Fundamentals of Quantum Theory

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If you are not confused by quantum physics then you haven't really understood it

—Niels Bohr

We live in a macroscopic world surrounded by macroscopic objects, which adhere to the laws of classical mechanics and are very comfortable with it. From the trajectory of a humble pebble thrown into a pond and the ripples thus created by it, to the motion of the great planets can all be quite satisfactorily explained within the domain of classical physics.

However, apart from this macroscopic scale, there exist numerous other phenomena around us, especially on the microscopic scale, which seem to defy most conventional "common-sense" beliefs. The key to the understanding of the workings of this amazing microscopic world lies with quantum physics.

According to classical physics and also our everyday understanding a ping-pong ball thrown at a brick wall has absolutely no chance of somehow "magically" going through it and re-appearing on the other side. However in the world of quantum mechanics the almost analogous event of an electron incident upon an energy barrier, does have a finite non-zero probability of appearing on the other side of the barrier (not by some "magic" but rather by a commonplace quantum phenomena called tunneling). What may seem rather absurd (sometimes bordering on ridiculous) in the macroscopic world may be a very common phenomena in the quantum domain.

1 Origins of Quantum Physics

At the beginning of the twentieth century three major issues stood in front of the scientific community that could not be properly explained within the framework of classical physics. First there was the Blackbody radiation problem, which could not

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be satisfactorily explained by the Rayleigh-Jeans law, especially for high frequencies (the so called "UV catastrophe"). Then there was the photo-electric effect, where the stopping potential for photo-current (electron emission) from an irradiated emitter was found to be dependent on frequency rather than intensity. This was contrary to the classical predictions that for the same frequency higher intensities should produce a higher stopping potential. Thirdly there was the Compton shift, where monochromatic X-rays scattered by a material block always seemed to shift by a certain discrete amount (for a fixed angle of incidence). All these seemed to vaguely point that energy emitted or absorbed in these processes were somehow related to the frequency.

The existence of such fixed amounts of energy or 'quanta of energy' was proposed by Max Planck in his theory of blackbody radiation to successfully explain the radiation spectra. Also in the theory of specific heat of solids, Einstein had considered oscillators vibrating at fixed frequencies to successfully explain the variation of specific heats of solids over a wide range of temperature. Another proof of energy quantization (i.e. having specific discrete levels or 'states' of energy in a system) was given by the success of the Bohr model of the Hydrogen atom. All these theories and experimental evidences were combining to pave the way towards a new theory.

2 The Wave Particle Duality

Between 1924 and 1927 two most significant and very radical ideas emerged, which were to become the cornerstones of what was to emerge as the quantum theory. In 1924 Louis de Broglie, in his thesis titled *Recherches sur la théorie des quanta* proposed the wave-particle duality, a revolutionary concept that hypothized the association of any material particle with an associated matter wave and vice-a-versa.

According to de Broglie hypothesis a material particle travelling with momenta p is associated with a matter-wave of wavelength λ as

$$\lambda = \frac{h}{p} \tag{1}$$

This is also in corroboration with the dual nature of light as observed by various experiments. While classical experiments like the Young's double slit experiment demonstrated the wave nature of light which is responsible for diffraction and interference, the works by Einstein on the photo electric effect is hard evidence of particle nature of light (the particle associated with light energy being known as the photon). In this regard it would be relevant to mention that in 1660–1675 first Pierre Gassendi and thereafter Sir Isaac Newton had hypothized light to be made up of particles (termed as 'corpuscules' by Newton). These ideas had been discarded in favor of the wave theory, which envisioned light to propagate as mechanical waves

through a 'luminiferous aether' medium. The existence of the aether was discarded after the famous Michelson-Morely experiment in 1887. With the subsequent discovery of photo-electric effect in 1887 by Heinrich Hertz and its successful theoretical explanation in 1905 by Albert Einstein, the particle theory of light was revived in a whole different avatar and the dual-nature of light emerged.

3 The Uncertainty Principle

In 1927, Werner Heisenberg put forward his uncertainty principle which put rather simply states that there exists a fundamental limit of precision, to which extent specific pairs of complementary variables (also known as canonically conjugate variables) such as position and momenta can be simultaneously measured. To put it mathematically in the form of an equality, let us consider a simultaneous measurement of the position x and the momenta p of a particle. Then Heisenberg's uncertainty principle states that the uncertainty or error in the measurement of position (say Δx) and that of momentum (Δp) must be such that

$$\Delta x \Delta p \geq h \tag{2}$$

This error in measurement is a fundamental limit in nature itself and cannot be improved upon.

