

Big idea #1: Quantum mechanics explains light/matter interactions and the behavior of small objects more effectively than classical mechanics. Quantum mechanics is fundamentally different from classical mechanics in that the state of an object is described by a wavefunction, not just vectors.

Learning target: At the beginning of the 20th century, matter was seen as consisting of particles, and light was seen as consisting of waves.

Sample success criteria:

- Given the wavelength or frequency of an electromagnetic wave, find the other. Identify which region of the electromagnetic spectrum the wave is in (from a figure – don't memorize).

Learning target: In order to explain experiments – the behavior of blackbodies, the photoelectric effect, and the emission spectra of atoms – light, in addition to being wave-like, is also appropriately viewed as packets of energy called photons.

Sample success criteria:

- Explain how the concept of quantized energy rationalizes the behavior of blackbodies.
- Given the workfunction of a metal and the wavelength of an incoming photon, predict whether electrons are ejected from the surface of the metal, and if so, what their speed is.
- Given a wavelength of light emitted by an atom, find the energy difference between two orbits in the Bohr model of the atom.

Learning target: In order to explain other experiments (e.g., electron diffraction), matter at the small scale should also be seen as having a particle/wave duality.

Sample success criteria:

- Use the de Broglie relation to explain which types of objects – heavy or light – have a large wavelength (i.e., significant uncertainty in their position).

Learning target: Because matter is inherently wave-like, classical mechanics is incomplete. In the more complete set of rules (quantum mechanics), the position and momentum of an object are described by a wavefunction. The probability of finding an object at a given point is proportional to the square of its wavefunction.

Sample success criteria:

- Normalize a given wavefunction, and find the probability that its position will be measured in a specified region of space.
- Describe what it physically means for a wavefunction to have a node, and how this contradicts our intuition of how objects move around in space.

Big idea #2: Every observable property (position, momentum, energy, etc.) corresponds to a mathematical operator, and the possible outcomes of a measurement are the eigenvalues of that operator. The eventual outcome can be predicted only in terms of probabilities.

Learning target: For an operator \hat{A} , the eigenfunctions ψ and eigenvalues a are the functions and values that satisfy the equation $\hat{A}\psi = a\psi$.

Sample success criteria:

- For a given operator \hat{A} , determine whether a function ψ is an eigenfunction of \hat{A} . If so, find the corresponding eigenvalue.

Learning target: Every observable property (position, momentum, energy, etc.) corresponds to a mathematical operator. (The energy operator is called the Hamiltonian operator.) Possible outcomes of a measurement are the eigenvalues of that operator.

Sample success criteria:

- Recognize common quantum mechanical operators (position, momentum, energy).
- Given the numerical eigenvalues of an operator, predict the possible values of a measurement of the corresponding property.

Learning target: If the wavefunction ψ is already an eigenfunction of a given property, the result of a measurement of that property is (with 100% probability) the eigenvalue corresponding to ψ .

Sample success criteria:

- For a property corresponding to operator \hat{A} , predict the outcome when that property is measured for an object in wavefunction ψ (which happens to be an eigenfunction of \hat{A}).

Learning target: If the wavefunction ψ is not an eigenfunction of a given property, the possible results of a measurement of that property (predictable only in terms of probability) are the eigenvalues corresponding to the eigenfunctions that comprise ψ . The process of measurement causes ψ to collapse to an eigenfunction.

Sample success criteria:

- If told that wavefunction ψ is a sum of eigenfunctions ($\psi = a\psi_a + b\psi_b + \dots$), predict the possible outcomes of a measurement and their respective probabilities. Describe what happens to ψ when the property is measured.

Learning target: This set of rules carries surprising implications. Measurement in quantum mechanics changes the state of an object, and certain pairs of properties cannot be known simultaneously.

Sample success criteria:

- Calculate the commutator of two properties (e.g., position and momentum), and describe the physical implications of the result.

Big idea #3: For a given potential energy environment (particle in a box, hydrogen atom, etc.), one can solve the Schrödinger equation to find the possible outcomes of an energy measurement and the corresponding wavefunctions.

Learning target: The particle in a box is a model for translational motion in a confined space. The potential energy operator $V(x)$ is flat inside the box and infinite outside the box. Energies are quantized, while wavefunctions are sine functions that reach zero at the edges of the box.

Sample success criteria:

- State the relationship between quantum number n and the number of nodes in a wavefunction. Sketch wavefunctions for several values of n .
- Explain how the quantization of energy arises from the boundary conditions of the box.
- Determine what particle masses and box sizes (large or small) lead to energy levels that are farthest apart.
- Determine whether energy levels for the particle in a box are equally spaced, or whether they get closer together or farther apart as levels get higher.

Learning target: The harmonic oscillator is a model for vibrational motion. The potential energy operator $V(x)$ is parabolic, like a classical spring. Energies are quantized, while wavefunctions oscillate and decay toward zero on both sides.

