4.S: Quantum Mechanics (Summary)

Key Terms

anti-symmetric function	odd function
Born interpretation	states that the square of a wave function is the probability density
complex function	function containing both real and imaginary parts
Copenhagen interpretation	states that when an observer *is not* looking or when a measurement is not being made, the particle has many values of measurable quantities, such as position
correspondence principle	in the limit of large energies, the predictions of quantum mechanics agree with the predictions of classical mechanics
energy levels	states of definite energy, often represented by horizontal lines in an energy “ladder” diagram
energy quantum number	index that labels the allowed energy states
energy-time uncertainty principle	energy-time relation for uncertainties in the simultaneous measurements of the energy of a quantum state and of its lifetime
even function	in one dimension, a function symmetric with the origin of the coordinate system
expectation value	average value of the physical quantity assuming a large number of particles with the same wave function
field emission	electron emission from conductor surfaces when a strong external electric field is applied in normal direction to conductor’s surface
ground state energy	lowest energy state in the energy spectrum
Heisenberg’s uncertainty principle	places limits on what can be known from a simultaneous measurements of position and momentum; states that if the uncertainty on position is small then the uncertainty on momentum is large, and vice versa
infinite square well	potential function that is zero in a fixed range and infinitely beyond this range
momentum operator	operator that corresponds to the momentum of a particle
nanotechnology	technology that is based on manipulation of nanostructures such as molecules or individual atoms to produce nano-devices such as integrated circuits
normalization condition	requires that the probability density integrated over the entire physical space results in the number one
odd function	in one dimension, a function antisymmetric with the origin of the coordinate system
position operator	operator that corresponds to the position of a particle
potential barrier	potential function that rises and falls with increasing values of position
principal quantum number	energy quantum number
probability density	square of the particle’s wave function

quantum dot	small region of a semiconductor nanocrystal embedded in another semiconductor nanocrystal, acting as a potential well for electrons
quantum tunneling	phenomenon where particles penetrate through a potential energy barrier with a height greater than the total energy of the particles
resonant tunneling	tunneling of electrons through a finite-height potential well that occurs only when electron energies match an energy level in the well, occurs in quantum dots
resonant-tunneling diode	quantum dot with an applied voltage bias across it
scanning tunneling microscope (STM)	device that utilizes quantum-tunneling phenomenon at metallic surfaces to obtain images of nanoscale structures
Schrödinger's time-dependent equation	equation in space and time that allows us to determine wave functions of a quantum particle
Schrödinger's time-independent equation	equation in space that allows us to determine wave functions of a quantum particle; this wave function must be multiplied by a time-modulation factor to obtain the time-dependent wave function
standing wave state	stationary state for which the real and imaginary parts of Ψ(x,t)Ψ(x,t) oscillate up and down like a standing wave (often modeled with sine and cosine functions)
state reduction	hypothetical process in which an observed or detected particle "jumps into" a definite state, often described in terms of the collapse of the particle's wave function
stationary state	state for which the probability density function, $\lvert\Psi(x,t)\rvert^2$, does not vary in time
time-modulation factor	factor $e^{-i\omega t}$ that multiplies the time-independent wave function when the potential energy of the particle is time independent
transmission probability	also called tunneling probability, the probability that a particle will tunnel through a potential barrier
tunnel diode	electron tunneling-junction between two different semiconductors
tunneling probability	also called transmission probability, the probability that a particle will tunnel through a potential barrier
wave function	function that represents the quantum state of a particle (quantum system)
wave function collapse	equivalent to state reduction
wave packet	superposition of many plane matter waves that can be used to represent a localized particle

Key Equations

Normalization condition in one dimension	$P(x=-\infty,+\infty)=\int_{-\infty}^{\infty}\mid\Psi(x,t)\mid^2 dx=1$
Probability of finding a particle in a narrow interval of position in one dimension $(x, x+dx)$	$P(x,x+dx)=\Psi^*(x,t)\Psi(x,t)dx$
Expectation value of position in one dimension	$\langle x\rangle=\int_{-\infty}^{\infty}\Psi^*(x,t)x\Psi(x,t)dx$
Heisenberg's position-momentum uncertainty principle	$\Delta x\Delta p\geq\frac{\hbar}{2}$

