CLASSICAL MECHANICS VS. QUANTUM MECHANICS
Q.M. IS THE BRANCH OF PHYSICS NEEDED TO UNDERSTAND
THE PERIODIC TABLE
CHEMICAL BONDS
MOLECULAR MOTIONS
INTERACTION OF LIGHT W/MATTER (SPECTROSCOPY)
* LIGHT IS OUR BEST PROBE OF THE NANO-WORLD WHERE
Q.M. APPLIES

BUT WHERE DOES CLASSICAL PHYSICS FAIL?
WHY DOESN'T CLASSICAL PHYSICS APPLY TO ALL PHENOMENA?
SHORT ANSWER:
* SYSTEMS WITH SHORT LENGTH SCALES (Å - mm)
* LOW TEMPERATURES / SMALL ENERGIES (FEW K
  \(10^{-18}\) J)
* SMALL MASSES (PROTONS/E- \(10^{-27}\) kg / \(10^{-31}\) e)

WE DON'T ALWAYS NEED SOPHISTICATED INSTRUMENTS
TO OBSERVE Q.M. EFFECTS.
IN LATE 1800'S PHYSICISTS THOUGHT EVERYTHING WAS
UNDER CONTROL - MATTER WAS DESCRIBED BY
NEWTONIAN MECHANICS (OR MATHEMATICAL EQUIVALENTS)
LIGHT WAS DESCRIBED BY MAXWELL'S EQUATIONS
MATTER \(\rightarrow\) PARTICLES \(\rightarrow\) LIGHT \(\rightarrow\) WAVE
(TRAJECTORIES) \(\rightarrow\) \(\rightarrow\) \(\rightarrow\) \(\rightarrow\) \(\rightarrow\)
(REFRACTION, DIFFRACTION, INTERFERENCE).

WHERE DID CLASSICAL PHYSICS BEGIN TO UNRAVEL?
1. BLACKBODY RADIATION (PLANCK 1900)
2. STRUCTURE OF ATOMS & ATOMIC SPECTROSCOPY
3. PHOTOELECTRIC EFFECT (EINSTEIN 1905)

MAX PLANCK WAS TRYING TO CALCULATE COLOR OF LIGHT
EMITTED BY HOT METALS, TO IMPROVE
DIRECTIONALITY OF GERMAN STEEL MANUFACTURING
As explained in textbooks, it was impossible to explain the spectrum of light emitted by a blackbody unless one assumed that light was quantized, packed into "energy quanta." In 1873, James Clerk Maxwell proposed that light was an electromagnetic wave. He showed that the electric and magnetic fields of the wave propagated perpendicular to each other and to the direction of propagation.

\[ E = \frac{1}{\lambda} \text{V/m} \]

\[ c = 2.998 \times 10^8 \text{ m/s} \]

\[ \lambda = \frac{c}{f} \]

\[ E = 1.25 \text{ V/m} \]

\[ f = 10 \text{ Hz} \]

\[ c = 3.40 \times 10^8 \text{ m/s in vacuum} \]

\[ N = \frac{E}{h} \]

\[ N = \frac{1.25}{6.62 \times 10^{-34}} \]

\[ N = 1.88 \times 10^{34} \]

The energy \( E \) is the energy of each quantum, and the frequency \( f \) is the frequency at which the light is emitted. The energy \( E \) is given by Planck's constant \( h \) times the frequency \( f \). The number of quanta \( N \) is the total energy \( E \) divided by the energy of each quantum.
THE PHOTOELECTRIC EFFECT (HERTZ 1887)

BASIS FOR NIGHT-VISION GOGGLES & PMTs

INTERACTION OF LIGHT WITH METAL SURFACE CAN CAUSE E\textsuperscript{-} TO BE Emitted - USuALy UV LIGHT

Let's say we have a vacuum system set up with a clean Cu surface.

\[ \text{CONTROL INTENSITY + WAVELENGTH} \rightarrow \text{MEASURE \# AND KINETIC ENERGY OF E}^{-} \]

\[ / / \text{Cu} / / / \]

PREDICTION OF CLASSICAL PHYSICS - INCREASED LIGHT INTENSITY CAUSES E\textsuperscript{-} IN METAL TO "VIBRATE" WITH LARGER AMPLITUDE, AND THEREFORE ESCAPE METAL

- QUANTITATIVE MODEL: COLLECTION OF DAMEN OSCILLATORS

PREDICTIONS:

\( \text{LIKE DOING WORK ON E}^{-} \)

- KINETIC ENERGY OF PHOTOELECTRONS INCREASES WITH LIGHT INTENSITY
- PHOTODESIS SHOULD BE OBSERVED FOR ANY FREQUENCY OF LIGHT, IF INTENSITY IS HIGH ENOUGH

CLEAN METAL

\[ \text{DETECTOR} \]

SIMPLE 1-D MODEL:

\* E\textsuperscript{-} EMMITED WITH KINETIC ENERGY E\textsubscript{kin}

\* APPLY VOLTAGE \( U > 0 \) TO METAL / DETECTOR AT GROUND

\* MEASURE \( E\text{kin} \) BY TUNING U.

\( \text{1} \) \( U=0 \rightarrow \text{CURRENT} \)

\( \text{2} \) IF \( E\text{kin} < e \cdot U \) (ELECTROSTATIC POTENTIAL ENERGY)

E\textsuperscript{-} PULLED BACK TO SURFACE \( \rightarrow \) NO CURRENT

\* MEASURE DEPENDING POTENTIAL DIFFERENCE AT WHICH CURRENT \( \rightarrow 0 \), AS A FUNCTION OF FREQUENCY \( U \).
PHOTOELECTRIC EFFECT

**Observations**

* $U_0$ increases with $U$ of light
* For a particular $U$, $U_0$ does not depend on intensity, i.e., $E_{kin}$ not dependent on intensity
* Photoelectrons only observed for $U > U_0$
  
  Where $U_0$ is threshold dependent on metal
* Photocurrent ($e^-$/sec) is proportional to light intensity

**Einstein's Explanation (1905) Based on Planck's Hypothesis**

* Photon energy $E = hU$
* $E_{kin}$ determined by energy conservation
  \[ E_{kin} = \frac{1}{2}mv^2 = hU - \Phi \quad (\text{photon energy} - \text{work function}) \]

