Mandatory Assignment 1

FYS-2000 - Quantum Mechanics

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10. mars 2018

Contains 11 pages, frontpage included

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Task 1

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

We have the one dimensional Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi$$

Since we have definite value E we can use TISE (Time independent Schrödinger equation and separate the wave equation.

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)} \tag{1}$$

Time independent Schrödinger equation for one dimension, (TISE)

guessing the equation:

$$\psi(x) = Ae^{ikx} + B^{-ikx}$$

Using the euler identity:

$$e^{i\theta} = Cos(\theta) + iSin(\theta)$$

This gives:

$$\psi(x) = A(Cos(kx) + iSin(kx)) + B(Cos(kx) - iSin(kx))$$

$$\psi(x) = (A+B)(Cos(kx) + (A-B)iSin(kx) \tag{2}$$

This has to be equal to zero at $\psi(0)$ so we get

$$A = -B$$

Putting this back into (2) yield:

$$\psi(x) = i2ASin(kx)$$

We set i2A = C, and since $\psi(x)$ has to be zero at 0 and a, the sine function has to have $k = \frac{n\pi}{a}$ so that sine is always zero at every integer n (energy level) at 0 and a.

$$\psi(x) = CSin(\frac{n\pi x}{a})$$

The particle has to be in the well at each energy level so we normalize the wave function between 0 and a. We normalize the function:

$$\int_0^a |\Psi(x,t)|^2 \mathrm{dx} = 1$$

The $e^{iEt/\hbar}$ part cancels out and we get.

$$\int_0^a C^2 Sin^2(\frac{n\pi x}{a})\mathrm{dx} = 1$$

$$\frac{a}{2} = \frac{1}{C^2}$$

$$C = \sqrt{\frac{2}{a}}$$

$$\boxed{< x >= \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 \mathrm{dx}} \tag{3}$$

Expectation value for one dimension

We now have

$$\psi(x) = \sqrt{\frac{2}{a}} Sin(\frac{n\pi x}{a})$$

To find the expectation value we have to solve: Using Eq (3)

$$< x >= C^2 \int_0^a Sin^2(\frac{n\pi x}{a}) \mathrm{dx}$$

Use the trigonometric identity

$$Sin^2(x) = \frac{1}{2}(1 - Cos(2x))$$

$$< x >= \frac{1}{2a} \int_0^a (x - xCos(2x)) \mathrm{dx}$$

$$< x >= \frac{2}{a} \int_0^a (x(\frac{1}{2} - \frac{1}{2} Cos(\frac{2n\pi x}{a})) \mathrm{dx}$$

$$< x >= \frac{1}{a} \int_0^a x \mathrm{dx} - \frac{1}{a} \int_0^a x Cos(\frac{2n\pi x}{a}) \mathrm{dx}$$

The last integral becomes zero because sine function with $n\pi$ where n is a integer is always zero, so we get:

$$< x >= \frac{a}{2}$$

$$\boxed{< x^2 >= \int_{-\infty}^{\infty} x^2|\Psi(x,t)|^2 \mathrm{dx}} \tag{4}$$

Squared x of expectation value x, one dimension

$$< x^2 >= C^2 \int_0^a x^2 Sin^2(kx) dx$$

Here $k = \frac{n\pi}{a}$ and i use integration by parts where i define F $= x^2$, G $= \frac{x}{2} - \frac{Sin(2kx)}{4k}$, dF $= 2xdx$, dG $= Sin^2(kx)dx$

$$< x^2 >= C^2 \Big[FG \Big]_0^a \int_0^a GdFdx = \int_0^a FdGdx$$

$$C^2(x^2(\frac{x}{2} - \frac{Sin(2kx}{4k})) \Big|_0^a - \int_0^a 2x(\frac{x}{2} - \frac{Sin(2kx)}{4k})dx$$

$$C^2(\frac{a^3}{2} - \int_0^a x^2 dx - \int_0^a \frac{xSin(2kx)}{2k}dx$$

Do another integration by parts where F = x, G = $\frac{-Cos(2kx)}{4k^2}$,
dF = $1dx$, dG = $\frac{Sin(2kx)}{2k}dx$

$$< x^2 >= C^2(\frac{a^3}{2} - \int_0^a x^2 dx - FG\Big|_0^a - \int_0^a GdFdx)$$

$$< x^2 >= C^2(\frac{a^3}{2} - \frac{1}{3}a^3 + \left[x(-\frac{-Cos(2kx)}{4k^2})\right]_0^a - \int_0^a -\frac{Cos(2kx)}{4k^2}dx)$$

