Computational Physics – Lecture 17: Time-dependent Schrödinger equation I

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Computational Physics – Lectures 17 - 18: Time-dependent Schrödinger equation

Erwin Schrödinger
1887 - 1961

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- Why quantum theory?
- Potential barrier
  - Classical forbidden region
  - Quantum tunneling
- Tunneling
  - Thought experiment
  - Application: Electron focusing
- How to solve the time-dependent Schrödinger equation numerically?
  - Discretization →Matrix equation
  - Formal solution → time evolution operator

Contents

  - Product formula approach
- Exercise

Why quantum theory?

- Prior to 1900 all physical phenomena were believed to be explicable in terms of what we now call classical physics.
- Newtonian mechanics (1687):
  - explanation for the motion of mechanical objects (celestial and terrestrial scales)
  - Application to the motion of molecules → kinetic theory of gases.
  - J.J. Thomson´s discovery of the electron (1897) → behavior is described by Newton´s equations of motion.

Why quantum theory?

- Light:
  - Wave nature had been suggested by the diffraction experiments of Young (1803)
  - Wave nature became more obviously so by Maxwell´s discovery in 1864 of the connection between optical, magnetic and electrical phenomena.

→Thought at the end of the 19th century: all interesting questions have been asked and finding the right answers is merely a matter of time

Why quantum theory?

- Pre-quantum era: three critical experiments which could NOT be explained by a straightforward application of classical physics
  - Black-body radiation (Planck, 1900)
  - The photoelectric effect (Einstein, 1905)

  → Planck & Einstein: energy of electromagnetic waves is quantized into particles called photons (The word photon was introduced by Gilbert Lewis in 1926)

Why quantum theory?

- Optical line spectra (Bohr´s atom model, 1913)

→ Bohr: atoms are also quantized, in the sense that they can only emit discrete amounts of energy

- Combined work of Planck, Einstein and Bohr is known as the Old Quantum Theory, which relied heavily on the Newtonian mechanics, but sought to supplement it with supplementary conditions
- Early 1920´s: quantum theory as it then existed was unsatisfactory

Why quantum theory?

- Mid 1920´s two distinct and seemingly independent versions of a new quantum theory were presented:
  - Matrix mechanics (W. Heisenberg, 1925)
  - Wave mechanics (E. Schrödinger, 1926)

  Soon after their discovery these two formulations where shown to be equivalent, forming the basis of present-day quantum theory.

Quantum theory: Some concepts

- Quantum theory: asserts that with every possibility for an event in nature to take place, there is a quantity called amplitude associated with each alternative.
  - The amplitude associated with the overall event is obtained by adding the amplitudes of each of the alternatives.
  - The probability that the event will happen is equal to the square of the absolute value of the overall amplitude.

Quantum theory: Some concepts

→ If Φ_1 and Φ_2 are the amplitudes of the two possibilities for a particular event to take place

- the amplitude for the total event is $\Phi = \Phi_1 + \Phi_2$
- the probability for the event to occur is given by $P = \left|\Phi_1 + \Phi_2\right|^2$

- In the macroscopic world the total probability for an event to take place is given by

$$P = \left|\Phi_1\right|^2 + \left|\Phi_2\right|^2 = P_1 + P_2$$

Quantum theory: Some concepts

- In quantum theory

$$P = |\Phi_1|^2 + |\Phi_2|^2 + \Phi_1\Phi_2^* + \Phi_1^*\Phi_2 = P_1 + P_2 + \Phi_1\Phi_2^* + \Phi_1^*\Phi_2$$

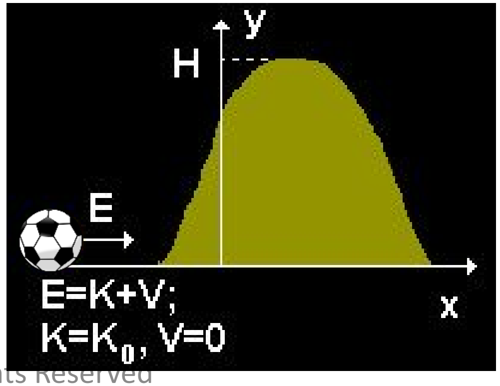
  - The two additional terms are due to the interference of alternatives.
  - If the event is interrupted before its conclusion, for example by determining if the event takes place through alternative 1, the amplitudes of all other alternatives can no longer be added to the total amplitude.

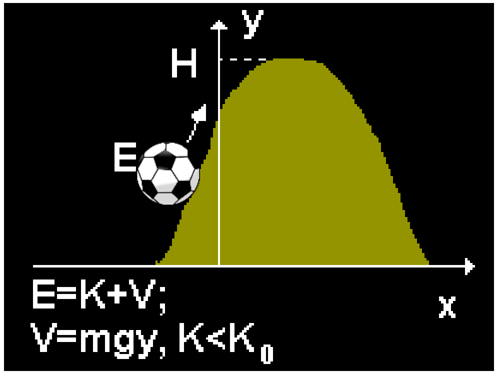
A quantum phenomenon:

Tunneling

Potential barrier: Classical forbidden region

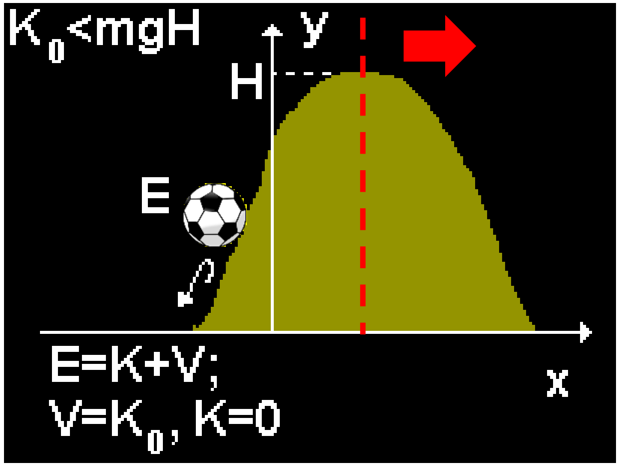
- Consider a classical particle (e.g. a ball) of mass m with a kinetic energy K moving toward a hill of height H. The ball rolls up the hill, transforming kinetic energy into potential energy given by $V = mgy$, where g is the acceleration due to gravitation.





