* Last time * Physical interpretation of the associated linear problem $\left(\frac{d^2}{dx^2} + u\right)\psi = \lambda\psi$ (9.1)

(time-dependent) Schrödinger equation for a particle (mass $1/2$) moving in potential $V(x)$:

$$i \frac{\partial}{\partial \tau} \Psi(x,\tau) = \left(- \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x,\tau) \qquad (11.2)$$

where $\Psi(x,\tau)$ is the wavefunction from which we construct a probability density $\rho = |\Psi(x,\tau)|^2$.

Key point to make contact with the associated linear problem:

separate variables: $\Psi(x,\tau) = \phi(\tau)\psi(x)$

(11.2) implies:

1. $\dot{\phi} = -ik^2\phi \quad \rightarrow \quad \phi(\tau) = e^{-ik^2\tau}$ (11.5) $\left[\dot{} = \frac{d}{d\tau}, \ ' = \frac{d}{dx} \right]$

↑ WLOG set constant $= 1$

2. $-\psi'' + V(x)\psi = k^2\psi$ - time independent Schrödinger equation for particle of energy $E = k^2$

This is our associated linear problem (9.1) upon the identifications:

$$u = -V$$

$$\lambda = -k^2$$

To define scattering data we need to study particle scattering! Now,

"scattering solutions" $\Leftrightarrow$ relax requirement $\int_{-\infty}^{\infty} |\psi|^2 \, dx < \infty$ to just require ψ bounded!

The scattering data is encoded in the asymptotics of ψ as $x \to \pm\infty$. Since $V \to 0$ as $x \to \pm\infty$:

$$-\frac{d^2}{dx^2}\psi \approx k^2\psi$$

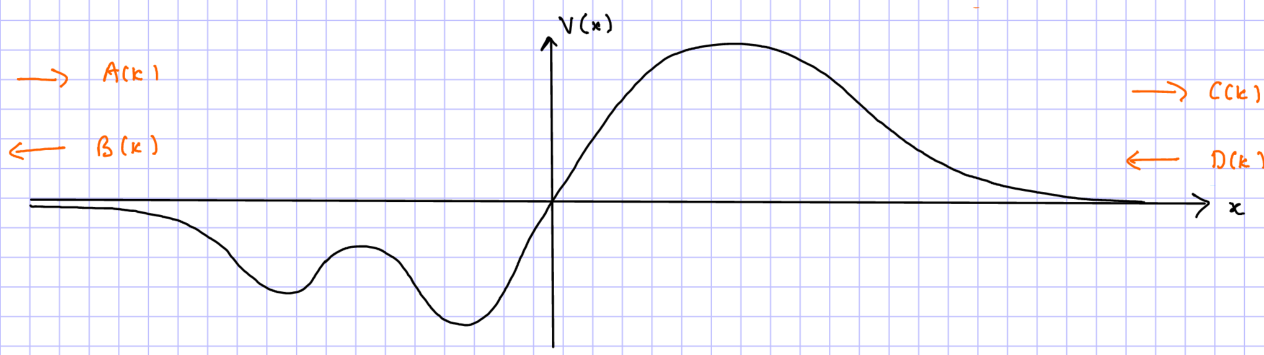
Hence:

$$\psi(x) \approx \begin{cases} A(k)e^{ikx} + B(k)e^{-ikx} & x \to -\infty \\ C(k)e^{ikx} + D(k)e^{-ikx} & x \to +\infty \end{cases} \qquad (11.9)$$

Reinstating τ:

$$\Psi(x,\tau) \approx \begin{cases} A(k)e^{+ik(x-k\tau)} + B(k)e^{-ik(x+k\tau)} & x \to -\infty \\ C(k)e^{ik(x-k\tau)} + D(k)e^{-ik(x+k\tau)} & x \to +\infty \end{cases} \qquad (11.10)$$

↑ right moving waves ↑ left moving waves



Consider first the case that the particles have positive energy $E = k^2 > 0$. So that $k \in \mathbb{R}$ and WLOG $k > 0$

To study scattering, by choice of convention we impose:

$D(k) = 0$ (incoming particles only from the left)

$$A(k) = 1 \qquad \text{(unit flux of incoming particles from the left)}$$

In this way, we can interpret:

$$B(k) =: R(k) \qquad \text{"reflection coefficient"} \qquad \text{(probability of reflection)}$$

$$C(k) =: T(k) \qquad \text{"transmission coefficient"} \qquad \text{(probability of transmission)}$$

