8/29/2023

- Uncertainty (last lecture)
  - Simultaneous specification of observables
  - Heisenberg and generalized uncertainty principles
- Time evolution of expectation values
  - General derivation
  - Ehrenfest's theorem
- Implications of the Schrödinger equation
  - Constraints on wavefunctions
  - Curvature
  - Penetration
  - Quantization
- Exercise 1: Introduction to Google Colab

Uncertainty

- This module is intended to help you achieve the following learning objectives:
  - Use the general uncertainty principle to evaluate limits on the simultaneous specification of a pair of quantities
- At the end of this module, you should be able to
  - answer the following questions:
    - What condition must be satisfied for two quantum observables to be simultaneously specified?
  - derive an uncertainty principle for an arbitrary pair of observables

Simultaneous specification

- Recall that two operators commute if $[\hat{\mathbf{A}}, \hat{\mathbf{B}}] = 0$.
- If two operators commute, then their corresponding observables can be simultaneously specified.
- If two operators do not commute, then their corresponding observables cannot be simultaneously specified. They are *complementary* observables.
  - This is counterintuitive.

Uncertainty

- Heisenberg uncertainty principle: $\Delta x \Delta p_x \geq \frac{1}{2}\hbar$
- General uncertainty principle: $\Delta A \Delta B \geq \frac{1}{2}\left|\left\langle [\hat{\mathbf{A}}, \hat{\mathbf{B}}] \right\rangle\right|$
- $\Delta A = \left\{ \left\langle A^2 \right\rangle - \langle A \rangle^2 \right\}^{\frac{1}{2}}$ is the root mean square deviation of the observable.

  The mean square deviation is,

  $$\left\langle (\delta A)^2 \right\rangle = \left\langle (A - \langle A \rangle)^2 \right\rangle = \left\langle A^2 - 2A \langle A \rangle + \langle A \rangle^2 \right\rangle$$
  $$= \left\langle A^2 \right\rangle - 2 \langle A \rangle \langle A \rangle + \langle A \rangle^2 = \left\langle A^2 \right\rangle - \langle A \rangle^2$$

- Uncertainty $\neq$ measurement error. Improved instruments do not reduce uncertainty beyond a certain point.

Proof

- The general uncertainty relation is based on Postulate 3
- To show this, we will
  - define spread operators
  - expand an integral that can be manipulated to the uncertainty relation

Spread operators

Suppose that $[\hat{\mathbf{A}}, \hat{\mathbf{B}}] = i\hat{\mathbf{C}}$ and the wavefunction is Ψ. Then expectations of A and B are, $\langle A \rangle = \left\langle \Psi \middle| \hat{\mathbf{A}} \middle| \Psi \right\rangle$ and $\langle B \rangle = \left\langle \Psi \middle| \hat{\mathbf{B}} \middle| \Psi \right\rangle$. Let the spread operators be,

$$
\begin{aligned}
\delta\hat{\mathbf{A}} &= \hat{\mathbf{A}} - \langle A \rangle \\
\delta\hat{\mathbf{B}} &= \hat{\mathbf{B}} - \langle B \rangle
\end{aligned}
$$

The commutation relation for the spread operators is $[\delta\hat{\mathbf{A}}, \delta\hat{\mathbf{B}}] = i\hat{\mathbf{C}}$.

Let $I = \int \left| \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \Psi \right|^2 d\tau$, where α is an arbitrary real number. I is non-negative. It can be written as,

