جامعة بنـها - كلية العلوم – قسم الرياضيــات

المستوى الثالث (شعبة رياضيات)

الفصل الدراسي الأول

يوم الامتحان: الخميس 21 / 1 / 2016 م

المادة : الأسس الرياضية لنظرية ميكانيكا الكم (M331)

أستاذ المادة : د . / خليل محمد خليل محمد

مدرس بقسم الرياضيات بكلية العلوم

صورة من الامتحان+ نموذج إجابته

Faculty of Science	Third level(Math.)	21 / 1 / 2016
Math. Department	(**Quantum &Statistical) Mechanics M331**	Time: 2 hours

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<u>First Part</u>: **Mathematical Foundations of Quantum Theory** (**one hour**)

Answer the following questions:

1.a	Show that: the eigenvalues of a unitary operator are complex numbers of unit modulus and its eigenvectors corresponding to unequal eigenvalues are mutually orthogonal? **(10 Marks)**
1.b	State the postulates of quantum mechanics. **(10 Marks)**
2.a	Prove that: $\underline{j}(x;t)=(\frac{\hbar}{\mu})\mathrm{Im}(\psi^*\frac{\partial\psi}{\partial x})$ where $\underline{j}(x;t)$ is the probability (particle) current density vector and ψ satisfy Schrödinger time dependent equation. **(10 Marks)**
2.b	A particle of a mass μ is located in a unidimensional square potential well with absolutely impenetrable walls $(0<x<l)$. Find (a) The energy eigenvalues and corresponding normalized eigenfunctions of the particle. (b) The probability of the particle with the lowest energy (ground state) being within the region $(\frac{l}{3}<x<\frac{2l}{3})$. **(10 Marks)**

<u>Look the Statistical Mechanics Exam</u>

Dr. Khalil Mohamed

إجابة السؤال 1.a:

Proof:

Let $\hat{U}$ be a unitary operator, where $\hat{U}\psi_i = \lambda_i \psi_i$; $\psi_i \neq 0$ *and* $\hat{U}\psi_j = \lambda_j \psi_j$; $\psi_j \neq 0$. Let

$\lambda_i \neq \lambda_j$ **for** $i \neq j$. Now

$(\hat{U}\psi_j, \hat{U}\psi_i) = \lambda_j^* \lambda_i (\psi_j, \psi_i) \qquad (i)$

By definition

$(\hat{U}\psi_j, \hat{U}\psi_i) = (\psi_j, \psi_i) \qquad (ii)$

from (i) *and* (ii)

$(1 - \lambda_i \lambda_j^*)(\psi_j, \psi_i) = 0 \qquad (iii)$

then $i = j$ *in* (iii) if $(1 - \lambda_i \lambda_i^*)(\psi_i, \psi_i) = 0$

Since $(\psi_i, \psi_i) \neq 0$ then $(1 - \lambda_i \lambda_i^*) = 0 \Rightarrow |\lambda_i|^2 = 1 \quad \therefore |\lambda_i| = 1$

Thus the eigenvalues are complex numbers of unit modulus.

by assumption $\lambda_i \neq \lambda_j$ then $i \neq j$ *in* (iii) if

Since $(\psi_i, \psi_i) \neq 0$ then $(1 - \lambda_i \lambda_i^*) = 0 \Rightarrow |\lambda_i|^2 = 1 \quad \therefore |\lambda_i| = 1$

$\lambda_i \neq \lambda_j \Rightarrow \lambda_i \lambda_j^* \neq \lambda_j \lambda_j^* = |\lambda_j|^2 = 1$ *then* $\lambda_i \lambda_j^* \neq 1$

from (iii) $\Rightarrow (\psi_j, \psi_i) = 0$

Therefore, eigenvectors corresponding to unequal eigenvalues are mutually orthogonal.

إجابة السؤال 1.b:

*The postulates of quantum mechanics are:

1)-Postulate I: Every physical state of a dynamical system (a particle) is represented at a given instant of time t by normed vector $|\psi\rangle_t$ in H. It is assumed that the state vector contains all the information which one can know about the state of the system at that instant of time. ψ and $e^{i\delta}\psi$ where $\delta^* = \delta$ represent the same physical state.