Potential barrier: Classical forbidden region

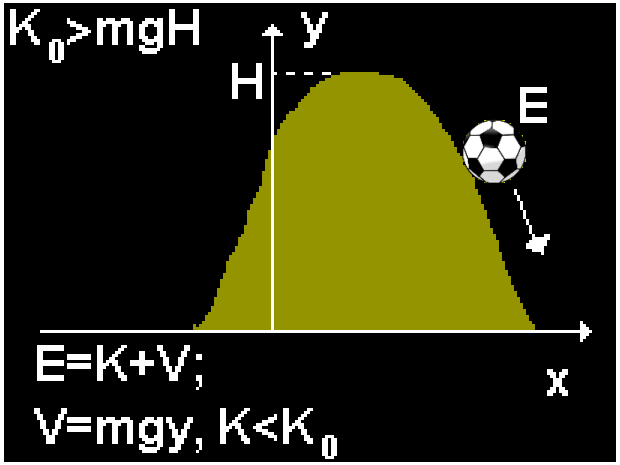
- If $K_0 < mgH$ the ball will not reach the top. At the point where $V = K_0$ the ball reverses its direction and rolls back from the slope.



Classical forbidden region

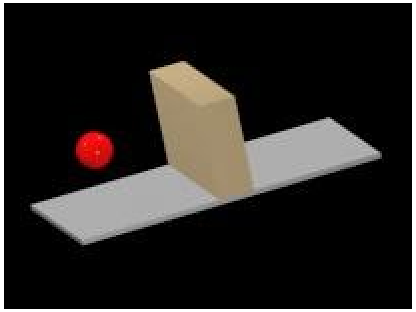
Potential barrier: Classical forbidden region

- If $K_0 > mgH$ the ball will roll over the top of the hill and will run down from the hill on the other side.



Potential barrier: Quantum tunneling

- Consider a particle with energy E approaching a potential step of height $V > E$



  - A classical particle will be reflected by the step
  - A quantum particle incident from the left has a nonzero probability for being found to the right of the step → tunneling

Potential barrier: Quantum tunneling

- The dynamics of the tunneling process can be studied by solving the time-dependent Schrödinger equation

Laplace operator (Laplacian)

$$i\hbar\frac{\partial}{\partial t}\Phi(\vec{r},t)=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})\right)\Phi(\vec{r},t)$$

- Measurements result in intensities which correspond to the probabilities

$$P(x,t)=\Phi^*(x,t)\Phi(x,t)=\left|\Phi(x,t)\right|^2$$

$$\nabla^2=\vec{\nabla}\cdot\vec{\nabla}=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\equiv\Delta$$

Intermezzo: Time-dependent Schrödinger equation (TDSE)

Erwin Schrödinger
1887 - 1961

- General:

$$i\hbar\frac{\partial}{\partial t}\Phi = H\Phi$$

where

  - H : Hamiltonian, operator corresponding to the total energy of the system. Its explicit form depends on the physical situation.
  - Φ : wave function (also called quantum state $\left|\Phi\right\rangle$ or state vector), a complex-valued function

Intermezzo: Time-dependent Schrödinger equation (TDSE)

- The TDSE (1926) describes how the quantum state of some physical system changes with time.

- What does Φ mean?
  - Copenhagen interpretation(s)
  - Ensemble interpretation (Einstein, Ballentine,…)
  - Many-world interpretation
  - …
  - No interpretation: mathematical/computational tool

Intermezzo: Time-dependent Schrödinger equation (TDSE)

- Here we consider the non-relativistic Schrödinger equation for a single particle moving in an electric field

$$i\hbar \frac{\partial}{\partial t}\Phi(\vec{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right)\Phi(\vec{r},t)$$

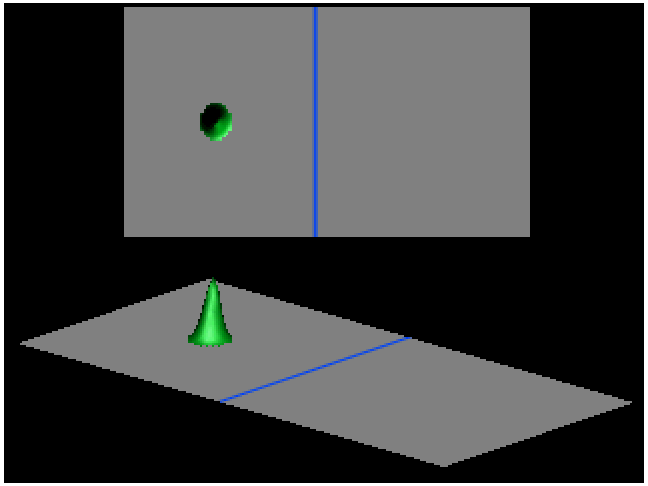
  where
  - m : mass of the particle
  - V : potential energy of the particle

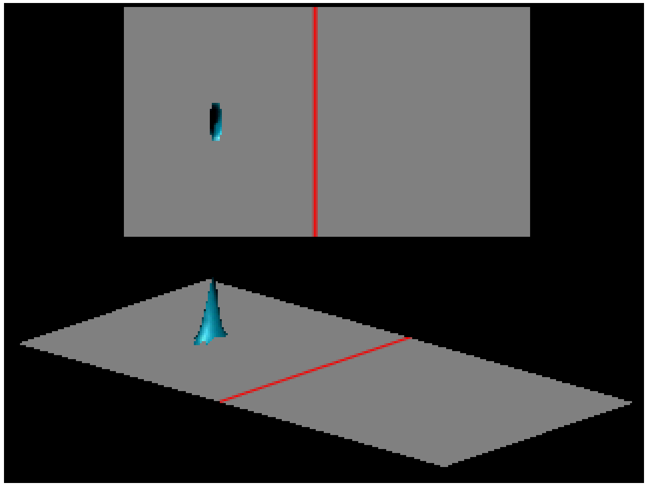
Potential barrier: Quantum tunneling

- A couple of 2D examples for initial values of the wave function $\Phi(\vec{r},t)$ being Gaussian wave packets with width $\sigma = (\sigma_x, \sigma_y)$ and rectangular barriers of width d
  - Movies (http://www.embd.be/quantummechanics) show the time-evolution of the probability

