Computer Simulations in Physics
Course for MSc physics students

Solving the time-dependent Schrödinger equation for 1-dimensional scattering of wavepackets

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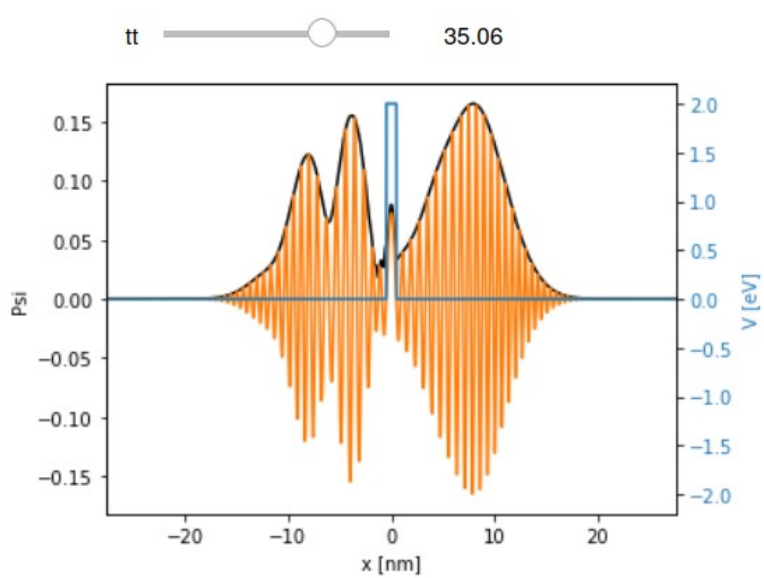
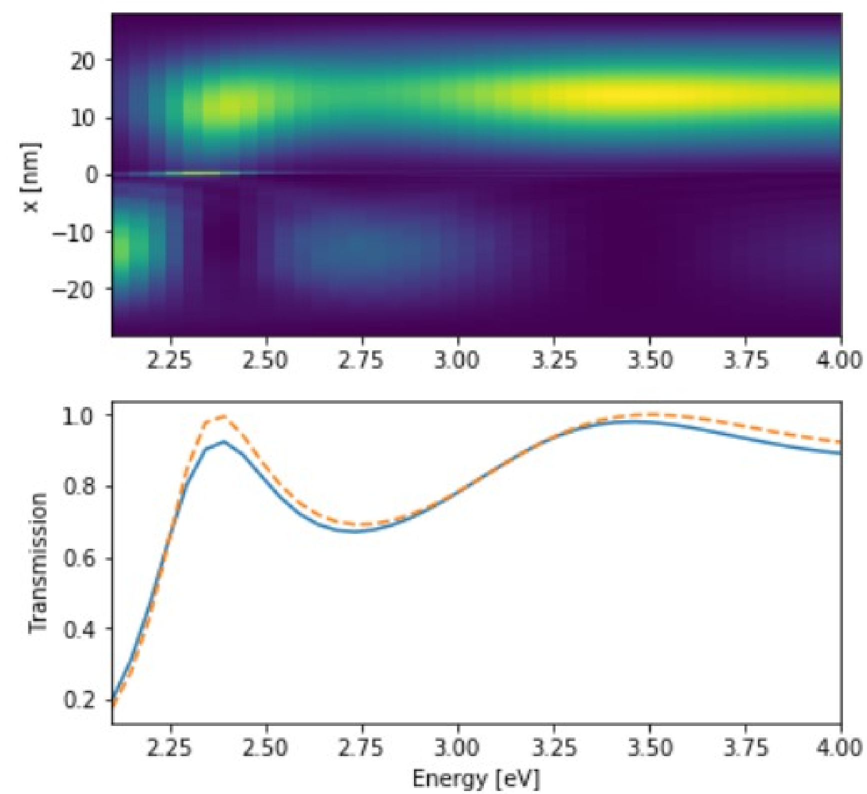
$$i\hbar\partial_t\Psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\Psi(x,t) + V(x)\Psi(x,t)$$