"scattering solution":

$$\psi(x) \approx \begin{cases} e^{ikx} + R(k)\, e^{-ikx}, & x \to -\infty \\ T(k)\, e^{ikx}, & x \to +\infty \end{cases} \qquad (11.13)$$

Exercise 60:

$$|R(k)|^2 + |T(k)|^2 = 1$$

"probability that a particle is either reflected or transmitted is equal to 1"

To prove such results, a convenient tool is the Wronskian

def^n: For two functions $f(x)$ and $g(x)$

$$W[f,g](x) := f'(x)\,g(x) - f(x)\,g'(x)$$

is called the Wronskian for f and g

Some properties

1. if f and g are linearly dependent then $W[f,g] = 0$ identically
2. if $W[f,g] = 0$ and f and g are both analytic (as will be the case for us) then f and g are linearly dependent.

Consider now the case that: $E = k^2 < 0$ (particles have negative total energy)

It's useful to write: $k = i\mu$ were $\mu \in \mathbb{R}$ and WLOG $\mu > 0$. Such that $E = -\mu^2 < 0$.

The general solution in this case has the following asymptotics

$$\psi(x) \approx \begin{cases} a(\mu)\, e^{-\mu x} + b(\mu)\, e^{\mu x}, & x \to -\infty \\ c(\mu)\, e^{-\mu x} + d(\mu)\, e^{\mu x}, & x \to +\infty \end{cases}$$

$$\psi \text{ is bounded} \iff a(\mu) = d(\mu) = 0$$

In this case are also satisfy the stronger constraint that $\int_{-\infty}^{\infty} |\psi|^2\, dx < \infty$ i.e. ψ is square integrable.

There might be no value of μ for which this is possible. But when they do exist such solutions are called bound state solutions

FACT : If $V(x) \to 0$ as $x \to \pm\infty$ bound state solutions exist for a finite (and possibly empty) set of μs

bound state solutions

$$\{\mu_k\}_{k=1}^{N} = \{\mu_1, \mu_2, \dots, \mu_N\} , \quad \mu_1 < \mu_2 < \dots < \mu_N$$

Summary

time independent Schrödinger equation

Find bounded solutions to T.I.S.E. with $V \to 0$ as $x \to \pm\infty$. Such solutions come in two flavours:

1. Positive energy $E = k^2 \in (0, \infty)$: "continuous spectrum" → "scattering solutions"

bounded and with "oscillatory asymptotics"

2. Negative energy $E = -\mu^2 \in \{-\mu_1^2, \dots, -\mu_N^2\}$:

"discrete spectrum" → "bound states"

square integrable with "damped asymptotics"

11.2 Examples

Example 1 : $V(x) = 0$ (everywhere)

In this case the T.I.S.E. is :

$$-\frac{d^2}{dx^2}\psi = E\psi \qquad \text{(everywhere)}$$

General solution : $\psi(x) = \alpha e^{ikx} + \beta e^{-ikx}$ for all x

Two cases :

1. $E = k^2 > 0$ and $k > 0$

Put back in τ dependence :

$$\Psi(x,\tau) = \alpha e^{ik(x-k\tau)} + \beta e^{-ik(x+k\tau)}$$

for all x not 'just' asymptotically.

To find the scattering solution compare with (11.13) :

$x \to -\infty$: $\alpha = 1$ and $\beta = R(k)$

$x \to +\infty$: $\alpha = T(k)$ and $\beta = 0$

these have to hold simultaneously!

$\Rightarrow$ $T(k) = 1$ and $R(k) = 0$

$\therefore$ Scattering solution : $\psi(x) = e^{ikx}$

" No particles are reflected i.e. all particles are transmitted with probability 1 "

2. Negative energy: $E = -\mu^2$ with $\mu > 0$

general solution: $\psi(x) = \alpha e^{-\mu x} + \beta e^{\mu x}$ for all x

This is only bounded if $\alpha = \beta = 0$. There are no bound state solutions

Conclusion to example 1: If $V = 0$ then the problem:

$$\left\{ \psi : \left(-\frac{\partial^2}{\partial x^2} + V \right) \psi = E \psi, \ \psi \text{ is bounded} \right\}$$

has a solution for all $E \geq 0$ and no solution if $E < 0$.

Energy spectrum of bounded solutions: