Computer Simulations in Physics
Course for MSc physics students

Solving the Schrödinger equation for 1-dimensional scattering

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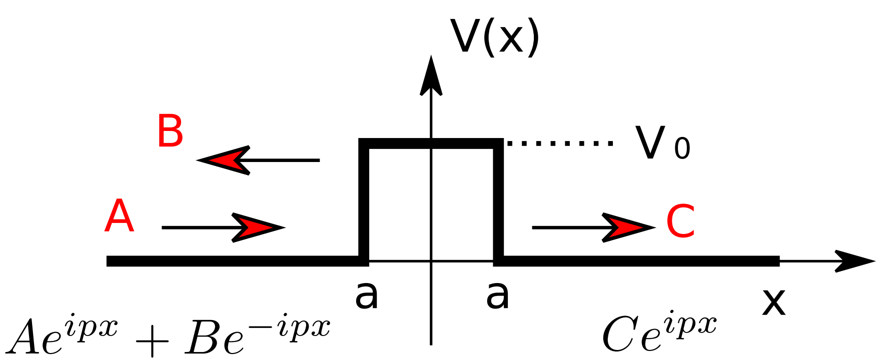
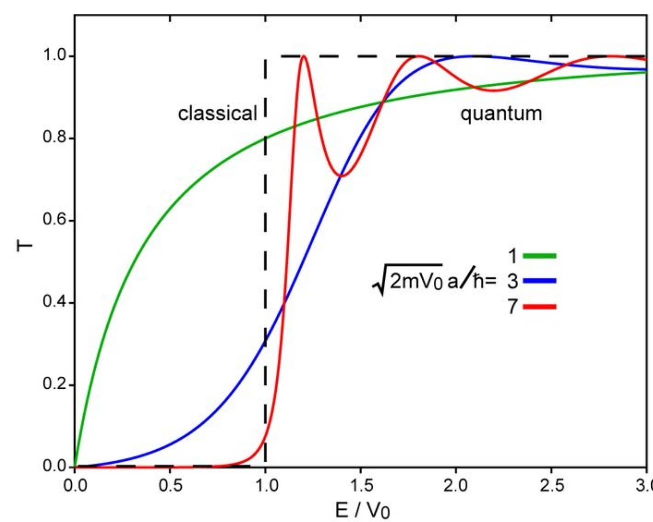
$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x)$$

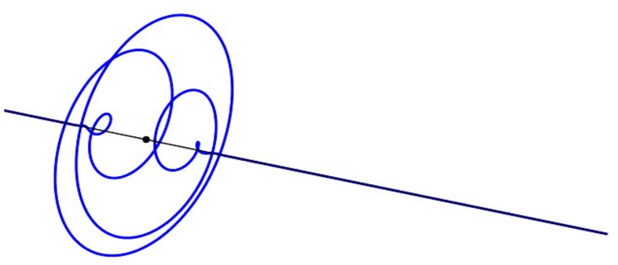




Literature

- Numerics: Computational Quantum Physics course at ETH Zurich SS 2008, by P. de Forcrand & M. Troyer
  - lecture notes online
- Quantum Scattering Theory: Any introductory Quantum Mechanics book, e.g., Griffiths

1-dimensional Quantum Mechanics, brief reminder



state of particle:
complex valued wavefunction $\Psi(x)$

position probability density: $|\Psi(x)|^2$

expectation value of position:

$$\langle x\rangle = \int dx\, |\Psi(x)|^2\, x = \int dx \Psi(x)^* x \Psi(x)$$

position operator: $\hat{x} = x\cdot$ $\quad \hat{x}\Psi(x) = x\Psi(x)$

momentum: $\hat{p} = -i\hbar\partial_x$ $\quad \langle p\rangle = \int dr \Psi(x)^* \hat{p}\Psi(x)$

Hamiltonian = operator of total energy: $\hat{H} = \frac{\hat{p}^2}{2m} + V$

time evolution, Schrodinger equation: $i\hbar\partial_t\Psi = \hat{H}\Psi$

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

1-dimensional quantum mechanics: eigenstates of Hamiltonian, time-independent Schrodinger equation

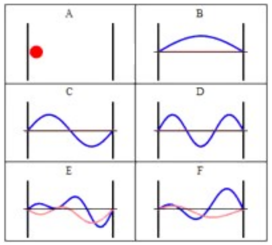
$$i\hbar\partial_t \Psi(x) = -\frac{\hbar^2}{2m}\partial_x^2 \Psi(x,t) + V(x)\Psi(x,t)$$

time evolution, Schrodinger equation: $$i\hbar\partial_t \Psi = \hat{H}\Psi$$

try it on eigenfunction of the operator H: $$\hat{H}\psi(x) = E\psi(x) \quad \rightarrow \quad \Psi(x,t) = e^{-iE/\hbar t}\psi(x)$$

This Ψ is a *stationary state*, position distribution $|\Psi(x,t)|^2$ independent of time