These two basic postulates of quantum mechanics can be correlated in a very interesting way. Let us consider a microscopic particle moving around freely in space and an observer equipped with a powerful microscope who is looking for it. Now we consider energetic photons colliding with the target particle and being reflected back into the microscope thus giving out the position of the particle. Now if a sole photon of wavelength λ were to collide with the particle, then according to de Broglie hypothesis the change in the momentum of the particle should be of the order of the photon momentum which is $p = h/\lambda$. Also considering the wavelength of the photon, the uncertainty in position should also be $\geq \lambda$. Which implies the product of the two uncertainties should be $\geq h$, which is essentially Heisenberg's uncertainty principle. Now if we look to minimize our error in measurement of position by minimizing lambda (say the hypothetical gamma-ray microscope) we would measure position much more accurately but in the process sacrifice accuracy in measuring the momenta.

4 The Wave Packet and the Wave Function Ψ

Now if we look to associate microscopic particles with a matter wave then we are to require a mathematical expression or simply a wave function which we call Ψ. This function is required to have both spatial and temporal dependence and therefore

$$\Psi(\vec{r},t) = \psi(\vec{r})\exp(-i\omega\cdot t) \tag{3}$$

For the 1-dimensional case this reduces to

$$\Psi(x,t) = \psi(x)\exp(-i\omega\cdot t) \tag{4}$$

With this wave function Ψ, we represent the matter wave associated with the microscopic particle under consideration. Now consider a wave group or a "wave packet" associated with a particle, which is this wave function Ψ confined in a small region of space. As a wave packet could be considered to be made by the superposition of a number of plane waves with infinitesimally differing k-values (wave vector) we could consider

$$\Psi(\vec{r},t) = \sum_{n=1}^{\infty} c_n(k)\Psi_n(\vec{r},t) \tag{5}$$

where $c_n(k)$ is the corresponding normalizing constant.

Now if we are to know the exact position of the particle within that wave packet then a narrower wave group (i.e. a smaller λ) would suit us better. But if λ becomes small, then the error in determining the momenta increases as $p = h/\lambda$ according to de Broglie hypothesis. Thus the concept of wave packets is consistent with Heisenberg's uncertainty principle as well.

As for the position of the particle, it may be considered that the particle is most likely to be at the center of the wave packet, but the probability of its existence in other regions of the wave packet are essentially non-zero. The probability of finding the particle at any particular position x is given by the quantity $\Psi^*\Psi$. Also since the particle does indeed exist, thus we could have the condition

$$\int_{-\infty}^{+\infty} \Psi^*\Psi \mathrm{d}\tau = 1 \tag{6}$$

which is famously known as the normalization condition. This essentially means that the probability of finding the particle over $-\infty$ to $+\infty$ is essentially 1. $\mathrm{d}\tau$ is a volume ensemble.

Another important quantity known as the probability current density is given by

$$J(\vec{r},t) = \frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi) \tag{7}$$

The significance of this quantity is the particle number conservation, (7) essentially means that if the probability of finding the particle increases in a specific region of space, then in other regions this probability must decrease.

The function Ψ should also fulfill the following conditions

1. It must be a finite and single valued function. This is essential because if the wave function is infinite then the probability of the finding the particle also becomes infinite which is impossible. Also the single valued-ness is essential so as to eliminate the un-physical concept that the particle has two different probabilities of existing at the same point.
2. The derivative of Ψ should be single valued and continuous. This is quite like the boundary conditions in electromagnetics where the derivative of the potential is considered continuous to properly account for interfaces and boundaries of different media. This is also true in most cases of quantum mechanical potential berries and finite wells. Even in the case of a particle confined within an infinite potential well there exists a small trailing edge of the wavefunction beyond the boundaries of the well.
3. $\Psi \to 0$ when $r \to \pm\infty$, which ensures $\int |\Psi|^2 \mathrm{d}\tau$ to be finite over all space.

With the rules of the game now laid down, we proceed to the equation that would describe the dynamics of the microscopic particle in the quantum realm, which is in fact the famous Schrödinger equation.

5 The Schrödinger Equation

It would be useful if we just recollect a little bit of operator algebra. Say we have a function $f(x)$ and an operator $\widehat{\Theta}$, and the operation be expressed as

$$\widehat{\Theta} f(x) = \alpha f(x) \tag{8}$$

then $f(x)$ is known as the eigenfunction of the operator $\widehat{\Theta}$, and α the eigenvalue of the same. In case of quantum mechanics, the measurement of any dynamical quantity g_n can be made from the wave function by means of an operation by a suitable operator $\widehat{\Gamma}$ corresponding to that quantity g_n.

$$\widehat{\Gamma}\Psi_n = g_n \Psi_n \tag{9}$$

Ψ_n is known as the eigenstate of the system and g_n the corresponding eigen-value. Now g_n can be various dynamical variable, depending on the operator $\widehat{\Gamma}$. We could measure quantities like position, momenta, energy, angular momenta etc. of the system by choosing suitable operators, as we shall soon see.

