جامعة بنها - كلية العلوم - قسم الرياضيات المستوى الثالث (شعبة رياضيات) الفصل الدراسي الأول

يوم الامتحان: السبت 2017/1/14 م

المادة: الأسس الرياضية لنظرية ميكانيكا الكم (M331)

أستاذ المادة : د . / خليل محد خليل محد

مدرس بقسم الرياضيات بكلية العلوم

صورة من الامتحان+ نموذج إجابته



Faculty of Science Third level (Math.) 14/1/2017 Math. Department Benha (Quantum & Statistical) Mechanics Time: 2 hours

First: Mathematical Foundations of Quantum Theory (M331) questions

1.a	Find the adjoint operator \hat{A}^+ if $\hat{A} = \frac{d}{dx}$ defined on L_2 i.e.
	$\hat{A}\varphi(x) = \frac{d}{dx}\varphi(x)$ with the boundary condition $\varphi(\pm \infty) = 0$. (6 Marks)
1.b	
	of unit modulus and its eigenvectors corresponding to unequal eigenvalues are mutually orthogonal? (7 Marks)
1.c	A particle of mass μ and energy E approaches a square potential barrier $U(x) = 0$, $x < 0$ and $U(x) = U_0$, $x \ge 0$ where $U_0 > 0$ from the left.
	Prove that the reflection coefficient R and the transmission coefficient T satisfy the relation $R+T=1$ if $E>U_0$. (7 Marks)
2.a	State the postulates of quantum mechanics. (10 Marks)
2.b	A particle whose Hamiltonian \hat{H} has discrete spectrum E_n , where
	$\hat{H}\varphi_n(x) = E_n \varphi_n(x), \langle \varphi_m(x) \varphi_n(x) \rangle = \delta_{mn}, E_n = (n + \frac{1}{2})\hbar\omega, \ n = 0, 1, 2, \dots$ is
	described at $t = 0$ by the normed state function
	$\psi(x;0) = \sqrt{\frac{1}{5}}\varphi_0(x) + \sqrt{\frac{1}{2}}\varphi_2(x) + C_3\varphi_3(x).$
	(i) Determine the numerical value of C_3 .
	(ii) Write out $\psi(x;t)$.
	(iii) What is $\langle E \rangle_{t=0}$ and $\langle E \rangle_{t=1}$. (10 Marks)

Look the Statistical Mechanics Exam

Dr. Khalil Mohamed

اجابة السؤال 1.2: Proof: To obtain the adjoint operator, we take the inner product

$$(\hat{A}\phi,\psi) = \int_{-\infty}^{\infty} (\hat{A}\phi(x))^* \psi(x) dx = \int_{-\infty}^{\infty} \frac{d}{dx} \phi(x)^* \psi(x) dx \quad \text{then by partial integration}$$

let
$$u = \psi(x)$$
 and $dv = \frac{d}{dx}\phi(x)^* dx$ this leads to $du = d\psi(x)$, $v = \phi(x)^*$ then

$$\int_{-\infty}^{\infty} \frac{d}{dx} \phi(x)^* \psi(x) dx = \psi(x) \phi(x)^* \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \phi(x)^* (\frac{d}{dx} \psi(x)) dx$$
. From the boundary condition

$$\phi(\pm \infty) = 0 \quad \text{then} \quad \int_{-\infty}^{\infty} \frac{d}{dx} \phi(x)^* \psi(x) dx = 0 + \int_{-\infty}^{\infty} \phi(x)^* (-\frac{d}{dx} \psi(x)) dx = (\phi, (-\frac{d}{dx}) \psi) = (\phi, \hat{A}^{\dagger} \psi)$$

$$\therefore \hat{A}^+ = -\frac{d}{dx}.$$

إجابة السؤال 1.b:

Proof:

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

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

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

by definition

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

from (i) and (ii)

$$(1 - \lambda_i \lambda_j^*)(\psi_j, \psi_i) = 0$$
 (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 $(1 - \lambda_i \lambda_i^*) = 0 \Rightarrow |\lambda_i|^2 = 1$ $\therefore |\lambda_i| = 1$

Thus the eigenvalues are complex numbers of unit modulus.

