PHYS 142/242

Lecture 02: Quantum Mechanics Refresher

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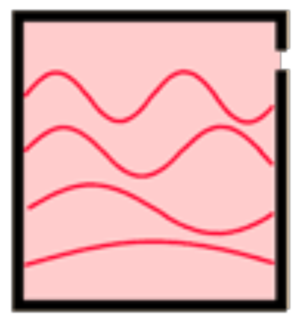
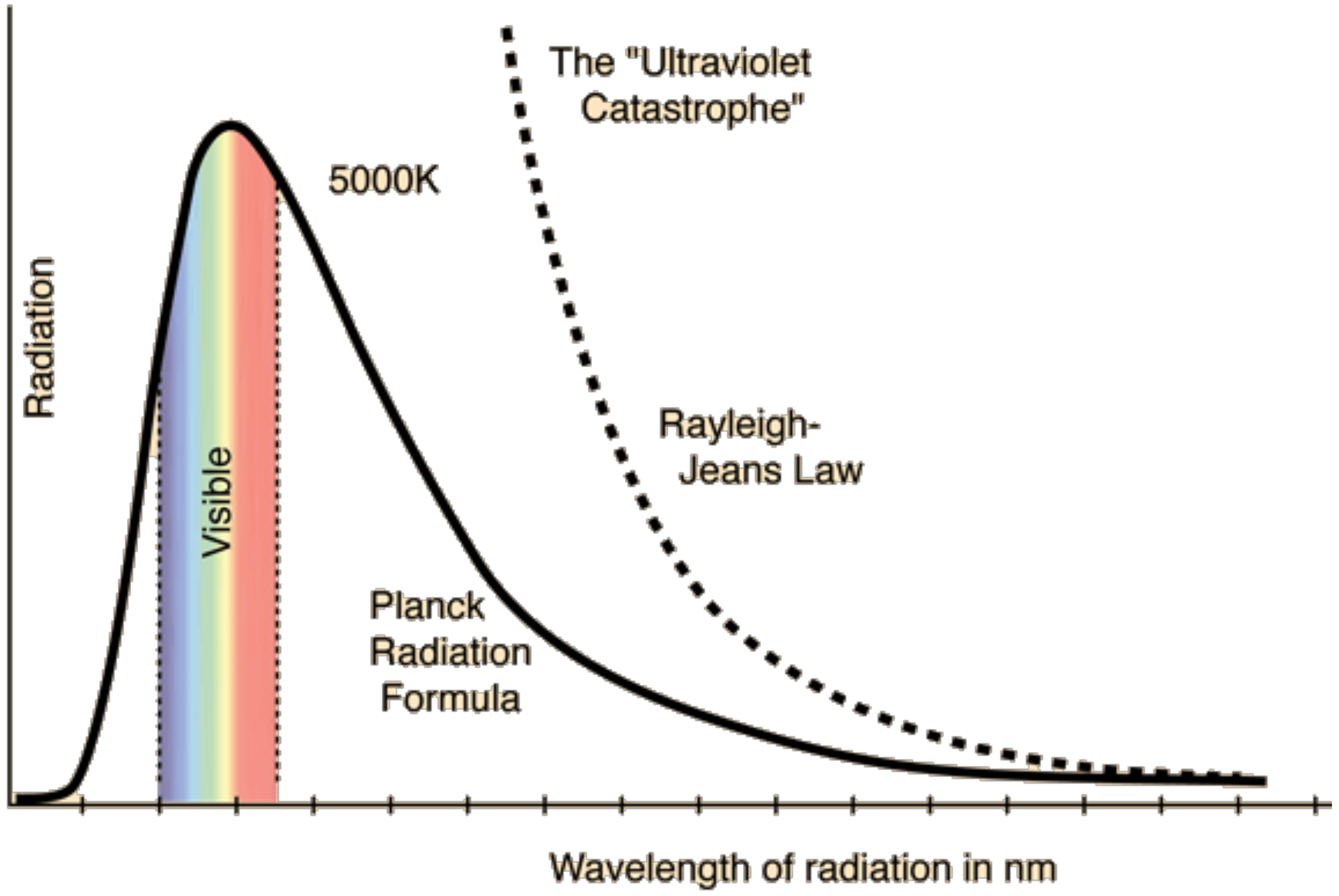
Quantum mechanics refresher

