Wave ftn

Note Title 9/7/2010

* Classical vs. Quantum Mechanics

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

[$ma = F$ Newton's 2nd law] [Schrödinger Eq.]

* In classical mechanics, we solve Newton's 2nd law to get "$x(t)$" out of $x(0)$ and $v(0)$
velocity

In quantum mechanics, we solve Schrödinger Eq. to get "$\Psi(x,t)$" out of $\Psi(x,0)$

Note: In QM, it is impossible to know both $x(0)$ and $v(0)$.

"$\Psi(x,t)$" is called the "wave function" of the particle.

* Meaning of $\Psi(x,t)$?

$$\int_a^b |\Psi(x,t)|^2 dx =$$ Probability of finding the particle between "a" and "b" at time "t"

; Born's Statistical Interpretation

* In general, $\Psi(x,t)$ is complex.

e.g. $\Psi(x,t) = \frac{1}{\sqrt{L}} e^{i(kx-\omega t)}$

$\Rightarrow |\Psi(x,t)|^2 = \frac{1}{L}$; real & non-negative

* Because $\Psi(x,t)$ is complex, it is generally not possible to plot it in a single graph; real and imaginary parts need to be plotted separately

e.g. $\Psi(x,t) = \frac{1}{\sqrt{L}} e^{i(kx-\omega t)}$

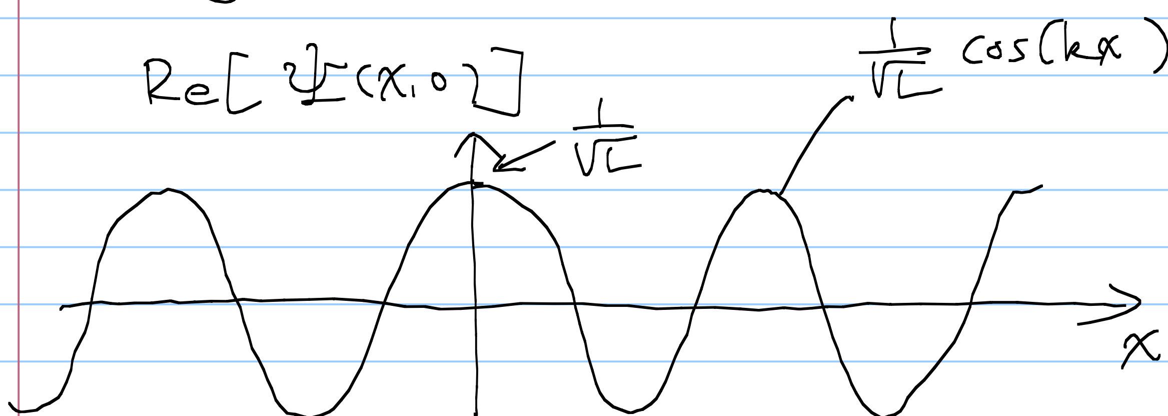
$$= \frac{1}{\sqrt{L}}\left(\cos(kx-\omega t) + i \sin(kx-\omega t) \right)$$

$$\Rightarrow \mathrm{Re}[\Psi(x,t)] = \frac{1}{\sqrt{L}} \cos(kx-\omega t)$$

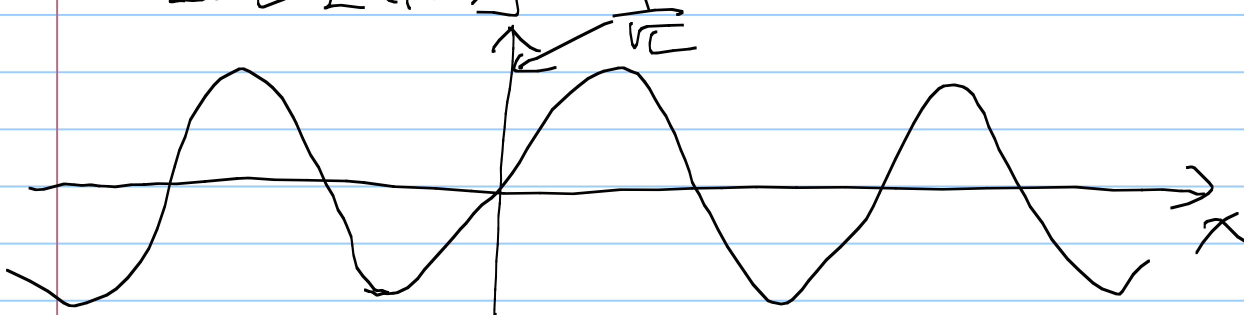
$$\mathrm{Im}[\Psi(x,t)] = \frac{1}{\sqrt{L}} \sin(kx-\omega t)$$