Example:
bound states in
a square well

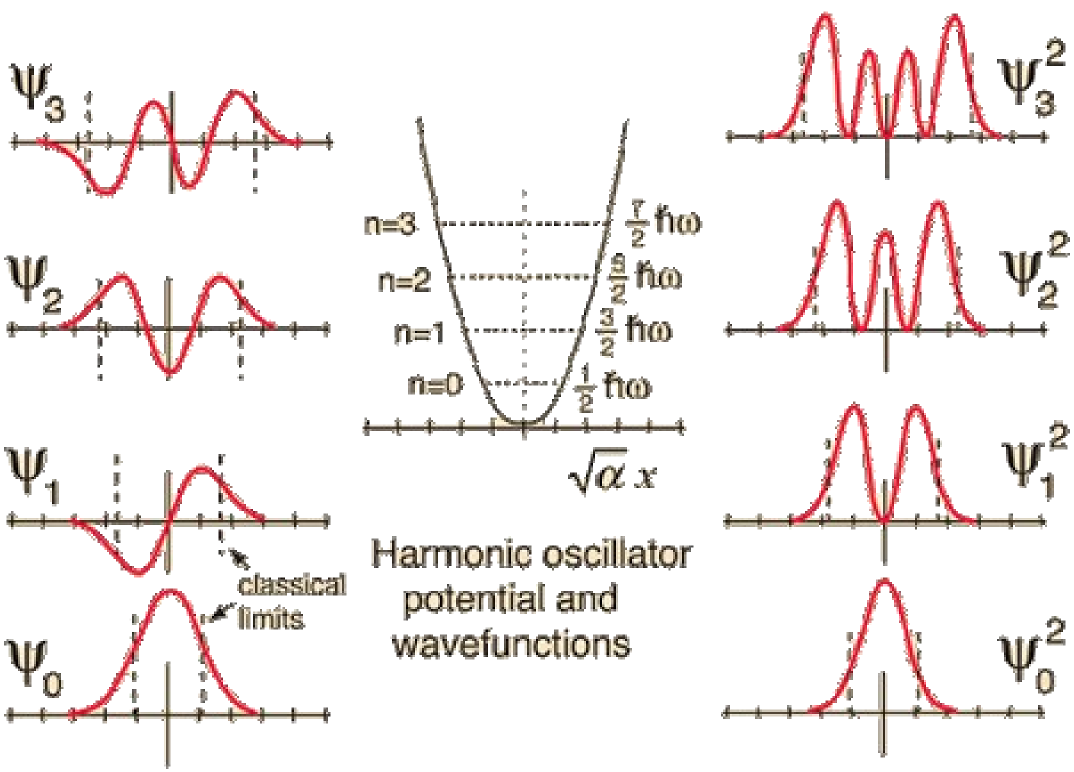


Some trajectories of a particle in a box according to Newton's laws of classical mechanics (A), and according to the Schrödinger equation of quantum mechanics (B–F). In (B–F), the horizontal axis is position, and the vertical axis is the real part (blue) and imaginary part (red) of the wavefunction. The states (B,C,D) are energy eigenstates , but (E,F) are not.

Bound states in 1D have real-valued wavefunctions, decrease fast enough as x→ infty

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x)+\underbrace{\frac{m\omega^2}{2}x^2}_{V(x)}\psi(x)=E\psi(x)$$

$$\Psi(x,t)\underset{x\to\pm\infty}{\longrightarrow}0$$ **particle does not escape**



First four harmonic oscillator normalized wavefunctions

$$\Psi_0=\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-y^2/2}$$

$$\Psi_1=\left(\frac{\alpha}{\pi}\right)^{1/4}\sqrt{2}y\,e^{-y^2/2}$$

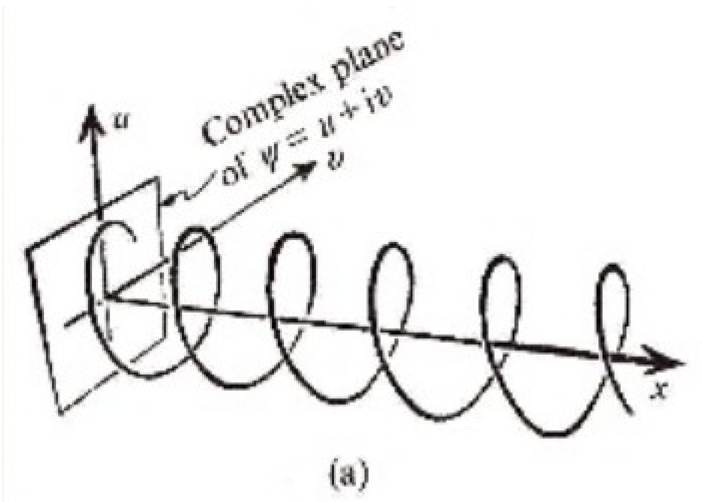
$$\Psi_2=\left(\frac{\alpha}{\pi}\right)^{1/4}\frac{1}{\sqrt{2}}(2y^2-1)\,e^{-y^2/2}$$

$$\Psi_3=\left(\frac{\alpha}{\pi}\right)^{1/4}\frac{1}{\sqrt{3}}(2y^3-3y)e^{-y^2/2}$$