Potential barrier: Quantum tunneling

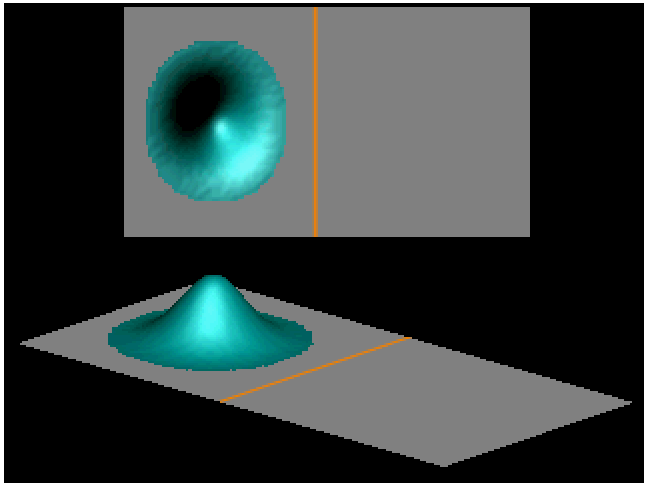
$V = 2E, d = \lambda$
$(\sigma_x, \sigma_y) = (2\lambda, 2\lambda)$

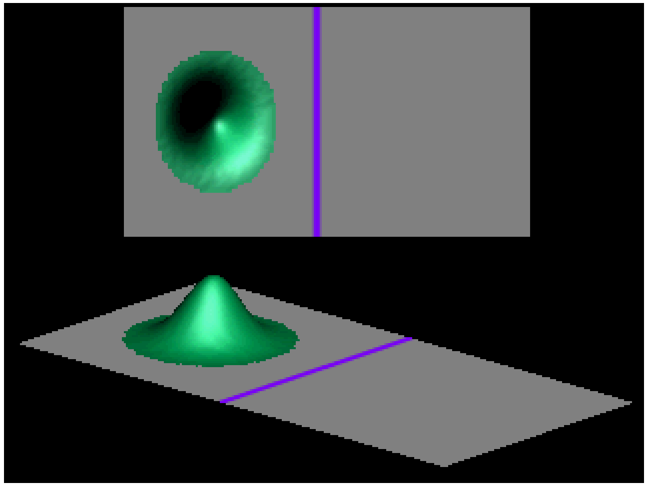




$V = 2E, d = \lambda$
$(\sigma_x, \sigma_y) = (\lambda, 2\lambda)$

$V = 2E, d = 2\lambda$
$(\sigma_x, \sigma_y) = (8\lambda, 8\lambda)$





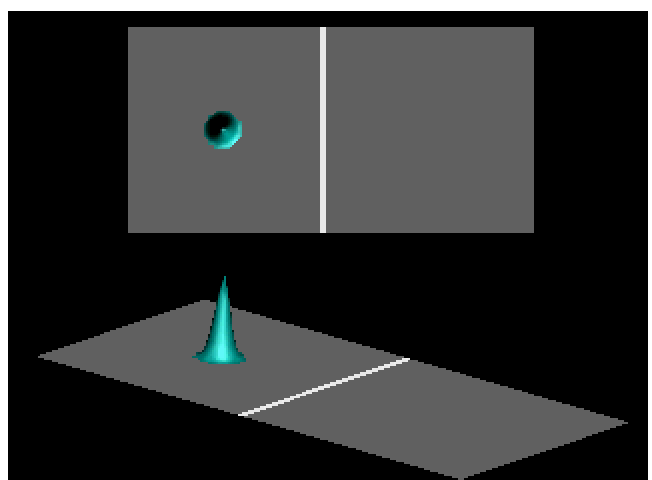
$V = 2E, d = \lambda$
$(\sigma_x, \sigma_y) = (10\lambda, 10\lambda)$

Potential barrier: Quantum tunneling

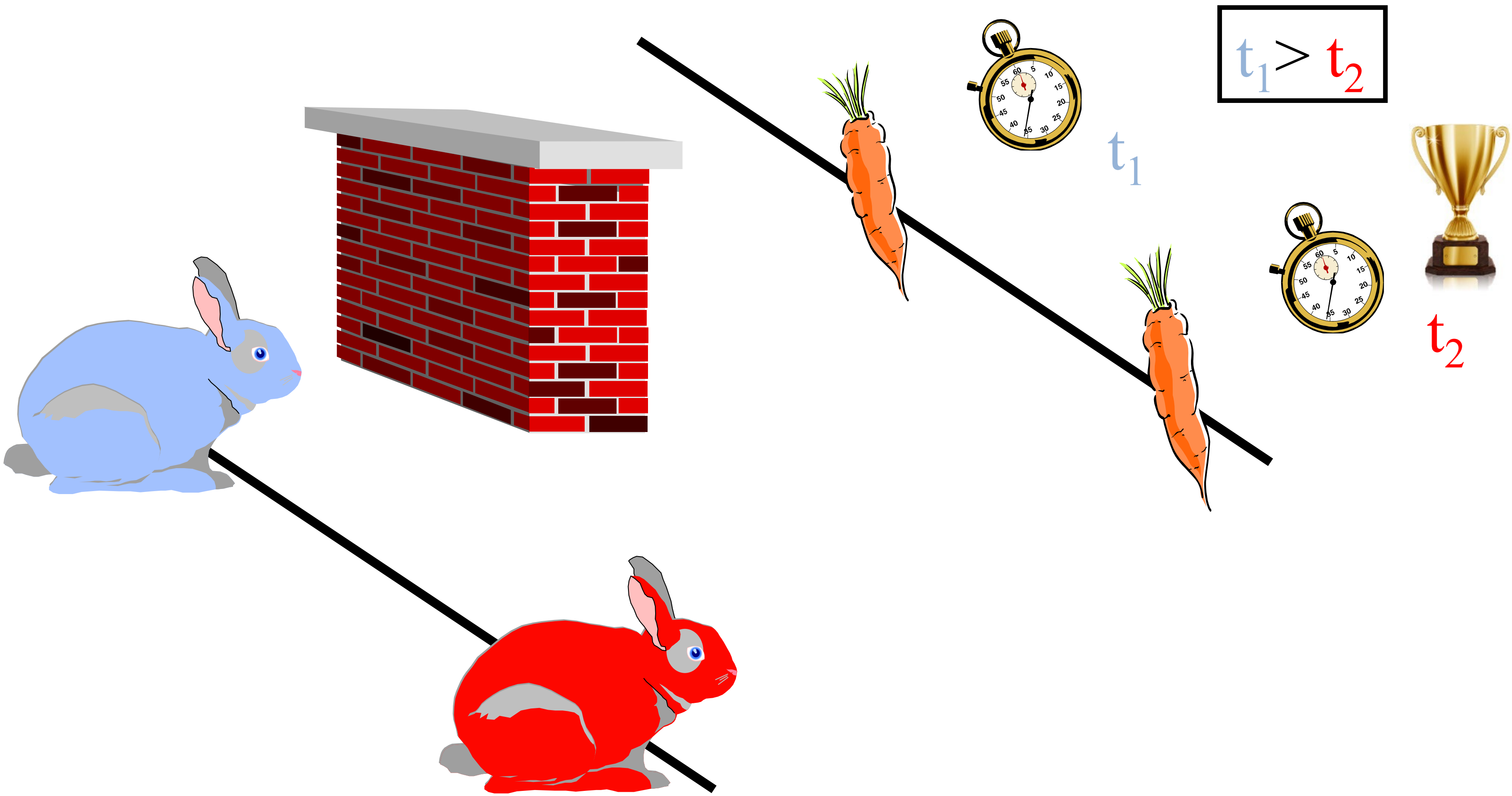
- Observations:
  - The shape of the transmitted wave packet depends on the width of the initial wave packet
  - The probability for tunneling vanishes exponentially with the thickness of the barrier
    - For $V = 2E$ and $d = 2\lambda$ the tunneling probability is less than 0.0000000001
  - Qualitatively the tunnel effect does not depend on the shape (rectangular, triangular, …) of the potential barrier