Another important thing that should be noted is that, as soon as we make a measurement on the system and find a particular eigenstate, the whole system collapses to that particular eigenstate. Any further measurements also give the same eigenvalue for the given operator.

Now in order to have a proper wave equation, we expect it to be a linear differential equation in $\Psi(\vec{r},t)$, as the wave function must be linear to preserve the superposition of waves. The equation should not also contain any dynamical variable so that we may continue to get wave functions of the packet corresponding to different dynamical variables. Also as a requirement, for a free particle the solution of the said equation should correspond to infinite plane waves. This is represented by

$$\Psi(\vec{r},t) = A(k)\exp\left\{i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right\} \tag{10}$$

From this plane wave function we can find out the energy and momentum operators easily. For this we use the wave vector k may be expressed as $k = p/\hbar$. Also from Einstein's theory of photo-electric emission the energy quanta for a radiation of frequency is given by $E = hv$ which gives, $\omega = \frac{E}{\hbar}$. Thus differentiating (10) w.r.t. time we find

$$\begin{aligned}\frac{\partial\Psi(x,t)}{\partial t} &= -\frac{i}{\hbar}E\cdot A\exp\left\{\frac{i}{\hbar}(px-Et)\right\}\\ &= -\frac{i}{\hbar}E\cdot\Psi(x,t)\end{aligned} \tag{11}$$

Equation (10) gives us the energy operator

$$\widehat{E} = i\hbar\frac{\partial}{\partial t} \tag{12}$$

With this operator the energy eigenvalue of a corresponding energy eigenstate can be found out. Similarly it is possible to find out the momentum operator form (10) by differentiating w.r.t. x as

$$\widehat{p} = -i\hbar\frac{\partial}{\partial x} \tag{13}$$

By taking the second derivative of (10) w.r.t. x, and rearranging and dividing by $2m$, we arrive at

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} &= \frac{p^2}{2m}\Psi(x,t)\\ &= E\Psi(x,t)\end{aligned} \tag{14}$$

thereafter using (11) we arrive at

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t} \tag{15}$$

In 3-dimensions this could be extended to

$$\nabla^2\Psi(\vec{r},t)+\frac{2mE}{\hbar^2}\Psi(\vec{r},t)=0 \tag{16}$$

this is the simplest form of the time dependent Schrödinger equation. If there exists a force field in which the particle is moving then the Schrödinger equation is modified to a more general form. The total potential associated with the field $V(x)$ adds to the energy $E=\frac{p^2}{2m}$ in this case and thus

$$E=\frac{p^2}{2m}+V(\vec{r},t) \tag{17}$$

Which combined with (16) leads to

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r},t)\right]\Psi(\vec{r},t) \tag{18}$$

From (18), we may define an operator which is known as the Hamiltonian operator or simply the Hamiltonian $\hat{H}$ of the system given by

$$\hat{H}=-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r},t) \tag{19}$$

The general form of (18) is written as

$$\nabla^2\Psi(\vec{r},t)+\frac{2m}{\hbar^2}[E-V(\vec{r},t)]\Psi(\vec{r},t)=0 \tag{20}$$

The Eq. (20) is known as the time dependent Schrödinger equation. In many cases the Hamiltonian may not explicitly depend on time, and for such cases V is a function of position only. In such cases the time independent form of the Schrödinger equation is used, which is

$$\nabla^2\psi(\vec{r})+\frac{2m}{\hbar^2}[E-V(\vec{r})]\psi(\vec{r})=0 \tag{21}$$

In $\psi(\vec{r})$ is the position dependent part of the wave function

$$\Psi(\vec{r},t)=A(k)\psi(\vec{r})\exp\left(-\frac{iEt}{\hbar}\right) \tag{22}$$

6 The Expectation Value

The solution of Schrödinger equation gives us results for various parameters of the system within the limits of the uncertainty principle. The quantities that result from a measurement performed are probabilities rather than exact values. Thus we consider the expectation value of a certain parameter, say position, which is like the average value of position obtained for a large number of particles described by the same wave function at a certain instant of time.

The expectation value of a certain quantity g associated with an operator $\hat{\Gamma}$ is defined as

$$\langle g \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{\Gamma} \Psi \mathrm{d}\tau \tag{23}$$

This indicates that at a certain instant of time t if we make a substantially large number of measurements over the wavefunction in order to extract the value of the quantity g (which could be position, momentum, energy etc.) we are most likely to arrive at this particular value of g, which is thus known as the expectation value.