$$\begin{aligned}
I &= \int \left\{ \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \Psi \right\}^* \left\{ \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \Psi \right\} d\tau \\
&= \int \left\{ \left([(\alpha\delta\hat{\mathbf{A}})\Psi]^* + i[(\delta\hat{\mathbf{B}})\Psi]^* \right) \right\} \left\{ \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \Psi \right\} d\tau \\
&= \int \Psi^* \left(\alpha\delta\hat{\mathbf{A}} + i\delta\hat{\mathbf{B}} \right) \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \Psi d\tau \; \textit{Hermitian} \\
&= \left\langle \left(\alpha\delta\hat{\mathbf{A}} + i\delta\hat{\mathbf{B}} \right) \left(\alpha\delta\hat{\mathbf{A}} - i\delta\hat{\mathbf{B}} \right) \right\rangle \\
&= \alpha^2 \left\langle (\delta\hat{\mathbf{A}})^2 \right\rangle + \left\langle (\delta\hat{\mathbf{B}})^2 \right\rangle - i\alpha \left(\left\langle \delta\hat{\mathbf{A}}\delta\hat{\mathbf{B}} - \delta\hat{\mathbf{B}}\delta\hat{\mathbf{A}} \right\rangle \right) \\
&= \alpha^2 \left\langle (\delta\hat{\mathbf{A}})^2 \right\rangle + \left\langle (\delta\hat{\mathbf{B}})^2 \right\rangle + \alpha \left\langle \hat{\mathbf{C}} \right\rangle \; \textit{Commutator}
\end{aligned}$$

$$
\begin{aligned}
I &= \alpha^2 \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle + \left\langle (\delta \hat{\mathbf{B}})^2 \right\rangle + \alpha \left\langle \hat{\mathbf{C}} \right\rangle \\
&= \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle \left(\alpha + \frac{\left\langle \hat{\mathbf{C}} \right\rangle}{2 \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle} \right)^2 + \left\langle (\delta \hat{\mathbf{B}})^2 \right\rangle - \frac{\left\langle \hat{\mathbf{C}} \right\rangle^2}{4 \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle} \quad \textit{Completing Squares} \\
&= \left\langle (\delta \hat{\mathbf{B}})^2 \right\rangle - \frac{\left\langle \hat{\mathbf{C}} \right\rangle^2}{4 \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle} \geq 0 \quad \textit{Special choice of } \alpha
\end{aligned}
$$

This can be rearranged into,

$$
\left\langle (\delta \hat{\mathbf{B}})^2 \right\rangle \left\langle (\delta \hat{\mathbf{A}})^2 \right\rangle \geq \frac{1}{4} \left\langle \hat{\mathbf{C}} \right\rangle^2
$$

Taking the square root yields the general uncertainty relation.

Review

- Check that you can
  - answer the following questions:
    - What condition must be satisfied for two quantum observables to be simultaneously specified?
  - derive an uncertainty principle for an arbitrary pair of observables

Time Evolution of Expectation Values

- This module is intended to help you achieve the following learning objectives:
  - Express time derivatives of expectation values
- At the end of this module, you should be able to
  - answer the following questions:
    - What condition must be satisfied for an observable to change with time?
    - How do classical and quantum observables correspond to one another?
  - determine how the expectation value of an observable changes with time

Time Evolution of Arbitrary Expectations

- $\dfrac{d\langle\Omega\rangle}{dt} = \dfrac{d\left\langle \Psi | \hat{\Omega} | \Psi \right\rangle}{dt}$, by a time derivative of the third postulate
- $\dfrac{d\langle\Omega\rangle}{dt} = \displaystyle\int \Psi^* \hat{\Omega} \left(\frac{\partial \Psi}{\partial t}\right) d\tau + \int \left(\frac{\partial \Psi^*}{\partial t}\right) \hat{\Omega} \Psi d\tau$ using differentiation by parts.

