psi_2(x) \text{ are by definition solutions to the TISE)} \\
\neq \;& \text{constant } \times (a_1\psi_1(x) + a_2\psi_2(x)) \text{ if } E_1 \neq E_2.
\end{aligned}
$$

RHS:

$$E\psi(x) = E\left[a_1\psi_1(x) + a_2\psi_2(x)\right]$$

Since there is no way to express the LHS into the form of constant $\times\left[a_1\psi_1(x) + a_2\psi_2(x)\right]$ (as what the RHS is) due to the fact that $E_1 \neq E_2$, we have shown that $\Psi(x) = a_1\psi_1(x) + a_2\psi_2(x)$ is NOT solution to the time-independent Schroedinger equation, $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$.

Q2(b)ii

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

3. (a) i. Explain, in your own words, why is the expectation value of a time-independent observable, $\hat{Q}$, as in the definition
[*Terangkan dalam ayat-ayat anda sendiri, kenapa nilai jangkaan suatu pembolehcerap tak bersandar masa, $\hat{Q}$, sebagaimana yang ditakrifkan oleh*]

$$\langle Q\rangle = \int_{-\infty}^{\infty}\Psi(x,t)^*\hat{Q}\Psi(x,t)dx$$

time independent
[*tak bersandar masa.*].

ii. "Stationary states" are states with definite energy. Explain what this means, and illustrate your explanation mathematically.
[*"Keadaan-keadaan pegun" adalah keadaan-keadaan yang pasti dalam tenaga. Terangkan apa yang dimaksudkan oleh kenyataan tersebut, dan ilustrasikan penjelasan anda secara matematik.*]

(8 marks)

(b) The most general solution to the time-dependent Schroedinger equation,
[*Penyelesaian paling am kepada persamaan Schroedinger bersandar masa,*]

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

is [*adalah*]

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

where $\Psi_n(x,t)$ are the stationary solutions. Show that
[*di mana* $\Psi_n(x,t)$ *adalah penyelesaian-penyelesaian pegun. Tunjukkan bahawa*]

$$\sum_n |c_n|^2 = 1.$$

Explain your steps clearly.
[*Terangkan langkah-langkah anda dengan jelas.*]

(12 marks)

Solutions
Q3(a)i
Short Answer: The complex time-dependence factor $e^{-iE_nt/\hbar}$ contained in $\Psi(x,t)$ gets canceled out when evaluating the inner product of $\Psi(x,t)$ with $\hat{Q}\Psi(x,t)$, $\langle\hat{Q}\rangle = \langle\Psi(x,t)|Q\Psi(x,t)\rangle$.

Detailed answer with mathematical proof: $\Psi(x,t)$, being a general solution, is a linear combination of stationary states,

$$\Psi(x,t) = \sum_n c_n\psi_n(x)\varphi_n(t),$$

with the time-dependence part carried by $\varphi_n(t) = e^{-iE_nt/\hbar}$.

Also, when a time-independent observable operator $\hat{Q}$ acts on a stationary state $\Psi_n(x,t) = \psi_n(x)\varphi_n(t)$, it ignores $\varphi_n(t)$:

$$\hat{Q}\Psi_n(x,t) = \hat{Q}\left[\psi_n(x)\varphi_n(t)\right] = \left[\hat{Q}\psi_n(x)\right]\varphi_n(t).$$

If we further assume the stationary states $\Psi_n(x)$ are also eigenstates of $\hat{Q}$,

$$\begin{aligned} \hat{Q}\Psi_n(x,t) &= q_n\Psi_n(x,t) \\ \hat{Q}\left[\psi_n(x)\varphi_n(t)\right] &= q_n\left[\psi_n(x)\varphi_n(t)\right] \\ \Rightarrow \hat{Q}\psi_n(x) &= q_n\psi_n(x). \end{aligned}$$