Thus depending upon the quantity for which the measurement is made, the expectation value is determined with the suitable operator. Let us take the case of position for example. Let the probability of finding a particle at a position x_j in the interval $\mathrm{d}x$ be given by P_j, thus

$$P_j = \left|\Psi(x_j)\right|^2 \mathrm{d}x \tag{24}$$

For a large number measurements, the expectation value would be

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x|\Psi|^2 \mathrm{d}x}{\int_{-\infty}^{+\infty} |\Psi|^2 \mathrm{d}x} \tag{25}$$

If Ψ is a normalized wave function then the denominator becomes unity and we have the expectation value for position

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\Psi|^2 \mathrm{d}x \tag{26}$$

Which can be written in as

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{x} \Psi \mathrm{d}x \tag{27}$$

where $\hat{x}$ is the position operator defined as $\hat{x}\Psi = x\Psi$.

7 The Free Particle Solution

The free particle such as an electron moving in free space can be described with the Schrödinger equation (for simplicity let's assume only the x component) as

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\psi = 0 \tag{28}$$

the solution for which is given by

$$\psi(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx} \tag{29}$$

where, $k = \sqrt{\frac{2mE}{\hbar^2}}$. The energy solution for this is given by

$$E = \frac{\hbar^2 k^2}{2m} \tag{30}$$

Which is essentially a parabola. When such an electron is confined within a region of space it can be modeled (ideally) as a particle within a rigid box (an infinite quantum well). Such a quantum well of length L in x direction can be represented by a potential

$$\begin{aligned} V(x) &= 0 \quad \text{for } 0 \le x \le L \\ V(x) &= \infty \quad \text{otherwise} \end{aligned} \tag{31}$$

In such cases, the solution of the Schrödinger equation gives quantized energy levels (as discussed in detail in the next chapter). It can also be elegantly deduced using the basic wave particle duality and the concept of standing matter waves (Fig. 1).

From the wave particle duality $\lambda = h/p$. For the matter waves within the well the situation is analogous to a standing waves in a string whose both ends are tied. For the classical tied string concept we know

$$n\lambda = 2L \tag{32}$$

n represents the mode of the vibration $(n = 1, 2, 3\ldots)$. Further if we consider the particle nature we know kinetic energy $E_\mathrm{K} = \frac{p^2}{2m}$. Which is the total energy in this case as inside the well $V(x) = 0$. Thus in terms of de Broglie wavelength of the particle we may write the energy of the

$$E_n = \frac{h^2}{2m\lambda^2} = \frac{n^2h^2}{8mL^2} \tag{33}$$

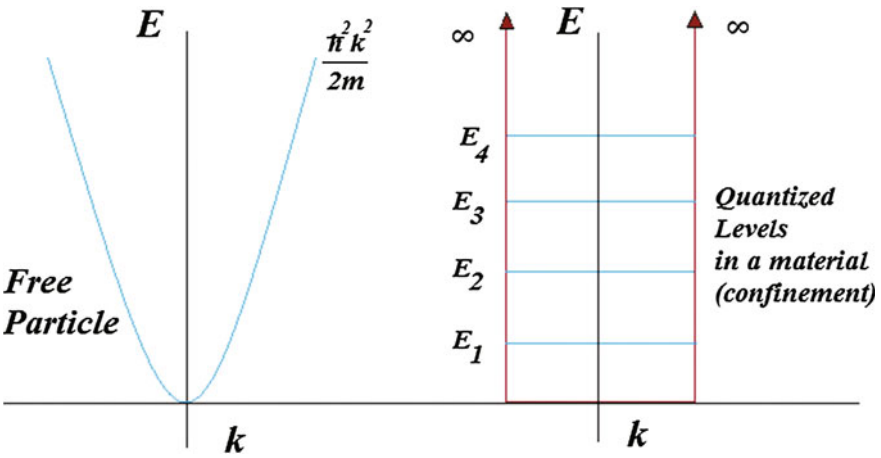


Fig. 1 The continuous energy solution for a free particle (such as electron in free space) becomes discrete energy levels for a confined system (such as an electron inside an infinite quantum well)

for $n = 1, 2, 3\ldots$. So we see how confining the electron within a rigid box can lead to the so-called energy quantization, which is a very fundamental concept in quantum mechanics. A more rigorous fully quantum mechanical proof by solution of the Schrödinger equation with boundary conditions for this particle in a box problem is provided in the next chapter.