So, say, for $t=0$

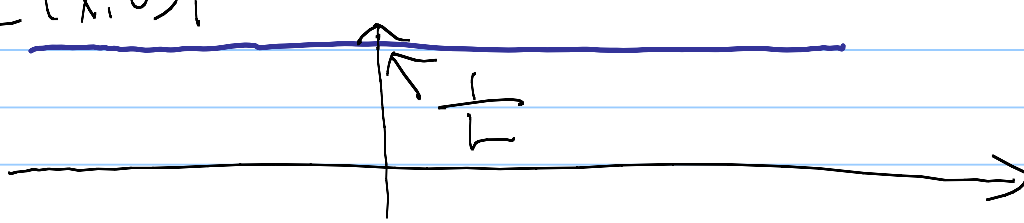
$\mathrm{Re}[\Psi(x,0)]$



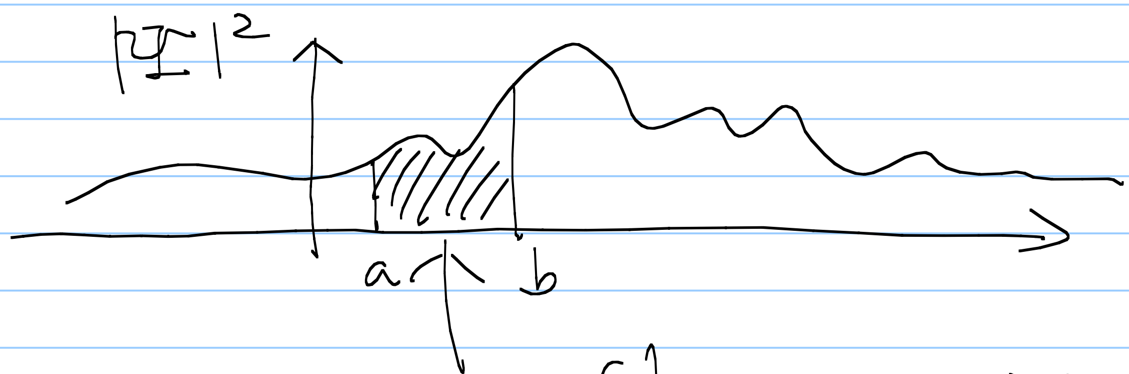
$\mathrm{Im}[\Psi(x,0)]$



$|\Psi(x,0)|^2$



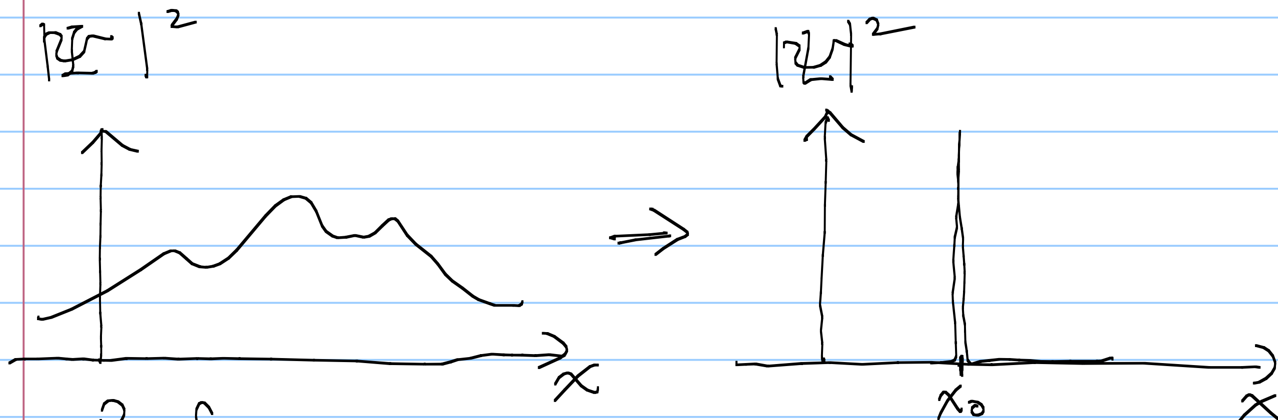
* Generally, what is physically measured is not $\Psi(x,t)$, but $|\Psi(x,t)|^2$