We have that C^2 is $\frac{2}{a}$, so we have

$$< x^2 >= \frac{2}{a}(\frac{3a^3 - 2a^3}{6} - \frac{a^3}{4k^2\pi^2})$$

Finally we have

$$< x^2 >= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$$

$$\boxed{< p >= \int_{-\infty}^{\infty} \Psi^*(x,t)(-i\hbar\frac{\partial}{\partial x})\Psi(x,t)\mathrm{dx}} \quad (5)$$

Expectation value for momentum

$$< p >= C^2(\int_0^a Sin(\frac{n\pi x}{a})(-i\hbar\frac{\partial}{\partial x})Sin(\frac{n\pi x}{a})dx)$$

Again we use k as previously defined.

$$-iC^2\hbar k\int_0^a (Sin(kx)Cos(kx)dx)$$

We have that

$$(Sin(kx)Cos(kx) = \frac{1}{2}Sin(2kx)$$

$$-iC^2\hbar k\int_0^a (\frac{1}{2}Sin(2kx)dx)$$

And

$$\int Sin(2kx)dx = -\frac{Cos(2kx)}{2k}$$

Therefore

$$-iC^2\hbar k[-1-(-1)] = 0$$

So we have

$$< p >= 0$$

$$\boxed{< p^2 >= \int_{-\infty}^{\infty} \Psi^*(x,t)(-i\hbar)^2 \frac{\partial^2}{\partial x^2})\Psi(x,t)\mathrm{dx}} \tag{6}$$

Squared p of expectation value p, one dimension

$$< p^2 >= \hbar^2 C^2 \int_0^a (Sin(kx)\frac{\partial^2}{\partial x^2}Sin(kx))dx$$

We have

$$\frac{\partial^2}{\partial x^2}Sin(kx) = -Sin(kx)k^2$$

So

$$< p^2 >= \hbar^2 C^2 k^2 \int_0^a -Sin^2(kx))dx$$

$$< p^2 >= \hbar^2 C^2 k^2 \left[\frac{Sin(2kx) - 2kx}{4k}\right]_0^a$$

Sinus becomes zero at 0 and a , therefore we have

$$< p^2 >= \hbar^2 C^2 k^2 (\frac{a}{2})$$

And finally

$$< p^2 >= \frac{\hbar^2 n^2 \pi^2}{a^2}$$

Lets find out if the uncertainty principle is satisfied.

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}} \tag{7}$$

Heisenberg uncertainty principle

And we have uncertainty given in x

$$\boxed{\Delta x = \sqrt{< x^2 > - < x >^2}} \tag{8}$$

Uncertainty in x

And we have the uncertainty in momentum given by

$$\boxed{\Delta p = \sqrt{< p^2 > - < p >^2}} \tag{9}$$

Uncertainty in momentum p

So first we need to solve for the uncertainty in x

$$\Delta x = \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}}$$

$$\Delta x = a\sqrt{\frac{n^2\pi^2 - 6}{12n^2\pi^2}}$$

and then the uncertainty in momentum p

$$\Delta p = \sqrt{\frac{\hbar^2 n^2 \pi^2}{a^2} - 0}$$

$$\Delta p = \frac{\hbar n \pi}{a}$$

Putting this into Eq(7) yields:

$$a\sqrt{\frac{n^2\pi^2 - 6}{12n^2\pi^2}}\frac{\hbar n \pi}{a} \geq \frac{\hbar}{2}$$

Squaring and multiplying both sides by 12:

$$n^2\pi^2 - 6 \geq 3$$

Solving for n

$$n \geq \frac{3}{\pi}$$

This satisfies the uncertainty equation if $\forall$ n $\epsilon\{\mathbb{N}\}$
We have the lowest uncertainty when we are in ground state 1, n = 1

Task 2

2a)