- $\Phi$ is a property of the material.
* Increasing photon energy $\rightarrow$ increases $E_{kin}$
* One photon $\rightarrow$ one photoelectron

---

**Diagram**

- Photon energy must exceed a threshold to result in photoemission
  
  * What happens to less energetic photons? (Reflected)
  
  
  Metal are shifted

**Show slide of night vision**

- Goggles - device with low work-function material (alkalis - e.g., C5 oxides) where $e^-$ are imaged onto a phosphor screen
In photoemission and related spectroscopies, a convenient unit of energy is \( eV \) "electron-volts" which is kinetic energy of an \( e^- \) accelerated from rest through a potential difference of 1 volt.

\[
\frac{1}{eV} = 1.602 \times 10^{-19} \text{ J}
\]

Values of \( eV \approx 0.1 - 10 \text{ eV} \)

Example problem with atomic ionization potential. 
At has \( I = 15.76 \text{ eV} \)
Let's say \( \lambda = 58.43 \text{ nm} \) photons from He discharge are used to ionize At - what is the speed of emitted \( e^- \)?

\[
58.43 \text{ nm} = 0.05843 \text{ cm} \]

\[
10^7/\lambda(\text{cm}) = \text{cm}^{-1} ; \quad 1/eV = 8065.5 \text{ cm}^{-1}
\]


\[
(10^7/58.43 \text{ cm})/8065.5 = 2.12 \text{ eV}
\]

\[
E_{kin} = 2.12 \text{ eV} - 15.76 \text{ eV} = 5.46 \text{ eV} = \frac{1}{2} m_e v^2
\]

\[
5.46 \text{ eV} \times \frac{1.602 \times 10^{-19} \text{ J}}{\text{eV}} = 8.75 \times 10^{-19} \text{ J}
\]

\[
v = \left( \frac{2 \times 8.75 \times 10^{-19} \text{ J}}{9.11 \times 10^{-31} \text{ kg}} \right)^{1/2} = 1.39 \times 10^6 \text{ m/s}
\]

So now we know that light must be described as both particle (photon) and as a wave to understand spectroscopy and optics.

This wave/particle duality is universal - not just for light, but for matter...
IN 1924, LOUIS DE BROGLIE POSTULATED THAT SINCE LIGHT IS A WAVE THAT BEHAVES LIKE A PARTICLE, WHICH HAS MOMENTUM, THEN MATTER SHOULD ALSO HAVE A WAVELENGTH ASSOCIATED WITH ITS MOMENTUM.

THE CONNECTION ARISES FROM EINSTEIN’S EQUATION FOR REST MASS AND ENERGY: 
\[ E = mc^2 \]

So photon "mass" = \( E/c^2 \)
\[ p = mv = (E/c^2) \frac{c}{E} = \frac{E}{c} = \frac{hc}{\lambda} \]

So \( p = \frac{h}{\lambda} \) for photons, and de Broglie suggested it also holds for matter!

WAVELENGTH OR (MOMENTUM)^{-1}

THIS IDEA IS COUNTERINTUITIVE BECAUSE WE USUALLY DON'T PERCEIVE MATTER TO HAVE WAVE PROPERTIES.

WHY? BECAUSE \( h \) IS SO SMALL! \( 6.626 \times 10^{-34} \text{ J} \cdot \text{s} \)

FOR EXAMPLE, A 1 kg IPAD TABLET THROWN 1 M/SEC
\[ \lambda = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{(1 \text{ kg})(1 \text{ m/s})} = 6.6 \times 10^{-34} \text{ m} \text{ WAVELENGTH} \]

FOR OBJECTS OF SUB-ATOMIC MASS, e.g., \( e^- \) \( W/KINETIC = 1 \text{ eV} \)
\[ v = \sqrt{\frac{2E}{m}} = \left( \frac{2 \times 1.602 \times 10^{-19} \text{ J}}{9.11 \times 10^{-31} \text{ kg}} \right)^{1/2} = 0.593 \times 10^6 \text{ m/s} \]
\[ \lambda = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{(3.11 \times 10^{-31} \text{ kg})(0.593 \times 10^6 \text{ m/s})} = 1.23 \times 10^{-9} \text{ m} \quad 1.23 \text{ nm} \]

THIS WAVELENGTH IS LARGE COMPARED TO THE SIZE OF AN \( e^- \) — VERY SIGNIFICANT!

\( e^- \) EXHIBIT DIFFRACTION FROM MOLECULES AND NANOSTRUCTURES.
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WAVES & INTERFERENCE

THE MATHEMATICAL FORMULATION OF Q.M. PREDICTS
WAVE-LIKE PHENOMENA FOR MATTER, e.g. INTERFERING

DOUBLE-Slit EXPT W/LIGHT WAS FIRST DONE BY
THOMAS YOUNG (1803)

HTTP://PHET.COLOrado.EDU/EN/SIMULATION/QUANTUM-WAVE-INTERFERENCE

PHET APP:

1. SET TO PHOTONS, DOUBLE SUTS ON, GREEN LIGHT, ADJUST SUTS
   → SHOW INTERFERENCE PATTERN
   HOW WOULD IT APPEAR IF LIGHT WERE CHANGED TO PARTICLES?

2. SET TO E−, ADJUST SUTS TO SHOW INTERFERENCE (SHALLER)
   HOW MANY E− ARE NECESSARY TO INTERFERE? MORE THAN 2?
   WHAT IF WE ENSURE ONLY ONE E− PASSES AT A TIME?

CAN WE TELL THROUGH WHICH SUT EACH E− PASSES?

3. PLACE DETECTOR ON ONE SUT → LOSS OF INTERFERENCE!
   ACT OF MEASURING PARTICLE PROPERTY CAUSES LOSS OF WAVE-
   LIKE EFFECTS... QUANTUM MEASUREMENTS AFFECT SYSTEM

TO DISCUSS THIS EXPT IN Q.M. TERMS, WE NEED TO
THINK IN TERMS OF A WAVEFUNCTION — THIS IDEA
HAS CLASSICAL ROOTS...