Sample success criteria:

- State the relationship between quantum number ν and the number of nodes in a wavefunction. Sketch wavefunctions for several values of ν .
- Determine what particle masses and spring constants (large or small) lead to energy levels that are farthest apart.
- Determine whether energy levels for the harmonic oscillator are equally spaced, or whether they get closer together or farther apart as levels get higher.

Learning target: The particle on a ring and shell are models for rotational motion. The potential energy operator $V(x)$ is flat, and motion is confined to a path or surface. Energies are quantized, while wavefunctions oscillate and depend on a quantum number or numbers.

Sample success criteria:

- For the particle on a ring and shell, state the relationships between quantum numbers l and m_l and the number of nodes in a wavefunction. Sketch wavefunctions for several values of l and m_l .
- For the particle on a ring and shell, explain how the quantization of energy arises from the continuity of the wavefunction.
- Determine whether energy levels for the particle on a ring and shell are equally spaced, or whether they get closer together or farther apart as levels get higher.

Learning target: The harmonic oscillator and particle on a shell have implications in the peak positions in vibrational and rotational spectroscopy.

Sample success criteria:

- Given a vibration-rotation spectrum of a diatomic molecule, assign initial and final values of ν and J to each peak.
- Use equations to illustrate why the fundamental peaks are approximately equally spaced.

Learning target: Hydrogen orbitals and their energies are solutions to the Schrödinger equation for the Coulombic potential of a point nuclear charge. Each orbital has quantum numbers n , l , and m_l , where the angular portion is the same as a wavefunction for the particle on a shell.

Sample success criteria:

- For a wavefunction to be a valid solution to the Schrödinger equation, state the restrictions on the values of n , l , and m_l .
- Given a mathematical wavefunction, sketch its nodal structure (radial and angular nodes).
- Given a mathematical wavefunction, determine its most probable position and radius of an electron.
- Given a picture of an orbital, determine the values of quantum numbers n and l .

Big idea #4: Trends in the periodic table and chemical reactivity arise from the laws of quantum mechanics.

Learning target: When a chemical system has more than one electron, the Schrödinger equation cannot be solved exactly. However, reasonable approximations can be made, and multi-electron orbitals qualitatively resemble hydrogen orbitals.

Sample success criteria:

- Explain in words how 1) the variational method and 2) perturbation theory can be used to find the approximate orbitals and energies of a multi-electron atom.

Learning target: The four quantum numbers (n , l , m_l , and spin quantum number m_s) fully specify the state of an electron within an atom or ion. The Pauli exclusion principle and Aufbau principle allow us to build up the ground-state electron configurations of multielectron atoms and ions.

Sample success criteria:

- Write the ground-state electron configuration of a specified atom or ion.
- To the extent that it is possible, determine the quantum numbers of an electron in a specified orbital.

Learning target: From electron configurations and electrostatic arguments, one can rationalize observed elemental trends such as atomic size, ionization energy, and electron affinity.

Sample success criteria:

- Explain in words why helium is the smallest neutral atom, helium has the highest ionization energy, and fluorine has the highest electron affinity.

Learning target: Valence-bond theory and molecular orbital theory determine the locations and energies of electrons with different levels of abstraction, detail, and accuracy. Molecular orbital theory is rooted in quantum mechanics, so it is the one we focus on in this course.

Sample success criteria:

- Weigh the pros and cons of illustrating a bonding pair of electrons as a line between two atoms (valence-bond theory) versus a filled bonding molecular orbital (molecular orbital theory).

Learning target: One can (approximately) solve the Schrödinger equation for a system with multiple nuclei, to find the orbitals and energy levels of a molecule. This is easiest to do for H_2 .

Sample success criteria:

- Draw a molecular orbital diagram for H_2 . Sketch pictures of the orbitals in your diagram, and fill in the appropriate number of electrons. Determine the bond order, showing that it is consistent with a Lewis structure.
- Using a molecular orbital diagram, explain why helium atoms tend not to form bonds with each other.

Learning target: With some approximations, molecular orbital theory helps us to gain insight into homonuclear and heteronuclear diatomic molecules: σ versus π bonds, bond order, magnetism, etc.

Sample success criteria:

- Draw a molecular orbital diagram for O_2 . Sketch pictures of the orbitals in your diagram, label them according to their σ/π and bonding/antibonding character, fill in the appropriate number of electrons, and classify the molecule as paramagnetic or diamagnetic. Determine the bond order, showing that it is consistent with a Lewis structure.

Learning target (probably in 462): Further simplifications (e.g., Hückel theory) make it possible to wrap our minds around the orbitals and energy levels of polyatomic molecules.

Sample success criteria:

- Write the Hückel Hamiltonian matrix of a conjugated hydrocarbon such as benzene.
- Given a Hückel Hamiltonian matrix, draw the Lewis structure of the corresponding molecule.
- Given the eigenvalues and eigenfunctions of a Hückel Hamiltonian matrix, draw a π molecular orbital diagram, including sketches of the orbitals.