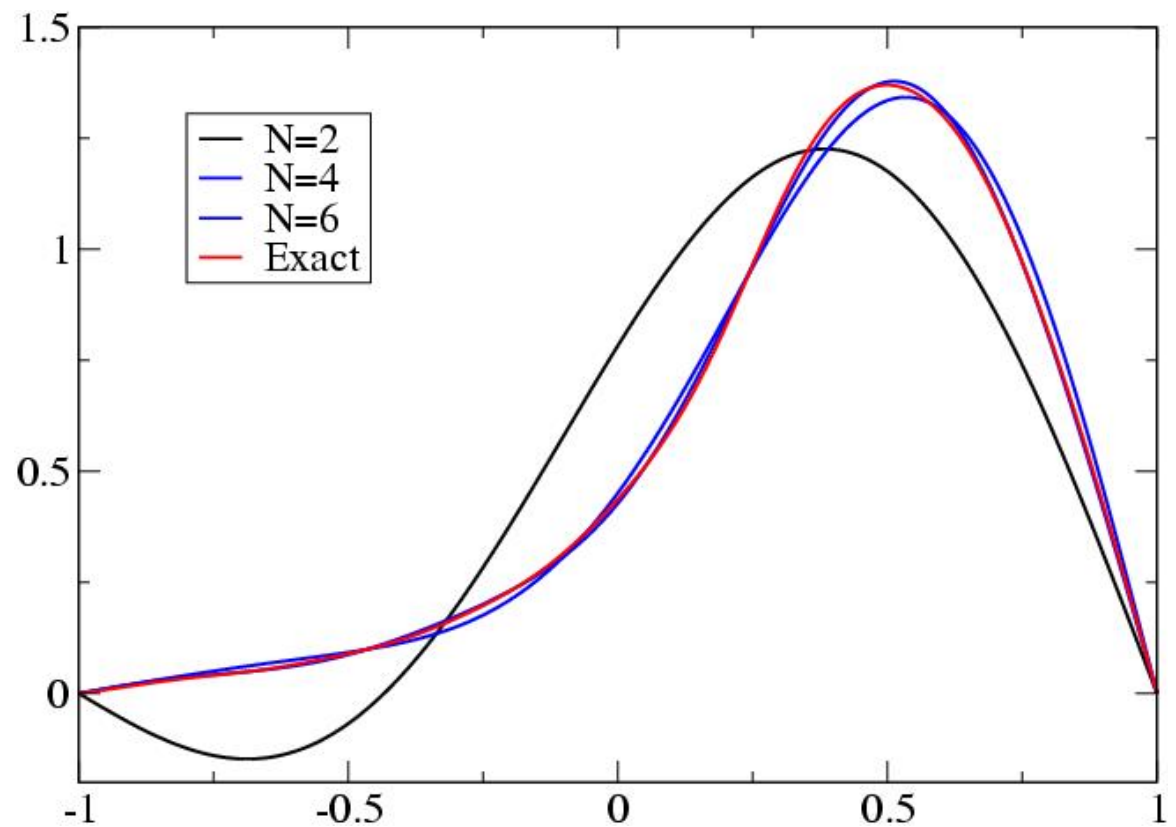
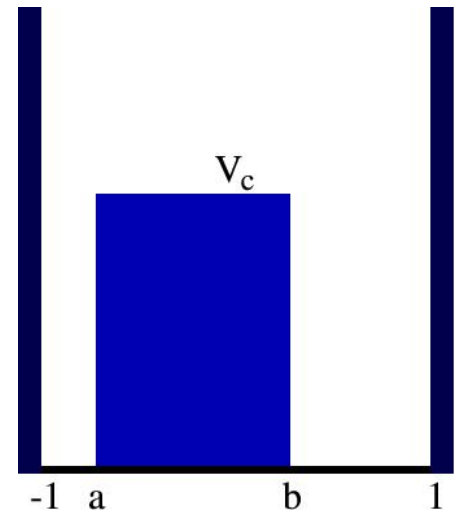


How about an asymmetric barrier?