  Using the Schrödinger equation and the properties of Hermitian operators,

  - $\displaystyle\int \Psi^* \hat{\Omega} \left(\frac{\partial \Psi}{\partial t}\right) d\tau = \frac{1}{i\hbar} \int \Psi^* \hat{\Omega} \hat{H} \Psi d\tau$
  - $\displaystyle\int \left(\frac{\partial \Psi^*}{\partial t}\right) \hat{\Omega} \Psi d\tau = -\frac{1}{i\hbar} \int \left(\hat{H}\Psi\right)^* \hat{\Omega} \Psi d\tau = -\frac{1}{i\hbar} \int \Psi^* \hat{H} \hat{\Omega} \Psi d\tau$
- $\dfrac{d\langle\Omega\rangle}{dt} = -\dfrac{1}{i\hbar}\left[\left\langle \Psi | \hat{H}\hat{\Omega} | \Psi \right\rangle - \left\langle \Psi | \hat{\Omega}\hat{H} | \Psi \right\rangle\right] = \dfrac{i}{\hbar}\left\langle \left[\hat{H}, \hat{\Omega}\right] \right\rangle$

Time Evolution of Position

- Given that $\frac{d\langle\Omega\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\hat{\mathbf{H}}, \hat{\boldsymbol{\Omega}}\right]\right\rangle$, then
  - If an operator commutes with the Hamiltonian, then its expectation value does not change with time
  - This can be used to prove Ehrenfest's theorem, an example of the correspondence principle - for large numbers and large energies, quantum calculations agree with classical calculations
    - $\frac{d}{dt}\left\langle p_x\right\rangle = -\left\langle\frac{dV}{dx}\right\rangle = \langle F\rangle$
    - $\frac{d}{dt}\langle x\rangle = \frac{\left\langle p_x\right\rangle}{m}$

Review

- Check that you can
  - answer the following questions:
    - What condition must be satisfied for an observable to change with time?
    - How do classical and quantum observables correspond to one another?
  - determine how the expectation value of an observable changes with time

Implications of the Schrödinger Equation

- This module is intended to help you achieve the following learning objectives:
  - Explain quantum penetration and tunneling
- At the end of this module, you should be able to
  - answer the following questions:
    - What are the requirements on the derivatives of a wavefunction for $|\Psi|^2$ to be a probability density and for Ψ satisfy the Schrödinger equation?
    - How does the potential and kinetic energy relate to the curvature of the wavefunction?
    - What is penetration? Is it permitted in classical mechanics? Is it permitted in quantum mechanics?
    - Under what conditions must energy be quantized?

Constraints on wavefunctions

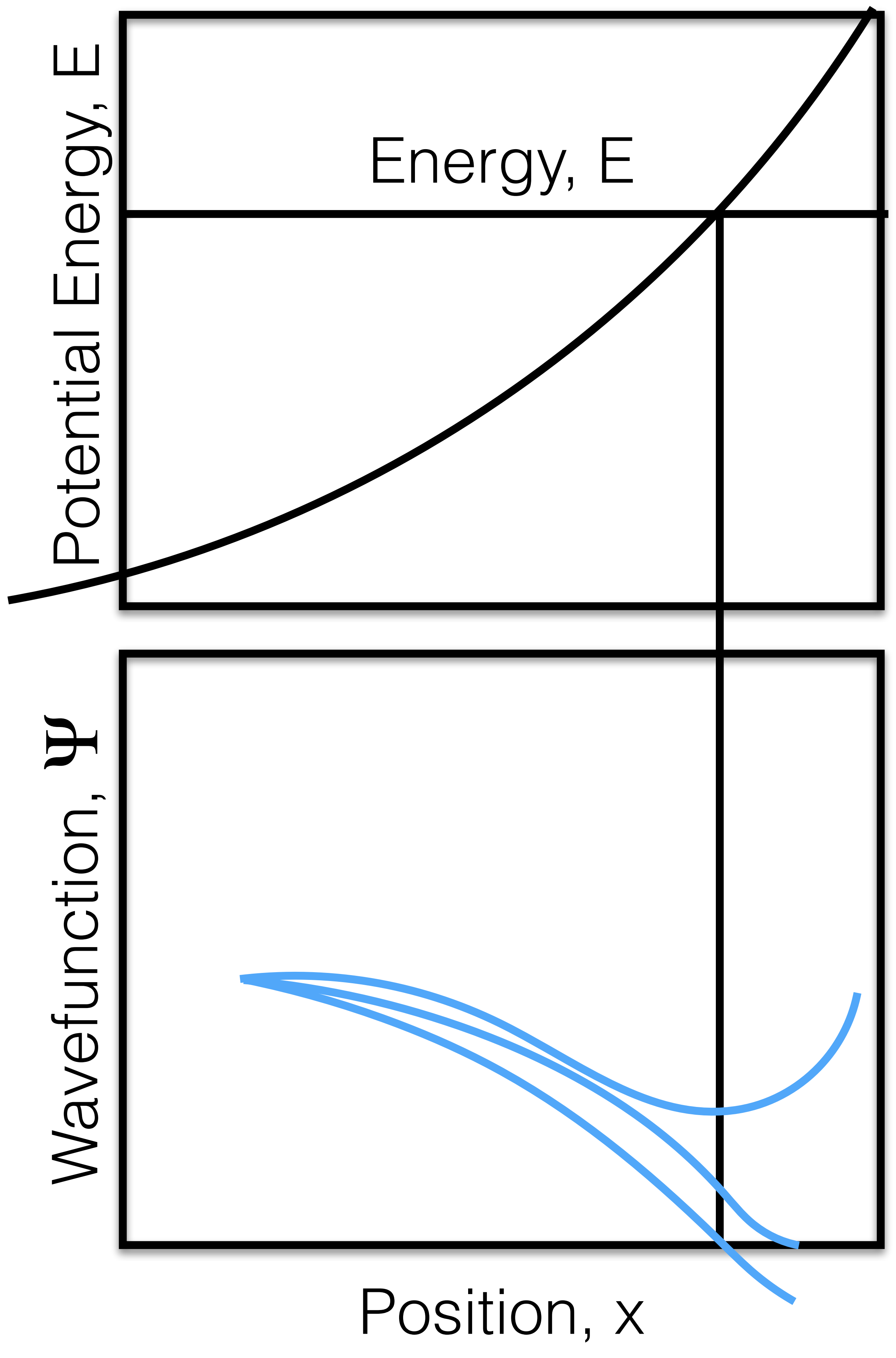
- $\int \Psi^* \Psi d\tau = 1$
- As $|\Psi|^2$ is a probability density, Ψ
  - Cannot be infinite over a finite region
  - Must be single-valued
  - In order for Ψ to be a solution to a second-order differential equation, it must have a second derivative. This implies that, except in ill-behaved regions of the potential, the function
    - is continuous and
    - has a continuous first derivative,

Curvature

- Colloquially, the second derivative can be thought of as the curvature
- The time-independent Schrödinger equation is
  - $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = E\Psi$
  - $\frac{\partial^2\Psi}{\partial x^2} = \frac{2m}{\hbar^2}(V - E)\Psi$
- Thus the curvature depends on the relative potential and total energy