8 The Linear Harmonic Oscillator Problem

Another one of the simplest problems in quantum physics that demonstrates key concepts such as energy quantization is the treatment of the linear harmonic oscillator. Physically such an oscillator can be thought of as a particle undergoing harmonic oscillations for small amplitudes in one dimension (say x). This can be described in line with the classical case of a particle under the influence of a parabolic potential represented by

$$V(x) = \frac{1}{2}kx^2 \tag{34}$$

k being the so-called spring constant. Classically such an oscillator would have frequency (Fig. 2)

$$v = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \tag{35}$$

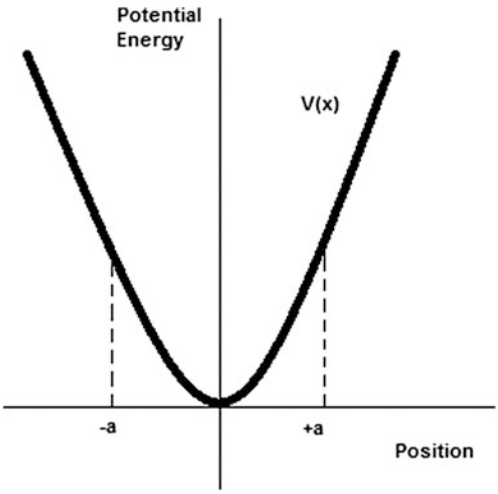


Fig. 2 Potential energy of a linear harmonic oscillator

For a quantum mechanical system under the influence of such a potential, the Schrödinger equation would be of the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0 \tag{36}$$

Equation (30) can be simplified by introducing the quantities λ and α given by

$$\lambda = \frac{2mE}{\hbar^2} \tag{37}$$

$$\alpha = \frac{2\pi mv}{\hbar} \tag{38}$$

Thus the Eq. (30) becomes

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \left(\lambda - \alpha^2x^2\right)\psi = 0 \tag{39}$$

For large values of x, i.e. $\alpha^2x^2 \gg \lambda$, (33) reduces to

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - \alpha^2x^2\psi = 0 \tag{40}$$

The general solution for which is

$$\psi(x) = \mathrm{e}^{\pm\frac{\alpha}{2}x^2} \tag{41}$$

as the solution $\psi(x) = e^{+\frac{\alpha}{2}x^2}$ blows up as $x \to \infty$, hence we take only the other solution

$$\psi(x) = e^{-\frac{\alpha}{2}x^2} \tag{42}$$

However in cases the value of x is small and the value of λ can no longer be neglected. In such cases, we can solve the problem using a power-series expansion of an introduced function $f(x)$ to express $\psi(x)$ as

$$\psi(x) = e^{-\frac{\alpha}{2}x^2} \cdot f(x) \tag{43}$$

Putting this value of $\psi(x)$ in (33) and rearranging, we arrive at

$$f'' - 2f'\alpha x + (\lambda - \alpha)f = 0 \tag{44}$$

Defining a variable $\rho = \sqrt{\alpha}x$, and rearranging, (38) can be recast as

$$\frac{d^2H}{d\rho^2} - 2\rho\frac{dH}{d\rho} + \left(\frac{\lambda}{\alpha} - 1\right)H = 0 \tag{45}$$

where $H(\rho)$ is the Hermite's polynomial and thus ψ is expressed as

$$\psi(\rho) = e^{\frac{-\rho^2}{2}}H(\rho) \tag{46}$$

The Hermite polynomial can be expressed as

$$H(\rho) = \sum_n a_n \rho^n \tag{47}$$

$n = 0, 1, 2, \ldots H(\rho)$ follows the recursion relation,

$$\frac{a_{n+2}}{a_n} = -\frac{\left(\frac{\lambda}{\alpha} - 2n - 1\right)}{(n+1)(n+2)} \tag{48}$$

From the general solution in (40), taking only the cases where the solution satisfies the requirement that $\psi(\rho) \to 0$ as $\rho \to \infty$, we arrive at the following condition using (40)–(42)

$$\frac{\lambda}{\alpha} = (2n + 1) \tag{49}$$

Since $\frac{\lambda}{\alpha} = \frac{2E}{h\nu}$, thus we have

$$\begin{aligned} E_n &= \left(n + \frac{1}{2}\right) h\nu \\ &= \left(n + \frac{1}{2}\right) \hbar\omega \end{aligned} \tag{50}$$

where n is 0, 1, 2, 3…. This is indeed an interesting solution, which implies that only certain energy values are allowed for a quantum linear harmonic oscillator. This revelation that in the quantum domain, the energy that a system may possess is not continuous but rather discretized lies at the heart of quantum physics.

For the case $n = 0$ the system possesses a non-zero energy given as

$$E = \frac{1}{2}\hbar\omega \tag{51}$$

This is the famous "zero-point energy". This concept is unique to quantum physics as classically the lowest possible energy of a harmonic oscillator should be zero. This indicates that when the system is at its lowest possible energy state (i.e. temperature nearing absolute zero) it is still supposed to have a non-zero energy value (Fig. 3).