$$\alpha=\frac{m\,\omega}{\hbar}\qquad y=\sqrt{\alpha}\,x$$

http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc5.html

Freely propagating particle: plane wave, wavepacket



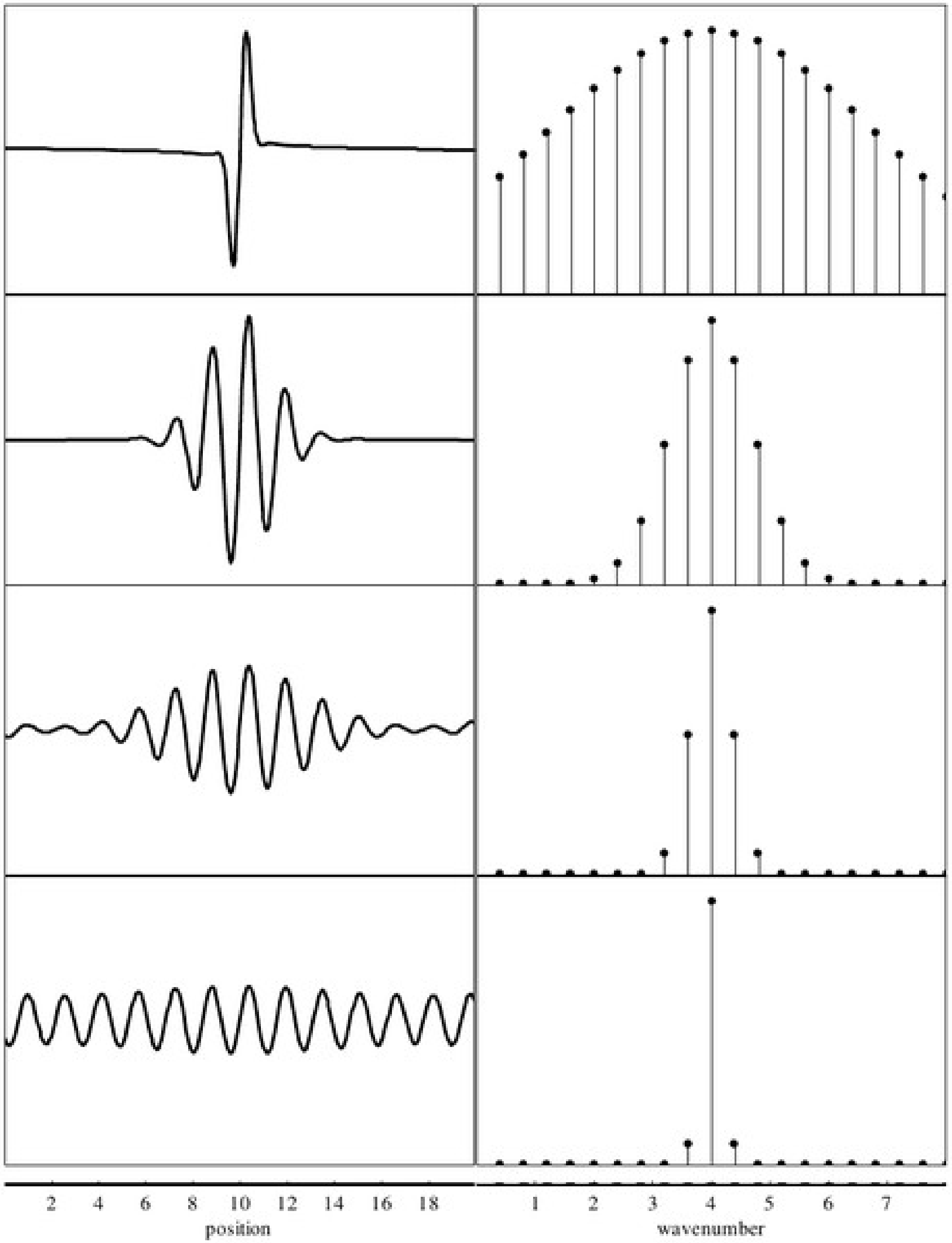
(a)

$$\Psi(x,t) = e^{ikx - iE/\hbar t}$$

Wavefunction not normalized for probability but for particle current

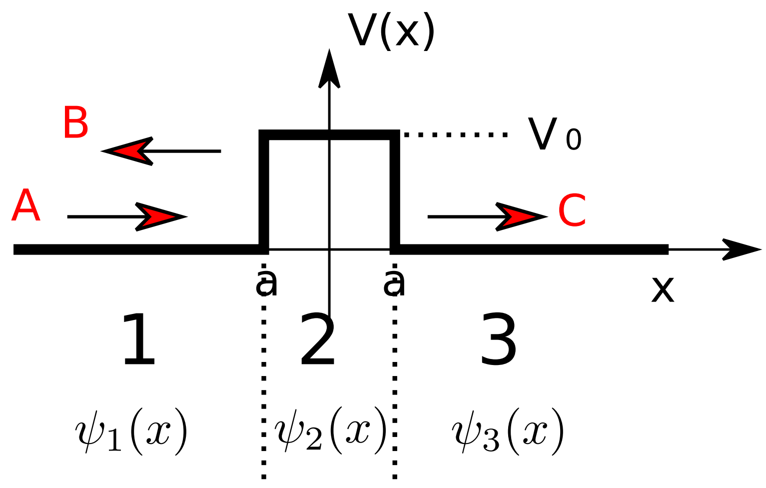
State of actual particle: wavepacket

Real space – momentum space: Fourier transform



Scattering states in 1D: incoming, reflected, transmitted plane wave + something in the middle

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



scattering state:
- a solution of Schrodinger eqn,
  = eigenstate of H
- with no incoming wave from right (D=0)

→ Away from scattering region (1,3):
superposition of plane waves
with wavenumber k_0

$$k_0 = \sqrt{2mE/\hbar^2}$$

→ In scattering region (2):
depends on potential

$$\psi_1(x) = Ae^{ik_0x} + Be^{-ik_0x} \qquad \psi_3(x) = Ce^{ik_0x} + De^{-ik_0x}$$

Solution over all x: fit solutions at a and -a:

$$\psi_1(-a) = \psi_2(-a) \qquad \psi_2(a) = \psi_3(a)$$

$$\psi_1'(-a) = \psi_2'(-a) \qquad \psi_2'(a) = \psi_3'(a)$$

reflection & transmission amplitudes:

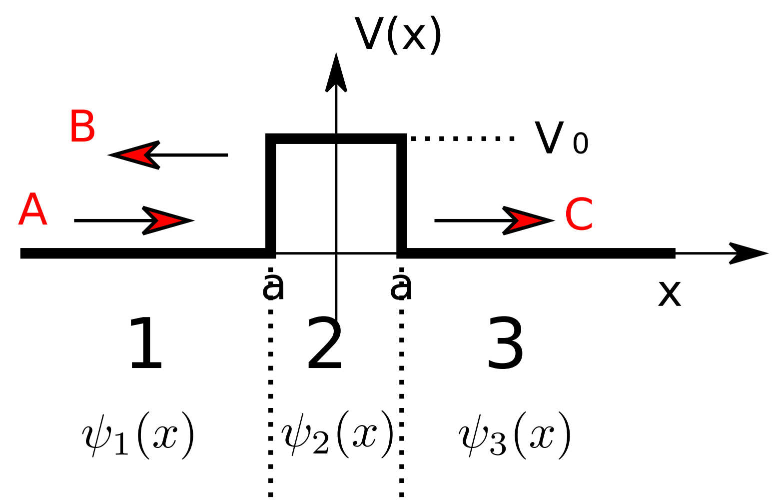
$$r = \frac{B}{A}; \quad t = \frac{C}{A}$$

reflection & transmission probabilities: $R = |r|^2| \quad T = |t|^2$

Example: scattering from Square barrier

Exactly solvable textbook problem (Griffiths Quantum Mechanics 2.6., or wikipedia, plane waves+fitting)

Solution simple in scattering region as well:



$$\psi_2(x) = Fe^{ik_1 x} + Ge^{-ik_1 x}$$

$$k_1 = \sqrt{2m(E - V_0)/\hbar^2}$$

$$k_0 = \sqrt{2mE/\hbar^2}$$

$$\psi_1(x) = Ae^{ik_0 x} + Be^{-ik_0 x}$$

$$\psi_3(x) = Ce^{ik_0 x} + De^{-ik_0 x}$$

Solution over all x: fit solutions at a and -a:

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reflection & transmission amplitudes:

$$r = \frac{B}{A}; \quad t = \frac{C}{A}$$

reflection & transmission probabilities: $R = |r|^2| \quad T = |t|^2$

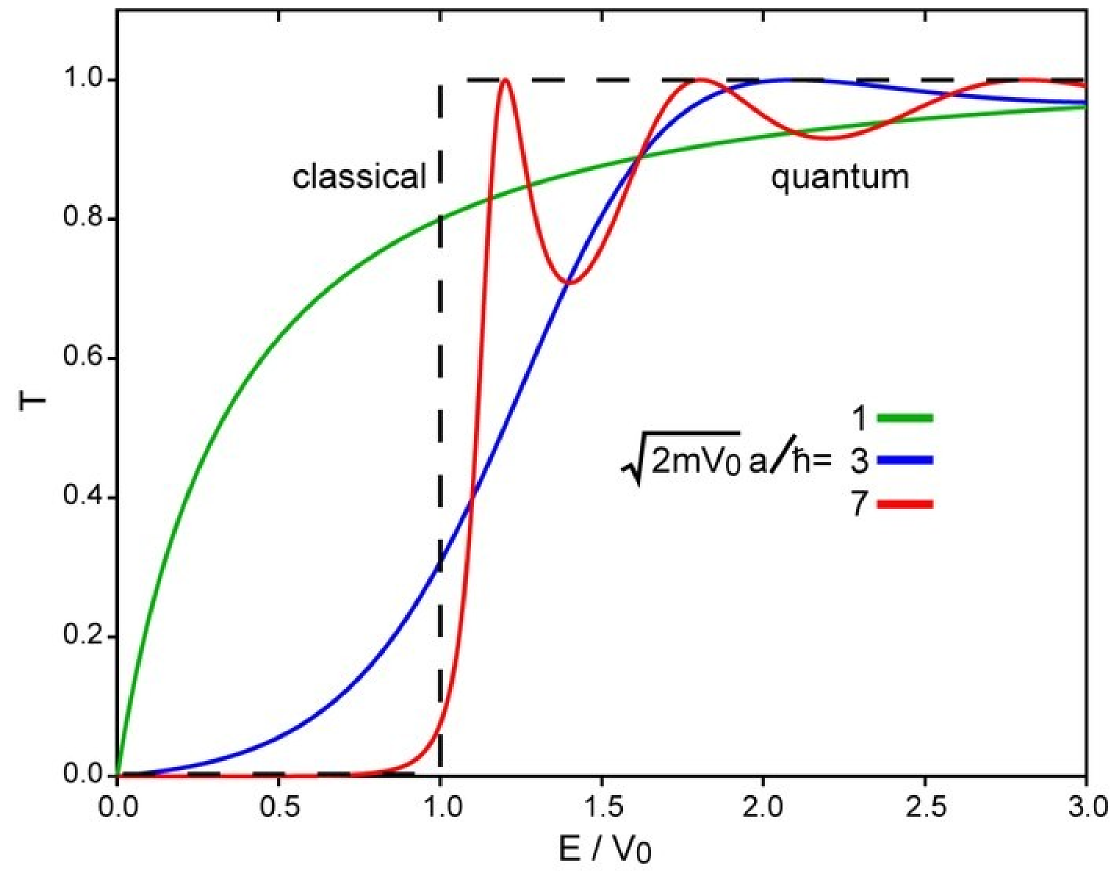
Transmission by tunneling and resonances in square barrier

Tunneling across barrier in classically forbidden regime:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sinh^2 2k_2 a}$$

Transmission across barrier in classically allowed regime:

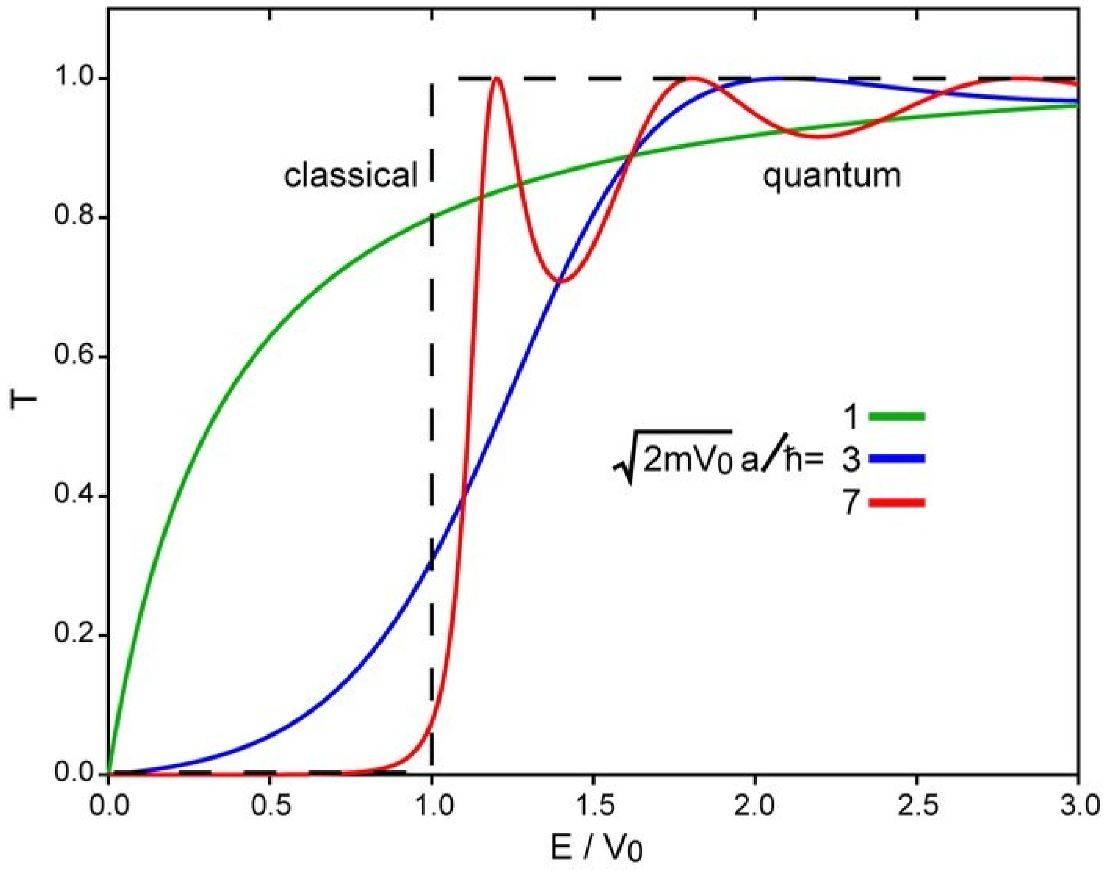
$$T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sin^2 2k_2 a}$$



Transmission resonances:
perfect transmission if 2a = n λ_2 / 2

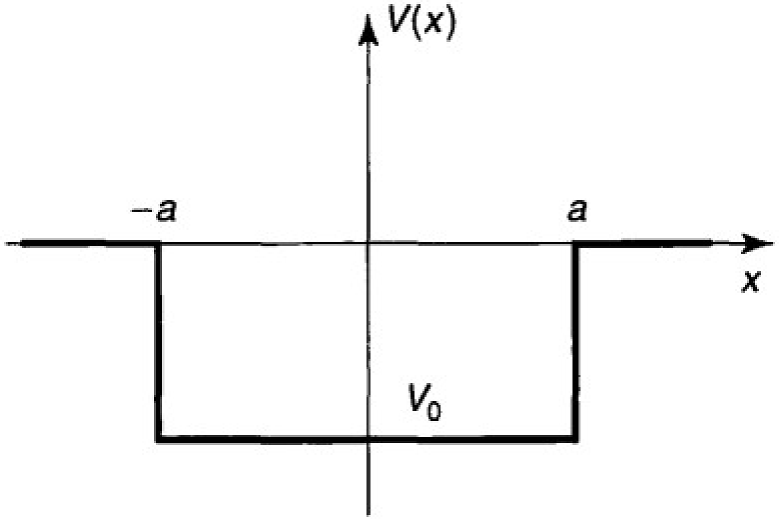
$$E_n = V_0 + \frac{\pi^2 \hbar^2}{8ma^2} n^2$$

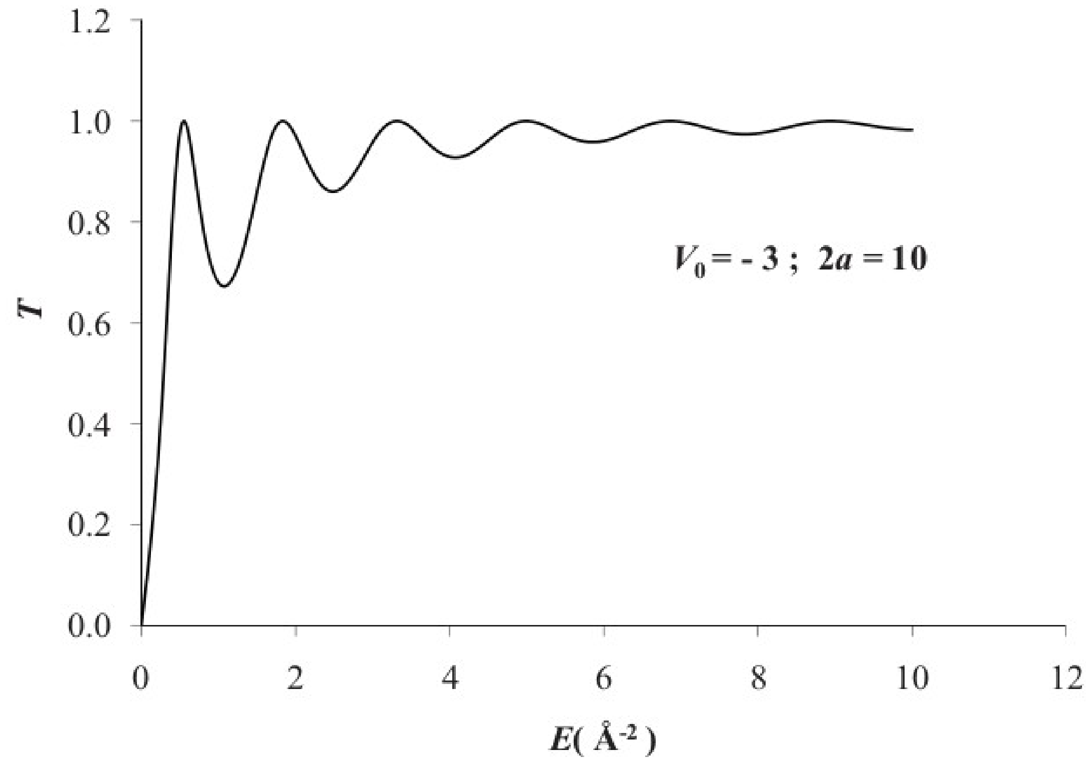
What is fundamental in quantum mechanics, what is only for square barrier?