We set L to be the width of the the box, so $L = 10^{-10}m$
As we found in previous task, we have that $k = \frac{n\pi}{L}$.
We use the solution

$$\psi(x) = Ae^{ikx}$$

By using Eq(1) we have

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

The derivative give us

$$\frac{d^2}{dx^2}\psi(x) = (i)^2k^2\psi(x)$$

therefore

$$\frac{\hbar^2}{2m}k^2\psi(x) + V(x)\psi(x) = E\psi(x)$$

Divide both sides by $\psi(x)$

$$\frac{\hbar^2}{2m}k^2 + V(x) = E$$

we have that $k = \frac{n\pi}{L}$ and the potential inside the box is zero. therefore we have the energy given:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

We then have the three first energy levels

$$E_1 = \frac{\hbar^2\pi^2}{2mL^2}$$

$$E_2 = \frac{2\hbar^2\pi^2}{mL^2}$$

$$E_3 = \frac{9\hbar^2\pi^2}{2mL^2}$$

2b)

The excitation energy needed to get from state 1 to level 3 is

$$\Delta E_{3,1} = \frac{9\hbar^2\pi^2}{2mL^2} - \frac{\hbar^2\pi^2}{2mL^2}$$

$$\Delta E_{3,1} = \frac{4\hbar^2\pi^2}{mL^2}$$

The relationship between energy and frequency is given by Using eq(10) we find the frequency

$$\boxed{E = hf} \tag{10}$$

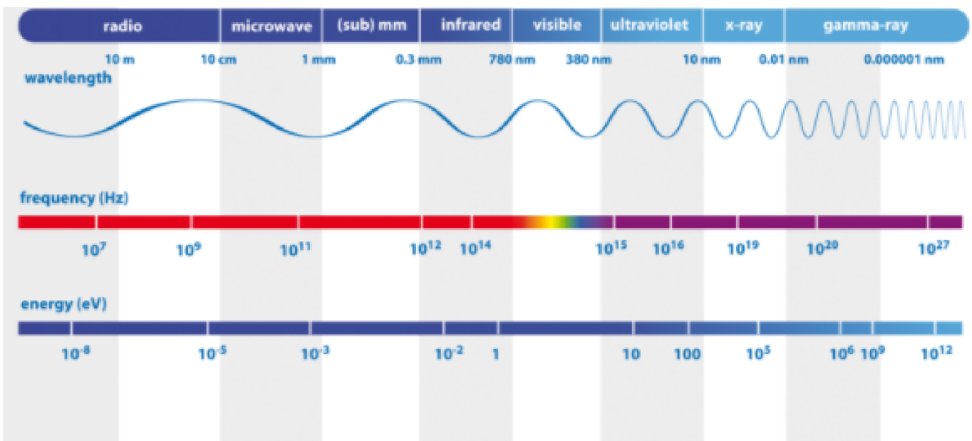
Energy given by frequency and plancks constant.

$$f = \Delta E_{3,1}/h$$

Using the m as the mass of electron we then have the following values $m = 9.109 \cdot 10^{-31} kg, h = 6.626 \cdot 10^{-34} Js, L = 10^{-}10$m and $\hbar = \frac{h}{2\pi}$
We get the frequency

$$f = 7.274 \cdot 10^{16} Hz$$

By look at the light spectrum in figure 1 we see that the light is in the ultraviolet frequency.



Figur 1: The light spectrum

Task 3

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\Psi(x,t)}{dx^2}+V(x)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)} \tag{11}$$

General Schrödinger equation for one dimension

Given the wave function for a state of definite energy we have the wave function in the form.

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}$$

Finding the derivative in terms of time yields:

$$\frac{\partial}{\partial t}\Psi(x,t)=-\frac{iE}{\hbar}\psi(x)e^{-iEt/\hbar}$$

Plugging this into eq(11)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)e^{-iEt/\hbar}+V(x)\psi(x)e^{-iEt/\hbar}=i\hbar(-\frac{iE}{\hbar})\psi(x)e^{-iEt/\hbar}$$

Here i can divide away $e^{-iEt/\hbar}$

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

This is the same as eq(1) which is the TISE

Task 4

Using eq(1) (TISE) and stationary-state wave functions given by $\psi(x)=Ae^{ikx}$

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

Dividing $\psi(x)$ and solving for the potential:

$$\frac{\hbar^2k^2}{2m}+V(x)=E$$

And since V(x) is real E is real.

