جامعة بنـها - كلية العلوم – قسم الرياضيـات

المستوى الثالث(رياضيات - ساعات معتمدة)

الفصل الدراسي الأول

يوم الامتحان: الأربعاء 14 / 1 / 2015 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 year Math. 14 / 1 / 2015
Math. Dept. Benha (**Quantum &Statistical) Mechanics** Time: 2 hours

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Mathematical Foundations of Quantum Theory (M331) questions:

Answer as you can:

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 $\varphi(\pm\infty)=0$.
1.b	Show that: the eigenvalues of a unitary operator are complex numbers of unit modulus and its eigenvectors corresponding to unequal eigenvalues are mutually orthogonal?
1.c	A particle of mass μ and energy E approaches a square potential barrier $U(x)=0,\ x<0$ and $U(x)=U_0,\ x\geq 0$ where $U_0>0$ from the left. Find the reflection coefficient R if $E<U_0$. Determine x_{eff} ?
2.a	State the postulates of quantum mechanics.
2.b	A particle of mass μ is located in a unidimensional square potential well with impenetrable walls $0<x<l$. The Hamiltonian of the particle comprise a discrete spectrum i.e. $\hat{H}\varphi_n(x)=E_n\varphi_n(x)$ where $\varphi_n(x)=\sqrt{\frac{2}{l}}\sin(\frac{n\pi}{l}x), 0<x<l,\ E_n=\frac{n^2\pi^2\hbar^2}{2\mu l^2}, n=1,2,3,...$ Find the normed state function $\psi(x,t)$ at $t>0$, if $\psi(x,0)=Ax(l-x),\ 0<x<l$. If at $t=0$, the energy is measured . determine the probability of the particle being in the n^{th} level. Hence calculate the probability for the first three levels?

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

Dr. Khalil Mohamed

:1.a إجابة السؤال

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

$$(\hat{A}\phi,\psi)=\int_{-\infty}^{\infty}(\hat{A}\phi(x))^{*}\psi(x)dx=\int_{-\infty}^{\infty}\frac{d}{dx}\phi(x)^{*}\psi(x)dx$$ 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

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

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

:1.b إجابة السؤال

Proof:

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

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

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

by definition

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

from (i) *and* (ii)

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

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

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.

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

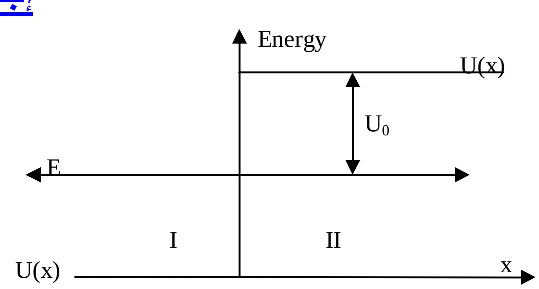
Since $(\psi_i,\psi_i)\neq 0$ then $(1-\lambda_i\lambda_i^{*})=0\Rightarrow|\lambda_i|^2=1$ $\therefore|\lambda_i|=1$

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

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

Therefore, eigenvectors corresponding to unequal eigenvalues are mutually orthogonal.

:1.c إجابة السؤال



The energy equation or Shrodinger equation my be written as:

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

Eqn(1) is

$$\left.\begin{aligned}&\psi_I''+k_0^2\psi_I=0, && k_0=\frac{1}{\hbar}\sqrt{2\mu E}, && x<0\\ &\psi_{II}''-\aleph^2\psi_{II}=0, && \aleph=\frac{1}{\hbar}\sqrt{2\mu(U_0-E)}, && x\geq 0\end{aligned}\right\} \qquad (2)$$

The general solution of system (2) is

$$\left.\begin{aligned}&\psi_I(x)=A\exp(ik_0x)+B\exp(ik_0x), && x<0\\ &\psi_{II}(x)=C\exp(\aleph x)+D\exp(-\aleph x), && x\geq 0\end{aligned}\right\} \qquad (3)$$

Since $\psi(x)$ has finite modulus for all x, then C must vanish.

<u>Continuity Conditions</u>

$$\left.\begin{aligned}&\psi_I(0)=\psi_{II}(0)\Rightarrow A+B=D\\ &\psi_I''(0)=\psi_{II}''(0)\Rightarrow k_0A-k_0B=i\aleph D\end{aligned}\right\} \qquad (4)$$

From (4)

$B=(\frac{k_0-i\aleph}{k_0+i\aleph})A$ and $D=(\frac{2k_0}{k_0+i\aleph})A$ Thus (3) becomes

$$\psi_E(x)=A\begin{cases}\exp(ik_0x)+(\frac{k_0-i\aleph}{k_0+i\aleph})\exp(-ik_0x) & x<0\\ (\frac{2k_0}{k_0+i\aleph})\exp(-i\aleph) & x\geq 0\end{cases}$$