$\varphi_n(t)$ is also x-independent. Therefore the time-dependence factor $\varphi_n(t)$ appearing in $\langle Q\rangle$ can be pulled out to cancel among themselves when summed over all states

m due to the orthogonality of $\psi_n(x)$:

$$\begin{aligned}
\langle Q\rangle &= \langle\Psi(x,t)|\hat{Q}\Psi(x,t)\rangle \\
&= \int_{-\infty}^{\infty}\left[\sum_n c_n\psi_n(x)e^{-iE_nt/\hbar}\right]^* \hat{Q}\left[\sum_m c_m\psi_m(x)e^{-iE_mt/\hbar}\right]dx \\
&= \sum_n\sum_m c_m c_n e^{iE_nt/\hbar}e^{-iE_mt/\hbar}\int_{-\infty}^{\infty}\psi_n(x)^*\hat{Q}\psi_m(x)dx \\
&= \sum_n\sum_m c_m c_n e^{i(E_n-E_m)t/\hbar}\int_{-\infty}^{\infty}\psi_n(x)^*(q_n\psi_m(x))dx \\
&= \sum_n\sum_m c_m c_n e^{i(E_n-E_m)t/\hbar}q_n\delta_{m,n} \\
&= \sum_n q_n|c_n|^2 \text{ ,which is time-independent}
\end{aligned}$$

Q3(a)ii

Stationary states are states with definite energy. This means that measurement for total energy done on a stationary state will always result in a definite value, say E. To prove this mathematically, we have to show that the variance of total energy of a stationary state $\sigma_H^2 = 0$:

The expectation value for total energy of a stationary state, $\Psi(x,t) = \psi(x)\varphi(t)$, is given by the expectation value of the Hamiltonian,

$$\langle H\rangle = \langle\Psi(x,t)|H\Psi(x,t)\rangle = \langle\psi(x)|H\psi(x)\rangle = E\langle\psi(x)|\psi(x)\rangle = E$$

since $H\psi(x) = E\psi(x)$, which is just the time-independent Schroedinger equation.

The expectation value for square of total energy of a stationary state is,

$$\langle H^2\rangle = \langle\psi(x)|H^2\psi(x)\rangle = E^2\langle\psi(x)|\psi(x)\rangle = E^2.$$

Variance in the total energy, $\sigma_H^2 = \langle H^2\rangle - (\langle H\rangle)^2 = (E^2) - (E)^2 = 0$.

4. (a) i. Explain why must the energy E as appear in the time-independent Schroedinger equation,
[*Terangkan mengapa tenaga E seperti yang muncul dalam persamaan Schroedinger tak bersandar masa*]

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar}\left[V(x) - E\right]\psi(x),$$

must be such that $E > V_{\min}$, where $V_{\min}$ the minimal of $V(x)$, $x \in (-\infty,\infty)$.
[*mesti sebegitu rupa supaya $E > V_{min}$, di mana V_{min} adalah minimum bagi $V(x)$, $x \in (-\infty,\infty)$.*]

ii. Explain what it means by the statement "a wavefunction is square-integrable".
[*Terangka apa yang dimaksudkan oleh kenyataan "fungsi gelombang adalah terkamirkan kuasa-dua"*]

(8 marks)

(b) In solving the time-dependent Schroedinger equation, separation of variable method is used. The time-dependent part of the separable solution is given by [*Dalam menyelesaikan persamaan Schroedinger bersandar masa, kaedah pemisahan pembolehubah digunakan. Bahagian bersandar masa penyelesaian terpisah adalah diberikan oleh*]

$$\frac{d\phi(t)}{dt} = -i\frac{E}{\hbar}\phi(t), \tag{1}$$

where E is the separable constant introduced during the procedure.
[*di mana E ialah pemalar pemisahan yang diperkenalkan dalam prosedur tersebut.*]

i. Show that [*Tunjukkan*]

$$\phi(t) = e^{-iEt/\hbar}$$

is the solution to Eq. (1).
[*adalah penyelesaian kepada Eq.* (1).]

ii. Evaluate $|\phi(t)|^2$.
[*Nilaikan* $|\phi(t)|^2$.]