— BASIC WAVE PHYSICS (1-DIMENSIONAL)

CONSIDER AMPLITUDE OF DISTURBANCE AS FUNCTION OF TIME & SPACE
→ U(X, T) THIS U IS A "WAVE-FUNCTION"

OBTAINED BY SOLVING THE CLASSICAL WAVE EQUATION
\[
\frac{\partial^2}{\partial x^2} U(x, t) = \frac{1}{\nu^2} \frac{\partial^2}{\partial t^2} U(x, t)
\]
WHERE \( \nu \) IS THE
WAVE FREQUENCY

— SOLVE WITH INITIAL CONDITIONS
   e.g. FIXED ENDPNTS, ETC.
AN INTERESTING PROPERTY OF THE WAVE EQUATION IS THAT THE SUM OF ANY TWO SOLUTIONS IS ALSO A SOLUTION — SUPERPOSITION PRINCIPLE — WAVES CAN PASS THROUGH EACH OTHER, CONSTRUCTIVELY/DESTRUCTIVELY INTERFERE

PARTICULAR SOLUTION TO WAVE EQUATION:

\[ u(x,t) = e^{i(kx - \omega t)} \]

\( \omega = 2\pi f \) CIRCULAR FREQ,

\( \omega / k \) IS PHASE VELOCITY OF WAVE

\( k = 2\pi / \lambda \) IS THE WAVE-VECTOR MAGNITUDE

RECALL \( \lambda = h / p \) SO \( k \) IS LIKE MOMENTUM

\( u(x,t) \) PROPAGATES FROM \(-\infty \rightarrow +\infty \) LEFT \( \rightarrow \) RIGHT

\( u^\prime(x,t) = e^{-i(kx - \omega t)} \) PROPAGATES FROM \(+\infty \rightarrow -\infty \)

FOR AN ELECTROMAGNETIC WAVE, WE WRITE THESE SOLUTIONS

\[ E(x,t) = E_0 e^{i(kx - \omega t)} \]

\( E_0 \) IS FIELD AMPLITUDE

\[ I = \left| E \right|^2 = E^* E(x,t)E(x,t) \] INTENSITY —

FOR MATTER WAVES, \( \lambda = h / p \)

\[ k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{h} \]

SO WAVEFUNCTION FOR A MATTER WAVE

\[ \psi(x,t) = A e^{i \left( \frac{p}{\hbar} \cdot x - \omega t \right)} \]

WHAT DOES IT MEAN?

1. AMPLITUDE (\( \psi \)) HAS NO DIRECT PHYSICAL INTERPRETATION
IT IS A COMPLEX QUANTITY, SO IT IS NOT DIRECTLY MEASURABLE
BUT THE COMPLEX NATURE ALLOWS FOR ADDITION OF \( \psi \)'S → INTERFERENCE PHENOMENA

2. \( |\psi(x,t)|^2 dx dt = \psi^* \psi dx dt \) IS "PROBABILITY DENSITY"
OF FINDING PARTICLE IN \([x,x+dx]\) AT \([t,t+dt]\)
IT'S ANALOGOUS TO INTENSITY IN E-M
3. Since $|\psi(x,t)|^2$ is a probability, physically meaningful wavefunctions must satisfy normalization condition:

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 \, dx = 1 \quad \text{in 1-dimension, analogous expressions in 3d, polar coords, etc.}$$

Why? Because particle must be 100% within all space.

4. $\psi$ must be "well-behaved" - defined over all space + time, continuous & infinitely differentiable, single-valued.

Back to the double-slit opt - Quantum particles interfere to form pattern beyond slit, but interference is destroyed if detector is placed in one or more slits.

For transmitted e$^{-}$: $\psi = \psi_{\text{left}} + \psi_{\text{right}}$ $\quad \ell/r\text{ slits}$

We observe interference by measuring probability density at the screen, so

$$|\psi|^2 = (\psi_{\text{left}} + \psi_{\text{right}})^* (\psi_{\text{left}} + \psi_{\text{right}})$$

$$|\psi|^2 = \psi_{\text{left}}^* \psi_{\text{left}} + \psi_{\text{right}}^* \psi_{\text{right}} + \psi_{\text{left}}^* \psi_{\text{right}} + \psi_{\text{right}}^* \psi_{\text{left}}$$

Interference terms.

If a detector is placed at one slit, e.g., left $\psi_{\text{right}} = 0$ if particle detected in left slit $\psi_{\text{left}} = 0$ if particle detected in right slit.

So for a single particle, $\psi = \psi_{\text{left}}$ or $\psi = \psi_{\text{right}}$ $\quad \rightarrow |\psi|^2 = |\psi_{\text{left}}|^2 \quad \text{or} \quad |\psi_{\text{right}}|^2$.

No interference terms.

Measurement is incompatible with interference. This phenomenon has no classical analog.

Action-at-a-distance "entanglement" allows slits to communicate with each other.
IMPORTANT APPLICATIONS OF MATTER WAVES - OPTICAL MICROSCOPY CAN ONLY RESOLVE FEATURES ON THE ORDER OF $\lambda/2$ DIMENSIONS $\lambda = 400-750$ nm OK FOR CELLS

BUT WITH SHORTER WAVELENGTH MATTER WAVES USING E- / NEUTRONS / HE-IONS, MUCH HIGHER RESOLUTION IS FEASIBLE - e.g., 10 keV ELECTRONS

$$v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2 \times 10^4 \text{eV} \times 1.602 \times 10^{-19} \text{J/eV}}{9.11 \times 10^{-31} \text{kg}}} = 5.93 \times 10^7 \text{ m/s}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{(9.11 \times 10^{-31} \text{kg}) (5.93 \times 10^7 \text{ m/s})} = 1.23 \times 10^{-12} \text{ m}$$

$\Rightarrow$ E- MICROSCOPES RESOLVES MUCH SMALLER STRUCTURES * SLIDE? NANOSTRUCTURES, VIRUSES, ORGANELLES, ETC.