Tunneling: Thought experiment

- Consider two identical wave packets which start moving at the same time.
  - The blue colored wave packet will hit a potential barrier ($V > E$)
  - The red colored one (initially invisible because hidden under the blue wave) will not feel the step

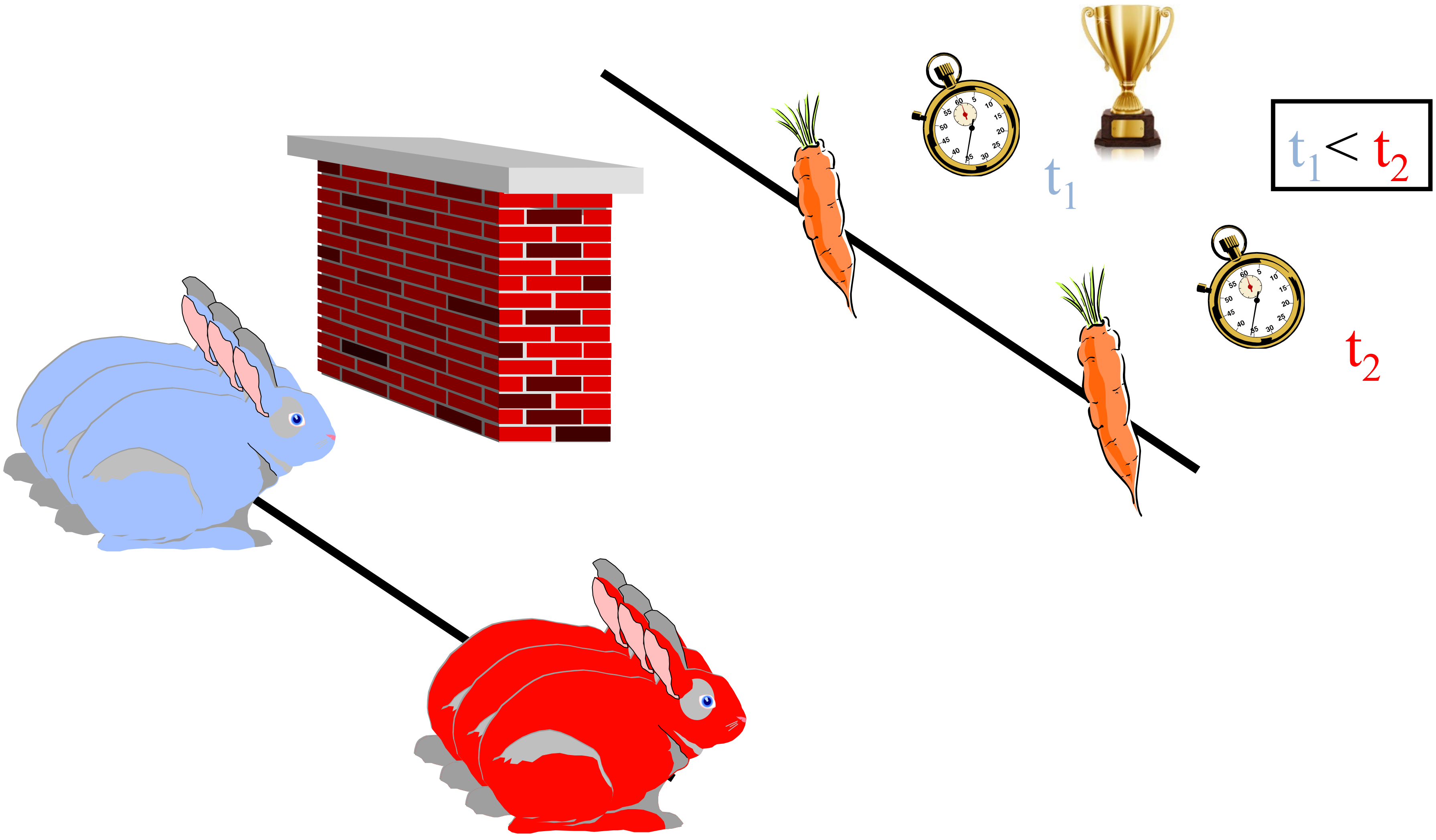


Intermezzo: Rabbit race

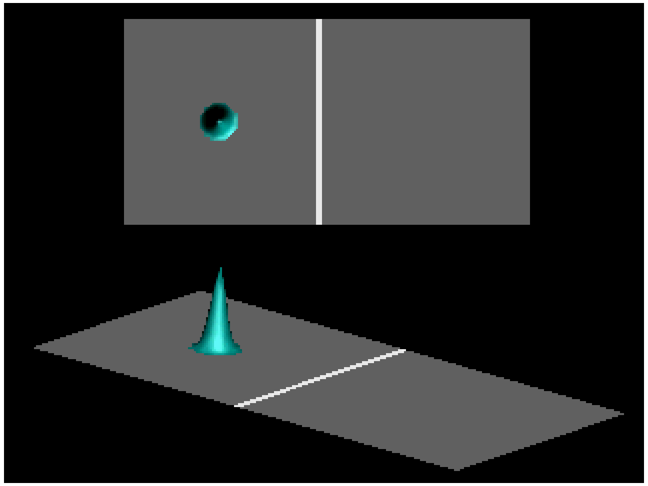


What if we would have quantum rabbits ?

Intermezzo: Rabbit race



Tunneling: Thought experiment



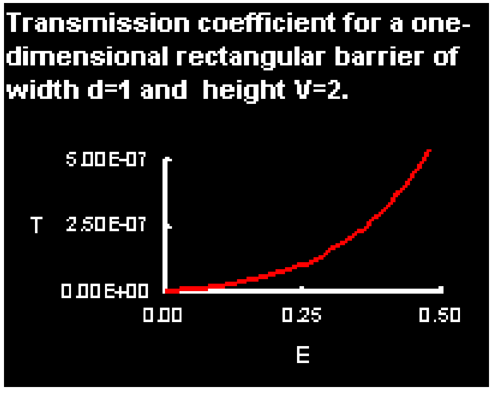
- Observation: The part of the wave packet that tunneled through the potential barrier (i.e. the blue wave to the right of the strip) runs ahead of the red-colored wave packet that did not feel any potential.

Tunneling: Thought experiment

- Explanation:
  - The initial Gaussian wave packet can be viewed as a superposition of plane waves with different momentum.
  - A tunnel barrier acts as a high-pass momentum filter: For increasing momentum perpendicular to the step, the probability for tunneling increases.

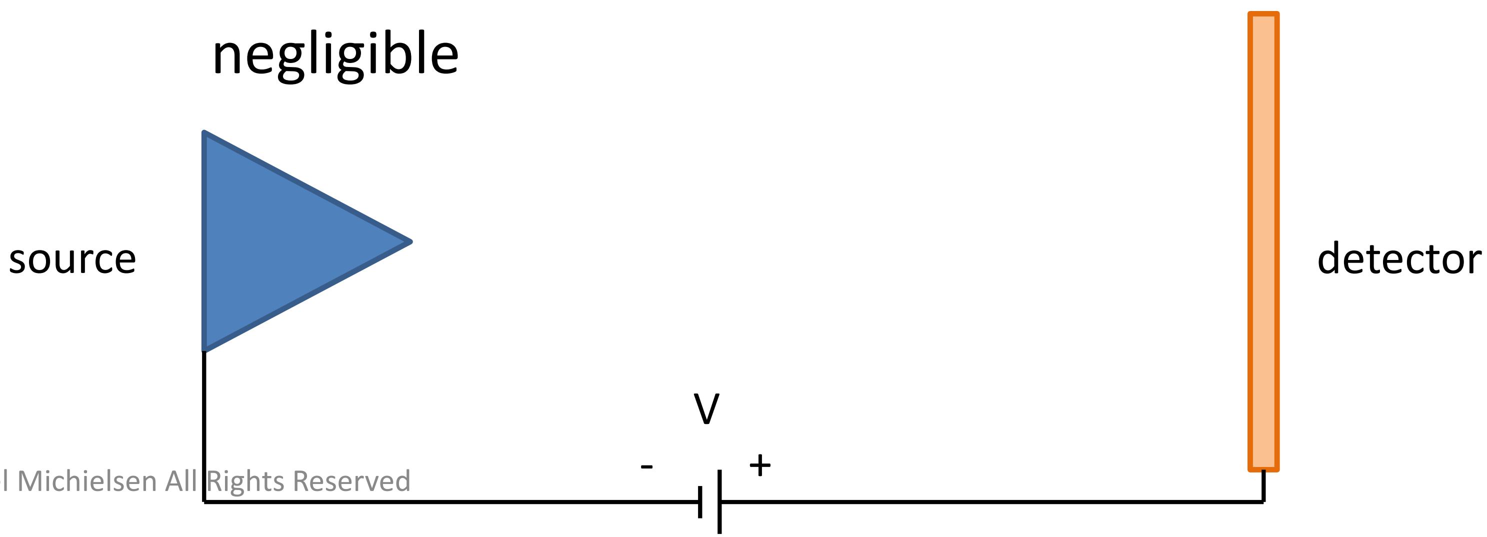
Tunneling: Thought experiment

- Filtering effect
  - also occurs if the motion of the particle is one-dimensional
  - is a direct consequence of the fact that the tunnel probability is a function of the energy
    - In free space the energy is proportional to the momentum squared



Tunneling: Application

- Coherent and focused electron beams
  - Simplest method: Apply large voltage between electron source and screen (detector)
    - Electrons leaving the source are accelerated.
    - If the acceleration is sufficiently large, the width of the electron beam in the direction of acceleration is negligible



Tunneling: Application

- Applications:
  - television displays
  - conventional electron microscopes
- Explanation: classical mechanical framework

– Other method: Reduction of the size of the aperture of the source

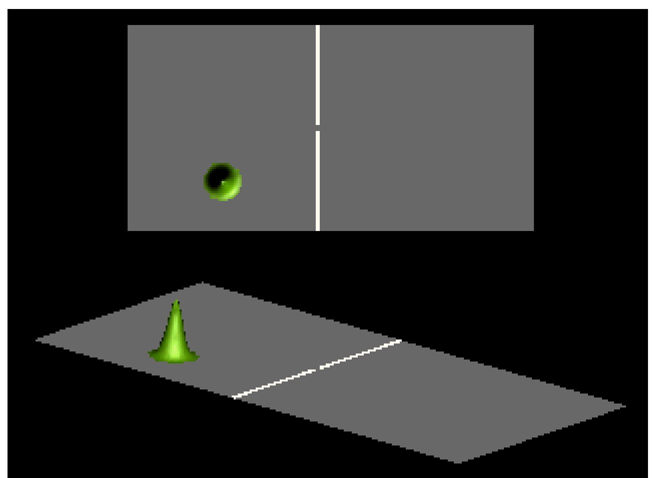
- Works well as long as this size is much larger than the typical wavelength of the emitted particles
- When the dimension of the aperture becomes comparable to the characteristic wavelength the beam will spread out due to diffraction.

