

A light INTRODUCTION TO QM

When spatial dimensions approach the atomic scale cannot be understood in terms of classical laws. :

- Atoms/molecules and their properties
- chemical bond
- the motion of charges in a crystal
- phonon dispersion relations

Moreover, many phenomena exhibited on a macroscopic scale reveal underlying quantum phenomena.

A transition then occurs from the classical laws to the quantum-mechanical laws of physics.

Quantum mechanics is therefore the basis of our present understanding of all natural phenomena studied and exploited in chemistry, biology, physics, materials science, engineering, etc.

➤ **Physical behaviour at the nanoscale is accurately predicted by quantum mechanics, as represented by the **Schrödinger Equation**, which therefore provides a quantitative understanding of the properties of low-dimensional structures.**

The Schrödinger Equation

The wave function of an uncharged particle with no spin satisfies the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right) \psi(\vec{r}, t) = i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t},$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator, $i = \sqrt{-1}$, and $V(\vec{r}, t)$ is the spatiotemporally varying potential influencing the particle's motion. The particle's mass m in the equation has to be carefully handled. For a particle (electron or hole) in a solid, this mass is its effective mass m , which is usually less than the mass of an isolated electron. In the above equation the action of Hamiltonian operator

$H(\vec{r}, t) \equiv -\hbar^2 / 2m \nabla^2 + V(\vec{r}, t)$ on the wave function yields the total energy of the particle. The first part of $H(\vec{r}, t)\psi(\vec{r}, t)$ is the kinetic energy, and the second part is the potential energy. For many real systems, the potential does not depend on time, ie $V(\vec{r}, t) = V(\vec{r})$. Then, the dependences on time and spatial coordinates of $\psi(\vec{r}, t)$ are separated as

$$\psi(\vec{r}, t) = \text{Re} \left[e^{-iEt/\hbar} \psi(\vec{r}) \right],$$

Where $\psi(r)$ is a complex-valued function of space only, and E is the energy of the system. Using this representation of the wave function in the Schrödinger equation, the time harmonic Schrödinger equation is obtained and can be written as,

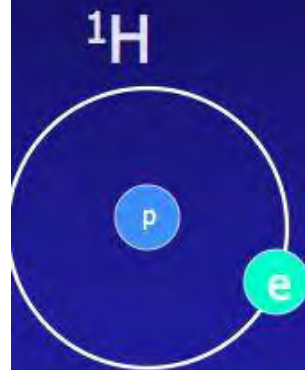
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r}) = E\psi(\vec{r}) \quad (4)$$

Analytical solutions of the time-harmonic Schrödinger equation can be obtained for a variety of relatively simple conditions. These solutions provide an insight into the nature of quantum phenomena and sometimes provide a reasonable approximation of the behaviour of more complex systems—e.g., in statistical mechanics, molecular vibrations are often approximated as harmonic oscillators. Several of the more common analytical solutions are for a free (isolated) particle: a particle in a box, finite potential well, 1D lattice, ring, or spherically symmetric potential; the hydrogen atom or hydrogen-like atom; the quantum harmonic oscillator; the linear rigid rotor; and the symmetric top.

- For many systems, however, there is no analytic solution to the Schrödinger equation, and the use of approximate solutions becomes necessary. Some commonly used numerical techniques are: perturbation theory, density functional theory, variational methods (such as the popular Hartree–Fock method which is the basis of many post-Hartree–Fock methods), quantum Monte Carlo methods, the Wentzel–Kramers–Brillouin (WKB) approximation, and the discrete delta- potential method.

! Solving the Schrödinger Equation for the Hydrogen Atom !

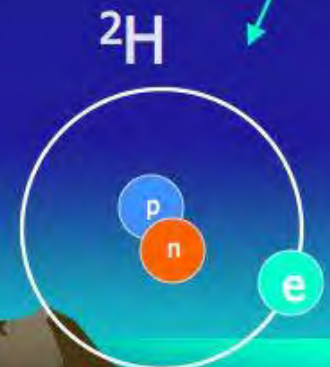
The Hydrogen Atom



- One electron orbiting a nucleus
- 1 proton = Z = atomic number
- Total mass = $A = Z + N = 1$
- Add a neutron and you have Deuterium = ${}^2\text{H} = \text{D}$



A water molecule



THE WAVE FUNCTION

In the Schrödinger description of quantum mechanics, an elementary particle - electron, a hole and a photon or even a physical system such as an atom is described by a wave function $\Psi(\mathbf{r}, \mathbf{t})$, which depends on the variables describing the degrees of freedom of the particle system.