NOTE THE ENORMOUS DIFFERENCE BETWEEN Q.M. + CLASSICAL MECH.
* IN CLASSICAL MECHANICS, WE CAN SPECIFY A TRAJECTORY WHICH DEFINES LOCATION + MOMENTUM OF A PARTICLE EXACTLY IN TIME/SPACE
* IN Q.M., WE CAN ONLY SPECIFY THE PROBABILITY THAT IT MAY BE FOUND AT $[x, x+dx]$ AT $[t, t+dt]$ $\Rightarrow \psi(x, t)$, $1/\psi(x, t)^2 dx dt$

CLASSICAL OBJECT:

\begin{align*}
\text{P}(x) & \\
\text{P}(x_0) & = 1 \\
\text{P}(x_0+dx_0) & = 0
\end{align*}

Q.M. OBJECT

\begin{align*}
\text{P}(x) & \\
\text{P}(x_0) & = \text{MAX}
\end{align*}

THERE IS ALWAYS INHERENT UNCERTAINTY IN POSITION OF A QUANTUM PARTICLE NOT A TECHNOLOGICAL ISSUE
HEISENBERG'S UNCERTAINTY PRINCIPLE

For Q.M. particles, there is inherent tradeoff between ability to specify position & momentum.

Heisenberg's Uncertainty Principle (1926) states that position & momentum of a particle cannot be simultaneously determined with infinite precision. The uncertainties are related by

\[ \Delta x \cdot \Delta p_x \geq \frac{\hbar}{2} \]

\( \Delta x, \Delta p_x \) position & momentum uncertainties

* There is no single, well-defined quantum trajectory along which a particle travels from point A to point B.

* There are other pairs of observables connected by uncertainty relations, e.g.

\[ \Delta L \geq \hbar, \quad \Delta t \cdot \Delta E > \frac{\hbar}{2} \]

* Position uncertainty \( \Delta x \) is typically on the order of the de Broglie wavelength for the particle, and is a natural consequence of the wave-nature of Q.M. particles. E.g., for a plane wave

\[ \psi = A_0 \exp \left[ i (p/x - wt) \right] \quad \lambda = \frac{\hbar}{p} \]

This particle exists in a well-defined momentum state (\( \hbar \)), but the position of the particle extends over all \( x \).

\[ \Psi \Psi^* = \cos^2 [p/x - wt] + \sin^2 [p/x - wt] = 1 \]

So a perfectly well-defined momentum \( \rightarrow \) complete uncertainty in position!
UNCERTAINTY PRINCIPLE

CONSIDER INTERMEDIATE CASES IN WHICH A PARTICLE IS SOMEWHAT LOCALIZED — "WAVE PACKETS"

FOURIER'S THEOREM STATES THAT ANY QUASI-PERIODIC FUNCTION CAN BE WRITTEN AS A SUM OF SIN/COS

APPLET

http://phet.colorado.edu/en/simulation/fourier

A SPATIALLY-LOCALIZED FUNCTION CAN ONLY BE FORMED AS A SUM OF COS/SIN FUNCTIONS WITH A DISTRIBUTION OF WAVELENGTHS (i.e. DISTRIBUTION OF MOMENTA)

— THE SCHRÖDINGER EQUATION — (TIME-INDEPENDENT)

ALL THE INFORMATION ABOUT DYNAMICS OF A Q.M. PARTICLE IS IN ITS WAVEFUNCTION, SO WE NEED THE Q.M. ANALOG OF THE CLASSICAL WAVE EQUATION \[ \frac{\partial^2 \psi}{\partial x^2} = \frac{1}{4\nu} \frac{\partial^2 \psi}{\partial t^2} \] TO OBTAIN THE Q.M.

THE TIME-INDEPENDENT SCHRÖDINGER EQ. WAS POSTULATED IN 1926 NOT DERIVED FROM CLASSICAL WAVE EQUATION. HE DIDN'T QUITE "DERIVE" IT — JUST TO SEE HOW HE CAME UP WITH IT, WE CAN CONSIDER THE FOLLOWING ARGUMENT:

ASSUME THAT CONSERVATION OF ENERGY APPLIES TO A PARTICLE

\[ E = E_{\text{kinetic}} + E_{\text{potential}} = \frac{p^2}{2m} + V(x) \] "HAMILTONIAN"

NOW, WE NEED AN EXPRESSION FOR \( p^2 \) TO GET \( E_{\text{kinetic}} \\)

CONSIDER A PLANE-WAVE: \[ \psi = e^{i\left( \frac{p}{h} \cdot x - \omega t \right)} \]

HIGHER MOMENTUM \( \rightarrow \) SHORT \( \lambda) \rightarrow \) HIGH CURVATURE
Which mathematical operation describes curvature?

\[ \frac{d^2 \psi}{dx^2} \rightarrow \text{slope} ; \quad \frac{d^4 \psi}{dx^4} \rightarrow \text{curvature} \]

So momentum \( p \) \( \propto \frac{d^2 \psi}{dx^2} \).

If we apply this operation to a plane wave function

\[ \frac{d^2 \psi}{dx^2} = \frac{\partial}{\partial x} \left( \frac{i}{\hbar} \psi e^{i(\frac{\hbar}{\hbar} x - \omega t)} \right) = -\frac{\hbar^2}{\hbar^2} e^{i(\frac{\hbar}{\hbar} x - \omega t)} = -\frac{\hbar^2}{\hbar^2} \psi \]

So \( p = -\frac{\hbar^2}{\hbar^2} \frac{d^2 \psi}{dx^2} \).

\[ \implies \quad E = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \quad \text{multiply all by} \ \gamma^2 \]

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \gamma^2 = E \gamma^2 \implies \hat{H} \gamma^2 = E \gamma^2 \]

Hamiltonian operator \( \hat{H} \)

Time-independent Schrödinger equation in 1-dimension

Mathematically, this is an eigenvalue problem. Operator \times function = value \times function

\* Wavefunctions are often called "eigenfunctions" and the energy of the system in the state described by this wave/eigen-function is the eigenvalue.

For many problems, we'll need to consider 3 dimensions

\[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) = \nabla^2 \quad \text{"d2-squared"} \]

Laplacian operator

So 3-D Schrödinger equation:

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \chi(r) = E \chi(r) \]

Where \( \chi(r) = A e^{i(\frac{\hbar}{\hbar} r \hat{\hbar} - \omega t)} \)

The Hamiltonian is the function for total energy.

So it might contain terms for electrostatics, etc.
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T.I. SCHRODINGER EQ + T.D.S.E.