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

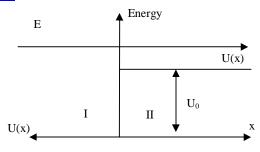
Since
$$(\psi_i, \psi_i) \neq 0$$
 then $(1 - \lambda_i \lambda_i^*) = 0 \Rightarrow |\lambda_i|^2 = 1$ $\therefore |\lambda_i| = 1$

$$\lambda_i \neq \lambda_j \Rightarrow \lambda_i \lambda_j^* \neq \lambda_j \lambda_j^* = \left| \lambda_j \right|^2 = 1 \text{ then } \lambda_i \lambda_j^* \neq 1$$

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

Therefore, eigenvectors corresponding to unequal eigenvalues are mutually orthogonal.

جابة السؤال 1.c:



The energy equation or Shrodinger equation may be written as:

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

According the potential regions, equation (1) becomes

$$\psi_{I}'' + k_{0}^{2} \psi_{I} = 0, k_{0} = \frac{1}{\hbar} \sqrt{2\mu E}, x < 0$$

$$\psi_{II}'' + k^{2} \psi_{II} = 0, k = \frac{1}{\hbar} \sqrt{2\mu (E - U_{0})}, x \ge 0$$
(2)

The general solution of system (2) is

$$\psi_{I}(x) = A \exp(ik_{0}x) + B \exp(ik_{0}x), \qquad x < 0$$

$$\psi_{II}(x) = C \exp(ikx) + D \exp(-ikx), \qquad x \ge 0$$
(3)

Since the beam incident from the left, then D must vanish.

Continuity Conditions

$$\overline{\psi_{I}(0) = \psi_{II}(0) \Rightarrow A + B = C}$$

$$\psi_{I}''(0) = \psi_{II}''(0) \Rightarrow k_{0}A - k_{0}B = kC$$
(4)

From (4)

$$B = (\frac{k_0 - k}{k_0 + k})A \qquad \text{and} \qquad C = (\frac{2k_0}{k_0 + k})A \qquad \text{Thus (3) becomes}$$

$$\psi_{E}(x) = A \begin{cases} \exp(ik_{0}x) + (\frac{k_{0} - k}{k_{0} + k})\exp(-ik_{0}x) & x < 0 \\ (\frac{2k_{0}}{k_{0} + k})\exp(ikx) & x \ge 0 \end{cases}$$

$$(5)$$

Since the reflection coefficient R and the transmission T coefficient satisfy the relations $R = \frac{|j_{ref}|}{|j_{inc}|}$

and
$$T = \left| \frac{j_{tran}}{j_{inc}} \right|$$
 respectively, where $j(x,t) = (\frac{\hbar}{\mu}) \operatorname{Im}(\psi^*(x,t) \frac{\partial \psi(x,t)}{\partial x})$.

Now, let us calculate R and T. From the values for A and B with equation (5), one gets

$$j_{inc} = \frac{\hbar k_0}{\mu} |A|^2, \qquad J_{ref} = -\frac{\hbar k_0}{\mu} |B|^2, \qquad J_{tran} = \frac{\hbar k}{\mu} |C|^2 \qquad \therefore R = \left| \frac{B}{A} \right|^2 = (\frac{k_0 - k}{k_0 + k})^2$$

And
$$T = \frac{k}{k_0} \left| \frac{C}{A} \right|^2 = \frac{4k_0 k}{(k_0 + k)^2}$$

Thus

$$R+T=(\frac{k_0-k}{k_0+k})^2+\frac{4k_0k}{(k_0+k)^2}=\frac{k_0^2-2k_0k+k^2+4k_0k}{(k_0+k)^2}=\frac{k_0^2+2k_0k+k^2}{(k_0+k)^2}=1\,.$$

*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 $|\psi\rangle$ 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:

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

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

3)- Postulate III: If a particle is in state $|\psi\rangle$, a measurement of a dynamical variable A represented by the observable \hat{A} in the discrete spectrum $\hat{A} | \varphi_n \rangle = a_n | \varphi_n \rangle, \ \langle \varphi_n | \varphi_n \rangle = \delta_{nm}, \quad \hat{1}_a = \sum_i | \varphi_i \rangle \langle \varphi_i | \quad \text{will}$