Formulas also hold for transmission across square well, transmission resonances

As before, with $V_0<0$.





Transmission across square well is always classically allowed:

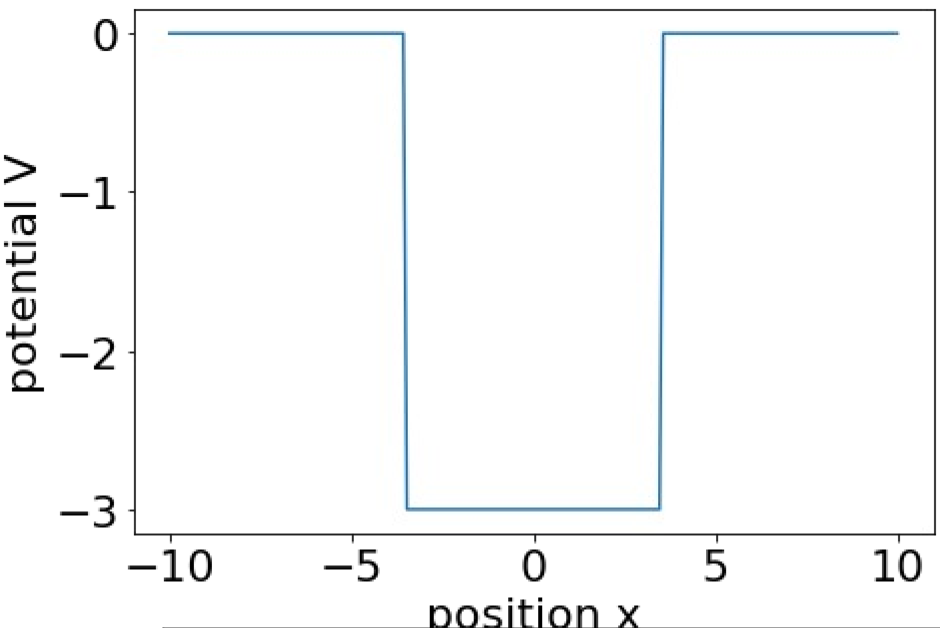
$$T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)}\sin^2 2k_1 a}$$

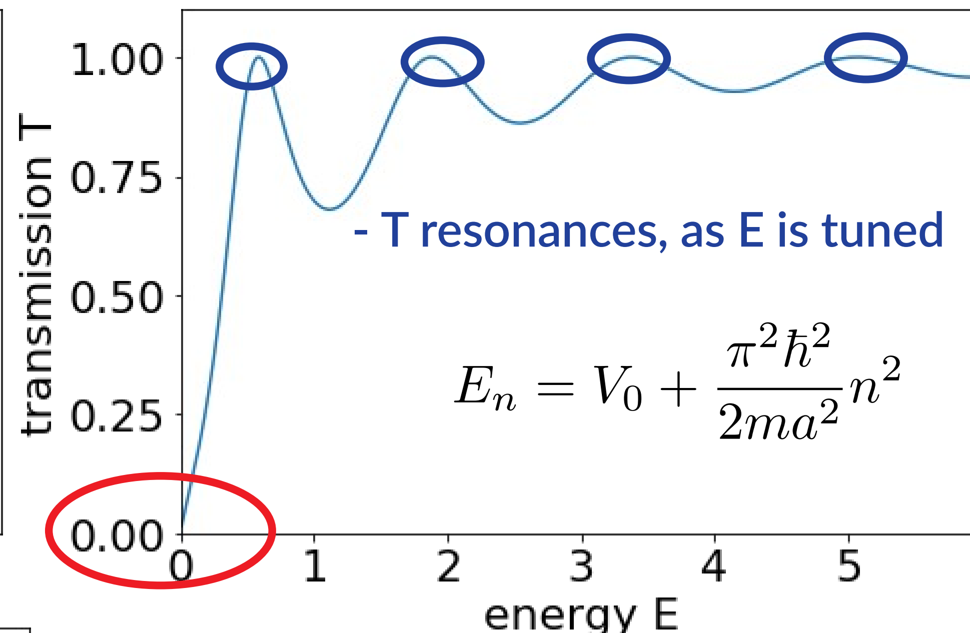
No transmission for $E \to 0$

$$E_n = V_0 + \frac{\pi^2\hbar^2}{8ma^2}n^2$$

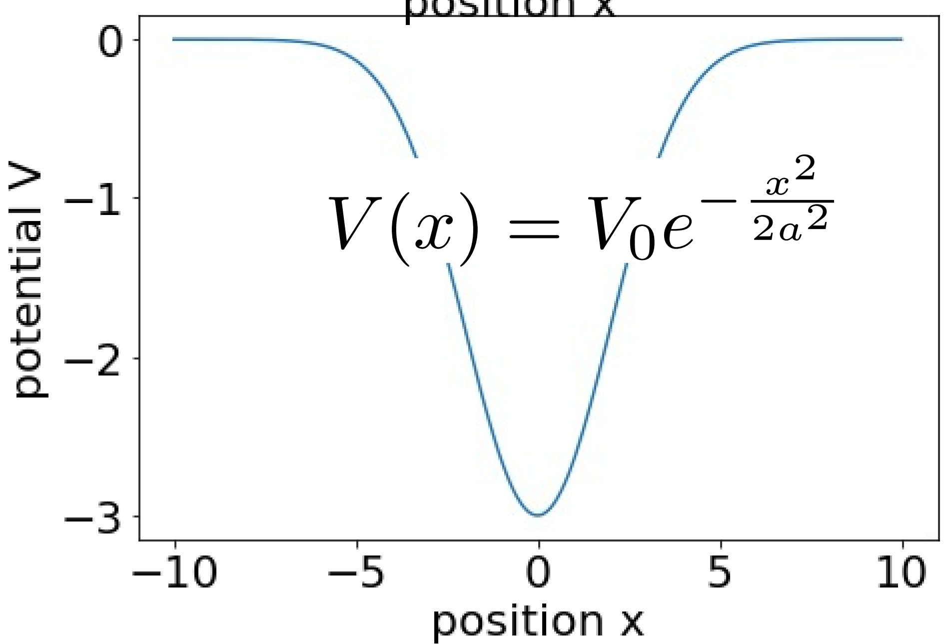
What about a transmission resonance at 0 energy?