N	energy
1	8.48449
2	6.01721
3	5.06098
4	5.01719
5	4.99315
6	4.96887
8	4.96195
10	4.95900
...	
20	4.95466
...	
50	4.95407
true:	4.95402



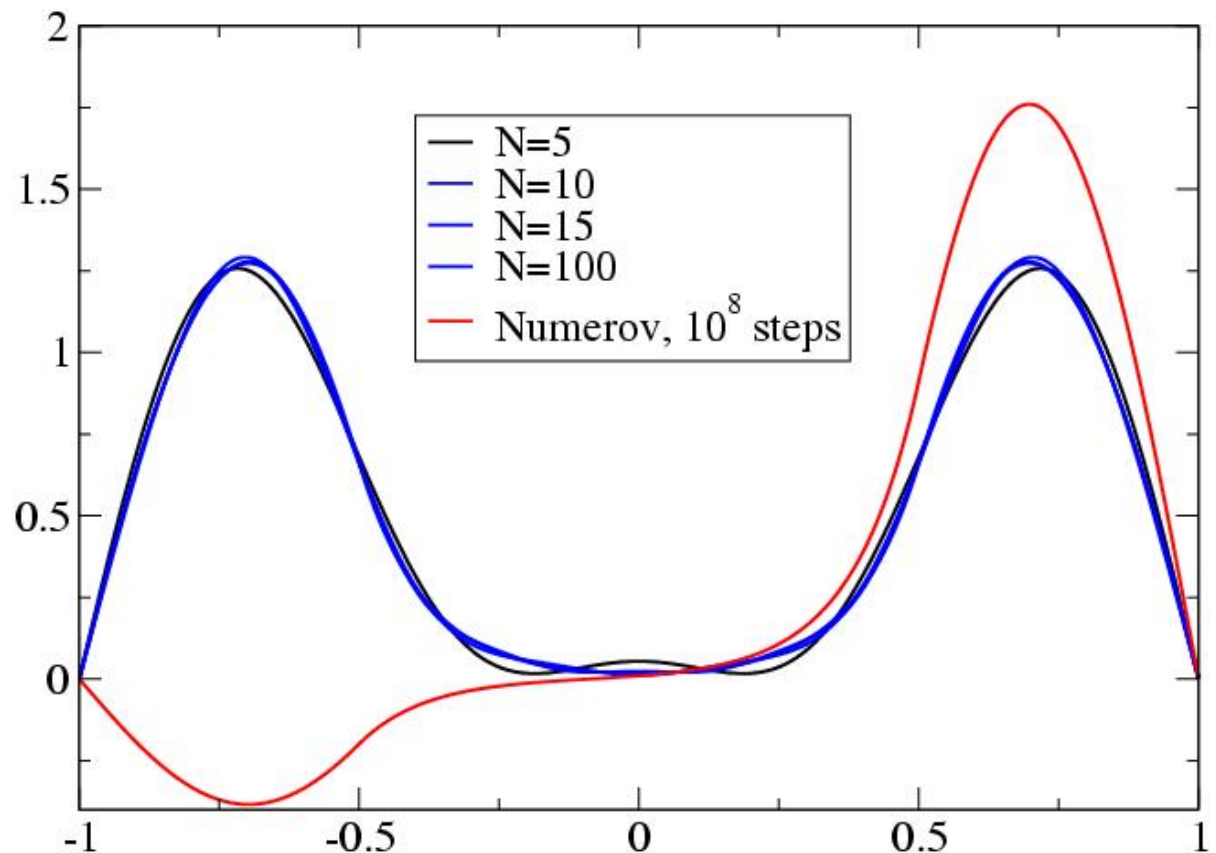
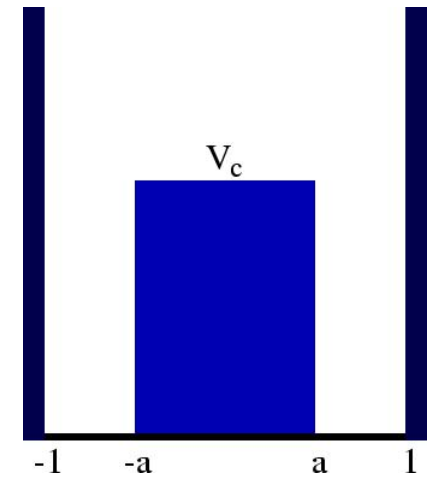
Let's do a large barrier; $V_c=50$

N	energy
2	29.93480
4	14.86237
6	13.79536
8	13.62645
10	13.56317
...	
20	13.48853
30	13.47853
...	
100	13.47439

Numerov: 13.45011
(based on 10^8 steps)

What's going on?

