

# PHYS 2210 Quantum Physics 1

## More 1D Special Cases

- Return to the Dirac Delta function
  - Properties
  - Representations
  - TISE solution
- Model molecules
  - Two Dirac Deltas
  - A double square well

# The Dirac Delta Function

- Definition:  $\int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx = f(x_0)$
- $\delta(x - x_0) = \begin{cases} 0 & \text{for } x \neq x_0 \\ \infty & \text{for } x = x_0 \end{cases}$
- $\int \delta(x - x_0) dx = 1$
- $\delta(x)$  is real
- $\delta(x)$  is even

# Some Dirac Delta Representations

- $\delta(x) = \lim_{\alpha \rightarrow \infty} \sqrt{\frac{\alpha}{\pi}} e^{-\alpha x^2}$
- $\delta(x) = \lim_{\alpha \rightarrow 0} \frac{1}{\pi} \frac{\alpha}{x^2 + \alpha^2}$
- $\delta(x) = \lim_{\alpha \rightarrow 0} \frac{1}{\pi} \frac{\sin \frac{x}{\alpha}}{x}$
- $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} dx$

# The delta function potential

$$\hat{H}\psi = E\psi$$
$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + \lambda \delta(x) \psi = E\psi$$

with  $\lambda$  negative, for an attractive potential.

$$\psi = Ae^{Kx} + Be^{-Kx}$$

So for negative x,  $\psi^- = Ae^{Kx}$

and for positive x,  $\psi^+ = Be^{-Kx}$

Continuity of the wavefunction gives  $\psi^- = \psi^+$  so  $A = B$ .

The slope on the two sides is discontinuous due to the infinite  $\delta$  function.

$$\left. \frac{d\psi}{dx} \right|_{-\beta} = KA; \quad \left. \frac{d\psi}{dx} \right|_{\beta} = -KA; \quad \text{for small } \beta, \text{ so } \left. \frac{d\psi}{dx} \right|_{-\beta} - \left. \frac{d\psi}{dx} \right|_{\beta} - \left. \frac{d\psi}{dx} \right|_{-\beta} = -2KA;$$

Returning to the Schrodinger equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + \lambda \delta(x) \psi = E\psi$$

We integrate both sides once in x, from  $-\beta$  to  $+\beta$ .

$$-\int_{-\beta}^{\beta} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi dx + \int_{-\beta}^{\beta} \lambda \delta(x) \psi dx = \int_{-\beta}^{\beta} E\psi dx$$

The rhs goes to zero as  $\beta \Rightarrow 0$  because the integrand is finite.

$$\text{so, } \int_{-\beta}^{\beta} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi dx = \int_{-\beta}^{\beta} \lambda \delta(x) \psi dx$$

$$\text{Doing both integrals separately, } \frac{\hbar^2}{2m} \frac{\partial \psi}{\partial x} \Big|_{-\beta}^{\beta} = \lambda \psi(0)$$

$$\text{and substituting } \frac{\partial \psi}{\partial x} \Big|_{-\beta}^{\beta} = -2AK \text{ (from the previous slide),}$$

$$\text{we have } -\frac{\hbar^2 K}{m} = \lambda$$

$$K = -\frac{\lambda m}{\hbar^2} \Rightarrow E = \frac{\hbar^2 K^2}{2m} = -\frac{m\lambda^2}{2\hbar^2}$$

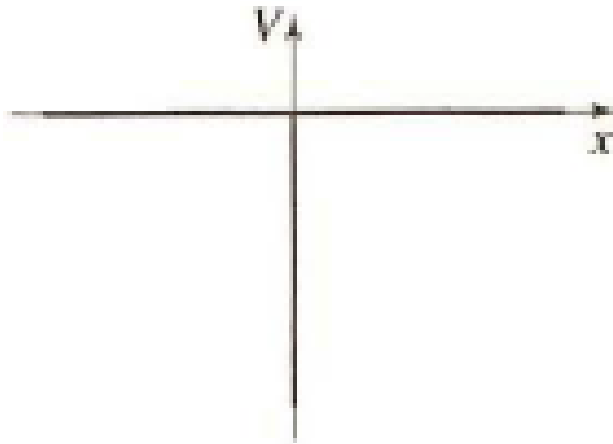


Figure 4.14 The Dirac delta function potential energy (4.77).

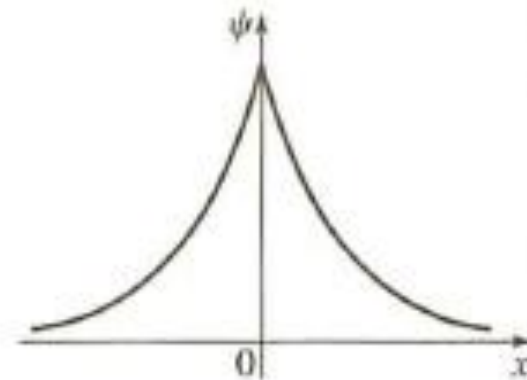


Figure 4.15 The wave function (4.85) for a particle bound in a Dirac delta function potential energy well.

$$\psi(x) = A \exp\left(-\frac{\lambda m}{\hbar^2} |x|\right)$$

is the only bound state.