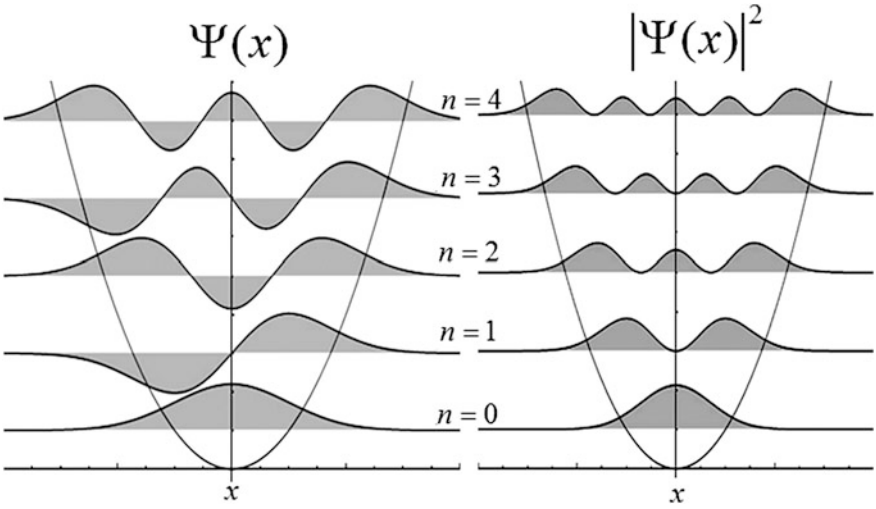


Fig. 3 Nature of wavefunctions and corresponding probabilities for the harmonic oscillator problem (Courtesy Wikimedia Commons. This is an edited version: original file © Alan McC, distributed under the creative commons license)

The wave functions for the different states are expressed as

$$\psi_n(\rho) = \left(\frac{2mv}{\hbar}\right)^{1/4} (2^n n!)^{-1/2} H_n(\rho) \mathrm{e}^{-\rho^2/2} \tag{52}$$

Interestingly there exists a small non-zero part of the wavefunction beyond the potential barrier. This tail of the wavefunction outside the bound system represents a probability that a particle may have a non-zero probability of existing beyond the confining potential, which is the basic concept of quantum mechanical tunneling.

9 The Kronig-Penney Model for Electron in a 1-Dimensional Lattice

In case of an electron confined in a rigid box since $V(x) = 0$ everywhere inside the box, it can be considered as an "empty solid" (i.e. just a confining potential without any atoms or molecules within it). In a real solid however atoms and molecules exist and the potential inside the boundaries is not zero but rather periodic according to the lattice (the concept of lattice and structure of solids are discussed in detail the subsequent chapters, for now we can assume lattice as a neatly arranged grid/blueprint where atoms/molecules are located in a solid material) (Fig. 4).

The simplest solid to consider would be a linear chain of equally spaced atoms. In such a linear chain the potential would look something as shown in the figure. Considering an infinite chain, this was approximated by a periodic square well potential by Kronig and Penney.

In such a periodic potential, where

$$U(x) = U(x + L) \tag{53}$$

The Bloch's theorem expresses the wavefunction with a periodic amplitude part $u(x)$ having the same periodicity as that of the potential (1-D lattice in this case). The wave function is represented as

$$\psi(x) = \mathrm{e}^{i\vec{k}\cdot\vec{x}} u(x) \tag{54}$$

The amplitude part satisfies the condition $u(x) = u(x + L)$, which ensures the continuity of the wavefunction in the periodic lattice (Fig. 5). This also means that a translation by the periodicity L, results in only a phase shift of the original wave by an amount $\mathrm{e}^{i\vec{k}\cdot\vec{L}}$. Mathematically this can be written as