GIVEN A HAMILTONIAN & BOUNDARY CONDITIONS, THE T.I.S.E. CAN BE SOLVED TO GIVE WAVEFUNCTIONS & ENERGIES OF A QUANTUM SYSTEM.

WHAT ABOUT TIME?

SCHRODINGER ASSUMED THAT PLANCK/ENSTEIN'S CIRCULAR-FREQUENCY ENERGY RELATION HOLDS FOR A PLANE WAVE, \( E = \frac{\hbar}{2}\pi \nu = \frac{\hbar}{\pi} \omega \)

so \[ \psi(x,t) = e^{i \left( \frac{p x}{\hbar} - \omega t \right)} = e^{i \left( \frac{p x}{\hbar} - E t \right)} = e^{\frac{i}{\hbar} \left( p x - E t \right)} \]

TO OBTAIN AN OPERATOR FOR \( E \), NOTE THAT

\[ \frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} \psi \left( \frac{p x - E t}{\hbar} \right) = \frac{-i}{\hbar} E \psi \]

so \[ \frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} E \psi \]

AND SINCE \( E \psi = \hat{H} \psi \) FROM TIME-INDEPENDENT EQUATION,

\[ i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi \] (TIME-DEPENDENT SCHRODINGER EQ)

NOTE THAT THESE EQUATIONS ARE POSTULATES - JUST LIKE

NEWTON'S LAWS OF MOTION - THEY CAN BE SUPPORTED BY EXPT

(OR DISPROVEN) BUT NEVER RIGOROUSLY PROVEN!

--- STATIONARY STATE WAVEFUNCTIONS ---

WE WILL MOSTLY LOOK AT WFS THAT ARE SOLUTIONS TO

TIME-INDEPENDENT SCHRODINGER EQ (STATIONARY STATES,

SOLUTIONS WILL TYPICALLY BE A SET OF WAVEFUNCTIONS

AND ENERGIES \( \psi_n, E_n \)

I ALREADY MENTIONED THAT \( |\psi_n|^2 \) IS A PROBABILITY DENSITY,

SO A WELL-BEHAVED PROBABILITY DENSITY MEANS THAT

\( \psi_n \) MUST BE FINITE-VALUED, CONTINUOUS, SINGLE-VALUED,

DEFINED OVER ALL COORDINATE SPACE, DIFFERENTIABLE

A FEW MORE PROPERTIES OF WAVEFUNCTIONS
A WAVEFUNCTION IS **NORMALIZED** IF \( \int dt |\psi|^2 = 1 \)

E.G., INTEGRATION FROM \(-\infty\) TO \(\infty\) IF 1-D PROBLEM

TWO WAVEFUNCTIONS ARE **ORTHOGONAL** IF \( \int dt \psi_i \psi_j = 0 \)

A SET OF WAVEFUNCTIONS \( \psi_i \) THAT SOLVES THE SCHRÖDINGER EQ.
FOR A PARTICULAR SYSTEM (E.G., PARTICLE IN A BOX OR HARMONIC OSCILLATOR) FORMS AN ORTHO-NORMAL BASIS SET OF FUNCTIONS

- ANALOGOUS TO \( \hat{x}, \hat{y}, \hat{z} \) VECTORS IN 3-D CARTESIAN SPACE

SO WE CAN WRITE

\[
\int dt \psi_i^* \psi_j = S_{ij} \quad S_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}
\]

**DIRAC-BRACKET NOTATION**

\[
\int \psi_i^* \psi_j \, dt = 0 \quad \rightarrow \quad \langle \psi_i | \psi_j \rangle = 0
\]

\[
\int \psi_i^* \psi_i \, dt = 1 \quad \rightarrow \quad \langle \psi_i | \psi_i \rangle = 1
\]

\( |\psi\rangle \) IS A WAVEFUNCTION \( \langle \psi | \) IS THE COMPLEX CONJUGATE OF \( |\psi\rangle \)

"KET" "BRA"

BRA + KET ASSEMBLED INTO \( \langle \psi | \psi \rangle \) MEANS AN INTEGRAL OVER ALL SPACE, \( \langle \psi_n | \psi_m \rangle = S_{nm} \)

**REMEmBER THAT TO MAKE THE COMPLEX CONJUGATE OF A FUNCTION, JUST REPLACE \( i \) WITH \( -i \) IN THE EXPRESSION**

IF THE FUNCTION IS REAL, IT IS EQUAL TO ITS COMPLEX CONJUGATE

WE WILL USE THIS NOTATION AGAIN...
Chem 4531 Fall 2015  Wavefunctions

Examples -

1. In 1-D, we can see graphically that \( \cos(x) \) and \( \sin(x) \) are orthogonal.

\[
\int_{0}^{2\pi} \cos(x) \sin(x) dx = 0
\]

Because it represents the sum of the area between the curves and the horizontal axis, so (+) and (-) areas cancel.

Same idea in 3-D space - e.g. \( p_x \) and \( p_y \) orbitals are wavefunctions → they are orthogonal.

2. Normalization. Sometimes, you will obtain a \( \psi \) and will need to normalize it.

E.g. \( \psi = a (a-x) \) over \( 0 \leq x \leq a \)

To normalize it, we multiply by a constant "\( N \)" and then calculate value of \( N \) from the integral that defines the normalization condition:

\[
N^2 \int_0^a \psi^* \psi dx = 1 = N^2 \int_0^a [a(a-x)]^2 dx = 1
\]

\[
N^2 a^2 \int_0^a (a^2 - 2ax + x^2) dx = 1
\]

\[
N^2 (a^4 - a^3 x^2 + \frac{1}{3} a^2 x^3) \bigg|_0^a = 1 \quad \Rightarrow \quad N^2 \frac{a^5}{3} = 1
\]

So \( N = \sqrt{\frac{3}{a^5}} \)

So normalized \( \psi = \sqrt{\frac{3}{a^5}} a(a-x) \)
CHEM 4531 FALL 2015 OPERATORS/OBSERVABLES

SO FAR, I'VE INTRODUCED THE IDEA OF A WAVEFUNCTION, \( \psi(t, x) \)

WHICH IS OBTAINED BY SOLVING THE SCHRÖDINGER EQUATION

(WE HAVE YET TO DO THIS!)

