PH253 Lecture 14: Schrödinger's equation

mechanics with matter waves

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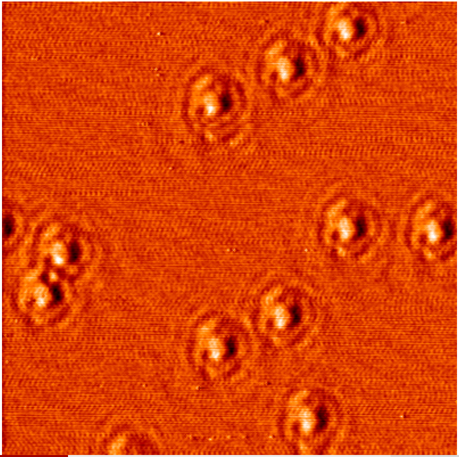
electron waves are a thing

Single atoms of Co on a Cu single crystal surface. Due to the differing number of electrons per atom, the Co atoms create a standing wave disturbance on the Cu surface. Courtesy O. Kurnosikov (unpublished, ca. 2001)



Outline

1. Overview of Schrödinger's equation

2. Free particles

3. Potential Step

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Time-dependent version:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

1. $\psi(x,t)$ = wavefunction for object, the "amplitude"
2. This equation gives the time evolution of system, given $\psi(x,t=0)$
3. 1st order in time, evolution of amplitude deterministic
4. Write out for discrete time steps ($\partial\psi/\partial t \rightarrow \Delta\psi/\Delta t$)

$$\Delta\psi = \psi(x,t+\Delta t) - \psi(x,t) = \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}\Delta t$$

Time-independent version:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

1. Time-independent version gives $\psi(t=0)$ and energy
2. Given potential $V(x,t)$ can find ψ
3. Typically: consider static cases, $V = V(x)$
4. What does the wave function tell us?

Properties of ψ

1. ψ gives probabilities: $|\psi(x,t)|^2\,dx = P(x,t)\,dx$
2. Probability particle is in $[x, x+dx]$ at time t
3. Normalization: particle is *somewhere:* $\int\limits_{-\infty}^{\infty} P(x)\,dx = 1.$
4. ψ is in general complex: $\psi = a + bi$ or $\psi = Ae^{iB}$
5. Phase is key for interference of 2 matter waves
6. $\psi_{\text{tot}} = a\psi_1 + b\psi_2$, but $|\psi_{\text{tot}}|^2 \neq |\psi_1|^2 + |\psi_1|^2$
7. Single particle or bound state - no interference, ψ can be real.

Time dependence

1. Let's say $V(x)$ is independent of time (static environment)
2. Then presume wave function is separable into t, x parts
3. I.e., $\Psi(x,t) = \psi(x)\varphi(t)$
4. V indep. of time required for conservative forces (see ph301/2)
5. Mostly what we will worry about anyway
6. If this is the case, plug into time-dep. Schrödinger
7. One side has only x, the other only t dependence

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

Time dependence

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

1. $\Psi(x,t) = \psi(x)\varphi(t)$. One side has only x, the other only t.
2. Each side must then be separately equal to the same constant E

$$i\hbar\frac{\partial\varphi}{\partial t} = E\varphi$$

Now separate & integrate (recall $1/i = -i$):

$$\frac{\partial\varphi}{\varphi} = -\frac{iE}{\hbar}\,\partial t \qquad \Longrightarrow \qquad \varphi = e^{iEt/\hbar}$$

With $E = \hbar\omega$, $\varphi = e^{-i\omega t}$ – simple oscillation; E is energy!

Spatial dependence

1. If V independent of time, amplitude oscillates with frequency ω
2. Then $\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$
3. Spatial part from time-independent equation - 2nd half of separation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

Can we make this look like something more familiar?

What is this equation?