Tunneling: Application

– Nanosource (atom-size tips): emitting electrons at fairly low applied voltages (a few thousand volts or less) with a small angular spread (of a few degrees)
  - Applications:
    - Electron holography
    - Electron interferometry
  - Main physical mechanism: Tunneling through surrounding metal-vacuum potential

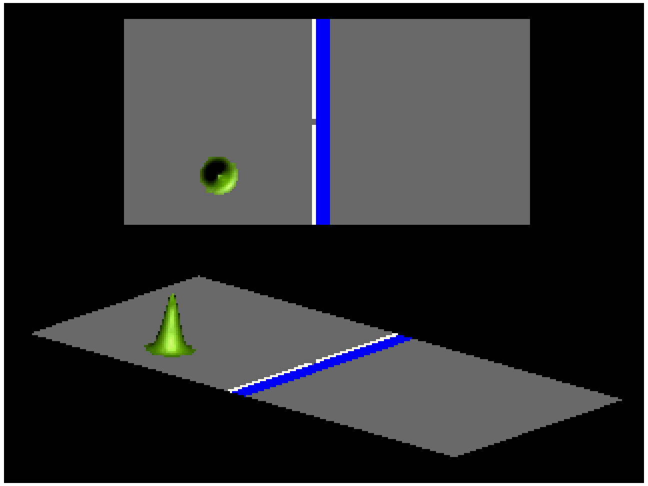
Tunneling: Application

- A wave passing through a narrow slit is scattered in many directions. Both the momentum parallel and perpendicular to the slit are no longer conserved.



Tunneling: Application

- Placing a tunnel barrier (e.g. triangular potential barrier) to the right of the slit can strongly modify the properties of the transmitted wave.



Simple model to describe the electron emission from nanoscale sources

How to solve the time-dependent Schrödinger equation numerically?

Time-dependent-Schrödinger equation

- Time-dependent-Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\Phi(\vec{r},t)=\left(-\frac{\hbar^2}{2M}\nabla^2+V(\vec{r})\right)\Phi(\vec{r},t)$$

  – Solution contains all dynamical information on the system

  – Formal solution:

$$\Phi(\vec{r},t)=e^{-itH}\Phi(\vec{r},t=0)$$

    - Explicit expression for the solution can in general not be written down in closed form

    → Rely on numerical techniques to solve the initial value problem

From continuum model to discrete model

- Time-dependent-Schrödinger equation (TDSE)

$$i\hbar \frac{\partial}{\partial t}\Phi(\vec{r},t) = \left(-\frac{\hbar^2}{2M}\nabla^2 + V(\vec{r}) \right)\Phi(\vec{r},t)$$

- 1D, we use

$$V(x) \rightarrow V(x = j\Delta)$$

$$\frac{\partial^2}{\partial x^2}\Phi(x,t) \rightarrow \frac{\Phi(x+\Delta,t) - 2\Phi(x,t) + \Phi(x-\Delta,t)}{\Delta^2}$$

to bring the equations in a form that is suitable for numerical simulation

From continuum model to discrete model

- Discretization ($\hbar = M = 1$)

$$i\frac{\partial}{\partial t}\begin{pmatrix}\Phi_1(t)\\ \Phi_2(t)\\ \Phi_3(t)\\ \vdots\\ \vdots\\ \Phi_L(t)\end{pmatrix} = \underbrace{\Delta^{-2}\begin{pmatrix}1+\Delta^2V_1 & -1/2 & 0 & & & 0\\ -1/2 & 1+\Delta^2V_2 & -1/2 & & & \\ 0 & -1/2 & 1+\Delta^2V_3 & & & \\ & & & \ddots & & 0\\ & & & & 1+\Delta^2V_{L-1} & -1/2\\ 0 & & & 0 & -1/2 & 1+\Delta^2V_L\end{pmatrix}}_{H}\begin{pmatrix}\Phi_1(t)\\ \Phi_2(t)\\ \Phi_3(t)\\ \vdots\\ \vdots\\ \Phi_L(t)\end{pmatrix}$$

  - Recall that Φ_j are complex numbers
  - $V_j = V(j\Delta)$

$\boxed{\text{Matrix equation}}$

Numerical method

- H can be brought in diagonal form
  - analytically
  - brute force numerical diagonalization
- Exact diagonalization of H (see Numerical Recipes)

  $$H\Psi = E\Psi$$

  Time-independent Schrödinger equation

  - Eigenvalues and eigenvectors:
    $(E_n, \Psi_n) \quad n = 1, \ldots, L$
    Matrix of eigenvectors: $U, \quad U^\dagger U = (U^*)^T U = U^{-1} U = I$
    Diagonal matrix with eigenvalues: D

    $$U^\dagger H U = D$$

  - Library: LAPACK

Numerical method

- Computer resources diagonalization:
  - # operations: $O(L^3)$
  - Memory: $O(L^2)$
    e.g. total available memory on IBM Blue Gene/Q, Forschungszentrum Jülich: 458752 GB = 458752 10^9 bytes
    - » Most ideal case:
      8 bytes for a real number (13-15 digit floating point arithmetic)
      → 16 bytes for a complex number
      → 28672 10^9 complex numbers can be stored
      → 5 10^6 x 5 10^6 matrix (2000 x 2000 matrix can be diagonalized on a desktop computer without too much effort)

Numerical method

- Computer resources time evolution:

$$
\begin{aligned}
e^{-itH} &= UU^{\dagger}e^{-itH}UU^{\dagger} \\
&= Ue^{-itU^{\dagger}HU}U^{\dagger} \\
&= Ue^{-itD}U^{\dagger}
\end{aligned}
$$

  - # operations:

$$
\begin{aligned}
\Phi(t+\tau) = e^{-i\tau H}\Phi(t) &= Ue^{-i\tau D}\boxed{U^{\dagger}\Phi(t)} && O(L\times L) \\
&= U\boxed{e^{-i\tau D}\Phi'(t)} && O(L) \\
&= \boxed{U\Phi''(t)} && O(L\times L)
\end{aligned}
$$

Numerical method

- Hidden problem in matrix equation TDSE:
  – If H cannot be brought in diagonal form
    - analytically
    - brute force numerical diagonalization
  – then it is impossible to calculate $e^{-itH}\Phi(\vec{r},t)$