(12 marks)

Solution

Q4(a)i

Given $\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar}[V(x) - E]\psi(x)$, if $E < V_{\text{min}}$, where V_{min} the minimal of $V(x)$, $x \in (-\infty, \infty)$, then ψ and $\frac{d^2\psi(x)}{dx^2}$ always have the same sign: If $\psi(x)$ is positive (negative), then $\frac{d^2\psi(x)}{dx^2}$ is also positive (negative). This means that ψ always curves away from the x-axis (see Figure 4). In either cases ($\psi(x)$ starts out positive or negative), $|\psi(x)| \to \infty$ as $x \to \pm\infty$. In order for $\psi(x)$ to remain normalisable, we must not allow $E < V(x)_{\text{min}}$, $\forall x \in (-\infty, \infty)$.

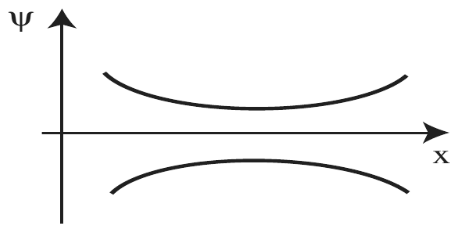


Figure 1: Behavior of $\psi(x)$ when ψ and $\frac{d^2\psi(x)}{dx^2}$ always have the same sign.

Q4(a)i

A wavefunction $\Psi(x,t)$ is square-integrable if

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx < \infty.$$

To be so, $\Psi(x,t)$ must go to zero faster than $1/\sqrt{|x|}$ as $|x| \to \infty$.

5. (a) i. What are the essential differences between the solutions for the time-dependent Schroedinger eqation (TDSE) in an infinite quantum well and that of a free particle? List your answers in the form of a comparison table.
[*Apakah perbezaan yang mustahak antara penyelesaian kepada persamaan Schroedinger berdandar masa (TDSE) bagi telaga kuantum tak terhingga dan penyelesaian untuk zarah bebas? Senaraikan jawapan anda dalam bentuk jadual perbandingan.*]

ii. Explain why the "stationary solution" to the time-dependent Schrodinger equation for a free particle in the form $\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}$, where $k \equiv \pm\frac{\sqrt{2mE}}{\hbar}$, is not physical.
[*Jelaskan mengapa " penyelesaian pegun" kepada persamaan Schrodinger bersandar masa bagi zarah bebas dalam bentuk $\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}$, di mana $k \equiv \pm\frac{\sqrt{2mE}}{\hbar}$, adalah tidak fizikal.*]

(8 marks)

(b) For a free particle, the most general solution to the TDSE is given by
[*Untuk zarah bebas, penyelesaian yang paling am untuk TDSE diberikan oleh*]

$$\Psi(x,t) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk,$$

where A is the normalisation constant.
[*di mana A adalah pemalar normalisasi.*]

i. Prove that $\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = A^2 \int_{-\infty}^{\infty} |\phi(k)|^2 dk$.
[*Buktikan bahawa $\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = A^2 \int_{-\infty}^{\infty} |\phi(k)|^2 dk$.*]

Hint: You may have to make use of the definition for Dirac delta function,
[*Mungkin anda perlu gunakan definisi bagi fungsi delta Dirac,*]

$$\int_{-\infty}^{\infty} e^{i(k'-k)x} dx = 2\pi\delta(k'-k).$$

ii. If $\phi(k) = \frac{\sin(ka)}{k}$, where a is a positve real constant, find the normalisation constant A.
[*Jika $\phi(k) = \frac{\sin(ka)}{k}$, di mana a pemalar bernilai benar positif, dapatkan pemalar normalisasi A.*]

Hint:

$$\int_{-\infty}^{\infty} \frac{\sin^2(ka)}{k^2} dk = a\pi.$$

(12 marks)

Solutions

Q5(a)i

Infinite quantum well	**Free particle**
Boundary conditions $\psi(x) = 0$ at the edges of the well are required.	No boundary conditions are required.
Energies are quantised.	Energies are not quantised.
Normalised.	Dirac normalised.
Always in a bounded state.	Always in a scattered state.
The general solution is a sum over discrete eigenstates, $\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$.	The general solution is an integration over continuous variable k, $\Psi(x,t) = \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$.
The probability density for the particle at the nodes and the boundaries is zero.	The probability density is everywhere the same and non-zero.
Stationary states trapped inside the infinite well.	Wave packet travels in all space.