2)- Postulate II: To every dynamical variable A there corresponds an observable $\hat{A}$. The observable $\hat{x}$ and $\hat{p}$ must satisfy $[\hat{x}, \hat{p}] = i\hbar$. The rules for constructing the observable $\hat{A}$ corresponding to the dynamical variable A, in the $x-rep$ are as follows:

$$(i) x \to \hat{x} = x,\ t \to \hat{t} = t,\ p \to \hat{p} = -i\hbar \frac{d}{dx}$$

$$(ii) A(x, p, t) \to \hat{A} = A(x, -i\hbar \frac{d}{dx}, t).$$

3)- Postulate III: If a particle is in state $|\psi\rangle_t$, a measurement of a dynamical variable A which is represented by the observable $\hat{A}$ and

$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle,\ \langle\varphi_n|\varphi_n\rangle = \delta_{nm},\ \hat{1}_a = \sum_i |\varphi_i\rangle\langle\varphi_i|$ will

*yield one of the eigenvalues a_i with probability

$$\rho_\psi(a_i) = \frac{|\langle \varphi_i | \psi \rangle|^2}{\langle \psi | \psi \rangle}$$

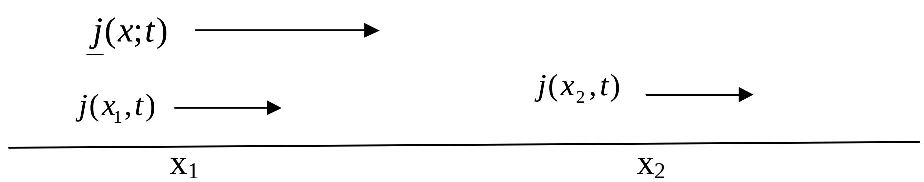
** If the result of measurement is a_k, then the state of the system will change from $|\psi\rangle$ to $|\varphi_k\rangle$ as a result of measurement.

4)- Postulate IV: The state function $\psi(x,t)$ describing the state of a dynamical system obeys the following" Schrodinger time-dependent" equation whose Hamiltonian $\hat{H}$ is

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

إجابة السؤال 2.a:

Probability (particle) current density vector $\underline{j}(x;t)$



The probability that a particle is inside the interval (x_1, x_2) at time t is:

$$\int_{x_1}^{x_2} \rho(x,t)dx = \int_{x_1}^{x_2} \psi^*(x,t)\psi(x,t)\,dx$$

The rate of change of probability for the particle to be inside (x_1, x_2)

$$j(x_1,t) - j(x_2,t) = \frac{d}{dt}\int_{x_1}^{x_2} \rho(x,t)dx = \frac{d}{dt}\int_{x_1}^{x_2} \psi^*(x,t)\psi(x,t)\,dx \qquad (1)$$

$$= \int_{x_1}^{x_2} \frac{\partial}{\partial t}(\psi^*(x,t)\psi(x,t))\,dx = \int_{x_1}^{x_2} (\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi)\,dx$$

Since $\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t}$ and $(\hat{H}\psi)^* = -i\hbar \frac{\partial \psi^*}{\partial t}$, then

$$\frac{\partial \psi}{\partial t} = \frac{i}{\hbar}[\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - U(x)]\psi \quad \text{and} \quad \frac{\partial \psi^*}{\partial t} = -\frac{i}{\hbar}[\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - U(x)]\psi^*; \; U^* = U$$

From which $\psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi = \frac{i\hbar}{2\mu}(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi)$. Substituting into (1)

$$j(x_1,t) - j(x_2,t) = \frac{i\hbar}{2\mu}\int_{x_1}^{x_2} (\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi)\,dx = \frac{i\hbar}{2\mu}\int_{x_1}^{x_2} \frac{\partial}{\partial x}(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi)\,dx$$

$$= \frac{i\hbar}{2\mu}(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi)\Big|_{x_1}^{x_2} \qquad (2)$$

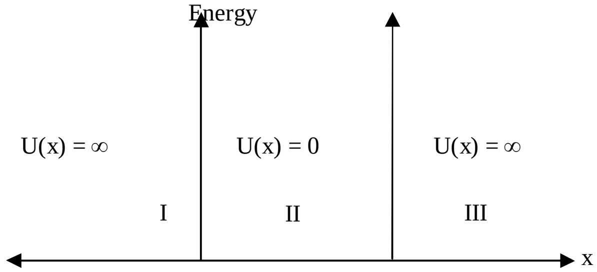
From (2)

$$j(x,t) = -\frac{i\hbar}{2\mu}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) \qquad (3)$$

$$\therefore \quad j(x,t) = \left(-\frac{i\hbar}{2\mu}\right)(2i)\,\mathrm{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right) = \left(\frac{\hbar}{\mu}\right)\mathrm{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right)$$

إجابة السؤال 2.b:

Number (a)



The energy equation or Shrodinger equation may be written as:

$$\left[\frac{d^2}{dx^2} + \frac{2\mu}{\hbar}(E - U(x))\right]\psi_E = 0 \qquad (1)$$

According the potential regions, equation (1) becomes

$$\left.\begin{aligned} &\psi_I'' = 0, && && -\infty < x < 0 \\ &\psi_{II}'' + k^2\psi_{II} = 0, && k = \frac{1}{\hbar}\sqrt{2\mu E}, && 0 < x < l \\ &\psi_{III}'' = 0, && && l < x < \infty \end{aligned}\right\} \qquad (2)$$

The general solution of system (2) is

$$\psi_{II}(x) = A\sin(kx) + B\cos(kx), \qquad 0 < x < l\} \qquad (3)$$

Continuity Conditions

$$\left.\begin{aligned} &\psi_I(0) = \psi_{II}(0) \Rightarrow 0 = A\sin(0) + B\cos(0) \Rightarrow B = 0. \\ &\psi_{II}''(l) = \psi_{III}''(l) \Rightarrow A\sin(kl) = 0 \end{aligned}\right\} \qquad (4)$$

For the non-trivial solution $A \neq 0 \Rightarrow \sin(kl) = 0 \Rightarrow kl = n\pi;\ n = 0,1,2,......$

$$k = \frac{n\pi}{l};\ n = 0,1,2,...... \quad \text{then } \frac{1}{\hbar}\sqrt{2\mu E} = \frac{n\pi}{l} \Rightarrow \frac{2\mu E_n}{\hbar^2} = \frac{n^2\pi^2}{l^2}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2\mu l^2}\ ;\ n = 1,2,3,...... \quad \text{is the eigenvalues.}$$

$$\psi_E(x) = A\sin\left(\frac{n\pi}{l}x\right) \quad ;\ n = 1,2,3,...... \qquad (5)$$

And the normed state is

$$\int_0^l |A|^2 \sin^2\left(\frac{n\pi}{l}x\right)dx = 1 \Rightarrow \frac{|A|^2}{2}\int_0^l \left(1 - \cos^2\left(\frac{n\pi}{l}\right)\right)dx = \frac{|A|^2}{2}\left(x - \frac{l}{2n\pi}\sin\left(\frac{2n\pi}{l}x\right)\right)\Big|_0^l \Rightarrow A = \sqrt[2]{2/l}$$

$$\psi_E(x) = \sqrt{2/l}\,\sin(\frac{n\pi}{l}x) \quad ; n = 1,2,3,\ldots\ldots \qquad 0 < x < l$$ is the normalized eigenfunctions

Number (b)

$$\because \;\; \psi_E(x) = \sqrt{2/l}\,\sin(\frac{n\pi}{l}x) \quad ; n = 1,2,3,\ldots\ldots \qquad 0 < x < l$$

In case of ground state $n = 1$, then $\psi_E(x) = \sqrt{2/l}\,\sin(\frac{\pi}{l}x) \qquad 0 < x < l$

And the probability that the particle is inside the interval $(\frac{l}{3} < x < \frac{2l}{3})$ become

$$\int_{l/3}^{2l/3} \rho(x)dx = \int_{l/3}^{2l/3} \psi^*(x)\psi(x)\,dx = \frac{2}{l}\int_{l/3}^{2l/3} \sin^2(\frac{\pi}{l}x)dx = \frac{2}{l}.\frac{1}{2}\int_{l/3}^{2l/3} (1-\cos(\frac{2\pi}{l}x))dx$$

$$= \frac{1}{3} + \frac{\sqrt{3}}{2\pi}.$$

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