Literature

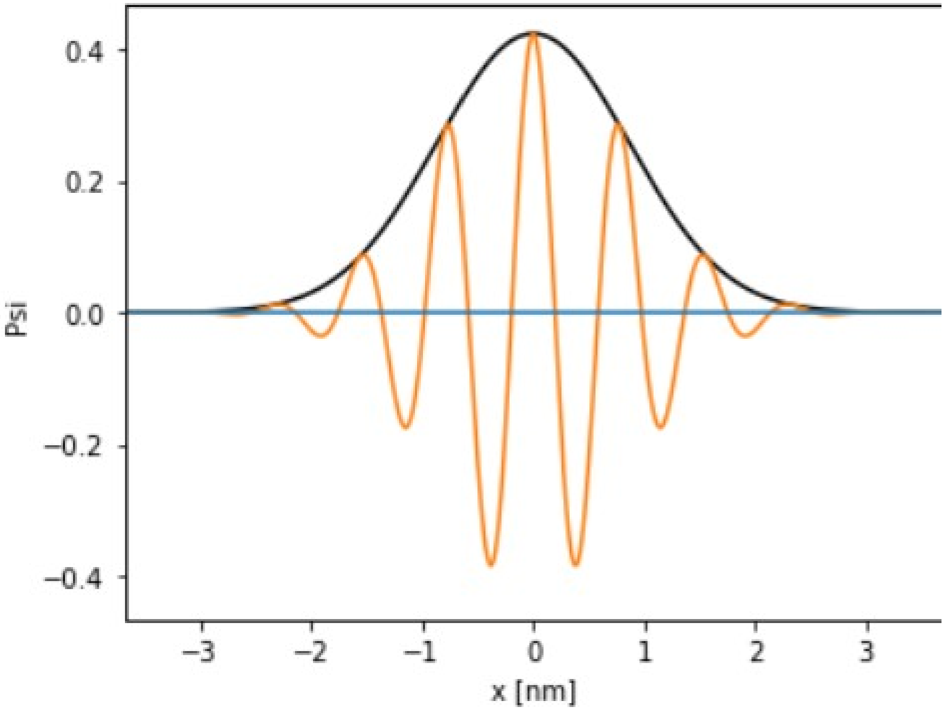
- Numerics: Computational Quantum Physics course at ETH Zurich SS 2008, by P. de Forcrand & M. Troyer
  - lecture notes online
- Quantum Scattering Theory: Any introductory Quantum Mechanics book, e.g., Griffiths

Wavepackets in momentum representation

Wavepacket: normalized superposition of plane waves

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk \equiv \mathcal{F}[\Phi]$$

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = \int_{-\infty}^{\infty} |\Phi(k)|^2 \, dk = 1$$



Reverse engineer amplitudes of plane waves by Fourier transform:

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx} dx \equiv \mathcal{F}^{-1}[\Psi]$$

Gaussian wavepackets are simple and minimum-uncertainty wavepackets

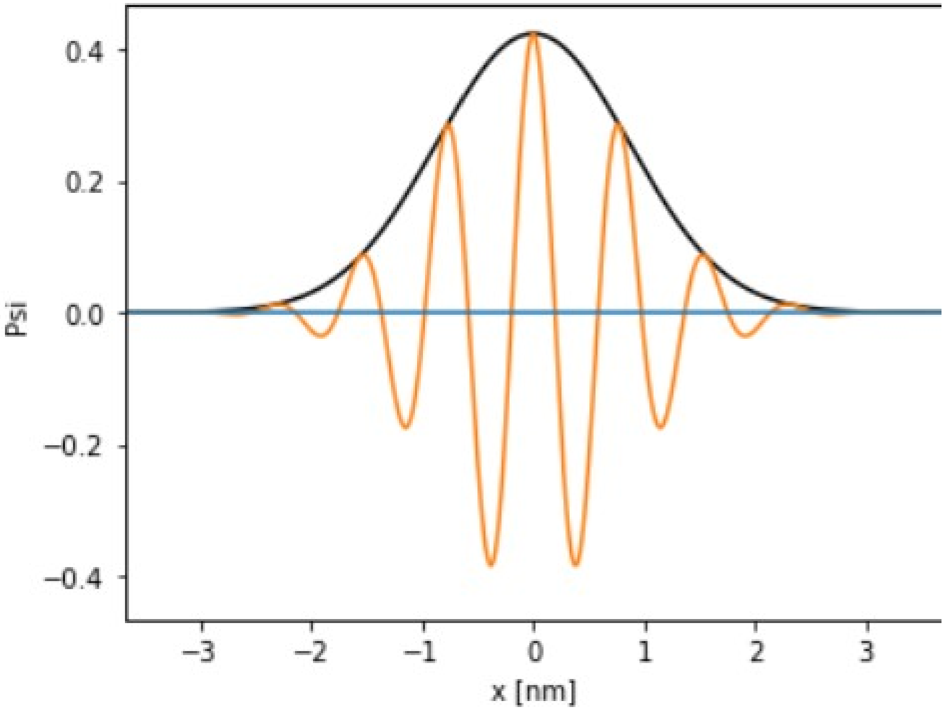
momentum boosted by k_0

$$\Psi(x) = \frac{1}{\sqrt[4]{2\pi s^2}} e^{\frac{-(x-x_0)^2}{4s^2}} e^{ik_0 x}$$

Momentum-space wave function also Gaussian, with transformed width

$$w = \frac{1}{2s}$$

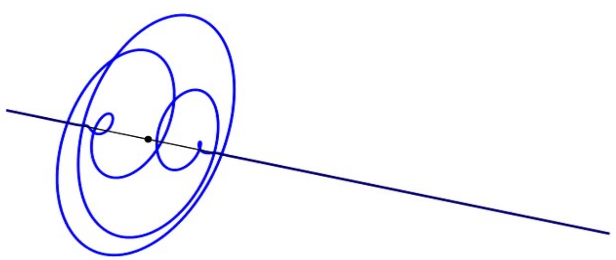
$$\Phi(k) = \frac{1}{\sqrt[4]{2\pi w^2}} e^{\frac{-(k-k_0)^2}{4w^2}} e^{ikx_0}$$



Saturates Heisenberg uncertainty $\Delta x \Delta p \geq \frac{\hbar}{2}$

Free time evolution of wavepackets is easy to compute in the momentum representation

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



$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}e^{-i\omega(k)t}dk$$

dispersion relation

$$\omega(k) = \frac{\hbar k^2}{2m}$$

Gaussian wavepackets propagate with group velocity v, twice faster than the waves they are composed of

$$v = \frac{d\omega}{dk} = \frac{\hbar k}{m} = 2\underbrace{\frac{\omega}{k}}_{v_{\mathrm{phase}}}$$

Gaussian wavepackets spread out in time, for t>>τ ballistic spread

$$s(t) = s_0\sqrt{1+\frac{t^2}{\tau^2}} \qquad \tau = \frac{2ms_0^2}{\hbar}$$

heavier particle → slower spread
tighter wavepacket → faster spread

For time evolution of wavepacket with some Hamiltonian, need to deconstruct wavepacket into eigenstates. Simple with discrete spectrum...

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

Start with a wavepacket with energy $E \approx E_0$

$$|\Psi\rangle = \Psi(x) = \frac{1}{\sqrt[4]{2\pi s^2}} e^{\frac{-(x-x_0)^2}{4s^2}} e^{ik_0 x}$$

Obtain a set of eigenstates of H around $E \approx E_0$

$$\hat{H}|n\rangle = E_n|n\rangle \quad \rightarrow \quad |n(t)\rangle = e^{-iE_n/\hbar t}|n\rangle$$

Reverse engineer the wavepacket

$$|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle \approx \sum_{n:E\approx E_0} \langle n|\Psi\rangle|n\rangle$$

Similar to momentum representation:

$$\Phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x)e^{-ikx}dx \qquad \Psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk$$

What about dx, dk?

For time evolution of wavepacket with some Hamiltonian, need to deconstruct wavepacket into eigenstates. For continuous spectrum, need dk, dx

Start with a wavepacket with energy $E \approx E_0$

Obtain a dense enough set of eigenstates of H around $E \approx E_0$ $\hat{H}|\Psi(k)\rangle = E_k|\Psi(k)\rangle \quad \rightarrow \quad |\Psi_k(t)\rangle = e^{-iE_k/\hbar t}|\Psi_k\rangle$

Eigenstates indexed by continuous parameter k, sampled at intervals dk

Real-space wavefunction sampled at intervals dx

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psi0 = exp(-(x-x0)**2/4./Dx**2) * exp(1.j*k0*x)
psi0 /= sqrt(sum(abs(psi0)**2) * dx)
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$$\Psi(x) = \frac{1}{\sqrt[4]{2\pi s^2}} e^{\frac{-(x-x_0)^2}{4s^2}} e^{ik_0 x}$$

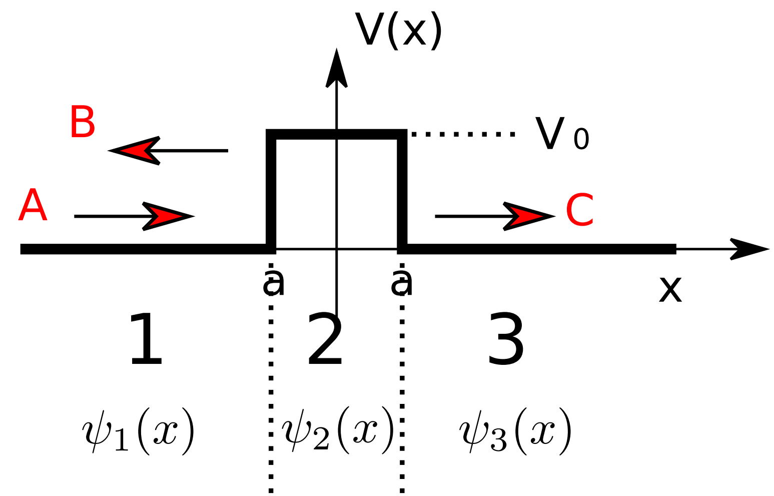
$$\Phi(k) = \frac{1}{\sqrt[4]{2\pi s^2}} e^{\frac{-(k-k_0)^2}{4s^2}} e^{ikx_0}$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k)\Psi_k(x)dk$$

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:

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

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

reflection & transmission amplitudes:

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

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

You can try this with scattering states for the square potential barrier!

1) Decide momentum and size of incident wavepacket (should be broad enough so energy well defined & slower spread)

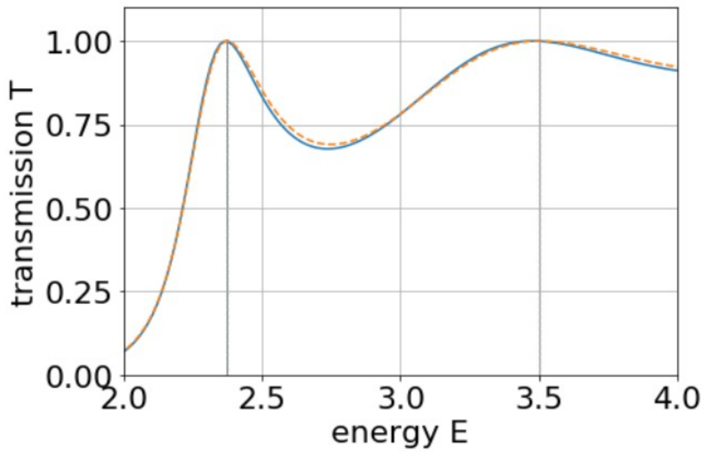
2) Take long enough leads, obtain a dense enough set of scattering states with $E \approx E_0$