- Today, we'll review the basic terminology and notation of quantum mechanics
- Without rehashing the full history, its beginnings are often traced to solving the "ultraviolet catastrophe"
    - "Blackbody radiation" refers to a system that absorbs all incident radiation and re-radiates energy characteristic of the system (e.g., resonant modes of the cavity)
    - Classically, this radiation blows up to infinity at higher frequencies (or lower wavelengths)
    - Plank resolved this by hypothesizing that energy is quantized in units of $E = h\nu$

Radiation modes in a hot cavity provide a test of quantum theory



	#Modes per unit frequency per unit volume	Probability of occupying modes	Average energy per mode
CLASSICAL	$\frac{8\pi\nu^2}{c^3}$	Equal for all modes	kT
QUANTUM	$\frac{8\pi\nu^2}{c^3}$	Quantized modes: require $h\nu$ energy to excite upper modes, less probable	$\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1}$



States and probabilities

- The state of a particle is a (column) vector, or **ket**, in **Hilbert space** $|\psi\rangle$
  - A **bra** $\langle\psi|$ is a (row) vector or linear operator
- Described by a complex-valued wavefunction in ***position space***

$\langle x|\psi\rangle \equiv \psi(x,t)$, where t denotes a (potential) time dependence

- States are **normalized**

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = \int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx = 1$$

- **The Born rule**: probability density p for the result of a measurement of the particle's position at time t is

$$p(x,t) = |\psi(x,t)|^2$$

Superposition

- A particle can exist in a **superposition**

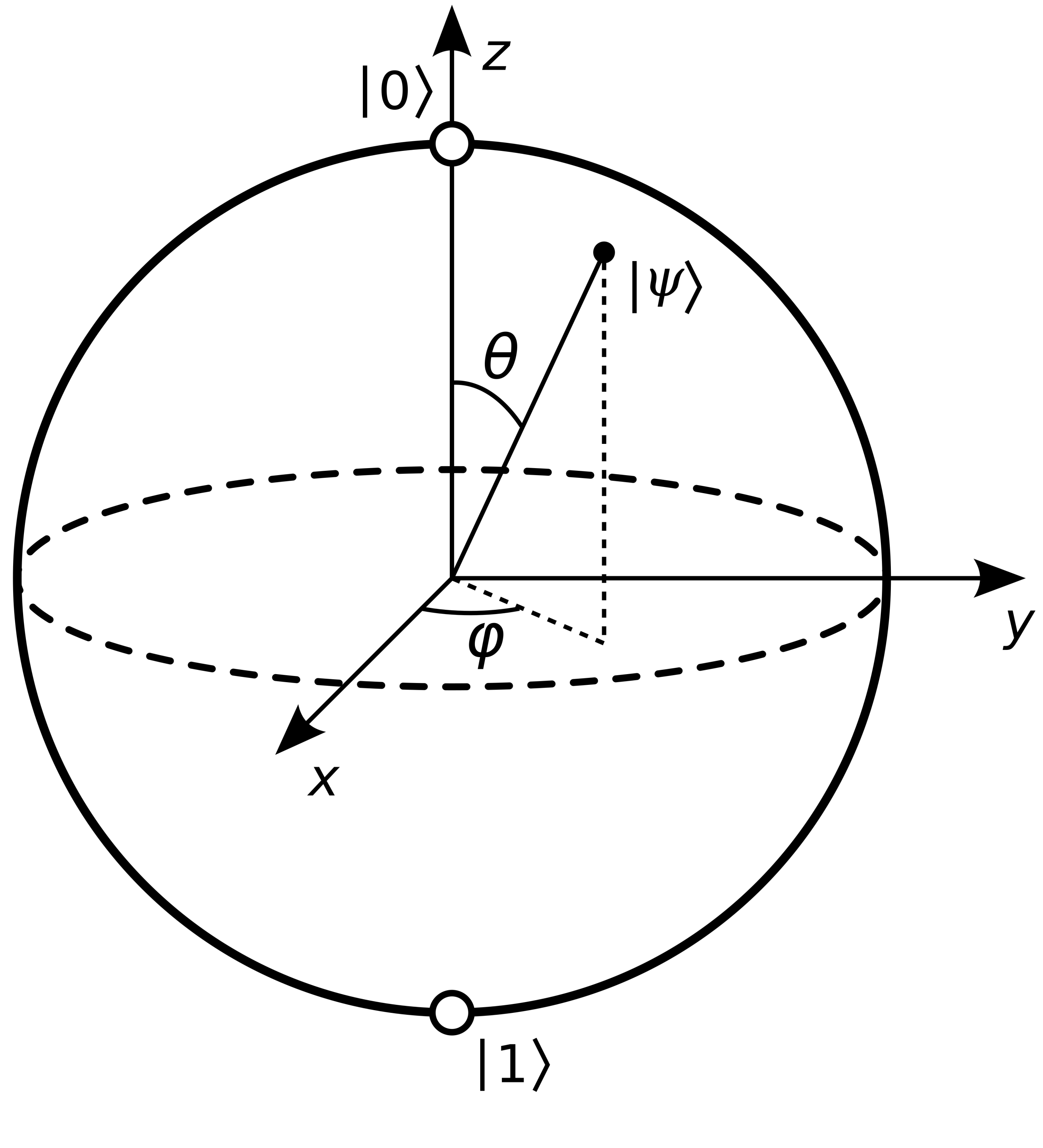
$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle$$

- Assuming $|0\rangle, |1\rangle$ form an **orthonormal basis**, normalization implies

$$\langle\psi|\psi\rangle = c_0^* c_0 + c_1^* c_1 = |c_0|^2 + |c_1|^2 = 1$$

- Useful representation is the **Bloch sphere**

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



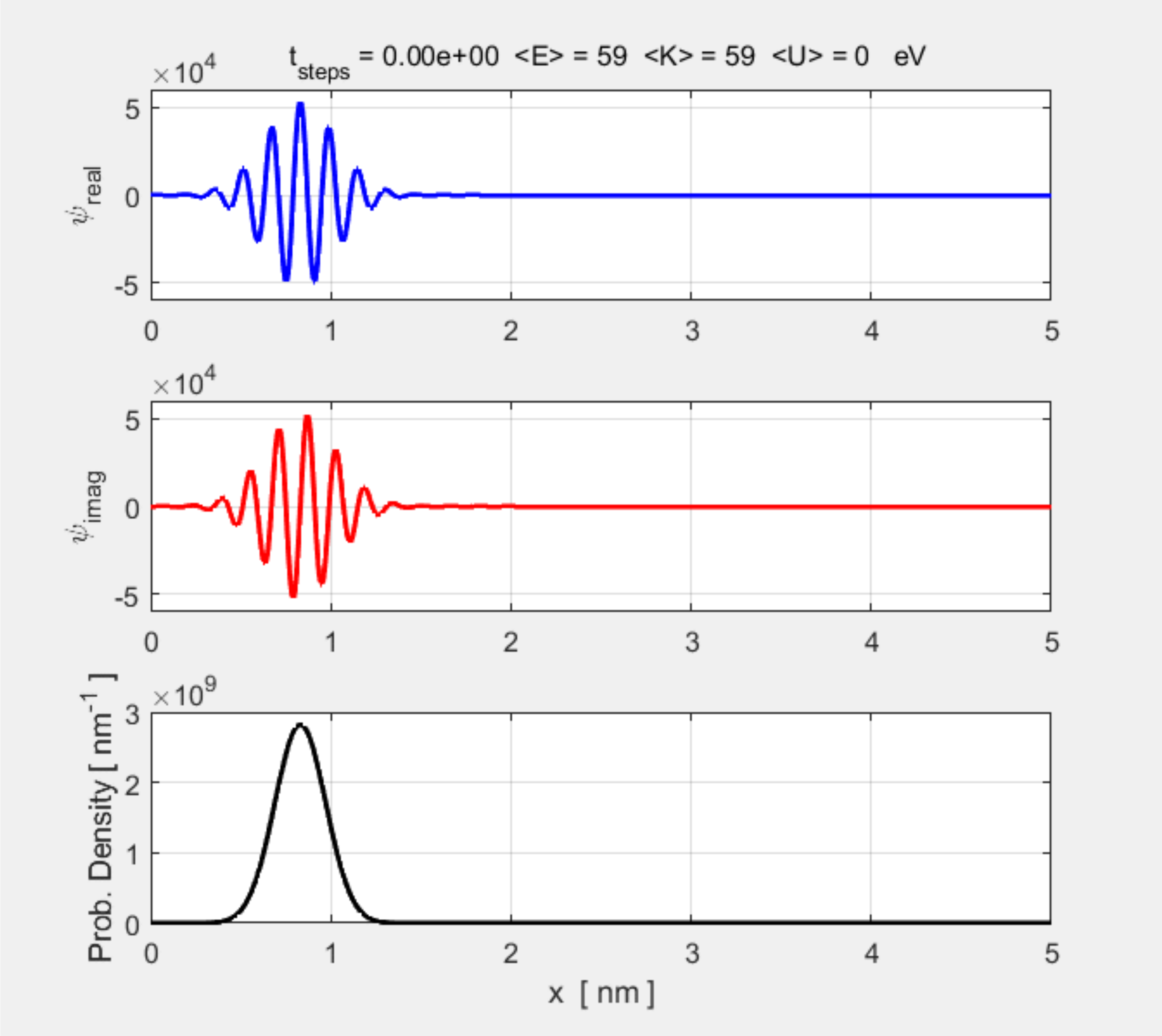
Expectation values

- The **expectation value** of an observable (say position), is given by:

$$\langle x \rangle = \langle \psi | x | \psi \rangle = \int_{-\infty}^{\infty} |\psi(x,t)|^2 x \, dx$$

- A useful notion of **uncertainty** is the variance:

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2$$



Operators

- Momentum operator is

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

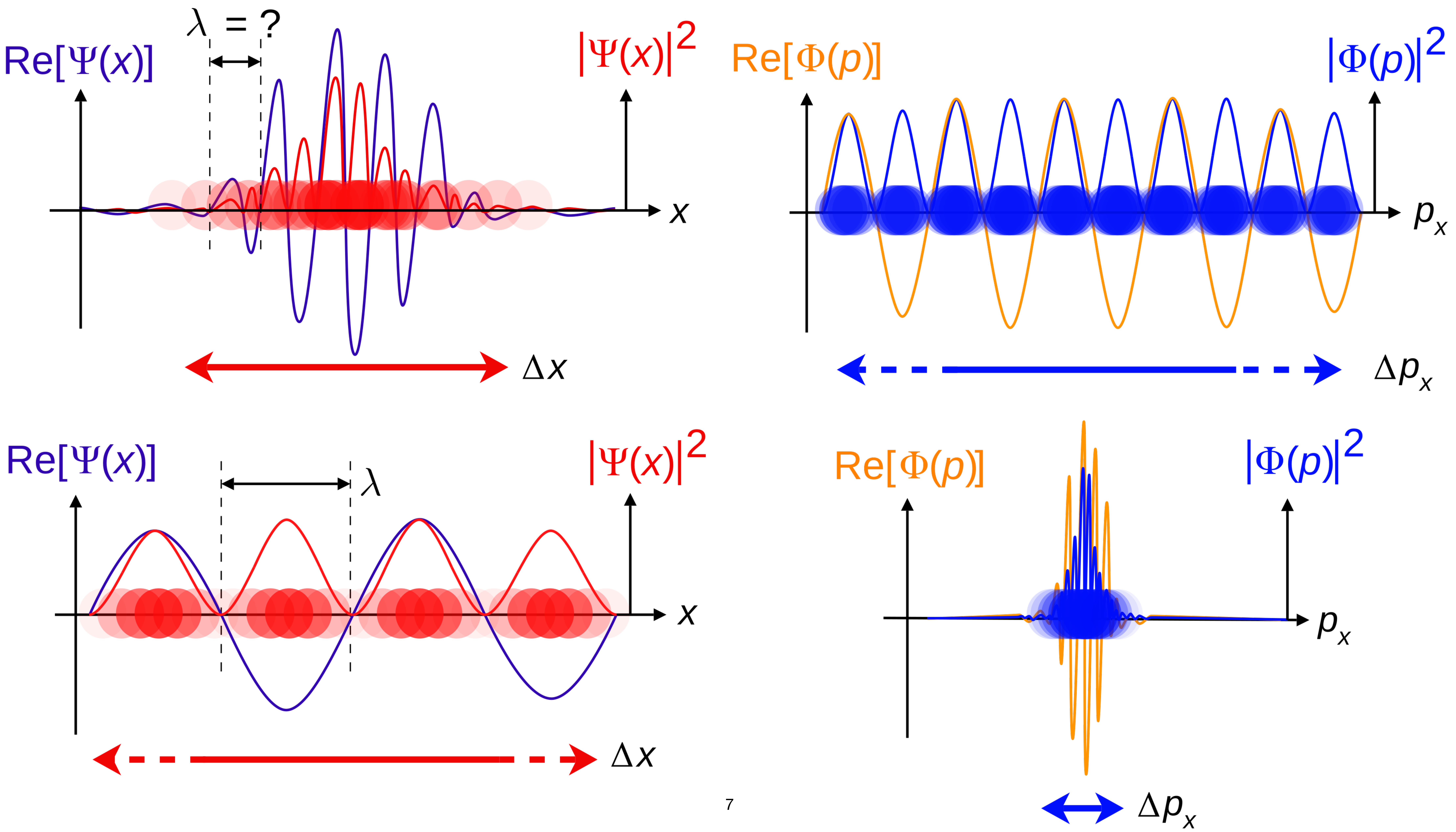
- Note: $\hat{p}$ and $\hat{x}$ do not commute:

$$[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

- From this property, we can derive Heisenberg's uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Uncertainty principle



Hamiltonian

- The **Hamiltonian** (energy) operator is

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

- **Eigenstates** of the Hamiltonian operator are also known as **stationary states**

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$$

  - Stationary states have a **definite energy**

Example: Plane waves

- **Plane wave** solution

$$\langle x | \psi \rangle = \psi(x, t) = C \exp[i(kx - \omega t)]$$

means particle has momentum $p = \hbar k$ and energy $E = \hbar \omega$

- Can check by applying operator definitions

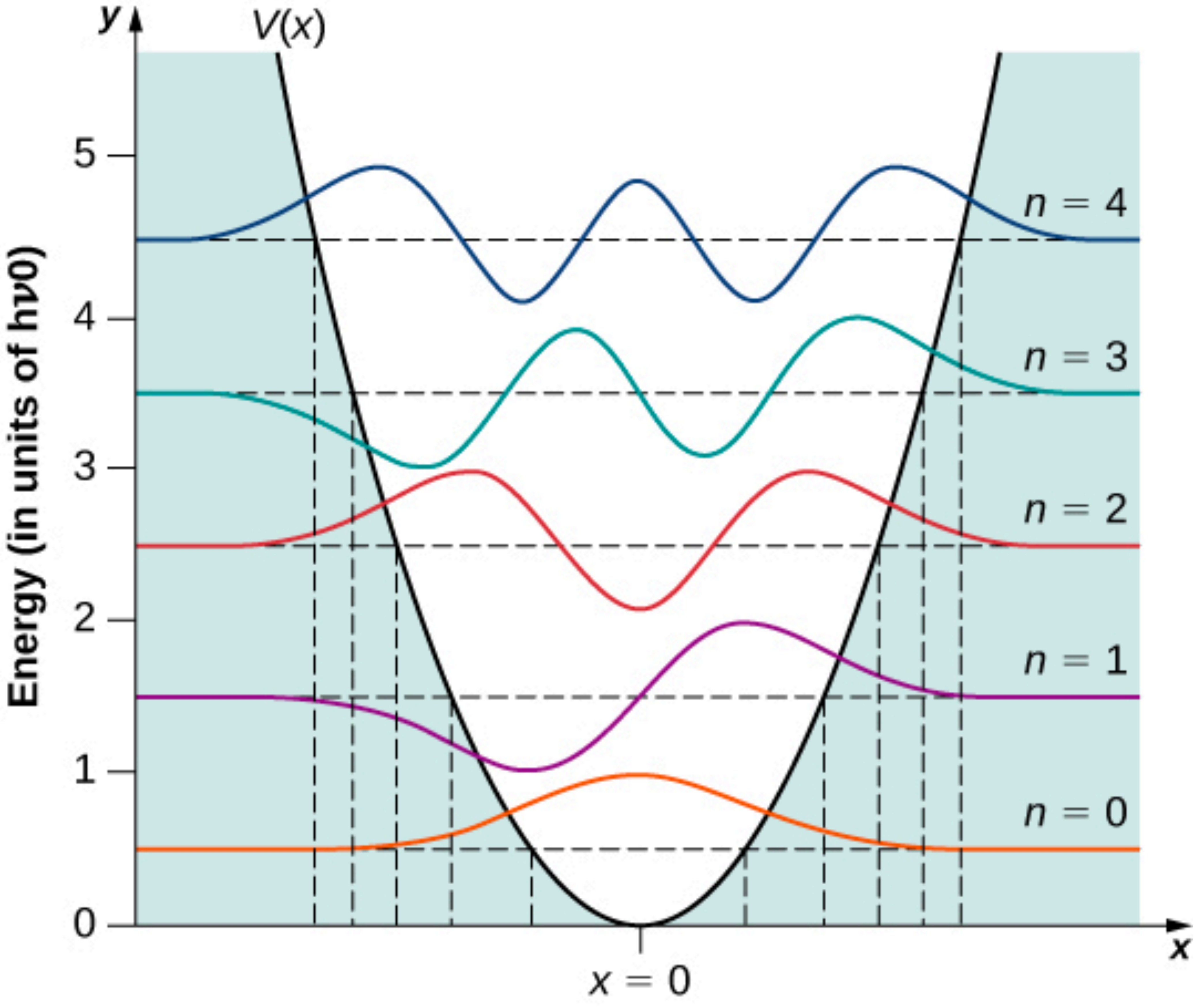
$$\hat{p} | \psi \rangle = (\hbar k) | \psi \rangle$$