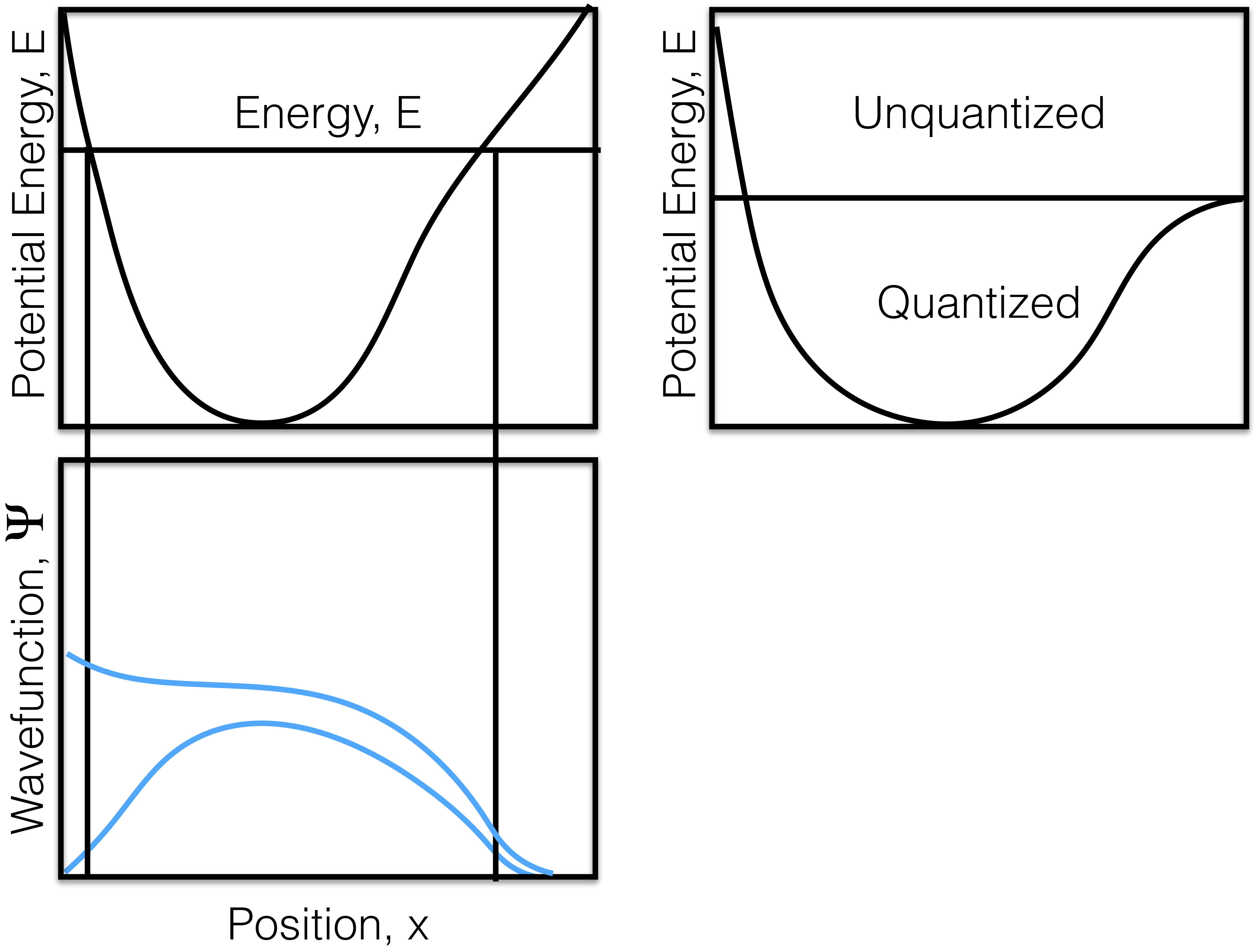
Curvature and Penetration

- Consider a particle moving right in a harmonic potential
  - In classical mechanics, what happens with the
    - potential and kinetic energy?
    - probability density? It is possible to see E < V?
- Based on $\dfrac{\partial^2\Psi}{\partial x^2} = \dfrac{2m}{\hbar^2}(V - E)\Psi$, what happens to the curvature and slope of the wavefunction if
  - E > V?
    - the curvature is negative; the slope decreases
  - E = V?
    - the curvature is zero; the slope is constant
  - E < V?
    - the curvature is positive; the slope increases
- In QM there is penetration into the classically forbidden region
- Kinetic energy is negative but the expectation value is positive



Quantization

- When there are two boundary conditions to satisfy (a particle is bounded), then it is possible to find acceptable solutions to $\hat{\mathbf{H}}\Psi = E\Psi$ for only certain values of E
- The need to satisfy two boundary conditions implies quantization of the energy
- Quantization is *not* required if there is only one boundary



Review

- Check that you can
  - answer the following questions:
    - What are the requirements on the derivatives of a wavefunction for $|\Psi|^2$ to be a probability density and for Ψ satisfy the Schrödinger equation?
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Exercise 1: Introduction to Google Colab

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