$$\text{area} = \int_a^b |\Psi(x,t)|^2 dx$$

$\Rightarrow$ Before any measurement, we know only the probability of what we will measure.

$\Rightarrow$ what happens after measurement?



Before position measurement

Immediately after position measured to be "x_0"

* **Measurement collapses the wavefctn to the measured state.**

Collapsed state remains the same as the state before measurement only if it is a stationary state

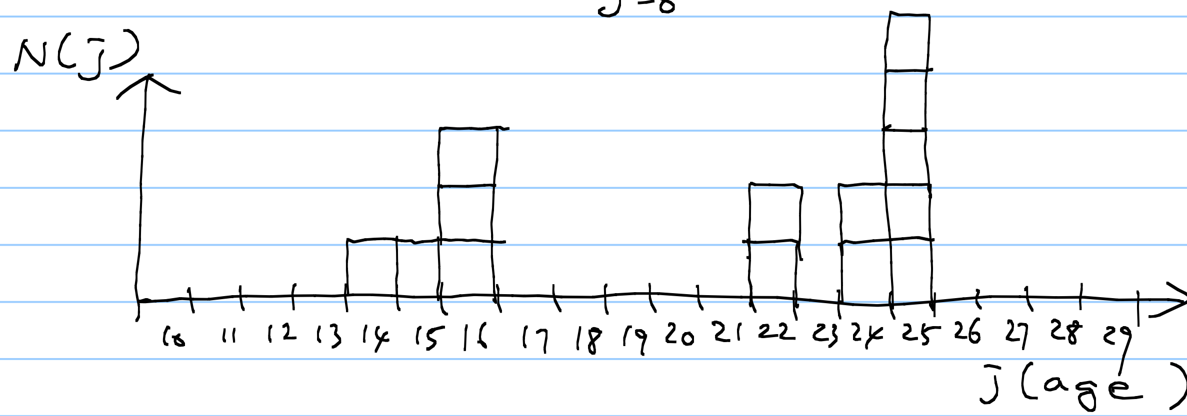
$\Rightarrow$ will be discussed in Chap. 2

Probability

* Discrete variables

probability $P(j) = \dfrac{N(j)}{N}$, $\quad 1 = \sum_{j=0}^{\infty} P(j)$

, where $N \equiv \sum_{j=0}^{\infty} N(j)$



Q1 : most probable age ? $j = 25$

Q2 : median age ? $\dfrac{22+24}{2} = 23$

Q3 : average age ? $\langle j \rangle = \dfrac{\sum j N(j)}{N}$

$$= \frac{14+15+3\times16+2\times22+2\times24+5\times25}{14}$$

$$= \frac{294}{14} = 21$$

Average of $f(j)$ is

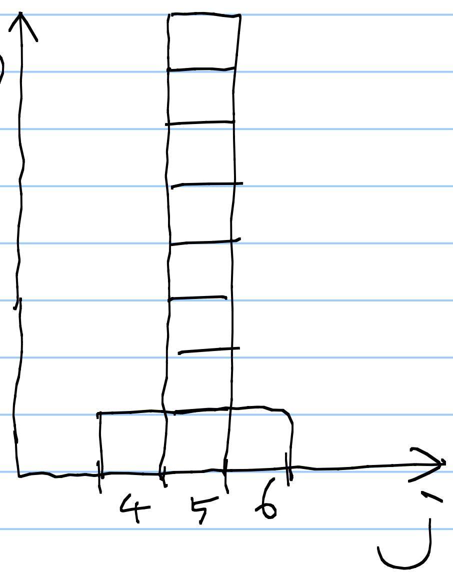
$$\langle f(j) \rangle \equiv \sum_{j=0}^{\infty} f(j) P(j)$$