Do some factoring. Treat $\partial^2/\partial x^2$ as an *operator*.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right)\psi=E\psi$$

Looks a little like $K+V=E$
Let $\mathbf{p}=-i\hbar\frac{\partial}{\partial x}$. Then $\mathbf{p}^2=-\hbar^2\frac{\partial^2}{\partial x^2}\ \ldots$

$$\left(\frac{\mathbf{p}^2}{2m}+V\right)\psi=E\psi$$

The time-independent equation is just conservation of energy!
Must be so: V independent of t requires conservative forces.
Classical *analogy*: $\mathbf{p}=m\frac{d}{dt}$, $\mathbf{p}x=p$ would give momentum.

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An electron alone in the universe

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

For a free isolated particle, $V = 0$. Thus,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \qquad \text{or} \qquad \frac{\partial^2\psi}{\partial x^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi$$

1. We know this equation, it is $a = \frac{d^2x}{dt^2} = -k^2x$
2. Know the solutions are oscillating functions. In general, noting time dependence already found:

$$\psi(x) = e^{-iEt/\hbar}\left(Ae^{ikx} + Be^{-ikx}\right)$$

An electron alone in the universe

$$\psi(x) = e^{-iEt/\hbar}\left(Ae^{ikx} + Be^{-ikx}\right)$$

Sum left- and right-going sinusoidal waves. What is k?
By analogy:

$$a = \frac{d^2x}{dt^2} = -k^2x \quad \text{and} \quad \frac{\partial^2\psi}{\partial x^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi$$

1. This implies $k^2 = 2mE/\hbar^2$, or $E = \hbar^2k^2/2m$.
2. For a free particle, $E = p^2/2m$, implying $|p| = \hbar k$
3. In agreement with de Broglie and classical physics so far
4. Since via Planck $E = \hbar\omega$, implies $\hbar\omega = \hbar^2k^2/2m$
5. Or $\omega = \hbar k^2/2m$

An electron alone in the universe

$$\omega = \frac{\hbar k^2}{2m}$$

1. Last time: group velocity of wave packet is $v_{\text{group}} = \partial\omega/\partial k$
2. $\partial\omega/\partial k = \hbar k/m = p/m = v$
3. Just what we expect for classical particle: $p = mv$, $E = p^2/2m$
4. Stickier question: where is the particle?

An electron alone in the universe

$$\psi(x) = e^{-iEt/\hbar}\left(Ae^{ikx} + Be^{-ikx}\right)$$

1. Probability it is in $[x, x+dx]$ is $P(x)\,dx = |\psi(x)|^2\,dx$
2. Probability in an interval $[a,b]$?
3. $P(\text{in } [a,b]) = \int\limits_a^b P(x)\,dx$
4. In our case equivalent to $\int\limits_{-\infty}^{\infty} \cos^2 x\,dx$ ...not defined
5. Plane wave solution is not *normalizable*, P has no meaning
6. Infinite uncertainty in position, because we know k & p precisely!
7. Makes sense, empty universe with no constraints. Can be anywhere.

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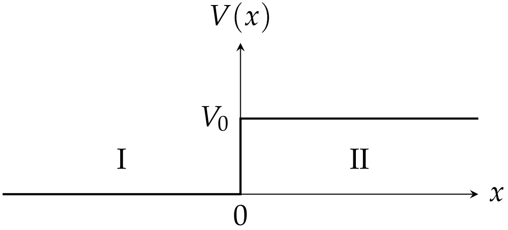
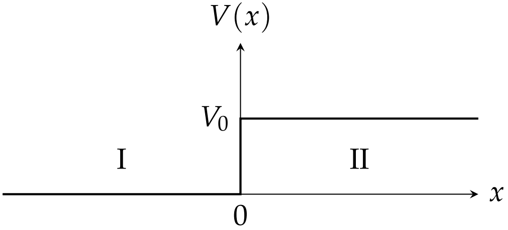
Slightly less empty universe



1. Particle of energy $E > V_o$ coming from **left** sees step in potential
2. $V(x) = 0$ for $x < 0$, $\quad V(x) = V_o$ for $x \geq 0$
3. Write down time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \quad \text{or} \quad \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