The **square of the wave function** is interpreted as the **probability** of finding a particle at spatial location $\mathbf{r} = (\mathbf{x}, \mathbf{y}, \mathbf{z})$ and instant of time \mathbf{t} .

The wave function **contains all the information** that may be obtained about a physical entity and is sufficient to describe a particle or system of particles.



Example: If the wave function of an ensemble of electrons in a device, is known, it is possible in principle to calculate all the macroscopic parameters that define the electronic performance of that device.



Quantum Conductance

WHY Wave Function?

A basic characteristic of all matter at the atomic/ nanoscale is the manifestation of the **wave–particle duality**—a fundamental quantum-mechanical principle that states that all matter (electrons, nuclei, photons, etc.) behaves as both waves and particles.

What is the scale reference?

The quantum effects of confinement become significant when at least one of the **dimensions of a structure is comparable in length to the de Broglie wavelength**. If at least one dimension of a solid is comparable to the de Broglie wavelength of the particle, a quantum-mechanical treatment of particle motion becomes necessary.

In quantum mechanics, the trajectory of a moving particle loses its meaning when the **distance over which potential energy varies** is on the order of the **de Broglie wavelength**.

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m^*E}} = \lambda_o \sqrt{\frac{m_o}{m^*}} \longrightarrow \lambda_{\text{deB}} \sim \frac{h}{\sqrt{mk_{\text{B}}T}}$$

Exercise 1: Deriving the de Broglie wavelength of a particle

De Broglie derived his equation using well established theories through the following series of substitutions. de Broglie first used Einstein's famous equation relating matter and energy:

$$E = mc^2, \quad E = \text{energy}, \quad m = \text{mass}, \quad c = \text{speed of light}$$

Using Planck's theory which states every quantum of a wave has a discrete amount of energy given by Planck's equation:

$$E = h\nu, \quad E = \text{energy}, \quad h = \text{Plank's constant } (6.62607 \times 10^{-34} \text{ J s}), \quad \nu = \text{frequency}$$

Since de Broglie believed particles and wave have the same traits, he hypothesized that the two energies would be equal: **$mc^2 = h\nu$**

Because real particles do not travel at the speed of light, De Broglie submitted velocity (v) for the speed of light (c): **$mv^2 = h\nu$**

de Broglie substituted v/λ for ν and arrived at the final expression that relates wavelength and particle with speed: **$mv^2 = h\nu/\lambda \Rightarrow$**

$$\lambda = h\nu/mv^2 = h/mv$$

Solving the Schrödinger Equation for QUANTUM WELLS

There are 2 approaches. The simplest approach is the infinite well model and the real approach is the finite well. The Schrödinger equation in the well is for each case:

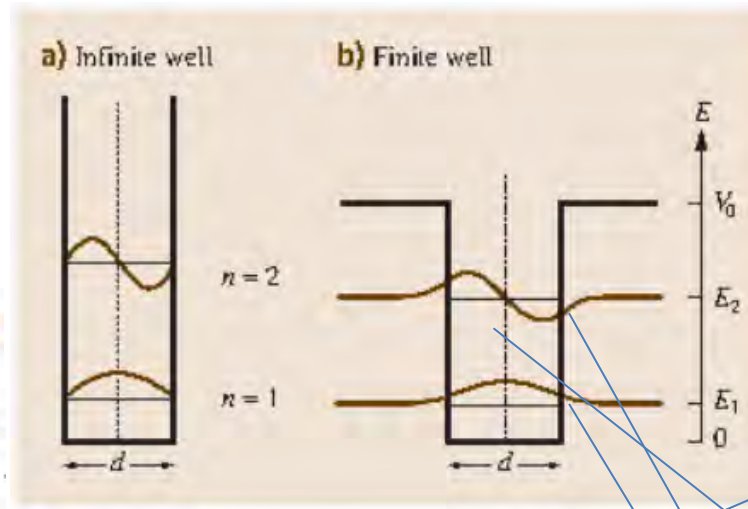
Infinite Well

$$-\frac{\hbar^2}{2m_w^*} \frac{d^2\psi(z)}{dz^2} = E\psi(z)$$

$$\psi_n(z) = \sqrt{\frac{2}{d}} \sin k_n z$$

$$k_n = (n\pi/d)$$

$$E_n = \frac{\hbar^2 k_n^2}{2m_w^*} = \frac{\hbar^2}{2m_w^*} \left(\frac{n\pi}{d}\right)^2$$