$$\psi(x + L) = \psi(x) \mathrm{e}^{i\vec{k}\cdot\vec{L}} \tag{55}$$

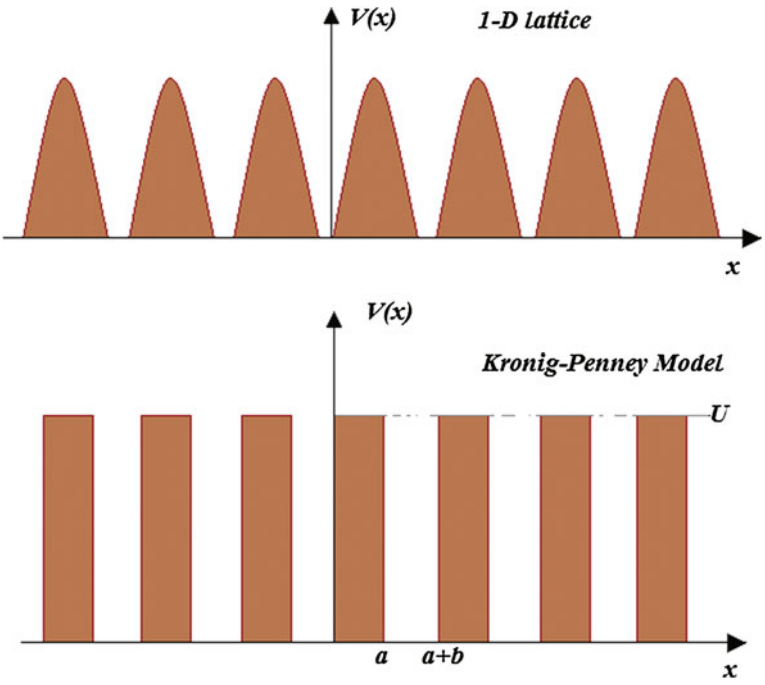
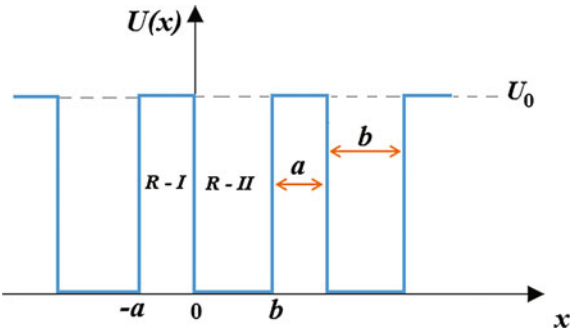


Fig. 4 Potential profile of 1-D lattice

We now direct our attention to a toy example of a 1-D linear chain of atoms. Let us consider the diameter of the positively charged ion-cores to be a and the inter-atomic spacing to be b. The lattice parameter in such a case can be written as $L = (a + b)$. For such a lattice the potential has two distinct regions being repeated along the x direction. The repeat unit being within $0 \leq x \leq (a + b)$. If we solve the Schrödinger equation for this repeat unit consistent with the Bloch's theorem, it is possible to have the solution for the whole 1-D lattice.

Fig. 5 A typical periodic potential in 1-D lattice



In region I (R-I i.e. $0 \leq x \leq a$) the potential is $U(x) = U_0$ which is constant. Thus in R-I the Schrödinger equation is given by

$$\frac{\mathrm{d}^2\psi_{\mathrm{I}}}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - U_0)\psi_{\mathrm{I}} = 0 \tag{56}$$

This has the general solution

$$\psi_{\mathrm{I}} = A\mathrm{e}^{\beta x} + B\mathrm{e}^{-\beta x} \tag{57}$$

In (56) $\beta = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$. The solution for the region-II (R-II) where the potential $U(x) = 0$ is given by

$$\psi_{\mathrm{II}} = C\mathrm{e}^{i\alpha x} + D\mathrm{e}^{-i\alpha x} \tag{58}$$

In (57) $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$. Using the boundary conditions

$$\begin{aligned} \psi_{\mathrm{I}}|_{x=0} &= \psi_{\mathrm{II}}|_{x=0} \\ \left.\frac{d\psi_{\mathrm{I}}}{dx}\right|_{x=0} &= \left.\frac{d\psi_{\mathrm{II}}}{dx}\right|_{x=0} \end{aligned} \tag{59}$$

We arrive at a the relations

$$\begin{aligned} A + B &= C + D \\ \beta(A - B) &= \alpha(C - D) \end{aligned} \tag{60}$$

Further as the solution in a periodic potential should be a Bloch wave, we may write

$$\psi_{\mathrm{I}}(-a) = \psi_{\mathrm{II}}(b)\mathrm{e}^{ikL} \tag{61}$$

Using (57)–(61), we arrive at the equality

$$\cos(kL) = \frac{\beta^2 + \alpha^2}{2\alpha\beta}\sinh(\alpha a)\sin(\beta b) + \cosh(\alpha a)\cos(\beta b) \tag{62}$$

By taking the limit $b \to 0$ and $U_0 \to \infty$ (which mathematically signifies a dirac delta type periodic potential) and taking the constant $P = \frac{m_{\mathrm{e}} a b U_0}{\hbar^2}$ (62) can be simplified to

$$\cos(ka) = \frac{P\sin(\alpha a)}{\alpha a} + \cos(\alpha a) \tag{63}$$

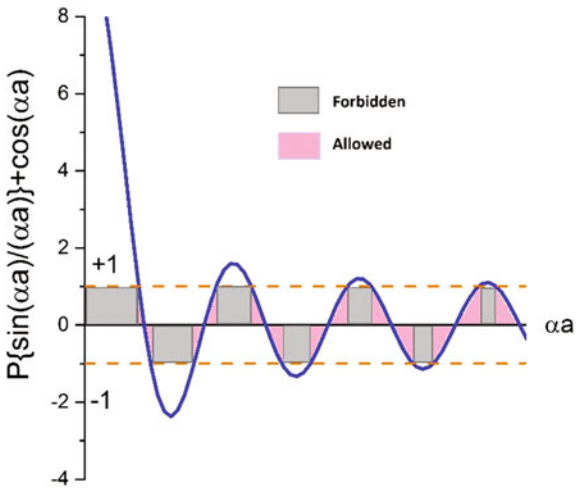


Fig. 6 The graphical solution of (63) showing the allowed and the forbidden regions of the solution