Q5(a)ii

Because the "stationary state" solutions $\Psi(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)}$ is not normalisable:

$$\begin{aligned}
\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx &= |A|^2 \int_{-\infty}^{\infty} |e^{ik\left(x - \frac{\hbar k}{2m}t\right)}|^2 dx \\
&= |A|^2 \int_{-\infty}^{\infty} \left[e^{ik\left(x - \frac{\hbar k}{2m}t\right)}\right]^* e^{ik\left(x - \frac{\hbar k}{2m}t\right)} dx \\
&= |A|^2 \int_{-\infty}^{\infty} e^{-ik\left(x - \frac{\hbar k}{2m}t\right)} e^{ik\left(x - \frac{\hbar k}{2m}t\right)} dx \\
&= |A|^2 \int_{-\infty}^{\infty} dx \rightarrow 0
\end{aligned}$$

Q5(b)i

$$
\begin{aligned}
& \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx \\
= & \left|\frac{A}{\sqrt{2\pi}}\right|^2 \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} \left[\phi(k) e^{i(kx - \frac{\hbar k^2}{2m} * 0)}\right]^* dk \cdot \int_{-\infty}^{\infty} \phi(k') e^{i(k'x - \frac{\hbar (k')^2}{2m} * 0)} dk' \right\} dx \\
= & \frac{|A|^2}{2\pi} \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ikx} e^{ik'x} \phi(k)^* \phi(k') dk dk' \right\} dx \\
= & \frac{|A|^2}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} e^{i(k'-k)x} dx \right\} \phi(k)^* \phi(k') dk dk' \\
& \Big\downarrow \int_{-\infty}^{\infty} e^{i(k'-k)x} dx = 2\pi\delta(k'-k) \\
= & \frac{|A|^2}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} 2\pi\delta(k'-k)\phi(k') dk' \right) \phi(k)^* dk \\
& \Big\downarrow \int_{-\infty}^{\infty} 2\pi\delta(k'-k)\phi(k') dk' = 2\pi\phi(k) \\
= & |A|^2 \int_{-\infty}^{\infty} \phi(k)\phi(k)^* dk \\
= & |A|^2 \int_{-\infty}^{\infty} |\phi(k)|^2 dk.
\end{aligned}
$$

Q5(b)ii

$$
\begin{aligned}
\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx &= |A|^2 \int_{-\infty}^{\infty} |\phi(k)|^2 dk. \\
&= |A|^2 \int_{-\infty}^{\infty} \frac{\sin^2(ka)}{k^2} dk. \\
&= |A|^2 a\pi = 1 \\
\Rightarrow A = \frac{1}{\sqrt{a\pi}}.
\end{aligned}
$$

6. (a) Give the definitions of [*Berikan takrifan bagi*]

   i. Hermitian operator $\hat{Q}$ [*Operator Hermit* $\hat{Q}$]

   ii. Its Hermitian conjugate, $\hat{Q}^\dagger$ [*Konjugat Hermitnya,* $\hat{Q}$].

   iii. Why are observable in quantum mechanics represented by Hermitian operators?
   [*Mengapakah pembolehcerap dalam mekanik kuantum diwakili oleh operator Hermitian?*]

iv. Prove that a Hermitian operator is equal to its conjugate.
[*Buktikan bahawa operator Hermit adalah bersamaan dengan konjugatnya.*]

(8 marks)

(b) A free particle, which is initially localised in the range $-a < x < a$, is released at time $t = 0$:
[*Satu zarah bebas, yang pada mulanya ditempatkan dalam julat* $-a < x < a$, *dilepaskan pada masa* $t = 0$:]

$$\Psi(x,0) = \begin{cases} A, & \text{if} -a < x < a, \\ 0, & \text{otherwise,} \end{cases}$$

where A and a is a real positive constant. Find $\Psi(x,t)$.
[*di mana A adalah pemalar bernilai benar positif. Dapatkan* $\Psi(x,t)$.]

(12 marks)

Solutions

Q6(a)i
Operators $\hat{Q}$ that have the property

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle \text{ for all } f(x), g(x)$$

are called Hermitian.

Q6(a)ii
Hermitian conjugate (or adjoint) of an operator $\hat{Q}$ is the operator $\hat{Q}^\dagger$ such that

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}^\dagger f|g\rangle$$

for all f and g.