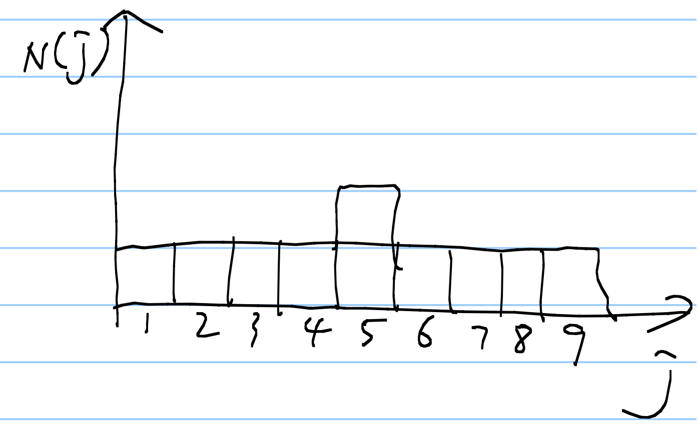
called "expectation value" of $f(j)$

Standard deviation

$$\sigma \equiv \sqrt{\langle (j - \langle j \rangle)^2 \rangle} = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

Ex.)





$$\langle j \rangle = 5$$

$$\langle j^2 \rangle = \frac{4^2 + 5^2 \times 8 + 6^2}{10} = \frac{252}{10} = 25.2$$

$\Downarrow$

$$\sigma = \sqrt{25.2 - 5^2} = 0.45$$

$\Downarrow$

$$\langle j \rangle = 5$$

$$\langle j^2 \rangle = \frac{1+4+9+16+25\times 2 + 36+49+64+91}{10} = \frac{310}{10} = 31.0$$

$$\sigma = \sqrt{31 - 5^2} = 2.5$$

* σ tells you how widely distributed the values are

Continuous Variable

probability density $\rho(x)$

$\rho(x)\,dx$ = probability that "x" lies between x and $x+dx$

$$1 = \int_{-\infty}^{\infty} \rho(x)\,dx,$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\,\rho(x)\,dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\,\rho(x)\,dx$$

$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$\boxed{\text{Ex}}$ $\rho(x) = A e^{-\lambda x^2}$

① A ? $\quad 1 = \int_{-\infty}^{\infty} A e^{-\lambda x^2}\,dx = A \cdot \sqrt{\pi} \cdot \frac{1}{\sqrt{\lambda}}$

$$\int_0^{\infty} e^{-x^2/a^2}\,dx = \sqrt{\pi} \cdot \frac{a}{2}$$

$$\Rightarrow A = \sqrt{\frac{\lambda}{\pi}}$$

② $\langle x \rangle$? $= A \int_{-\infty}^{\infty} x e^{-\lambda x^2}\,dx = 0$

③ $\langle x^2 \rangle$? $= A \int_{-\infty}^{\infty} x^2 e^{-\lambda x^2}\,dx$

$$= -A \frac{\partial}{\partial \lambda}\left[\int_{-\infty}^{\infty} e^{-\lambda x^2}\,dx\right]$$

$$= -A \cdot \frac{\partial}{\partial \lambda}\left[\sqrt{\frac{\pi}{\lambda}}\right]$$

$$= -\sqrt{\frac{\lambda}{\pi}} \cdot \sqrt{\pi} \cdot \left(-\frac{1}{2}\right) \lambda^{-\frac{3}{2}}$$

$$= \frac{1}{2}\frac{1}{\lambda}$$

$$\Rightarrow \sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{\sqrt{2\lambda}}$$

* Normalization of a wave ftn

$|\Psi(x,t)|^2$; probability density

$\Rightarrow \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$ for any "t".