The solution is a transcendental one, and it needs to be solved graphically. A graphical solution involves the plotting of the RHS and the LHS of (63) and finding the regions where solutions are possible.

The graphical solution shows that the relation in (63) is satisfied for only certain ranges of values of αa for which the value of the RHS is within +1 and −1 (i.e. the maximum and the minimum value of the cosine function on the LHS, indicated by the orange dashed lines) (Fig. 6). The regions in which the RHS value exceeds this limit, the corresponding values of αa are not allowed and these forbidden regions are highlighted in grey. Other regions having allowed values are highlighted in purpule.

As $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$, the significance of the solution of (63) means that for the 1-D lattice the energy E can't have continuous values as in the case of a free particle (i.e. the relation $E = \frac{\hbar^2 k^2}{2m_e}$ is not allowed for all values of the wave vector k). For certain values of k there exists a discontinuity in the E–k plot (Fig. 7).

Physically this existence of discontinuity in the energy band structure signifies the forbidden-gap in the bandstructure of a 1-D solid.

The points of discontinuity are $k = \pm\frac{n\pi}{a}$, where $n = 1, 2, 3\ldots$. These regions in the k-space for which there exists allowed values of E (e.g. within $k = \frac{n\pi}{a}$ to $-\frac{n\pi}{a}$) are known as the Brillouin Zones of the lattice. Physically the electron travelling in the lattice can be considered to be reflected back from the boundaries of the subsequent Brillouin Zones. A more detailed description of these zones are provided in the chapter on solid state physics.

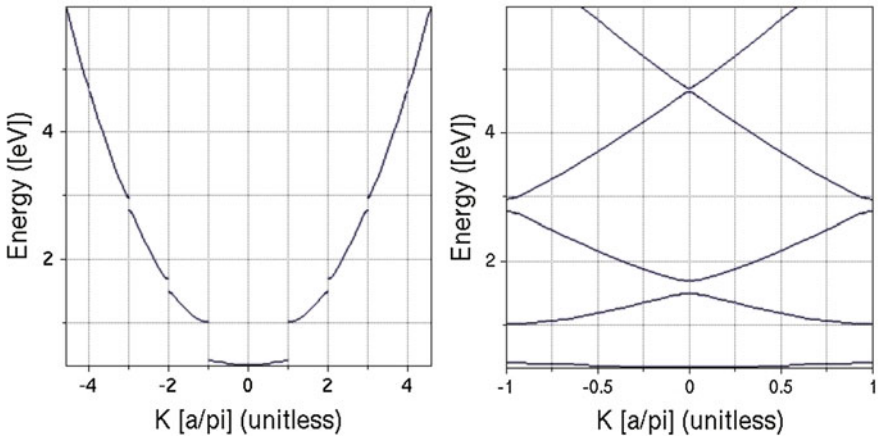


Fig. 7 *E–k* relation of 1-D periodic lattice plotted in **a** the extended and **b** the reduced zone scheme

This can be plotted in the extended zone scheme or the reduced zone scheme (i.e. by applying Bloch's theorem the *E–k* relation in regions outside $k = \pm\frac{\pi}{a}$, are "folded back" into the same by shifting the phase accordingly).

Thus the simple Kronig-Penney model gives an insight into the quantum mechanical origin of energy band gaps in a 1-D solid. In case of bulk (3-D) solids the potential is not as simple to visualize and involves electro-electron interactions as well. An accurate description of such materials can be obtained by tight binding or ab initio methods. However as a starting point in quantum physics of solids the Kronig-Penney model retains a special significance.

10 Chapter Summary

Here we have presented in brief the key concepts of quantum physics such as the uncertainty principle, wave particle duality, the basic laws that govern matter waves and seen how to set-up the Schrödinger equation for a quantum mechanical system. Quantum phenomenon such as energy quantization through confinement and origin of band gaps in solids has also been introduced. In the subsequent chapter we will explore more about the tunneling and other phenomena in quantum physics. With these very basic concepts of quantum physics we would progress further through the book to develop our understanding of nanomaterials and their physical properties and some novel nanoscale devices.

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