→ Numerical method:
  – Propose an approximation for the time-evolution operator $e^{-i\tau H}$ for a well-chosen time step τ
  – Integration of TDSE by repeated application of the approximate time-step operator $e^{-i\tau H} = \left(e^{-i\tau H/m}\right)^m$

Numerical method

– Quantum mechanics imposes some extra constraints: The total probability should be conserved
  - We do not want the algorithm to “create” or “remove” part of the particle

→ The approximate time-evolution operator U should be a unitary operator

$$U^{-1}(t) = (U^{*}(t))^{T} = U^{\dagger}(t)$$

Numerical method

– Crucial observation: If we change the wave function by any unitary transformation, the total probability (= Euclidean length of the vector) does not change

- Proof:

$$P = \sum_{i=1}^{L} \Phi_i^* \Phi_i = \sum_{i=1}^{L} \sum_{j=1}^{L} \Phi_i^* \delta_{i,j} \Phi_j = \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{k=1}^{L} \Phi_i^* U_{i,k}^{-1} U_{k,j} \Phi_j$$

$$= \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{k=1}^{L} U_{k,i}^* \Phi_i^* U_{k,j} \Phi_j = \sum_{k=1}^{L} \left(\sum_{i=1}^{L} U_{k,i}^* \Phi_i^* \right) \left(\sum_{j=1}^{L} U_{k,j} \Phi_j \right)$$

$$= \sum_{k=1}^{L} \Psi_k^* \Psi_k \quad \text{where} \quad \Psi_k = \sum_{j=1}^{L} U_{k,j} \Phi_j$$

Numerical method

- Unitarity of the approximate time-step operator implies unconditional stability of the numerical method
  $UU^{\dagger} = 1 \rightarrow \|U\| = 1$ whereas a necessary and sufficient condition for stability is $\|U\| \leq 1$
- Local error of the approximate time-step operator, i.e. maximum error made in taking a single step:
  $\left\| e^{-i\tau H} - U \right\|$
- Maximum global error after m time steps:
  $m \left\| e^{-i\tau H} - U \right\|$

Product formula approach

- Strategy: We search for a decomposition $H = A + B + \ldots$ such that $\exp(-itA)$, $\exp(-itB)$, … are unitary matrices
  - Why?

    Any product of unitary matrices is unitary
    - Proof

$$\left(U_1 U_2 \ldots U_p\right)^{-1} = U_p^{-1} \ldots U_2^{-1} U_1^{-1} = \left(U_p^*\right)^T \ldots \left(U_2^*\right)^T \left(U_1^*\right)^T$$

$$= \left(U_1^* U_2^* \ldots U_p^*\right)^T = \left(\left(U_1 U_2 \ldots U_p\right)^*\right)^T$$

H. De Raedt, "Product Formula Algorithms for Solving the Time-Dependent Schrödinger Equation", Comp. Phys. Rep. 7, 1 – 72 (1987)

Product formula approach

- This is easy…
- If $A = A^\dagger = \left(A^*\right)^T$ (Hermitian matrix) then

  $$\left(e^{iA}\right)^\dagger = e^{-iA^\dagger} = e^{-iA} = \left(e^{iA}\right)^{-1}$$

  is a unitary matrix
- Therefore, we can confine the search to matrices $A, B, C,$ which are Hermitian and for which $H = A + B + C$

Product formula approach

- Simple choice (assuming L is odd)

$$H = V + K_1 + K_2 = \Delta^{-2}\begin{pmatrix} 1+\Delta^2 V_1 & 0 & 0 & & & 0 \\ 0 & 1+\Delta^2 V_2 & 0 & & & \\ 0 & 0 & 1+\Delta^2 V_3 & & & \\ & & & \ddots & & 0 \\ & & & & 1+\Delta^2 V_{L-1} & 0 \\ 0 & & & 0 & 0 & 1+\Delta^2 V_L \end{pmatrix}$$

$$+\Delta^{-2}\begin{pmatrix} 0 & -1/2 & 0 & & & 0 \\ -1/2 & 0 & 0 & & & \\ 0 & 0 & 0 & & & \\ & & & \ddots & -1/2 & 0 \\ & & & -1/2 & 0 & 0 \\ 0 & & & 0 & 0 & 0 \end{pmatrix} + \Delta^{-2}\begin{pmatrix} 0 & 0 & 0 & & & 0 \\ 0 & 0 & -1/2 & & & \\ 0 & -1/2 & 0 & & & \\ & & & \ddots & & 0 \\ & & & & 0 & -1/2 \\ 0 & & & 0 & -1/2 & 0 \end{pmatrix}$$

Product formula approach

- Second-order product formula algorithm

$$e^{-i\tau H} \approx e^{-i\tau K_1/2} e^{-i\tau K_2/2} e^{-i\tau V} e^{-i\tau K_2/2} e^{-i\tau K_1/2}$$

- $e^{-i\tau V}$ is a diagonal matrix with elements that are the exponentials of the diagonal elements of V ➔very simple
- $e^{-i\tau K_1/2}, e^{-i\tau K_2/2}$ are block diagonal matrices of 2x2 matrices

$$\exp\left(ia \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) = \begin{pmatrix} \cos a & i \sin a \\ i \sin a & \cos a \end{pmatrix}$$

Product formula approach

- $e^{-i\tau K_1/2}, e^{-i\tau K_2/2}$: We have to calculate e^{iaX} with

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad a = \tau / 4\Delta^2$$

We use

$$e^{iaX} = \sum_{k=0}^{\infty} \frac{i^k a^k}{k!} X^k$$

Product formula approach

$$X^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv I$$

$$X^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^1 = X$$

$$X^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

$$X^3 = X$$

$$X^4 = X^2 = I$$

$$X^5 = X$$

$\ldots$

Product formula approach

$$\rightarrow\ e^{iaX} = I + iaX - \frac{a^2}{2!} I - i\frac{a^3}{3!} X + \frac{a^4}{4!} I + \dots$$

$$= \left(1 - \frac{a^2}{2} + \frac{a^4}{24} - \dots\right) I + i\left(a - \frac{a^3}{6} + \dots\right) X$$