Q6(a)iii
Hermitian operator arise naturally in QM because their expectation values are real, $\langle \hat{Q}\rangle = \langle \hat{Q}\rangle^*$.

Q6(a)iv
The proof that a Hermitian operator is equal to its conjugate, $\hat{Q}^\dagger = \hat{Q}$, can be shown via definitions given in **Q6(a)i** and **Q6(a)ii**:

The definition for a Hermitian operator $\hat{Q}$ is

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle \text{ for all } f(x), g(x). \tag{2}$$

By definition, Hermitian conjugate (or adjoint) of an operator $\hat{Q}$ is the operator $\hat{Q}^\dagger$ such that

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}^\dagger f|g\rangle \text{ for all } f(x), g(x). \tag{3}$$

Comparing the RHS of both Eqs. (2), (3),

$$\langle \hat{Q}f|g\rangle \equiv \langle \hat{Q}^\dagger f|g\rangle.$$

Hence,

$$\hat{Q} = \hat{Q}^\dagger.$$

Q6(b)

First find the normalisation constant A:

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

The most general solution to the TDSE for a free particle is

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk.$$

where $\phi(k)$ is the Fourier transform of $\Psi(x,0)$,

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx. \tag{4}$$

Then work out $\phi(k)$ using Eq.(4):

$$\begin{aligned}
\phi(k) &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx} dx \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \frac{ie^{-ikx}}{k}\bigg|_{-a}^{a} \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \cdot \frac{i}{k} \left(e^{-ika} - e^{ika}\right) \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \cdot \frac{i}{k} \left[(\sin ka - i\cos ka) - (\sin ka + i \cos ka)\right] \\
&= \frac{1}{\sqrt{a\pi}} \frac{\sin(ka)}{k}
\end{aligned}$$

Then put it back to $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$, and we obtain

$$\Psi(x,t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m}t)} dk.$$

7. (a) i. Explain what it means by the statement "a function $f(\mathbf{r})$ is spherically symmetric". $\mathbf{r}$ is a vector in 3D-space.
[*Terangkan apa yang dimaksudkan dengan kenyataan "fungsi $f(\mathbf{r})$ adalah bersimetri sfera". $\mathbf{r}$ adalah vektor dalam ruang 3D.*]

ii. Explain why is the hydrogen wavefunction, $\psi_{n\ell m}(r, \theta, \phi)$, spherically symmetric for $\{\ell, m\} = \{0, 0\}$.
[*Terangkan mengapa fungsi gelombang hidrogen, $\psi_{n\ell m}(r, \theta, \phi)$, adalah bersimetri sfera bagi $\{\ell, m\} = \{0, 0\}$.*]

(8 marks)

(b) The normalised hydrogen wave functions are given by
[*Fungsi gelombang hidrogen yang dinormalisasikan diberikan oleh*]

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^\ell \left[L_{n-\ell-1}^{2\ell+1}(2r/na)\right] Y_\ell^m(\theta, \phi),$$

where the associate Laguerre polynomials are given by
[*di mana polinomial Laguerre bersekutu diberikan oleh*]

$$L_{q-p}^q(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_q(x).$$

and [*dan*]

$$L_q(x) \equiv e^x \left(\frac{d}{dx}\right)^q (e^{-x} x^q),$$

is known as the q-th **Laguerre polynomial**. $Y_\ell^m(\theta, \phi)$ are the spherical harmonics.
[*dikenali sebagai* **polinomial Laguerre** *ke-q. $Y_\ell^m(\theta, \phi)$ adalah harmonik-harmonik sfera.*]

i. Show that the hydrogen ground state solution is given by
[*Tunjukkan bahawa penyelesaian keadaan dasar hidrogen diberikan oleh*]

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}.$$

ii. Show that the ground state solution above is normalised.
[*Tunjukkan bahawa penyelesaian keadaan dasar di atas adalah dinormalisasikan.*]

Hint: $\int_0^\infty y^2 e^{-y} dy = 2.$

(12 marks)

Solutions

Q7(a)i
The statement "$f(\mathbf{r})$ is spherically symmetric" means the value of the function $f(\mathbf{r})$ depends only on $|\mathbf{r}|$ only but not on the directions, namely, θ, ϕ: $f(\mathbf{r}) = f(|\mathbf{r}|)$.