\( \psi(t, x) \) COMPLETELY SPECIFIES THE STATE OF A Q.M. SYSTEM.

ALL THE INFORMATION ABOUT A SYSTEM IS IN \( \psi(t, x) \).

BUT HOW DO WE OBTAIN IT? IN Q.M., PHYSICAL QUANTITIES ARE CALLED "OBSERVABLES" - E.G. POSITION, MOMENTUM, KINETIC ENERGY, ETC.

* OBSERVABLES ARE MEASUREABLE QUANTITIES

* IN Q.M., OBSERVABLES ARE REPRESENTED BY OPERATORS WHICH ARE MATHEMATICAL RULES THAT DESCRIBES HOW TO TRANSFORM A WAVEFUNCTION \( \psi \rightarrow \hat{A} \psi \)

E.G. \( \hat{A} |\psi\rangle = 1\hat{A} |\psi\rangle \)

\( \hat{A} \) IS AN OPERATOR |

\( \hat{A} \) HAT

PHYSICALLY-RELEVANT OPERATORS ARE LINEAR:

\( \hat{A} (|\psi_1\rangle + |\psi_2\rangle) = \hat{A} |\psi_1\rangle + \hat{A} |\psi_2\rangle \)

Q.M OPERATOR FOR A CLASSICAL OBSERVABLE IS FORMED BY USING THESE TWO RULES:

1. POSITION OPERATOR IS MULTIPLICATION BY THAT COORDINATE: \( \hat{\hat{X}} = \hat{X} \)

2. COMPONENT OF MOMENTUM \( \hat{P}_x \) IS GIVEN BY

\( \hat{P}_x = -i\hbar \frac{\partial}{\partial x} \) (DERIVATIVE) \( \hbar = \frac{\sqrt{2\pi}}{2m} \)

SO, FOR EXAMPLE KINETIC ENERGY = \( \frac{1}{2}mv^2 = \hat{P}^2/2m \)

FOR A 1-D SYSTEM IS WRITTEN

\( \hat{T} = \frac{\hat{P}^2}{2m} = \frac{(-i\hbar \frac{\partial}{\partial x})^2}{2m} \)

\( \hat{T} = -\hbar^2 \frac{\partial^2}{\partial x^2} \)
Chem 4531 Fall 2015

Operators & Observables

I already mentioned the Hamiltonian operator $\hat{H}$

$$\hat{H} = \hat{T} + \hat{V}$$

(Kinetic + Potential Energies)

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$$

The $\hat{V}$ potential operator is a function of coordinate, so multiply by $V(x)$

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

is an eigenvalue equation, which means that operating on the wavefunction returns the wavefunction x constant

* In Q.M., the only possible result of a single measurement is an eigenvalue of the corresponding operator for that observable

$$\frac{d}{dx}(e^{-2x}) = -2e^{-2x}$$

Eigenvalue = -2

Eigenfunction = $e^{-2x}$

$$\frac{d}{dx}(x^3) = 3x^2$$

$x^2$ is not an eigenfunction of $d/dx$

* In Q.M., the average value of multiple measurements of an observable is given by

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi = \langle \psi | \hat{A} | \psi \rangle$$

"Expectation Value"

So, for example, if we solve the Schrödinger equation for a 1-d system, and get a set of $\psi_n$ and $E_n$,

$$E = \langle \psi_n | \hat{H} | \psi_n \rangle = \langle \psi_n | E_n | \psi_n \rangle = E_n \langle \psi_n | \psi_n \rangle = E_n$$

Note: $\hat{H}\psi = E\psi$

Another way of writing Schrödinger eq.
MEASUREMENTS ALWAYS GIVE REAL (AS OPPOSED TO COMPLEX) VALUES.

WAVEFUNCTIONS MAY BE COMPLEX, BUT WE CANNOT DIRECTLY MEASURE THEM. WE CAN ONLY MEASURE THE PROBABILITY DENSITY $|\Psi|^2$ WHICH IS REAL.

Q.M. OPERATORS FOR OBSERVABLES ONLY GIVE REAL EIGENVALUES, BECAUSE THESE OPERATORS ARE "HERMITIAN," WHICH MEANS THAT

$$<\Psi_n | A | \Psi_m> = <\Psi_m | A | \Psi_n>^*$$

$$a_m <\Psi_n | \Psi_m> = a_n^* <\Psi_m | \Psi_m>^* = a_n^* <\Psi_n | \Psi_m>$$

so

$$(a_m - a_n^*) <\Psi_n | \Psi_m> = 0$$

Which is true if $n \neq m <\Psi_n | \Psi_m> = 0$ ORTHOGONAL EIGENVECTORS!

$$n = m \quad a_n = a_n^* \quad \text{REAL EIGENVALUES}!$$

EXPECTATION VALUES + SUPERPOSITION STATES

IF A SYSTEM IS IN A STATE THAT CORRESPONDS TO AN EIGENSTATE $|\Psi_n> \neq 0$ OF AN OBSERVABLE $A$, THEN

$$A |\Psi_n> = a_n |\Psi_n>$$

SO VALUE $a_n$ IS ALWAYS OBTAINED. HOWEVER, A SYSTEM MAY NOT BE IN SUCH AN EIGENSTATE. IN THIS CASE, IT IS IN A

* SUPERPOSITION STATE.

WHAT IS THE RESULT OF MEASUREMENTS ON A SUPERPOSITION STATE?

I ALREADY MENTIONED THAT IT'S THE EXPECTATION VALUE $<\Psi | \hat{A} | \Psi>$. 