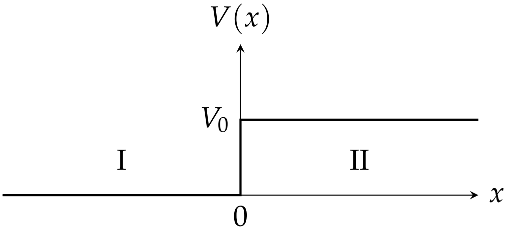
Solution still traveling waves



1. V is different in the two regions (I, II), solve separately
2. Since $E - V_0 > 0$ everywhere, same basic solution though.
3. Solution is still traveling waves like free particle

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \quad \text{or} \quad \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V\right)\psi = 0$$

Region I: free particle

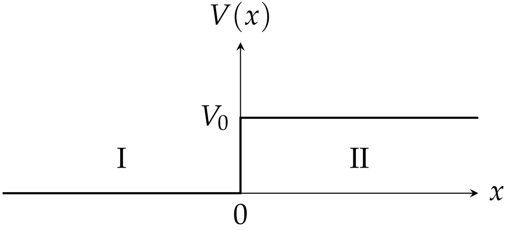


1. Let $k^2 = 2mE/\hbar^2$, same solution as free particle (ignore $e^{i\omega t}$)

$$\psi_I(x) = e^{ikx} + Re^{-ikx} \qquad \text{for } x < 0$$

1. Can choose constant of first term to be 1
2. First term is right-going wave, second is left-going wave.
3. Right-going wave is the *reflection* of incident wave

Region II: slightly less free particle

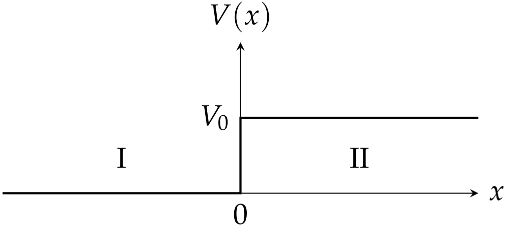


1. Second region: same! Let $q^2 = 2m(E - V_0)/\hbar^2$.
2. Need two constants now. (ignore $e^{i\omega t}$ still)

$$\psi_{II}(x) = Te^{iqx} + Ue^{-ikx} \qquad \text{for } x \geq 0$$

1. First term: transmitted portion.
2. Second term? Wave *coming from right* – unphysical, so $U = 0$
3. Overall: like any wave: incident = reflected + transmitted

Combining the solutions: continuity



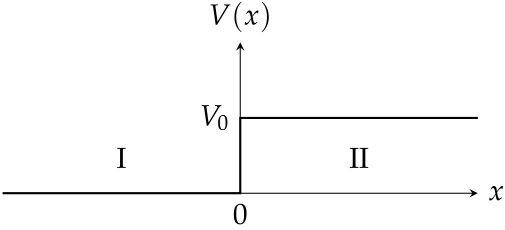
$$\psi_I(x) = e^{ikx} + Re^{-ikx} \qquad \psi_{II}(x) = Te^{iqx}$$

1. Continuity: match solutions at boundary!
2. ψ and its derivatives match at $x = 0$. So does $|\psi|^2$

$$\psi_I(0) = 1 + R = \psi_{II}(0) = T \qquad \Longrightarrow \qquad 1 + R = T$$

1. Total intensity for I and II match at the boundary

More continuity



$$\psi_I(x) = e^{ikx} + Re^{-ikx} \qquad \psi_{II}(x) = Te^{iqx}$$

1. Also match $\partial\psi/\partial x$ at boundary.

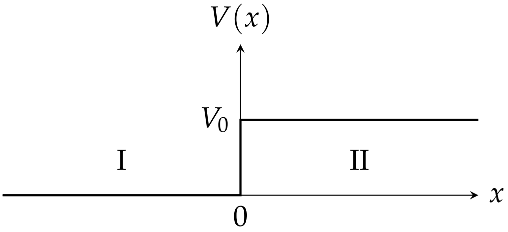
$$\left.\frac{\partial \psi_I}{\partial x}\right|_0 = \left.\frac{\partial \psi_{II}}{\partial x}\right|_0$$

$$ike^{ikx} + (-ik)Re^{-ikx} = iqTe^{iqx}$$

$$\text{at } x = 0: \quad ik - ikR = iqT$$

$$k(1-R) = qT$$

Coefficients for transmission & reflection



$$k(1-R) = qT$$

1. Also know $1 + R = T$ … algebra …

$$R = \frac{k-q}{k+q} \qquad T = \frac{2k}{k+q}$$

$$\psi(x) = \begin{cases} e^{ikx} + \left(\frac{k-q}{k+q}\right) e^{-ikx} & x < 0 \\ \left(\frac{2k}{k+q}\right) e^{iqx} & x \geq 0 \end{cases}$$