What happens to transmission resonances in smooth potentials?





- T resonances at E=0, as V0 is tuned?



- T resonances, as E is tuned?

- T resonances at E=0,
  as V0 is tuned?

Numerov: finite-difference method to solve Schrodinger equation (like Runge-Kutta)

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

discretize position: $x_n = n\Delta x$ $\psi_n = \psi(x_n)$

Taylor expand ψ:

$$\psi_{n\pm1} = \psi_n \pm \Delta x \psi_n' + \frac{\Delta x^2}{2}\psi_n'' \pm \frac{\Delta x^3}{6}\psi_n^{(3)} + \frac{\Delta x^4}{24}\psi_n^{(4)} \pm \frac{\Delta x^5}{120}\psi_n^{(5)} + \mathrm{O}(\Delta x^6)$$

Use a trick to get rid of all odd order derivatives:

$$\psi_{n+1} + \psi_{n-1} = 2\psi_n + (\Delta x)^2\psi_n'' + \frac{(\Delta x)^4}{12}\psi_n^{(4)}.$$

Approximate 4th derivative as a finite difference:

$$\psi_n^{(4)} = \frac{\psi_{n+1}'' + \psi_{n-1}'' - 2\psi_n''}{\Delta x^2}$$

Numerov method, summarized

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

dimensionless variables:

$$\psi''(x) + k(x)\psi(x) = 0$$

here, k(x) is short for

$$k^2(x) = \frac{2m(E - V(x))}{\hbar^2}$$

$$\left(1 + \frac{(\Delta x)^2}{12}k_{n+1}\right)\psi_{n+1} = \quad 2\left(1 - \frac{5(\Delta x)^2}{12}k_n\right)\psi_n - \left(1 + \frac{(\Delta x)^2}{12}k_{n-1}\right)\psi_{n-1} + \mathrm{O}(\Delta x^6)$$

locally accurate to 5th order

To calculate with Numerov method, need initial conditions: 2 neighboring values, to iterate

If potential is finite range, $V(x) = 0$ for $|x|>a$
→ use plane wave/decaying form

$$\psi(-a) = 1$$

(bound state at -E):

$$\psi(-a - \Delta x) = \exp(\Delta x \sqrt{2mE/\hbar})$$

scattering state at +E:

$$\psi(-a - \Delta x) = \exp(\pm i \Delta x \sqrt{2mE/\hbar})$$

Scattering problem by Numerov algorithm

$$\psi_L(x) = A\exp(-iqx) + B\exp(iqx) \qquad \psi_R(x) = C\exp(-iqx)$$

- Set $C = 1$ and use the two points a and $a + \Delta x$ as starting points for a Numerov integration.
- Integrate the Schrödinger equation numerically – backwards in space, from a to 0 – using the Numerov algorithm.
- Match the numerical solution of the Schrödinger equation for $x < 0$ to the free propagation ansatz (3.11) to determine A and B.

$$\begin{aligned} R &= |B|^2/|A|^2 \\ T &= 1/|A|^2 \end{aligned}$$

Choosing the right dimensionless variables is important before numerical work

commonly used Atomic Units:

- action $\hbar$ = 1.05 e-34 kgm^2/s
- charge e = 1.6 e-19 C
- length: Bohr radius: a = 52.9 pm
- mass: m_e = 9.11 e-31 kg

We find out the unit of energy by expressing

$$\frac{\hbar^2}{m_e a^2} = 1E_0 = 27.2\text{eV}$$

Better for us to measure energy in eV:

- action $\hbar$ = 1.05 e-34 kgm^2/s
- mass: m_e = 9.11 e-31 kg
- energy: E_0 = 1 eV

giving us as unit of time and length,

- time: t_0 = $\hbar$/eV = 6.58 e-16 sec = 0.658 femtosec
- length: $l_0 = \sqrt{E_0 t_0^2 / m_e}$ = 0.276 nm

shorthand k(x) in Numerov becomes:

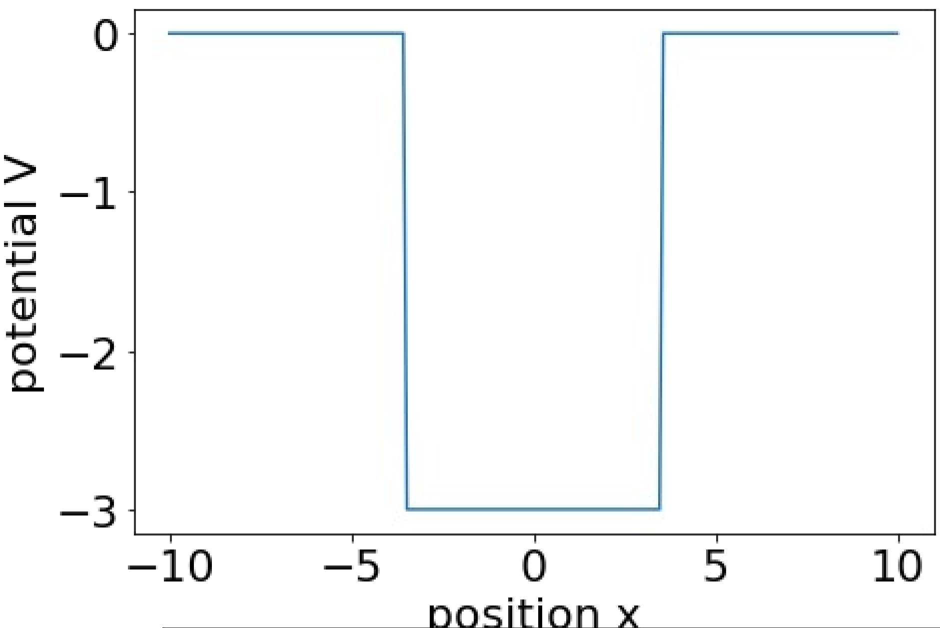
$$"k(x)" = k^2(x) = 2[E - V(x)]$$

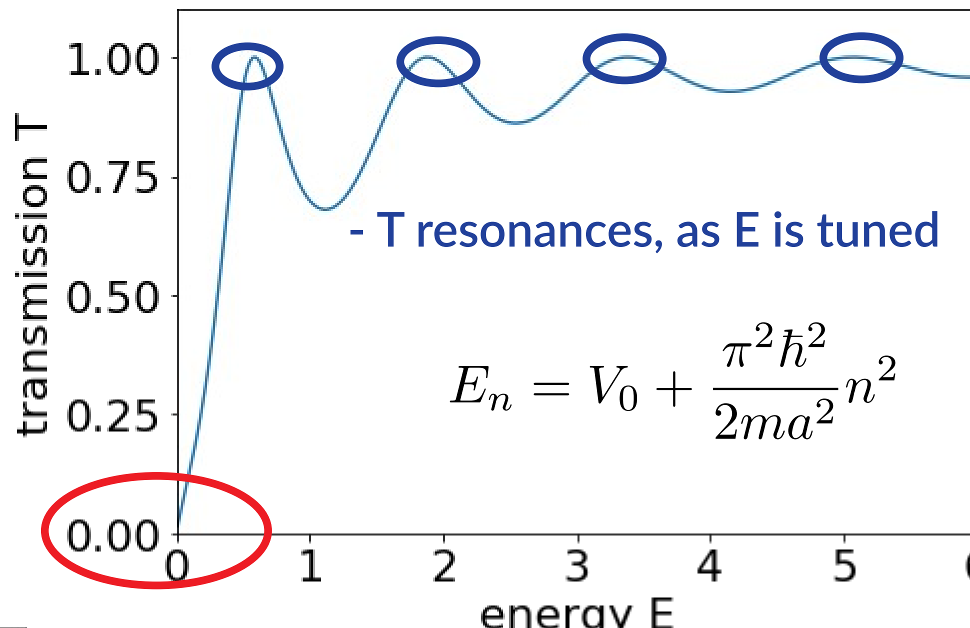
Exercises for today

- Calculate scattering from a square potential barrier by integration of Schrodinger equation using Numerov
  - Plot transmission as a function of energy, for a barrier height 2 eV, size 1nm
    - Compare with analytical curves

- Calculate scattering from a Gaussian potential barrier by the same method
  - Plot transmission as before, with a barrier height 2eV, size 1nm
  - What happened to the transmission resonances?

Homework: what happens to transmission resonances in smooth potentials?





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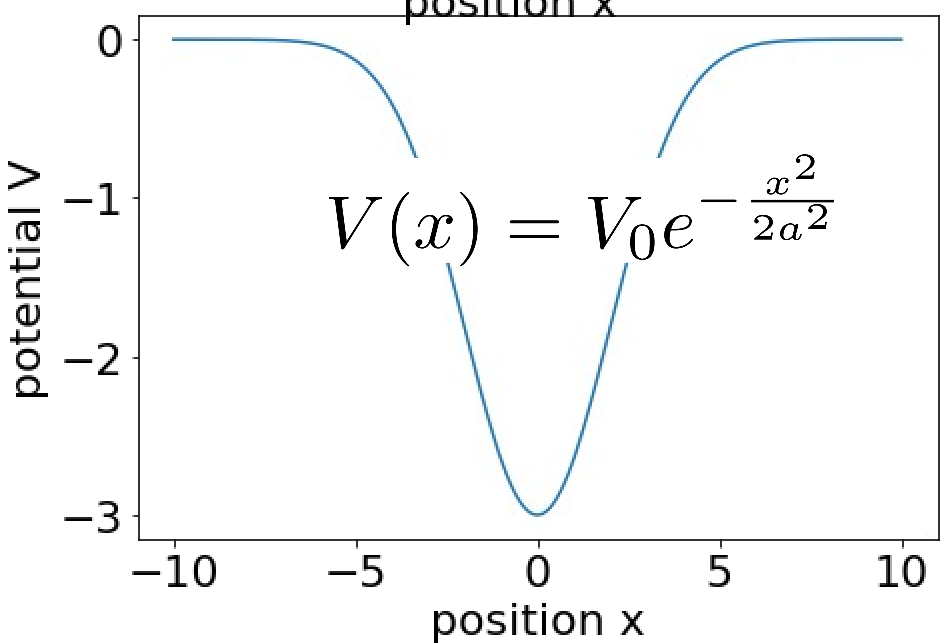

- T resonances, as E is tuned?

- T resonances at E=0,
  as V0 is tuned?

Homework exercises

- Calculate scattering from a square potential well by integration of Schrodinger equation using Numerov
  - Plot transmission as a function of energy, for a well depth 2 eV, size 2a=1nm.
    - Also plot analytical curves
  - Plot transmission as a function of well depth (4 eV→ 0 eV), at energy 0.1 eV, well size a=0.5 nm
- Change the shape of the potential well to Gaussian. What happens to the resonances in the two cases above?
  - Plot transmission as a function of energy, for a well depth 2 eV, size a=0.5nm
  - Plot transmission as a function of well depth (4 eV→ 0 eV), at energy 0.1 eV, well size a=0.5nm