Heisenberg's energy-time uncertainty principle	$\Delta E\Delta t \geq \frac{\hbar}{2}$
Schrödinger's time-dependent equation	$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+U(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}$
General form of the wave function for a time-independent potential in one dimension	$\Psi(x,t)=\psi(x)e^{-i\omega}$
Schrödinger's time-independent equation	$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$
Schrödinger's equation (free particle)	$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}=E\psi(x)$
Allowed energies (particle in box of length L)	$E_n=n^2\frac{\pi^2\hbar^2}{2mL^2}, n=1,2,3,\ldots$
Stationary states (particle in a box of length L)	$\psi_n(x)=\sqrt{\frac{2}{L}}sin\frac{n\pi x}{L}, n=1,2,3,\ldots$
Potential-energy function of a harmonic oscillator	$U(x)=\frac{1}{2}m\omega^2x^2$
Schrödinger equation (harmonic oscillator)	$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\psi(x)=E\psi(x)$
The energy spectrum	$E_n=(n+\frac{1}{2})\hbar\omega, n=0,1,2,3,\ldots$
The energy wave functions	$\psi_n(x)=N_ne^{-\beta^2x^2/2}H_n(\beta x), n=0,1,2,3,\ldots$
Potential barrier	$U(x)=\begin{cases}0, & \text{when } x<0\\ U_0, & \text{when } 0\leq x\leq L\\ 0, & \text{when } x>L\end{cases}$
Definition of the transmission coefficient	$T(L,E)=\frac{\lvert\psi_{tra}(x)\rvert^2}{\lvert\psi_{in}(x)\rvert^2}$
A parameter in the transmission coefficient	$\beta^2=\frac{2m}{\hbar^2}(U_0-E)$
Transmission coefficient, exact	$T(L,E)=\frac{1}{cosh^2\beta L+(\gamma/2)^2sinh^2\beta L}$
Transmission coefficient, approximate	$T(L,E)=16\frac{E}{U_0}(1-\frac{E}{U_0})e^{-2\beta L}$

Summary

7.1: Wavefunctions

- In quantum mechanics, the state of a physical system is represented by a wave function.
- In Born's interpretation, the square of the particle's wave function represents the probability density of finding the particle around a specific location in space.
- Wave functions must first be normalized before using them to make predictions.
- The expectation value is the average value of a quantity that requires a wave function and an integration.

7.2: The Heisenberg Uncertainty Principle

- The Heisenberg uncertainty principle states that it is impossible to simultaneously measure the *x*-components of position and of momentum of a particle with an arbitrarily high precision. The product of experimental uncertainties is always larger than or equal to $\hbar/2$.
- The limitations of this principle have nothing to do with the quality of the experimental apparatus but originate in the wave-like nature of matter.

- The energy-time uncertainty principle expresses the experimental observation that a quantum state that exists only for a short time cannot have a definite energy.

7.3: The Schrödinger Equation

- The Schrödinger equation is the fundamental equation of wave quantum mechanics. It allows us to make predictions about wave functions.
- When a particle moves in a time-independent potential, a solution of the time-dependent Schrödinger equation is a product of a time-independent wave function and a time-modulation factor.
- The Schrödinger equation can be applied to many physical situations.

7.4: The Quantum Particle in a Box

- Energy states of a quantum particle in a box are found by solving the time-independent Schrödinger equation.
- To solve the time-independent Schrödinger equation for a particle in a box and find the stationary states and allowed energies, we require that the wave function terminate at the box wall.
- Energy states of a particle in a box are quantized and indexed by principal quantum number.
- The quantum picture differs significantly from the classical picture when a particle is in a low-energy state of a low quantum number.
- In the limit of high quantum numbers, when the quantum particle is in a highly excited state, the quantum description of a particle in a box coincides with the classical description, in the spirit of Bohr's correspondence principle.

7.5: The Quantum Harmonic Oscillator

- The quantum harmonic oscillator is a model built in analogy with the model of a classical harmonic oscillator. It models the behavior of many physical systems, such as molecular vibrations or wave packets in quantum optics.
- The allowed energies of a quantum oscillator are discrete and evenly spaced. The energy spacing is equal to Planck's energy quantum.
- The ground state energy is larger than zero. This means that, unlike a classical oscillator, a quantum oscillator is never at rest, even at the bottom of a potential well, and undergoes quantum fluctuations.
- The stationary states (states of definite energy) have nonzero values also in regions beyond classical turning points. When in the ground state, a quantum oscillator is most likely to be found around the position of the minimum of the potential well, which is the least-likely position for a classical oscillator.
- For high quantum numbers, the motion of a quantum oscillator becomes more similar to the motion of a classical oscillator, in accordance with Bohr's correspondence principle.

7.6 The Quantum Tunneling of Particles through Potential Barriers

- A quantum particle that is incident on a potential barrier of a finite width and height may cross the barrier and appear on its other side. This phenomenon is called 'quantum tunneling.' It does not have a classical analog.
- To find the probability of quantum tunneling, we assume the energy of an incident particle and solve the stationary Schrödinger equation to find wave functions inside and outside the barrier. The tunneling probability is a ratio of squared amplitudes of the wave past the barrier to the incident wave.
- The tunneling probability depends on the energy of the incident particle relative to the height of the barrier and on the width of the barrier. It is strongly affected by the width of the barrier in a nonlinear, exponential way so that a small change in the barrier width causes a disproportionately large change in the transmission probability.
- Quantum-tunneling phenomena govern radioactive nuclear decays. They are utilized in many modern technologies such as STM and nano-electronics. STM allows us to see individual atoms on metal surfaces. Electron-tunneling devices have revolutionized electronics and allow us to build fast electronic devices of miniature sizes.