Alternatively.
We have the Hamilton operator

$$\boxed{\hat{H}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]} \tag{12}$$

The Hamiltonian operator

This is shown in the TISE. The Hamiltonian operator is an hermitian operator which means that the operator is the same as its hermitian conjugate.

$$\boxed{\hat{H}=\hat{H}^\dagger} \tag{13}$$

Identity of hermitian operator

Now let me introduce bra-ket notation. We have

$$< \Psi|\hat{A}|\Psi >= \int_{-\infty}^{\infty} \Psi^* \hat{A}\Psi dx$$

where $< \Psi$ is the complex conjugate of the vector $\Psi >$ and $|$ means the dot product and we have that $H|\Psi >=< \Psi|H^\dagger$
and if we use the operator on a eigenfunction we get the eigenvalue $H|\psi >= \lambda|\psi >$
Lets use the operator on a eigenfunction

$$\hat{H}|\psi >= E\psi >$$

Since the operator is hermitian, we can switch its position if we alter it to its hermitian conjugate given by a dagger, and complex conjugate its eigenvalue, but since the operator is hermitian it will still be the same, therefore:

$$\hat{H}|\psi >= E|\psi >$$

is the same as

$$< \psi|\hat{H}^\dagger =< \psi|E^*$$

,now if we form the inner product with $< \psi$ in the first equation and second with $\psi >$, we have

$$< \psi|\hat{H}|\psi >= E < \psi|\psi >$$

$$< \psi|\hat{H}^\dagger|\psi >= E^* < \psi|\psi >$$

and since the operator is hermitian we have

$$< \psi|\hat{H}|\psi >= E < \psi|\psi >$$

$$< \psi|\hat{H}|\psi >= E^* < \psi|\psi >$$

now since the equations are equal the eigenvalue E^* must be real.

Task 5

We have from last task that

$$\hat{H}|\psi_n >= E_n|\psi_n > \tag{14}$$

and one for $|\psi_m >$

$$\hat{H}|\psi_m >= E_m|\psi_m >$$

this is the same as

$$< \psi_m|\hat{H}^\dagger =< \psi_m|E_m* \tag{15}$$

lets take equation 14 and form the inner product with $< \psi_m$ and take equation 15 and form the inner product with $\psi_n >$. We now have

$$< \psi_m|\hat{H}|\psi_n >= E_n < \psi_m|\psi_n >$$

and

$$< \psi_m|\hat{H}^\dagger|\psi_n >= E_m^* < \psi_m|\psi_n >$$

We know from last task that the eigenvalue is real and that the hermitian conjugate is the same so we can clean up to

$$< \psi_m|\hat{H}|\psi_n >= E_n < \psi_m|\psi_n > \tag{16}$$

and

$$< \psi_m|\hat{H}|\psi_n >= E_m < \psi_m|\psi_n > \tag{17}$$

Now lets subtract eq 17 from the eq 16

$$(E_n - E_m) < \psi_m|\psi_n >= 0$$

Now if $E_n \neq E_m$ we know that

$$< \psi_m|\psi_n >= 0$$

The inner product is equal to zero, so we have that the eigenfunctions are orthogonal.

Task 6

To make the calculations a bit friendlier i will use Dirac Bra-Ket notations as done in task 4 and 5. So we have that

$$< \Psi|\hat{A}|\Psi >= \int_{-\infty}^{\infty} \Psi^* \hat{A}\Psi dx$$

as the sandwich integral we know. Therefore by replacing $\hat{A}$ with the momentum operator we have

$$< \Psi|\hat{P}|\Psi >= \int_{-\infty}^{\infty} \Psi^* (-i\hbar\frac{\partial}{\partial x})\Psi dx$$

which is also known as

$$< p >= \int_{-\infty}^{\infty} \Psi^* (-i\hbar\frac{\partial}{\partial x})\Psi dx \tag{18}$$

We know from the time dependent Schrödinger equation(eq 11) that

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

dividing by i and $\hbar$ on both sides give us:

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

and for the complex conjugate we have

$$\frac{\partial}{\partial t}\Psi^* = \frac{i}{\hbar}\Psi^*\hat{H}^\dagger$$

Now lets take the equation we started with in this task and take the time derivative which will give us the following by the product rule

$$\frac{d}{dt} < \Psi|\hat{A}|\Psi >=< \frac{d}{dt}\Psi|\hat{A}|\Psi > + < \Psi|\hat{A}|\frac{d}{dt}\Psi > + < \Psi|\frac{d}{dt}\hat{A}|\Psi >$$

this will give us

$$\frac{d}{dt} < \Psi|\hat{A}|\Psi >= \frac{i}{\hbar} < \Psi|\hat{H}\hat{A}|\Psi > -\frac{i}{\hbar} < \Psi|\hat{A}\hat{H}|\Psi > + < \Psi|\frac{d}{dt}\hat{A}|\Psi >$$

Which is

$$\frac{i}{\hbar} < \Psi|[H,A]|\Psi > + < \Psi|\frac{dA}{dt}|\Psi >$$

The $[\hat{H},\hat{A}]$ means the commutative of H with A which is $[\hat{H},\hat{A}] = \hat{H}\hat{A} - \hat{A}\hat{H}$ of course this would ordinarily be zero, but since since these are operators this is not necessary true.
So if we know that the operator A itself doesn't depend on time (like the momentum operator) we can remove the last part

$$\frac{d}{dt} < \Psi|\hat{A}|\Psi >= \frac{i}{\hbar} < \Psi|[\hat{H},\hat{A}]|\Psi >$$

This is also known as

Now lets use the momentum operator, but first lets make some connections with the Hamiltonian.

$$\hat{H} = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi$$

$$\boxed{\frac{d}{dt} < \Psi|\hat{A}|\Psi >= \frac{i}{\hbar} < \Psi|[\hat{H}, \hat{A}]|\Psi >} \tag{19}$$

Ehrenfest's Theorem

Now if we look at the part with the double derivative we can see some similarity with the momentum operator

$$\hat{P} = -i\hbar\frac{\partial}{\partial x}$$

therefore

$$\hat{P}^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

So change that part in the Hamiltonian

$$\hat{H} = [\frac{\hbar^2}{2m}\hat{P}^2 + V(x)]\Psi$$

So if we use this in the commutative we get

$$\frac{d}{dt} < \Psi|\hat{P}|\Psi >= \frac{i}{\hbar 2m} < \Psi|[\hat{P^2}, \hat{P}]|\Psi >$$

Now we don't have the potential part in the equation so lets add that as a commutative with P

$$\frac{d}{dt} < \Psi|\hat{P}|\Psi >= \frac{i}{\hbar 2m} < \Psi|[\hat{P^2}, \hat{P}]|\Psi > + \frac{i}{\hbar} < \Psi|\hat{V}, \hat{P}]|\Psi >$$

The potential is added as a operator since it operates on the state of the system Ψ. Now since the operator commutes with itself the commutes becomes zero. (This also means that it can be observed at the same time, which must be true because they are both momentum.

$$\frac{d}{dt} < \Psi|\hat{P}|\Psi >= \frac{i}{\hbar} < \Psi|\hat{V}, \hat{P}]|\Psi >$$

Now lets use more friendly term, as we know $\frac{d}{dt} < \Psi|\hat{P}|\Psi >= \frac{d}{dt} < \hat{P} >$ therefore

$$\frac{d}{dt} < \hat{P} >= \frac{i}{\hbar} < [\hat{V}, \hat{P}] >$$

Lets solve the right hand side, since the operator operates on the state of the system we find

$$< [\hat{V}, \hat{P}] > \psi(x) = V(x)(-i\hbar\frac{d}{dx}\psi(x) - (-i\hbar\frac{d}{dx})V(x)\psi(x)$$

By using the product rule $v'u + u'v$ on the last term and divide by ψ we get

$$[\hat{V}, \hat{P}] = i\hbar\frac{d}{dx}V(x)$$

Plugging this into

$$\frac{d}{dt} < \hat{P} >=< \frac{i}{\hbar}[\hat{V}, \hat{P}] >$$

we get

$$\frac{d}{dt} < \hat{P} >=< -\frac{d}{dx}V(x) >$$

Which is the what we wanted to find.