THE EXPECTATION VALUE IS A WEIGHTED AVERAGE 
CALCULATED FROM THE SQUARES OF THE COEFFICIENTS 
IN AN EXPANSION OF \( |\psi\rangle \) IN TERMS OF NORMALIZED 
EIGENFUNCTIONS OF \( \hat{A} \) \( (|\phi_n\rangle) \)

i.e. \( |\psi\rangle = \sum_n C_n |\phi_n\rangle \)

WHERE \( C_n = \langle \psi | \phi_n \rangle \) AND \( \hat{A} |\phi_n\rangle = \omega_n |\phi_n\rangle \)

SO \( P(\omega_n) = |C_n|^2 = C_n^* C_n \)

THESE \( C_n \) REPRESENT PROJECTIONS OF \( |\psi\rangle \) ONTO EACH 
EIGENFUNCTION \( |\phi_n\rangle \)

THE EIGENFUNCTIONS ARE AN ORTHONORMAL, COMPLETE 
Basis—other wavefunctions can be written 
AS A LINEAR COMBINATION WITHIN THE COMPLEX 
VECTOR SPACE OF THESE EIGENFUNCTIONS 

ANALOGY:

3-D SPACE \hspace{2cm} \text{WAVEFUNCTION (HILBERT) SPACE}

\( \hat{\mathbf{e}}, \hat{\mathbf{j}}, \hat{\mathbf{k}} \) BASIS VECTORS \hspace{2cm} \( |\phi_n\rangle \) BASIS VECTORS

\( \mathbf{\hat{r}} = x \hat{\mathbf{e}} + y \hat{\mathbf{j}} + z \hat{\mathbf{k}} \) VECTOR \hspace{2cm} \( |\psi\rangle = \sum_n C_n |\phi_n\rangle \)

\( \hat{\mathbf{r}} \cdot \hat{\mathbf{r}} = (x, y, z)^2 \cos \theta \) (SCALAR PRODUCT) \hspace{2cm} \langle \psi | \phi_n \rangle = \int d^3 r \, \psi^* (\mathbf{r}) \phi_n (\mathbf{r}) \)

\( x = \hat{\mathbf{r}} \cdot \hat{\mathbf{e}} ; y = \hat{\mathbf{r}} \cdot \hat{\mathbf{j}} ; z = \hat{\mathbf{r}} \cdot \hat{\mathbf{k}} \)

SO THE \( C_n \) ARE REALLY JUST COORDINATES WITHIN THE 
SPACE OF EIGENFUNCTIONS, \( \langle \psi | \phi_n \rangle \) REPRESENTS 
THE CONTRIBUTION OF EACH BASIS FUNCTION TO 
THE SUPERPOSITION STATE

STOP HERE 9/9/15
"EXPECTATION VALUE" \(\leftrightarrow\) "AVERAGE VALUE"

Just as we would calculate the average/mean value over a probability distribution,

\[
\langle x \rangle = \sum x \cdot p_x
\]

**Average value of** \(x\): \(\langle x \rangle\)

**Probability of obtaining** \(x\): \(p_x\)

\[
\langle x \rangle = \int dx \cdot x \cdot |\psi(x)|^2
\]

WHERE \(|\psi(x)|^2\) = **PROBABILITY**

We can also ask, if the average, "expectation" value for an observable is \(\langle x \rangle\), then what is the spread or distribution of this value?

\[
\sigma_x^2 = \langle (x-\langle x \rangle)^2 \rangle
\]

\[
\sigma_x = \sqrt{\sigma_x^2}, \text{ which is the standard deviation}
\]

We will return to this topic later, but the variance can be calculated from the expectation values:

\[
\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2
\]

For a state \(|\psi\rangle\):

\[
\sigma_x^2 = \langle \psi | x^2 | \psi \rangle - \langle \psi | x | \psi \rangle^2
\]

---

**PARTICLE IN A BOX**

To solve the Schrödinger equation, we need to write the Hamiltonian and we need boundary conditions, and luck!

It's a 2nd-order differential eq:

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x) = \epsilon \psi(x)
\]

So it has two linearly independent solutions \(\phi_1(x) \phi_2(x)\)

The general solution is a linear combination:

\[
\psi(x) = C_1 \phi_1(x) + C_2 \phi_2(x)
\]

\(C_1 \text{ and } C_2\) set by boundary conditions on \(\psi \) and \(\psi'\)
SIMPLEST EXAMPLE - FREE PARTICLE IN 1-D \( V(x) = 0 \)

\[
\frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi(x) \quad \frac{d^2 \psi}{dx^2} = \frac{-2mE}{\hbar^2} \psi(x)
\]

We know \( E = p^2 / 2m \), define \( p = \hbar k \) \((k = \text{wave-vector})\)

\[ 2mE = p^2 = \hbar^2 k^2 \quad \text{so} \quad k^2 = \frac{2mE}{\hbar^2} \]

\[ \frac{d^2 \psi(x)}{dx^2} = -k^2 \psi(x) \quad \text{which has the general solution} \]

\[ \psi(x) = Ae^{-ikx} + Be^{ikx} \quad \text{superposition of left- and right-traveling waves} \]

No boundary conditions, so any \( A, B \), and \( E = \frac{\hbar^2 k^2}{2m} \) are satisfactory.

As we saw recently, this wavefunction can't be normalized.

*Another way of writing solution: \( \psi(x) = A \cos(kx) + B \sin(kx) \)*

MORE INTERESTING CASE - PARTICLE IN A BOX

**Boundary conditions \( \rightarrow \text{physically reasonable solutions} \)**

\[
\begin{align*}
V(x) &= 0 \quad 0 < x < a \\
V(x) &= 0 \quad x < 0, \ x > a
\end{align*}
\]

First of all, what does this potential mean? Not a physical wall, but it implies no force on particle in box.

\( \text{Force at } x = 0, x = a \text{ pushes it back into potential well} \)

(Recall that \( F = -\frac{dV}{dx} \); \( F = -\frac{d\psi}{dx} \))

So particle cannot be located anywhere \( V(x) = 0 \)

\[ \psi(x) = 0 \quad x < 0, x > a \]

\[ \psi(x) = A \cos(kx) \text{ for } 0 < x < a \text{ - exactly like free particle} \]

To obtain physically reasonable \( \psi \), we need a continuous function.
Continuity means \( \psi'(0) = \psi'(a) = 0 \) because \( \psi = 0 \) on box

Substitute into \( \psi(x) \)

\[
\psi(x) = A \cos(x) + B \sin(x) = 0 \implies A = 0
\]

\[
\psi(x) = B \sin(kx) = 0
\]

\( B \neq 0 \) because particle must be somewhere

\[ \sin(kx) = 0 \text{ at } x = n\pi \text{ so } \sin(k\pi/a) = 0 \text{ at } k\pi/a = n\pi \]