From the values for A and B with equation (3), one gets

$$j_{inc}=\frac{\hbar k_0}{\mu}|A|^2, \qquad J_{ref}=-\frac{\hbar k_0}{\mu}|B|^2 \qquad \therefore R=\left|\frac{B}{A}\right|^2=\left|\frac{k_0-i\aleph}{k_0+i\aleph}\right|^2=1$$

Thus for energy region all incident particles are reflected.
And for finding the effective penetration depth x_{eff} in this case

$\because |\psi(x)|^2_{x_{eff}}=\frac{1}{e}|\psi(x)|^2_{x=0}$ where the barrier at $x=0$

With $\psi(x)=A(\frac{2k_0}{k_0+i\aleph})\exp(-\aleph x)$, $\quad \aleph=\frac{1}{\hbar}\sqrt{2\mu(U_0-E)}$

$$\therefore \left|\frac{2k_0}{k_0+i\aleph}A\exp(-\aleph x)\right|^2_{x_{eff}}=\frac{1}{e}\left\|\frac{2k_0}{k_0+i\aleph}A\exp(-\aleph x)\right\|^2_{x=0}$$

$$\frac{4k_0^2}{k_0^2+\aleph^2}A^2\exp(-2\aleph x_{eff})=\frac{1}{e}\frac{4k_0^2}{k_0^2+\aleph^2}A^2$$

$$-2\aleph x_{eff}=\ln(\frac{1}{e})=-1 \qquad \Rightarrow x_{eff}=\frac{1}{2\aleph}.$$

إجابة السؤال 2.a:

*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 $\hat{A}$

$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle,\ \langle\varphi_n|\varphi_n\rangle = \delta_{nm},\ \ \hat{1}_a = \sum_i |\varphi_i\rangle\langle\varphi_i|$ 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 whose Hamiltonian is $\hat{H}$ obeys the following" Schrodinger time-dependent" equation

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

إجابة السؤال 2.b:

$$\because \psi(x,0) = Ax(l-x), \qquad 0 < x < l$$

$$\Rightarrow \|\psi(x,0)\|^2 = 1 = <\psi(x,0)|\psi(x,0)> = \int_0^l |A|^2 x^2 (l-x)^2 dx = 1$$

$$\therefore A = \sqrt{\frac{30}{l^5}} \Rightarrow \psi(x,0) = \sqrt{\frac{30}{l^5}} x(l-x)\ \ (normalized).$$

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

$$\psi(x,t)=\sum_n \exp(-iE_n t/\hbar)\phi_n(x)<\phi_n(x)|\psi(x,0)>$$

$$\because\ <\phi_n(x)|\psi(x,0)>=\int_0^l \phi^*{}_n(x)\psi(x,0)dx=\sqrt{\frac{60}{l^6}}\int_0^l \sin(\frac{n\pi}{l}x)x(l-x)dx$$

$$=\sqrt{\frac{60}{l^6}}[\int_0^l lx\ \sin(\frac{n\pi}{l}x)dx-\int_0^l x^2\ \sin(\frac{n\pi}{l}x)dx$$

$$\sqrt{\frac{60}{l^6}}[\frac{-2l^3}{(n\pi)^3}(\cos(\frac{n\pi}{l}x)|_0^l]=\frac{2\sqrt{60}}{(n\pi)^3}[1-(-1)^n]$$

$$\therefore <\phi_n(x)|\psi(x,0)>=\begin{cases}\dfrac{4\sqrt{60}}{(n\pi)^3} & n=1,3,5,.........odd\\ 0 & n=0,2,4,.........even\end{cases}$$

$$\therefore \psi(x,t)=\sum_n \exp(-iE_n t/\hbar)\phi_n(x).\frac{4\sqrt{60}}{(n\pi)^3}\qquad 0<x<l\qquad ,n=1,3,5,..$$

$$=\frac{8\sqrt{30}}{\pi^3\sqrt{l}}\sum_n\frac{1}{n^3}\exp(-iE_n t/\hbar)\sin(\frac{n\pi}{l}x).\qquad 0<x<l\qquad ,n\ \ odd$$

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

$$\rho_{\psi(x,0)}(E_n)=|<\phi_n(x)|\psi(x,0)|^2=\left|\int_0^l \phi_n{}^*(x)\psi(x.0)dx\right|^2$$

$$=\left|\int_0^l\sqrt{\frac{2}{l}}\sin(\frac{n\pi}{l}x).\sqrt{\frac{30}{l^5}}(xl-x^2)dx\right|^2=\frac{240}{(n\pi)^6}\left|1-(-1)^n\right|^2,\ n\ \ odd$$

$$=\begin{cases}\dfrac{960}{(n\pi)^6} & n=1,3,5,.....\\ 0 & n=0,2,4,.......\end{cases}$$

$$\rho_{\psi(x,0)}(E_1)=\frac{960}{\pi^6},\qquad \rho_{\psi(x,0)}(E_2)=0,\qquad \rho_{\psi(x,0)}(E_3)=\frac{960}{(3\pi)^6}.$$

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