Finite Well

$$-\frac{\hbar^2}{2m_b^*} \frac{d^2\psi(z)}{dz^2} + V_0\psi(z) = E\psi(z)$$

$$\tan\left(\frac{kd}{2}\right) = \frac{m_w^* \kappa}{m_b^* k}$$

and

$$\tan\left(\frac{kd}{2}\right) = -\frac{m_b^* k}{m_w^* \kappa}$$

V_0 is the potential barrier and m_b^* is the effective mass in the barrier.

The boundary conditions require that the wave function and particle flux $(1/m^*)d\psi/dz$ must be continuous at the interface. This gives a series of even and odd parity solutions that satisfy these conditions.

inside

$$\frac{\hbar^2 k^2}{2m_w^*} = E_n$$

Exponential decay constant at the barrier.

$$\frac{\hbar^2 \kappa^2}{2m_b^*} = V_0 - E_n$$

Exercise 2: The de Broglie wavelength at a temperature T is approximately given by :
Why?

Answer

Same reasoning as before but now equal to thermal energy.

$$\lambda_{\text{deB}} \sim \frac{h}{\sqrt{mk_{\text{B}}T}}$$

Exercise 3: For an electron in GaAs with an effective mass of $0.067 m_0$, we find $\lambda_{\text{deB}} \approx 42 \text{ nm}$ at 300 K. In order to observe quantum confinement effects at room temperature for this material how thick should the structures be?

Answer

Thickness $\ll 42 \text{ nm}$ / $\sim 20\text{-}10 \text{ nm}$

Exercise 4: As an example, we consider a typical GaAs/Al_{0.3}Ga_{0.7}As QW with $d = 10$ nm. The confinement energy is 245 meV for the electrons and 125 meV for the holes. Determine E_1 and E_2 for electrons and holes in **(a)** Infinite Well model; **(b)** Finite Well model.

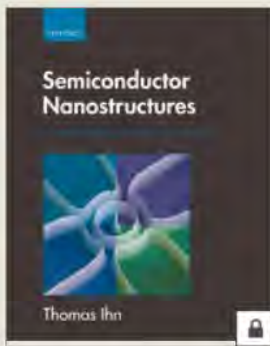
Answers

- (a) Infinite well model predicts $E_1 = 56$ meV and $E_2 = 224$ meV for the electrons, and for the heavy (light) holes, 11 meV (40 meV) and 44 meV (160 meV)
- (b) Finite Well model predicts $E_1 = 30$ meV and $E_2 = 113$ meV for electrons; 7 meV (21 meV) and 29 meV (78 meV) for the heavy (light) holes.

Exercise 5: Are the quantization effects already observed at room temperature?

Answer

$k_B T = 26$ meV at 300 K $\Rightarrow kT < E_1, E_2 \Rightarrow$ the quantization effects will be observable at room temperature.



Semiconductor Nanostructures: Quantum states and electronic transport

Thomas Ihn

ABSTRACT

This book presents the physics of semiconductor nanostructures with emphasis on their electronic transport properties. At its heart are five fundamental transport phenomena: quantized conductance, tunneling transport, the Aharonov–Bohm effect, the quantum Hall effect, and the Coulomb blockade effect. The book starts out with basics of solid state and semiconductor physics, such as crystal structure, band structure, and effective mass approximation, including spin-orbit interaction effects important for research in semiconductor spintronics. It deals with material aspects such as band engineering, doping, gating, and a selection of nanostructure fabrication techniques. The book discusses the Drude–Boltzmann–Sommerfeld transport theory as well as conductance quantization and the Landauer–Büttiker theory. These concepts are extended to mesoscopic interference phenomena and decoherence, magnetotransport, and interaction effects in quantum-confined systems, guiding the reader from fundamental effects to specialized state-of-the-art experiments.

Keywords: semiconductor nanostructures, electronic transport, quantized conductance, tunneling transport, Aharonov–Bohm effect, quantum Hall effect, Coulomb blockade effect, spintronics

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Full Quantum description of Semiconductor Physics