3) Decompose incident wavepacket at t=0 into scattering states

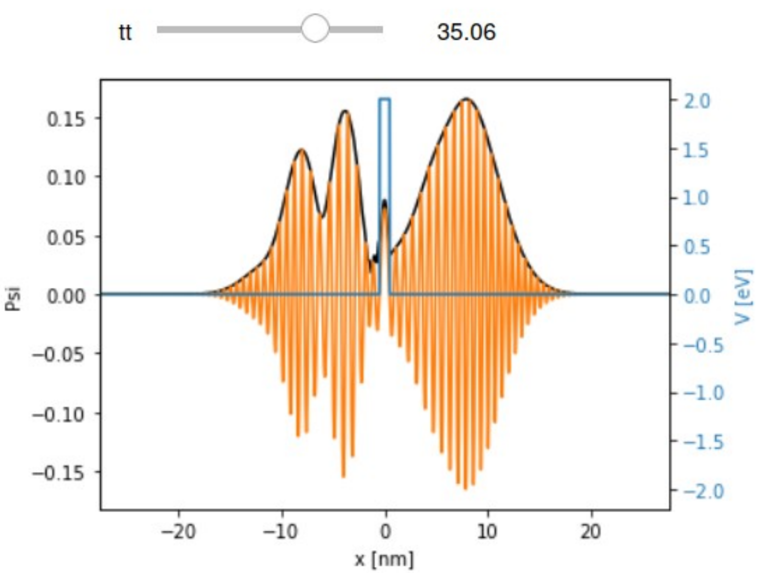
4) Build up time evolution of wavepacket

Expected plots:

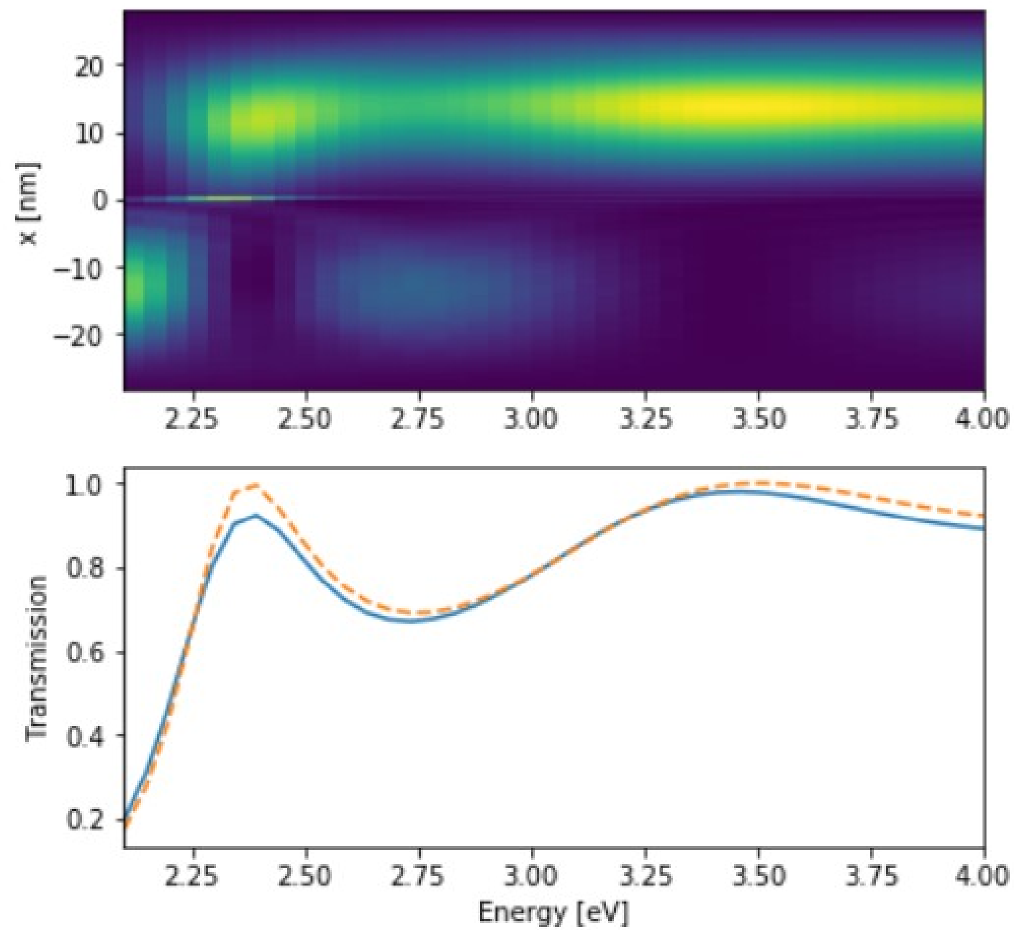
scattering resonances from last week:



wavepacket time evolution:



Homework: scattering resonances measured from snapshots after scattering event:



This spectral decomposition method is expensive if potential is time-dependent

Obtain a dense enough set of eigenstates of H around $E \approx E_0$

$$\hat{H}|n\rangle = E_n|n\rangle \quad \rightarrow \quad |n(t)\rangle = e^{-iE_n/\hbar t}|n\rangle$$

Best approach for time dependent potential: split operator method

$$i\hbar\partial_t|\Psi\rangle = \hat{H}(t)|\Psi\rangle \qquad \Delta_t = t/N \qquad \hat{H}_j = \hat{H}((j-1/2)\Delta_t)$$

Formal solution of Schrödinger equation:

$$\hat{U}(t) = \lim_{\Delta_t \to 0} e^{-\frac{i}{\hbar}\hat{H}_N\Delta_t} e^{-\frac{i}{\hbar}\hat{H}_{n-1}\Delta_t} \dots e^{-\frac{i}{\hbar}\hat{H}_1\Delta_t} \equiv \mathcal{T} e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'}$$

If Hamiltonian is sum of kinetic and potential energy: $\hat{H}(t) = \underbrace{-\frac{\hbar^2}{2m}\partial_x^2}_{\hat{T}} + \underbrace{V(x,t)}_{\hat{V}}$

1) Starting idea: T and V separately are diagonal in momentum/real space basis. Fast Fourier Transform is cheap, O(N log(N)) way to switch back and forth. Therefore, should use

$$e^{-i\Delta_t\hat{H}/\hbar} = e^{-i\Delta_t\hat{T}/\hbar} e^{-i\Delta_t\hat{V}/\hbar} + \mathcal{O}(\Delta_t^2)$$

2) Only ≈ because T and V don't commute. Improve error term by Strang splitting:

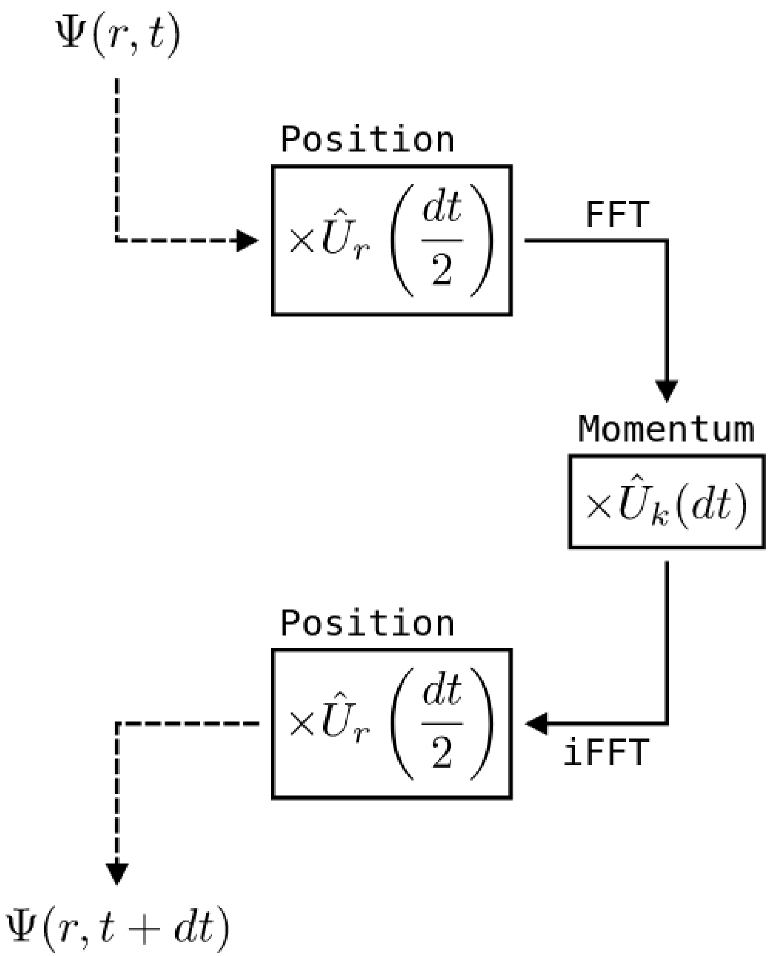
$$e^{-i\Delta_t\hat{H}/\hbar} = e^{-i\Delta_t\hat{V}/(2\hbar)} e^{-i\Delta_t\hat{T}/\hbar} e^{-i\Delta_t\hat{V}/(2\hbar)} + \mathcal{O}(\Delta_t^3)$$

can check by series expansion of exponentials

Explicit calculation of why Strang splitting is good

Split operator method, recipe

single timestep:



complete N cycles, n=1,...,N:

$$\Psi_1(x) = e^{-i\Delta_t V(x,t=0)/2}\Psi_0(x)$$

$$\underline{\Phi_{2n-1}} = \mathcal{F}(\underline{\Psi_{2n-1}})$$

$$\Phi_{2n}(k) = e^{-i\Delta_t k^2/(2m)}\Phi_{2n-1}(k)$$

$$\underline{\Psi_{2n}} = \mathcal{F}^{-1}(\underline{\Phi_{2n}})$$

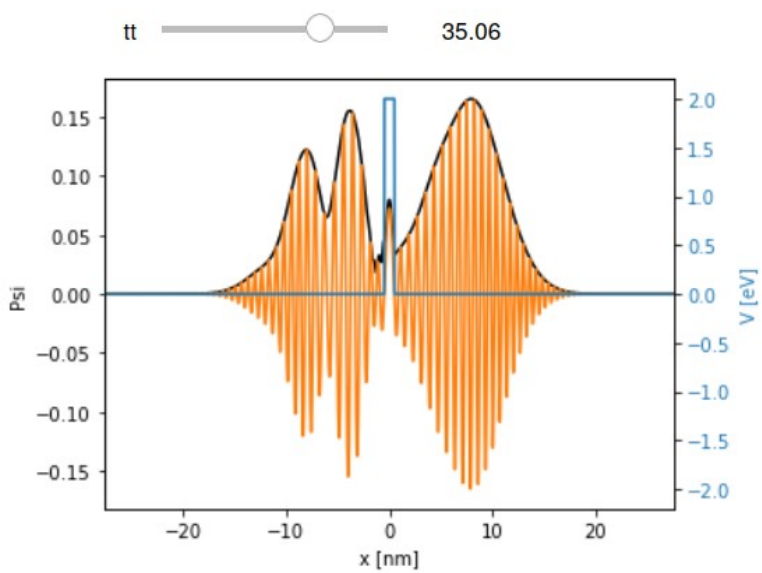
$$\Psi_{2n+1}(x) = e^{-i\Delta_t V(x,t=n\Delta_t)}\Psi_{2n}(x)$$

last step should be replaced by:

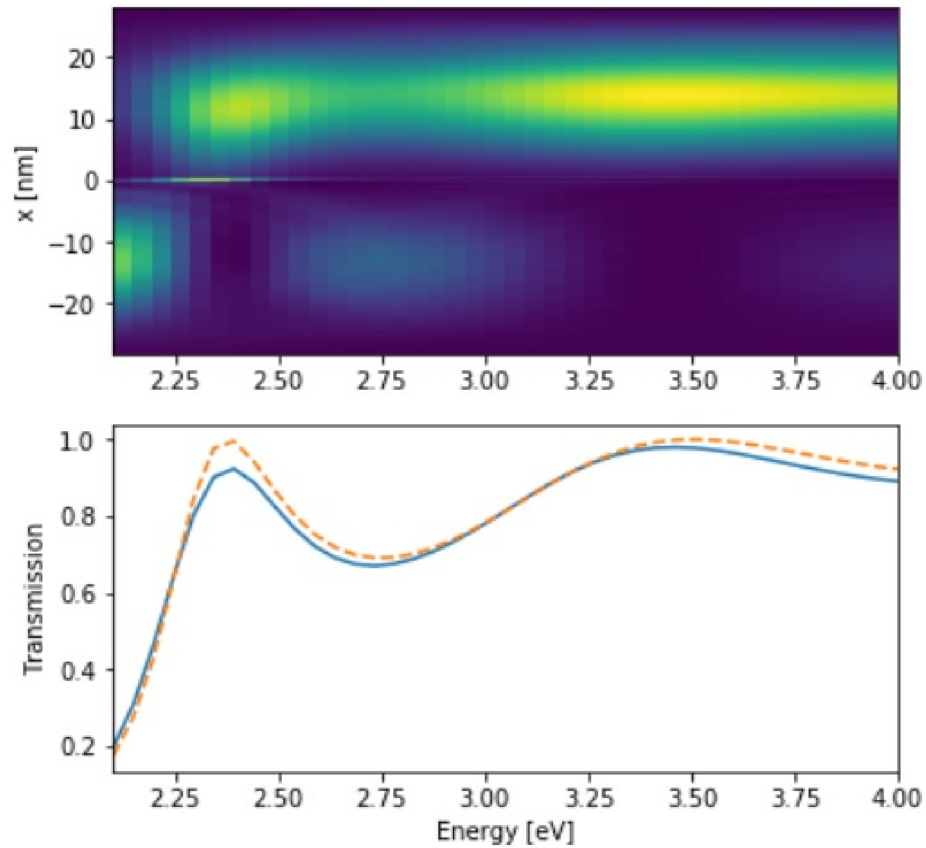
$$\Psi_{\mathrm{end}}(x) = e^{-i\Delta_t V(x,t=N\Delta_t)/2}\Psi_{2N}(x)$$

Implement split operator method and debug by comparing scattering wavepackets to Numerov

wavepacket time evolution:



Homework: scattering resonances measured
by wavepacket transmission:



Exercises for today and homework

- 1) Calculate scattering of a wavepacket of energy 2.5 eV, width in energy 0.5 eV, from a square potential barrier by the split operator method. Plot snapshots of wavepacket before/during/after scattering.
- Barrier parameters: height 2 eV, size 1nm
- if you feel extra enthusiastic: Same as above, but by decomposing the initial wavepacket into a superposition of scattering states (obtained by analytical solution).

- 1) Measure transmission as a function of energy (2.1 eV→ 5 eV) using time evolution of wavepackets, for a square potential barrier, using the split operatorspectral method. Barrier parameters: height 2 eV, size 1nm. Compare with analytical curves.
- +) if you feel extra enthusiastic: Same as above, but by decomposing the initial wavepacket into a superposition of scattering states (obtained by analytical solution).