Reflection & Transmission Probabilities

Probability of reflection? Magnitude of reflected wave! Note $|e^{iA}| = 1$.
Reflected wave: $|Re^{-ikx}|^2 = R^2$.

$$\begin{aligned} P_{\text{refl}} &= R^2 = \left(\frac{k-q}{k+q}\right)^2 && \text{reflection probability} \\ P_{\text{trans}} &= 1 - P_{\text{refl}} && \text{only 2 things can happen} \\ \implies \quad P_{\text{trans}} &= \frac{4kq}{(k+q)^2} && \text{transmission probability} \end{aligned}$$

1. Probability of transmission + reflection = 1
2. Like light, some amplitude is reflected and some transmitted
3. But not like particle - reflection *even if you clear the step*

Transmission is highly energy-dependent

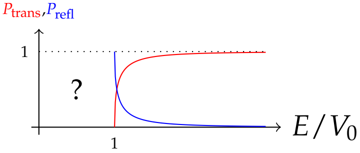
$$P_{\text{refl}} = \left(\frac{k-q}{k+q}\right)^2 \qquad \text{reflection}$$

$$P_{\text{trans}} = \frac{4kq}{(k+q)^2} = \sqrt{\frac{E-V_0}{E}}|T|^2 \qquad \text{transmission}$$

1. Degree of transmission depends on k, q, i.e., E compared to V_o
2. High energy: $k \sim q$ gives $P_{\text{refl}} \sim 0$, $P_{\text{trans}} \sim 1$
3. Low energy: $k \gg q$ gives significant P_{refl}
4. Check: $k = q$, $P_{\text{trans}} = 1$ – there is no step!
5. Check: $q = 0$, $P_{\text{trans}} = 0$ – zero energy there!
6. $E = V_0$? $P_{\text{trans}} = 0$, perfect reflection

Some interesting aspects

1. Classical: go over step, slow down to conserve E, never reflect
2. Quantum: chance of reflection, even if E high enough.
3. Note: we have not considered $E < V_0$.



1. If $E < V_0$? q is purely imaginary! Then iq is purely real.
2. Let $iq = \kappa$.

$$\psi_{II}(x) = Te^{-iqx} = Te^{-\kappa x} \qquad E < V_0 \tag{1}$$

1. Now exponentially decaying in region II

What comes next

1. If $E < V_0$, exponentially decaying in region II
2. Meaning there is some penetration of the "particle" into barrier

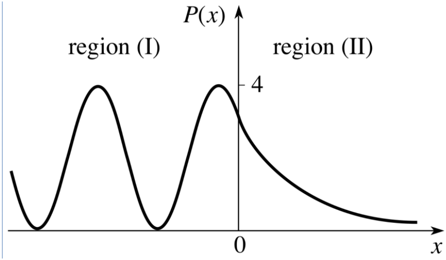


Figure: `http://www.met.reading.ac.uk/pplato2/h-flap/phys11_1.html`

What comes next

1. Thin barrier? *Tunnel effect* - jumping through walls!
2. Incoming wave doesn't have enough energy to go over barrier.
3. Decays into "forbidden" region, but if thin enough?
4. Some intensity leaks through! Particle goes through barrier.

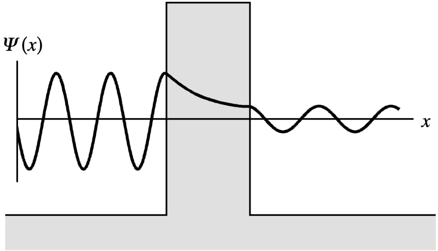


Figure: LeClair, Moodera, & Swagten in *Ultrathin Magnetic Structures III*