$$= (\cos a) I + i(\sin a) X$$

Product formula approach

→The expressions for $e^{-i\tau K_1/2}$ and $e^{-i\tau K_2/2}$ are

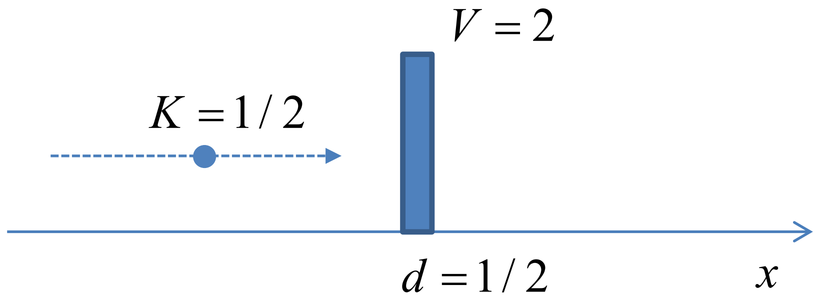
$$e^{-i\tau K_1/2}=\begin{pmatrix} c & is & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ is & c & 0 & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & c & is & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & is & c & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 & c & is & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & is & c & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 & \ddots & is & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & is & \ddots & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix} \quad e^{-i\tau K_2/2}=\begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & c & is & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & is & c & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & c & is & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & is & c & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 & c & is & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & is & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 & \ddots & is \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & is & c \end{pmatrix}$$

where $c=\cos\left(\tau/4\Delta^2\right)$ and $s=\sin\left(\tau/4\Delta^2\right)$

$\boxed{O(L)\text{ method}}$

Exercise

- Task: Solve the time-dependent Schrödinger equation for a particle impinging on a potential barrier → tunneling
- Kinetic energy K is less than the potential barrier V ➔ in classical mechanics, the particle has no chance to appear on the right hand side of the barrier
  - In quantum theory it has!



Exercise

- Solve the TDSE

$$i\hbar \frac{\partial}{\partial t}\Phi(x,t) = \left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V(x) \right)\Phi(x,t)$$

  by means of the product formula approach with the initial value of the wave function

$$\Phi(x,t=0) = (2\pi\sigma^2)^{-1/4} e^{iq(x-x_0)} e^{-(x-x_0)^2/4\sigma^2}$$

  a Gaussian wave packet centered around x_0 with a width σ and wave vector q
- Use units such that $M = \hbar = 1$

Exercise

- Set

$$0 \le x \le 100$$

$$\sigma = 3 \quad , \quad x_0 = 20 \quad , \quad q = 1$$

$$V(x) = \begin{cases} \quad 0 & \text{no barrier} \\ \hline \begin{cases} 2 & 50 \le x \le 50.5 \\ 0 & \text{otherwise} \end{cases} & \text{barrier} \end{cases}$$

$$\Delta = 0.1 \quad , \quad L = 1001 \quad , \quad \tau = 0.001 \quad , \quad m = 50000 \quad , \quad \text{discretization}$$

- Center of wave packet will move from $x = 20$ to about $x = 70$

Exercise

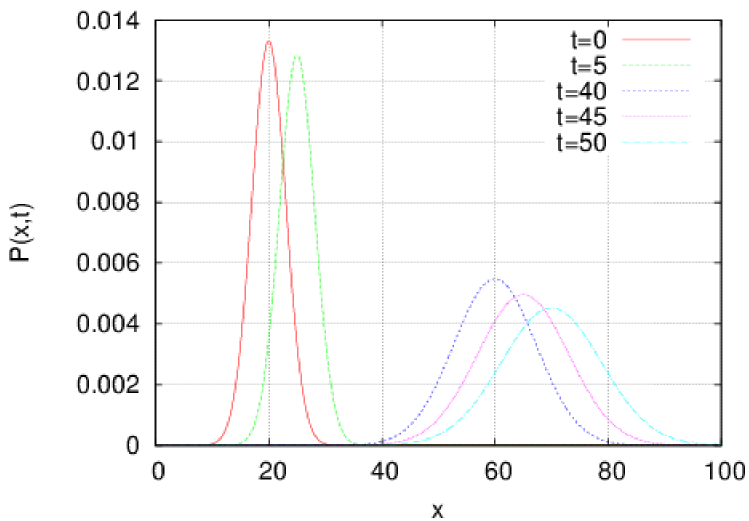
- Show snapshots of the probability distribution
- Explain why the center of the wave packet that tunnels through the barrier seems to have gained speed

Exercise

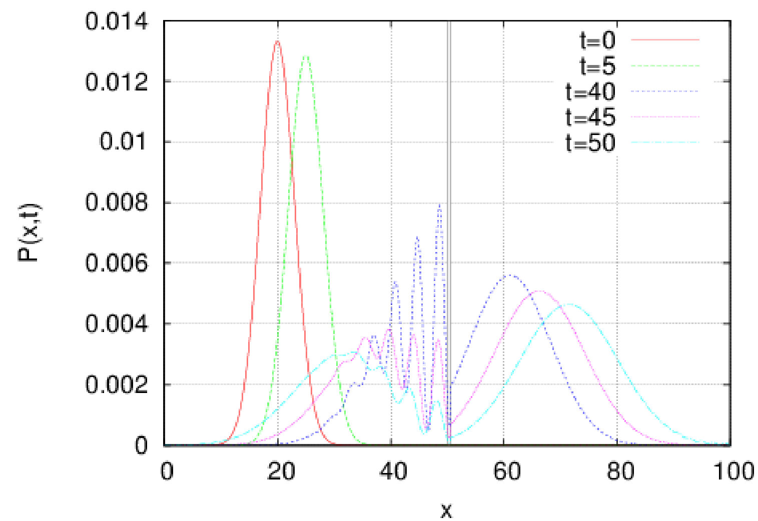
- Important "details":
  - Plot the probability $P(x,t) = \Phi^*(x,t)\Phi(x,t) = \left|\Phi(x,t)\right|^2$ not the wave function
  - The part of the wave that "tunnels" through the barrier has very little probability
    - Compute the total probability for $x > 50.5$ at the times at which snapshots are taken.
      Normalize the probabilities $P(x > 50.5, t)$ by the maximum of the total probability for $x > 50.5$

Exercise

- No potential barrier



- Potential barrier



The wave packet that tunnels through the barrier moves faster than the wave packet that moves in free space!

Report

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- Filename: Report_8_Surname1_Surname2.pdf, where Surname1 < Surname2 (alphabetical order).
  Example: Report_8_Jin_Willsch.pdf (Do not use "umlauts" or any other special characters in the names)
- Content of the report:
  - Names + matricle numbers + e-mail addresses + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 10 AM, July 3, 2023