

# Quantum Mechanics – Chapter 2

Daniel Wysocki and Kenny Roffo

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- 1 The Free Particle
- 2 The Delta-Function Potential
- 3 The Finite Square Well

# The Free Particle

# Wave Function

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$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k := \frac{\sqrt{2mE}}{\hbar}$$

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$$\Psi(x, t) = A \exp\left[\imath k \left(x - \frac{\hbar k}{2m} t\right)\right] + B \exp\left[-\imath k \left(x + \frac{\hbar k}{2m} t\right)\right]$$

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- the first term represents a wave travelling to the right, and the second to the left

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- now we may rewrite the wave function as

$$\Psi_k(x, t) = A \exp \left[ i \left( kx - \frac{\hbar k^2}{2m} t \right) \right]$$

# Normalization

- we cannot normalize  $\Psi_k$ , because  $\Psi_k^* \Psi_k = |A|^2$ , giving

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k dx = |A|^2 \int_{-\infty}^{+\infty} dx = |A|^2 \cdot \infty$$

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$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) \exp \left[ i \left( kx - \frac{\hbar k^2}{2m} t \right) \right] dk$$

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- in essence,  $(1/\sqrt{2\pi})\phi(k) dk$  is taking the place of the coefficients  $c_n$  in the discrete summation



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- we only now have to solve for  $\phi(k)$

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk$$

# General Solution

- this is a classic problem in Fourier analysis, whose answer is provided by **Plancherel's theorem**

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$$

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- now we can find  $\Psi(x, t)$

# de Broglie Wavelength and Speed

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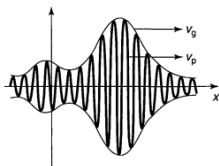
$$v_{\text{quantum}} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

- this is contrary to *classical* speed, which can be determined, for a free particle, by kinetic energy  $E = (1/2)mv^2$

$$v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2v_{\text{quantum}}$$

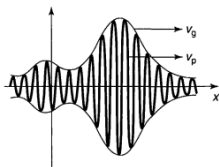


# Group and Phase Velocity



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- the classical velocity corresponds to the *group velocity*, the velocity of the *envelope*

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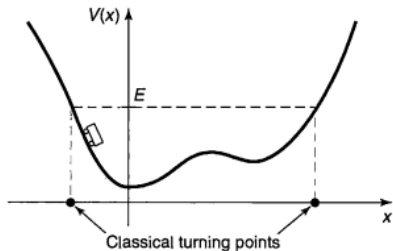
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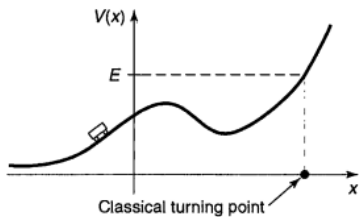
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# Classical Bound and Scattering states



(a)



(b)

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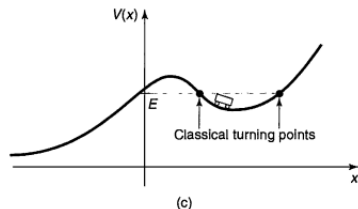
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- in practice, most potentials go to *zero* at infinity, simplifying the criterion to

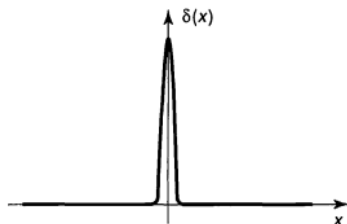
$$\begin{cases} E < 0 \implies & \text{bound state,} \\ E > 0 \implies & \text{scattering state.} \end{cases}$$

# Quantum Bound States and Scattering States



- *bound* state for classical particle, but *scattering* state for quantum particle

# The Delta–Function Well



- the **Dirac delta function** has infinite height, infinitesimal width, and an *area* of 1

$$\delta(x) := \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}, \quad \text{with } \int_{-\infty}^{+\infty} \delta(x) dx = 1.$$



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- multiplying by a function  $f(x)$  is equivalent to multiplying by  $f(a)$ , as it is zero everywhere outside of  $a$

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- the probability of transmission is proportional to the energy

# The Finite Square Well

# Problem

- consider the *finite* square well potential, where  $V_0$  is a positive real potential

$$V(x) = \begin{cases} -V_0, & \text{for } -a \leq x \leq a, \\ 0, & \text{for } |x| > a, \end{cases}$$

# General Solution

- the general solution is given by

$$\begin{cases} Fe^{-\kappa x}, & \text{for } x > a, \\ D \cos(lx), & \text{for } 0 < x < a, \\ \psi(-x), & \text{for } x < 0. \end{cases}$$

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- continuity of  $\psi(x)$  and  $\frac{d\psi}{dx}$  at the boundaries imply  $\kappa = l \tan(la)$ , where

$$\kappa := \frac{\sqrt{-2mE}}{\hbar}$$
$$l := \frac{\sqrt{2m(E + V_0)}}{\hbar}$$

# Energy of the Finite Square Well

- $\kappa$  and  $l$  are both functions of  $E$ , so to solve for  $E$  we first define:

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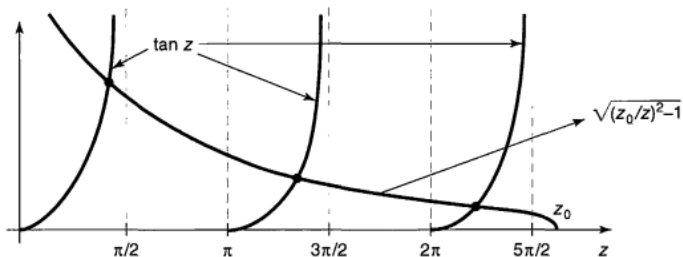
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- can only be solved numerically

# Energy of the Finite Square Well



# Wide, Deep Well

- if  $z_0$  is very large, the intersections occur just below  $z_n = n\pi/2$ , where  $n$  is odd

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- there are a finite number of bound states, but as  $V_0 \rightarrow \infty$ , it approaches the infinite square well, with infinite bound states

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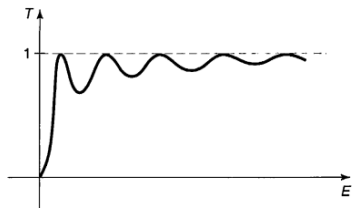
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- this reaches a limit at  $z_0 < \pi/2$ , where the lowest *odd* state disappears, leaving a single state
- no matter how small  $z_0$  becomes, the number of bound states is always at least one



# Transmission

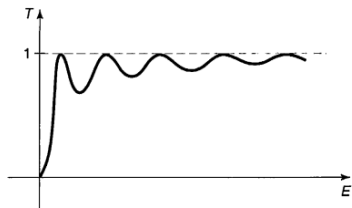


$$T^{-1} = 1 + \frac{V_0^2}{4E(E + V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right)$$

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- these are the allowed energies of the infinite square well

Thank you!