*yield one of the eigenvalues with probability a,

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

- ** 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 \hat{H} whose Hamiltonian is

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

إجابة السؤال 2.b:

(i)
$$: \|\psi(x,0)\|^2 = 1$$
, (normalized)

(i) :
$$\|\psi(x,0)\|^2 = 1$$
, (normalized) : $\frac{1}{5} + \frac{1}{2} + |c_3|^2 = 1$ $\Rightarrow \frac{7}{10} + |c_3|^2 = 1$

$$\therefore |c_3| = \sqrt{\frac{3}{10}}$$

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For finding $\psi(x,t)$ then

$$\psi(x,t) = \sum_{n} \exp(-iE_{n}t/\hbar)\phi_{n}(x) < \phi_{n}(x) | \psi(x,0) > and$$

$$\psi(x,0) = \sqrt{\frac{1}{5}}\phi_{0}(x) + \sqrt{\frac{1}{2}}\phi_{2}(x) + \sqrt{\frac{3}{10}}\phi_{3}(x)$$

$$\psi(x,t) = \sqrt{\frac{1}{5}}\exp(-iE_{0}t/\hbar) \phi_{0}(x) + \sqrt{\frac{1}{2}}\exp(-iE_{2}t/\hbar)\phi_{2}(x) + \sqrt{\frac{3}{10}}\exp(-iE_{3}t/\hbar)\phi_{3}(x)$$

From (1) and (2), we get

 $\therefore E_0 = \frac{\hbar\omega}{2}, E_2 = \frac{5\hbar\omega}{2}, E_3 = \frac{7\hbar\omega}{2}$

$$\psi(x,t) = \sqrt{\frac{1}{5}} \exp(-i\omega t/2) \ \phi_0(x) + \sqrt{\frac{1}{2}} \exp(-i5\omega t/2) \phi_2(x) + \sqrt{\frac{3}{10}} \exp(-i7\omega t/2) \phi_3(x)$$

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(2)

For finding the probability for particles that exist in the n level

$$\rho_{\psi(x,0)}(E_n) = \left| \langle \phi_n(x) | \psi(x,0) \right|^2 = \left| \langle \phi_n(x) | \sqrt{\frac{1}{5}} \phi_0(x) + \sqrt{\frac{1}{2}} \phi_2(x) + \sqrt{\frac{3}{10}} \phi_3(x) \rangle \right|^2$$

$$where \quad n = 0,1,2,....$$

$$\therefore \quad \rho_{\psi(x,0)}(E_0) = \frac{1}{5}, \qquad \rho_{\psi(x,0)}(E_2) = \frac{1}{2}, \qquad \rho_{\psi(x,0)}(E_3) = \frac{3}{10}.$$

$$\therefore \quad \langle E \rangle_{t=0} = \sum_{n=0}^{\infty} \rho(E_n) E_n = \frac{1}{5} E_0 + \frac{1}{2} E_2 + \frac{3}{10} E_3$$

بالمثل

$$\begin{split} \rho_{\psi(x,t)}(E_n) &= \left| <\phi_n(x) \, | \, \psi(x,t) \right|^2 \\ &= \left| <\phi_n(x) \, | \, \sqrt{\frac{1}{5}} \exp(-i\omega t/2) \, \phi_0(x) + \sqrt{\frac{1}{2}} \exp(-i5\omega t/2) \phi_2(x) + \sqrt{\frac{3}{10}} \exp(-i7\omega t/2) \phi_3(x) > \right|^2 \\ where \ n &= 0,1,2,..... \end{split}$$

$$\therefore \quad \rho_{\psi(x,t)}(E_0) = \frac{1}{5}, \qquad \rho_{\psi(x,t)}(E_2) = \frac{1}{2}, \quad \rho_{\psi(x,t)}(E_3) = \frac{3}{10}.$$

$$\therefore \langle E \rangle_{t>0} = \sum_{n=0}^{\infty} \rho(E_n) E_n = \frac{1}{5} E_0 + \frac{1}{2} E_2 + \frac{3}{10} E_3$$

$$\therefore \langle E \rangle_{t=0} = \langle E \rangle_{t>0}$$

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