# A Model Molecule

We will use the Dirac Delta function as a simplified representation of an electron bound to an atom.

We will address the case of an electron bound to a proton in a Coulomb potential later in this course.

Consider two delta function potentials near one another.

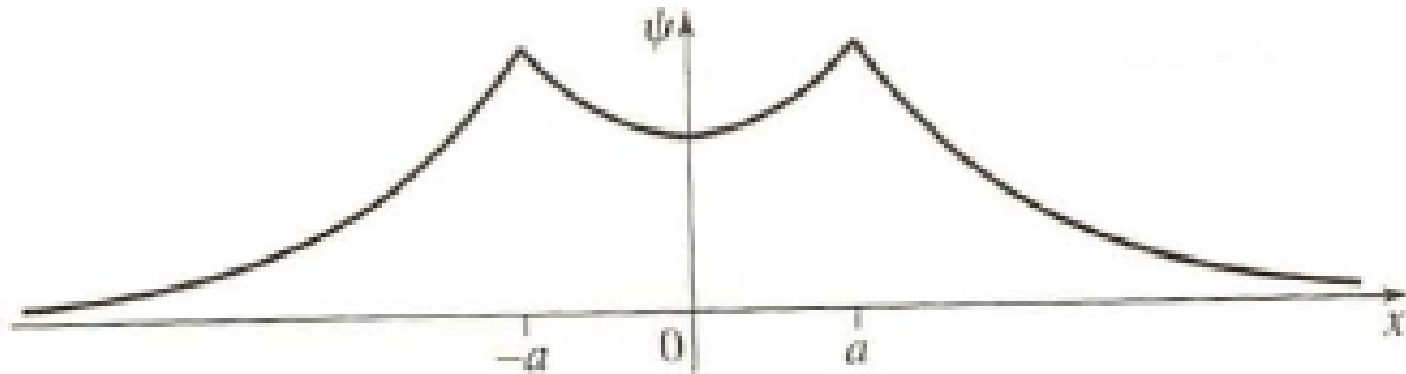


$$\frac{2m}{\hbar^2} V(x) = -\frac{\lambda}{a} [\delta(x - a) + \delta(x + a)]$$



# Model Molecule Wavefunction Shape

- We expect that the solution will look something like this:.



# Model Molecule Wavefunction

- Since  $E < V$  everywhere except for the two points  $a$  and  $-a$ , and the wavefunction must be normalizable, the solutions must be of the form:

$$\psi(x) = \begin{cases} C e^{Kx} & \text{for } x < -a \\ A \exp(Kx) + B \exp(-Kx) & \text{for } -a < x < a \\ D \exp(-Kx) & \text{for } a < x \end{cases}$$

- Where  $K = \sqrt{\frac{2m|E|}{\hbar^2}}$
- The lowest energy solution must be an even function, so  $C=D$  and  $A=B$ .

## Model Wavefunction (2)

Applying the symmetry conditions:

$$\psi(x) = \begin{cases} C e^{Kx} & \text{for } x < -a \\ A \cosh Kx & \text{for } -a < x < a \\ C e^{-Kx} & \text{for } a < x \end{cases}$$

Continuity at  $x=a$  yields:

$$A \cosh Ka = C e^{-Ka}$$

And the condition on the discontinuity in the derivative at  $x=a$  yields:

$$-KC e^{-Ka} - AK \sinh Ka = -\frac{\lambda}{a} A \cosh Ka$$

Putting the two conditions together:

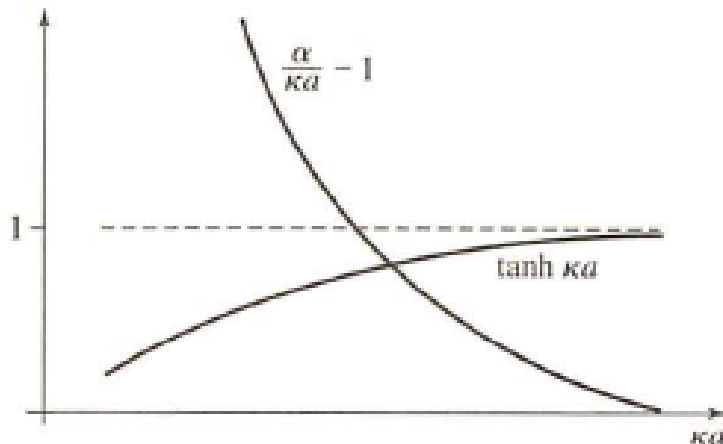
$$-KA \cosh Ka - A \sinh Ka = -\frac{\lambda}{a} A \cosh Ka$$

And dividing by  $A \cosh Ka$

$$\tanh Ka = \frac{\lambda}{a} - 1$$

Which can be solved numerically.

Here is a graphical representation to illustrate



Where the dashed line is the energy for a single well. The particle has lower energy when bound to two wells near one another – binding.

The solution above yields the eigenstate energy and wavefunction for the ground state.

This process can be repeated with the assumption that the eigenstate is odd about the center to search for a second state.

It is not surprising that it is found that the odd state is at higher energy than the ground state.

There are no other bound states.

Discuss covalent bonding and LCAO.

Discuss finding the kinetic energy expectation value.