$$\hat{H} | \psi \rangle = (\hbar \omega) | \psi \rangle$$

Example: Quantum harmonic oscillator

- Time-independent Schrödinger equation:

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



- **Ladder** of allowed energy levels

$$E_n = (n + \frac{1}{2})\hbar\omega \text{ with } n = 0,1,2,3,\ldots$$

- Wave functions for each energy level $\psi_n(x) = N_n e^{-\beta^2 x^2/2} H_n(\beta x)$
  - Note $H_0(y) = 1$ so ground state is a Gaussian

Time-dependent Schrödinger equation

- Time-dependent Schrödinger equation:

$$\hat{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle \Leftrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x) = i\hbar\frac{\partial\psi}{\partial t}$$

- **Time evolution** (stationary states pick up a phase): $\psi(x, t) = e^{-iE_n t/\hbar}\phi_n(x)$
  - Note: overall phase doesn't affect measurement probabilities because $|\psi(x, t)|^2 = |\phi_n(x)|^2$

- Stationary states form a **complete basis**, so we can write a general state as

$$\psi(x, t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(x)$$

In-class question

- Is $|\psi\rangle = (|\phi_0\rangle + |\phi_1\rangle)/\sqrt{2}$ a stationary state?

- No! Because each state picks up a different phase so you can't write the time evolution as an overall phase factor (i.e., no definite energy)

$$
\begin{aligned}
|\psi(t)\rangle &= (e^{-iE_0 t/\hbar}|\phi_0\rangle + e^{-iE_1 t/\hbar}|\phi_1\rangle)/\sqrt{2} \\
&= e^{-iE_0 t/\hbar}(|\phi_0\rangle + e^{-i(E_1 - E_0)t/\hbar}|\phi_1\rangle)/\sqrt{2}
\end{aligned}
$$

- ***Caveat***: Except if $E_0 - E_1 = 0$, i.e., the energy eigenstates are degenerate!

More Dirac notation

- Position eigenstates are **orthogonal**

$$\langle x | x' \rangle = \delta(x - x')$$

- Position eigenstates are **complete**

$$\int_{-\infty}^{\infty} |x\rangle\langle x| \, dx = 1$$

Propagator preview

- As a preview, we will study the **propagator**

  $$K(x_B, t_B; x_A, t_A) = \langle x_B | e^{-i\hat{H}(t_B - t_A)/\hbar} | x_A \rangle,$$

  which represents the amplitude for a particle to get from point A to point B

- Determines the wave function at a later time from an initial condition

  $$\psi(x_B, t_B) = \int_{-\infty}^{\infty} K(x_B, t_B; x_A, t_A)\, \psi(x_A, t_A)\, dx_A$$

  - As $t_B - t_A \to 0$, the propagator $K(x_B, t_B; x_A, t_A) \to \delta(x_B - x_A)$

- **Composition**: $K(x_C, t_C; x_A, t_A) = \int K(x_C, t_C; x_B, t_B)\, K(x_B, t_B; x_A, t_A)\, dx_B$

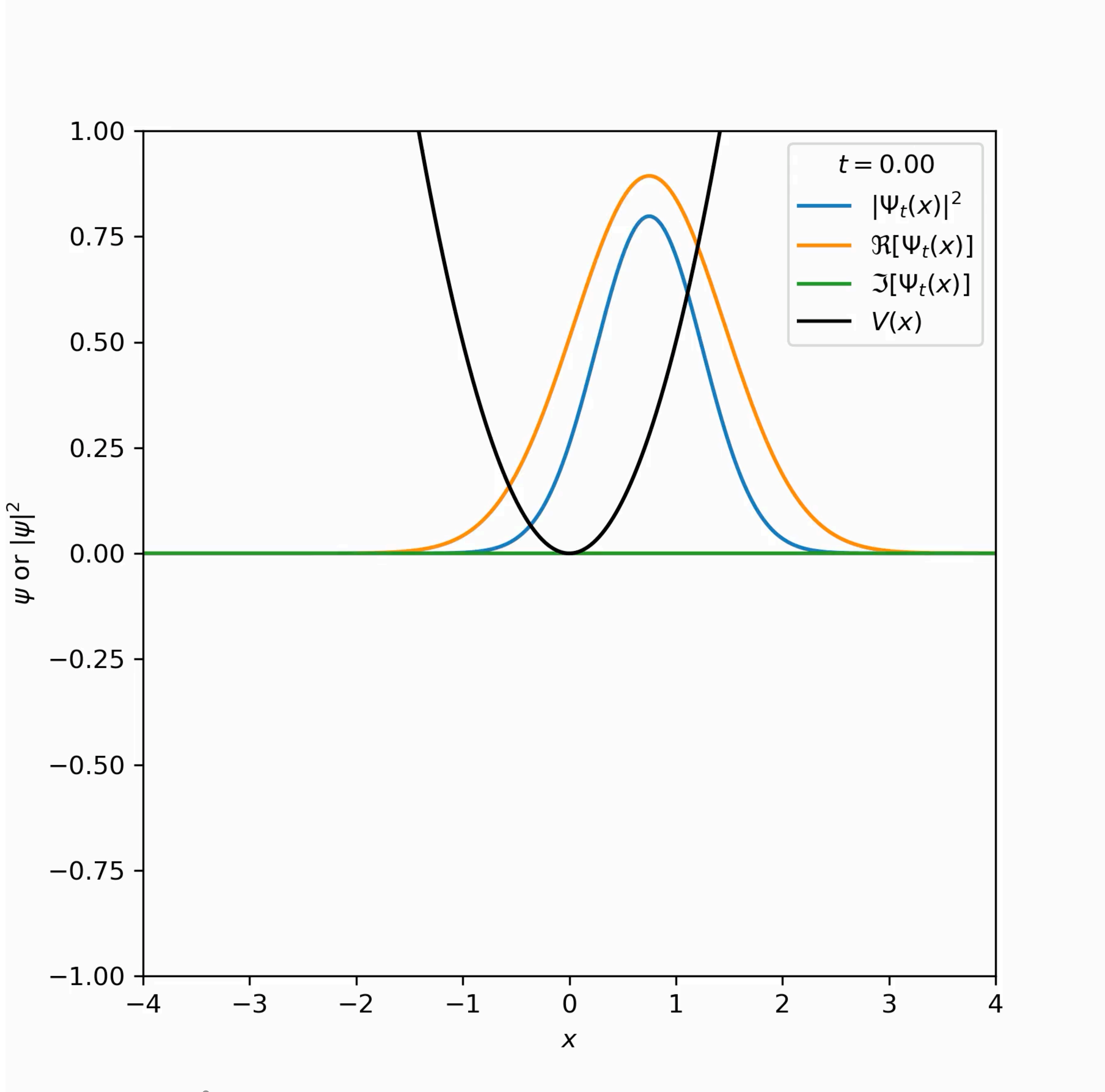
Propagator preview

- Applying composition N times:

$$K(x_N, t_N; x_1, t_1) = \int \cdots \int\int K(x_N, t_N; x_{N-1}, t_{N-1}) \cdots K(x_3, t_3; x_2, t_2) K(x_2, t_2; x_1, t_1)\, dx_2\, dx_3 \cdots dx_{N-1}$$

- Very high dimensional integral!
  We can use **Monte Carlo** methods
  to perform this integration

- Using this approach, you will solve the
  quantum harmonic oscillator
  (assignment 1)



Additional reading

- Feynman Lectures Vol. III, chapters 1–3
- Feynman–Hibbs, chapters 2–3