If $\Psi(x,t)$ is a solution of the Schrödinger Eq., then $A \cdot \Psi(x,t)$ is also a solution with any arbitrary complex constant "A".

$\Rightarrow$ Pick "A" to satisfy $\int_{-\infty}^{\infty} |A\Psi|^2 dx = 1$

; called "normalizing".

Normalizable $\Psi(x,t)$ is called "square-integrable"; All physically realizable states are square-integrable

$\boxed{\text{Ex.}}$ $\Psi(x, t=0) = Ax,\ A,\ \frac{A}{x},\ Ae^{-|x|}$

which of these are square-integrable?

$$\int_{-\infty}^{\infty} |Ax|^2 dx = 2|A|^2 \cdot \frac{x^3}{3}\Big|_0^{\infty} = \infty \quad \times$$

$$\int_{-\infty}^{\infty} |A|^2 dx = 2|A|^2\, x\Big|_0^{\infty} = \infty \quad \times$$

$$\int_{-\infty}^{\infty} \frac{|A|^2}{x^2} dx = 2|A|^2 \left[-x^{-1}\right]\Big|_0^{\infty} = \infty \quad \times$$

$$\int_{-\infty}^{\infty} |A|^2 e^{-2|x|} dx = 2|A|^2 \int_0^{\infty} e^{-2x} dx$$

$$= 2|A|^2 \frac{e^{-2x}}{-2}\Big|_0^{\infty}$$

$$= |A|^2 = 1 \quad \text{if } A = 1$$

$\Rightarrow Ae^{-|x|}$ is square-integrable

* If $\int_{-\infty}^{\infty} |\Psi(x, t=0)|^2 dx = 1$ at $t=0$,

Schrödinger Eq. guarantees that $\Psi(x,t)$ remains normalized at any other time. See Griffiths page 13-14 for the proof.

$\boxed{\text{Momentum}}$; $p \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}$

* $\langle x \rangle = \int_{-\infty}^{\infty} x \, |\Psi(x,t)|^2 dx$
; expectation value of x
; implies the average of repeated measurement of "x" on an ensemble of identically prepared systems.

* We will introduce the momentum operator "p" through $\langle p \rangle = m\langle v \rangle = m\frac{d\langle x \rangle}{dt}$.

Let's first check how to get $\frac{d\langle x\rangle}{dt}$.

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\left[\int x |\Psi|^2 dx\right]$$

$$= \int x \frac{\partial}{\partial t}|\Psi|^2 dx = \int x \frac{\partial}{\partial t}[\Psi\Psi^*]dx$$

$$= \int x\left[\left(\frac{\partial}{\partial t}\Psi\right)\Psi^* + \Psi\frac{\partial}{\partial t}\Psi^*\right]dx \; ; \; **$$

Schröd. Eq. gives $\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi\right)$

$$\frac{\partial \Psi^*}{\partial t} = \frac{-1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + V\Psi^*\right)$$

assume V is real

So $\left(\frac{\partial}{\partial t}\Psi\right)\Psi^* + \Psi\frac{\partial}{\partial t}\Psi^*$

$$= \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}\Psi^* + \frac{\hbar^2}{2m}\frac{\partial^2 \Psi^*}{\partial x^2}\Psi + \cancel{V\Psi\Psi^*} - \cancel{V\Psi^*\Psi}\right)$$

$$= \frac{i\hbar}{2m}\left(\frac{\partial^2 \Psi}{\partial x^2}\Psi^* - \frac{\partial^2 \Psi^*}{\partial x^2}\Psi\right)$$

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

Now

$$** = \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left(\frac{\partial \Psi}{\partial x}\Psi^* - \frac{\partial \Psi^*}{\partial x}\Psi\right)dx$$

$$= \frac{i\hbar}{2m}\left\{\cancel{\left[x\left(\frac{\partial \Psi}{\partial x}\Psi^* - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right]_{-\infty}^{\infty}} \to 0 - \int\left(\frac{\partial \Psi}{\partial x}\Psi^* - \frac{\partial \Psi^*}{\partial x}\Psi\right)dx\right.$$

Assume

$$\left[\int_{-\infty}^{\infty} u\,v'\,dx = uv\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} u'v\,dx\right]$$

$$= -\frac{i\hbar}{2m}\left[\int \Psi^*\frac{\partial}{\partial x}\Psi\,dx - \left[\cancel{\Psi^*\Psi\Big|_{-\infty}^{\infty}} \to 0 - \int \Psi^*\frac{\partial}{\partial x}\Psi\,dx\right]\right]$$

$$= -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial}{\partial x}\Psi\,dx$$

So

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int \Psi^*\frac{\partial}{\partial x}\Psi\,dx$$

Now considering

$$\langle x \rangle = \int x \Psi^* \Psi \, dx = \int \Psi^*(x) \Psi \, dx$$

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi \, dx ,$$

We define the momentum operator in position space, $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$.

Trivially $\hat{x} = x$ in position space.

These are called "operators".

For any arbitrary operator that can be expressed by x and p, $Q(x, p)$

$$\langle Q(x,p) \rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) \Psi \, dx$$

Ex. $T = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$

$$\Rightarrow \langle T \rangle = -\frac{\hbar^2}{2m} \int \Psi^* \frac{\partial^2}{\partial x^2} \Psi \, dx$$

Ex. $\Psi(x,0) = A e^{-\frac{x^2}{2a^2}}$

What is $\langle x \rangle$? $\langle p \rangle$? $\langle T \rangle$?

[Use $\int_0^\infty e^{-\frac{x^2}{a^2}} dx = \frac{a}{2}\sqrt{\pi}$

$\int_0^\infty x^2 e^{-\frac{x^2}{a^2}} dx = \frac{a^3}{4}\sqrt{\pi}$]

First, normalize

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

$$= |A|^2 a\sqrt{\pi} \Rightarrow A = \sqrt{\frac{1}{a\sqrt{\pi}}}$$

$$\langle x \rangle = |A|^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}} x \, e^{-\frac{x^2}{2a^2}} dx$$

$$= 0 \quad (\because \text{ odd integrand })$$

$$\langle p \rangle = |A|^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}} \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) e^{-\frac{x^2}{2a^2}} dx$$

$$= |A|^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}} \left(\frac{\hbar}{i}\left(-\frac{x}{a^2}\right)\right) e^{-\frac{x^2}{2a^2}} dx$$

$$= 0 \quad (\because \text{ odd integrand })$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}|A|^2 \int e^{-\frac{x^2}{2a^2}} \frac{\partial^2}{\partial x^2} e^{-\frac{x^2}{2a^2}} dx$$

$$\left[\frac{\partial}{\partial x} e^{-\frac{x^2}{2a^2}} = -\frac{x}{a^2} e^{-\frac{x^2}{2a^2}} \right.$$

$$\left. \frac{\partial^2}{\partial x^2} e^{-\frac{x^2}{2a^2}} = -\frac{1}{a^2} e^{-\frac{x^2}{2a^2}} + \left(-\frac{x}{a^2}\right)^2 e^{-\frac{x^2}{2a^2}} \right]$$

$$= -\frac{\hbar^2}{2m}|A|^2 \left[-\frac{1}{a^2}\int e^{-\frac{x^2}{a^2}} dx + \frac{1}{a^4}\int x^2 e^{-\frac{x^2}{a^2}} dx \right]$$

$$= \frac{\hbar^2}{2m} \frac{1}{a\sqrt{\pi}} \left[\frac{1}{a^2} a\sqrt{\pi} - \frac{1}{a^4} \frac{a^3}{2}\sqrt{\pi} \right]$$

$$= \frac{\hbar^2}{2m} \cdot \frac{1}{2a^2} = \underline{\frac{\hbar^2}{4ma^2}}$$