Q7(a)ii
The wavefunction for hydrogen has angular part and radial parts, $\psi_{n,\ell,m}(r,\theta,\phi) = R_{n,\ell}(r)Y_\ell^m(\theta,\phi)$, where the angular dependence is contained in the spherical harmonics $Y_\ell^m(\theta,\phi)$, which are characterised by the indices $\{\ell, m\}$. If $\{\ell, m\} = \{0, 0\}$, the spherical harmonics $Y_0^0(\theta,\phi)$ is just a constant and has no angular dependence. It means $\psi_{n,0,0}(r,\theta,\phi)$ has no angular dependence. Hence, $\psi_{n,0,0}(r,\theta,\phi) = \psi_{n,0,0}(r)$ is spherically symmetric.

Q7(b)i Given

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^\ell \left[L_{n-\ell-1}^{2\ell+1}(2r/na)\right] Y_\ell^m(\theta,\phi),$$

the ground-state wavefunction is

$$\begin{aligned}\psi_{1,0,0} &= \sqrt{\left(\frac{2}{a}\right)^3 \frac{(1-0-1)!}{2[(1+0)!]^3}} e^{-r/a} \left(\frac{2r}{a}\right)^0 \left[L_{1-0-1}^{2*0+1}(2r/a)\right] Y_0^0(\theta,\phi) \\ &= \frac{2}{\sqrt{a^3}} e^{-r/a} L_0^1(2r/a) Y_0^0(\theta,\phi)\end{aligned}$$

$Y_0^0(\theta,\phi) =$ constant, which can be determined via normalisation:

$$\begin{aligned}\int_{\theta=0}^{\theta=\pi} \int_{\phi=0}^{\phi=2\pi} |Y_0^0(\theta,\phi)|^2 \sin\theta d\theta d\phi &= 1 \\ \text{constant}^2 \int_{\theta=0}^{\theta=\pi} \int_{\phi=0}^{\phi=2\pi} \sin\theta d\theta d\phi &= 1 \\ \Rightarrow \qquad \text{constant} &= \frac{1}{\sqrt{4\pi}}.\end{aligned}$$

$$L_0^1(x) \equiv L_{q-p}^q(x), \quad q \equiv 1, \quad p \equiv 1$$

$$L_0^1(x) = (-1)^1 \left(\frac{d}{dx}\right)^1 L_1(x) = -\frac{d}{dx} L_1(x)$$

$$\begin{aligned}L_1(x) &= e^x \frac{d}{dx}^1 (e^{-x} x^1) = e^x(e^{-x} - xe^{-x}) = (1-x) \\ L_0^1(x) &= -\frac{d}{dx}(1-x) = 1.\end{aligned}$$

Put everything together,

$$\psi_{1,0,0} = \frac{2}{\sqrt{a^3}} e^{-r/a} \frac{1}{\sqrt{4\pi}} = \frac{e^{-r/a}}{\sqrt{a^3\pi}}.$$

Q7(b)ii

$$\int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \int_{r=0}^{r\to\infty} |\psi_{1,0,0}|^2 r^2 dr \sin\theta d\theta d\phi = \frac{4\pi}{a^3\pi} \int_{-\infty}^{\infty} r^2 e^{-2r/a} dr$$

Let $y = \frac{2r}{a}$, $\frac{dy}{dr} = \frac{2}{a}$, $r \to \infty, y \to \infty$.

$$\begin{aligned}
\int_0^\infty r^2 e^{-2r/a} dr &= \int_0^\infty r^2 e^{-2r/a} dr \\
&= \frac{a^3}{8} \int_0^\infty y^2 e^{-y} dy \\
&= \frac{a^3}{8} \cdot 2 = \frac{a^3}{4}.
\end{aligned}$$

Putting everything together,

$$\int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\pi} \int_{r=0}^{r\to\infty} |\psi_{1,0,0}|^2 r^2 dr \sin\theta d\theta d\phi = 1$$

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:

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

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

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

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