Where \( n = 1, 2, 3 \ldots \) so \( k = n\pi/a \) is quantized

\[
\frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2} \implies \frac{E}{\hbar^2} = \frac{n^2 \pi^2}{2ma^2} \quad \text{particle in box energy levels}
\]

Wavefunction: \( \psi(x) = B \sin(\frac{n\pi x}{a}) \)

To determine \( B \), we need to normalize \( \psi \)

\[
1 = \int_0^a |\psi|^2 dx = \int_0^a |B \sin(\frac{n\pi x}{a})|^2 dx = 1
\]

Some algebra \( \implies B = \frac{\sqrt{2}}{a} \)

So \( \psi(x) = \frac{\sqrt{2}}{a} \sin(\frac{n\pi x}{a}) \) where \( n = 1, 2, 3 \ldots \)

Properties of the solutions

* Discrete energy levels with \( \Delta E \) between levels

  That increases with \( n \)

  \[
  E_{n+1} - E_n = \frac{(n+1)^2 \pi^2}{2ma^2} - \frac{n^2 \pi^2}{2ma^2} = \frac{(n+1)^2 - n^2}{2} \frac{\hbar^2}{8ma^2}
  \]

  Show slide with energy levels (Chem 4521 Mar 13-18 lectures)


  \( \Delta E \) between levels increases as box size decreases

  \( E \propto \frac{1}{a^2} \) "Quantum confinement" \( \implies \) discrete levels

* \( E_i = \frac{\hbar^2}{8ma^2} \neq 0 \)

  Zero-point energy \( \implies \)

  Confined particle cannot be at rest
Part 1: Wavefunction in 1-D Box

- Wavefunction $\psi(x)$ is sinusoidal with # of nodes (points of zero probability) increasing as $n$ increases.
- $|\psi(x)|^2$ is also symmetric about center of box.
- High $n \rightarrow$ shorter $\lambda$ (higher momentum).

Part 2: Transition to Classical Behavior

- Large box or large $n \rightarrow$ transition to classical behavior of continuous energies $+ \frac{p(x)^2}{a}$.

Part 3: Particle in a Box Wavefunctions

- Wavefunctions are not eigenstates of the position operator (not surprising), but one can calculate probability of being localized to particular regions of the box.

Example: What is the probability of finding a $\mathrm{e}^-$ within 0.2 m of a wall in a 1.0 m box? Assume system is in lowest energy state.

- $\int_{0}^{0.2} |\psi_{n}(x)|^2 \, dx$ is probability of finding particle in dx.
- Integrate over interval $0 \rightarrow 0.2$.
- $\psi_{n}(x) = \sqrt{\frac{a}{\pi}} \sin \left(\frac{\pi nx}{a}\right)$.
- $P = \int_{0}^{0.2} \psi_{1}^2 \, dx$.
- $P = \frac{2}{a} \int_{0}^{0.2} \sin^2 \left(\frac{\pi nx}{a}\right) \, dx = \frac{1}{2} - \frac{1}{2\pi} \sin \left(\frac{2\pi nx}{a}\right)$.
- For $x = 0.2$, $a = 1.0$ $\Rightarrow$ $P = 0.05$ (5%).
- What is the classical probability? $(0.2/1.0) = 0.20$ (20%).

Part 4: Note on Classical Limit

- Note that as $n \rightarrow \infty$, $\frac{1}{2\pi n} \sin \left(\frac{2\pi nx}{a}\right) \rightarrow 0$.
- So $P \propto \frac{n}{a}$, which is the classical result.

"Correspondence Principle" - At high quantum numbers, classical result is obtained.
CHEM 1531  FALL 2015  PARTICLE IN A BOX

That was an example of directly using the probability density to calculate where the particle is located. We could also calculate expectation values of position \( \langle x \rangle \) and second moment of position \( \langle x^2 \rangle \)

\[
\langle x \rangle = \langle x | \hat{x} | x \rangle = \int_0^a dx \sqrt{\frac{a}{\pi \hbar^2}} x \sin^2 \left( \frac{\pi x}{a} \right)
\]

We could use a table of integrals or software to integrate this expression, but it's simplest to realize that \( | \psi_n \rangle \) is symmetric, centered in box, so the average position of the particle must be \( \langle x \rangle = a/2 \) for all \( n \).

Similarly, work through S.A.B. examples 9.12 + 9.13

Let's do an example to show \( \chi = 1 \) particle-in-a-box level satisfies the Heisenberg uncertainty principle

\[ \Delta x \Delta p \geq \frac{\hbar}{2} \quad \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \text{ etc.} \]

\[
\langle x^2 \rangle = \frac{1}{a} \int_0^a x^2 \sin^2 \left( \frac{\pi x}{a} \right) dx = \left( \frac{a}{2m} \right)^2 \left( \frac{\pi^2}{3} - 2 \right)
\]

\[ \Delta x = a \left[ \frac{a}{2} \cdot \frac{1}{2} - \frac{a}{2} \right] = a \left[ \frac{1}{2} - \frac{\hbar^2}{4m^2} \right] \]

\[ \Delta p = \left( \langle p^2 \rangle - \langle p \rangle^2 \right)^{1/2} ; \quad \langle p^2 \rangle = 2m \langle E \rangle \quad \frac{p^2}{2m} = E \]

\[ E = \frac{\hbar^2 a^2}{8m} \text{ so } \langle p \rangle = (2m) \cdot \frac{\hbar^2 a^2}{8ma^2} = \frac{\hbar}{2m} \]

\( \langle p \rangle \) is easy to evaluate; \( \langle p \rangle = 0 \) because particle is equally likely to move right or left: it's in \( -k \) superposition.

So \( \Delta p = \left( \frac{\hbar}{2m} \right)^{1/2} = \frac{\hbar}{2m} \)

So \( \Delta p \Delta x = a \left[ \frac{1}{2} - \frac{\hbar^2}{4m^2} \right] \cdot \frac{\hbar}{2m} = \frac{\hbar}{2} \left[ \frac{1}{2} - \frac{\hbar^2}{4m^2} \right] \]

\[ \Delta p \Delta x = 0.0904 \cdot \hbar > \frac{\hbar}{4\pi} = 0.0796 \]