- No agreement
- Wrong symmetry?
(comp with Numerov)



Explanation

Two almost degenerate states (symmetric/anti-symmetric)

- Numerical accuracy problems; Numerov mixes them
- The variational method easily keeps them separated (but larger errors in the energy)

N=20

$E_0 = 13.4885$

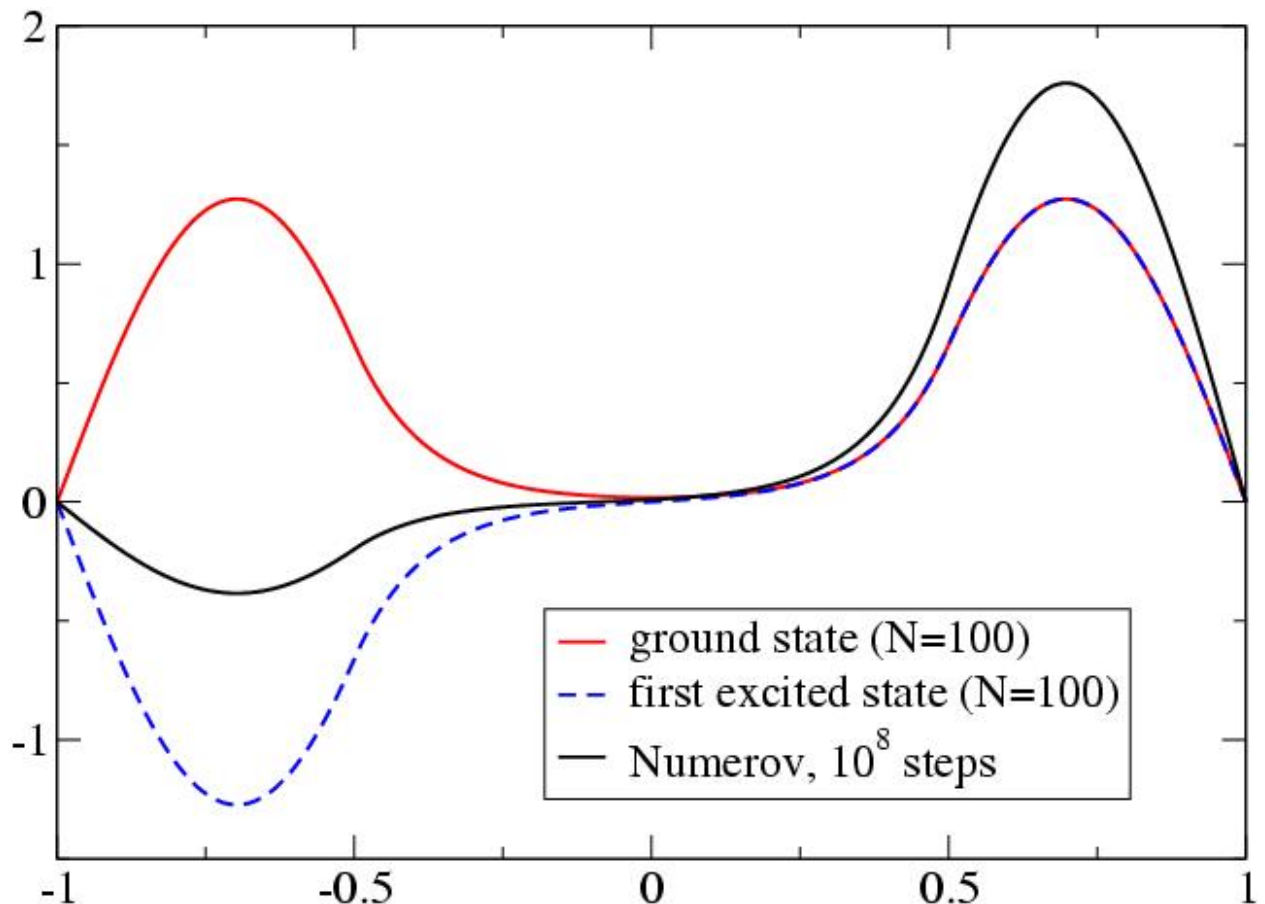
$E_1 = 13.4904$

N=100

$E_0 = 13.4744$

$E_1 = 13.4773$

Numerov: 13.45011
(based on 10^8 steps)



The Schrodinger equation in discretized real space

Example of grid-based method for 2D and 3D problems

Basis of states localized in small volume element

- large number of such states needed in 2D and 3D
- the resulting $N \times N$ matrix is too big to be fully diagonalized
- special methods exist for lowest states of sparse matrices
 - N up to several million (even 10s or 100s of millions)

Cubic d-dimensional space elements;

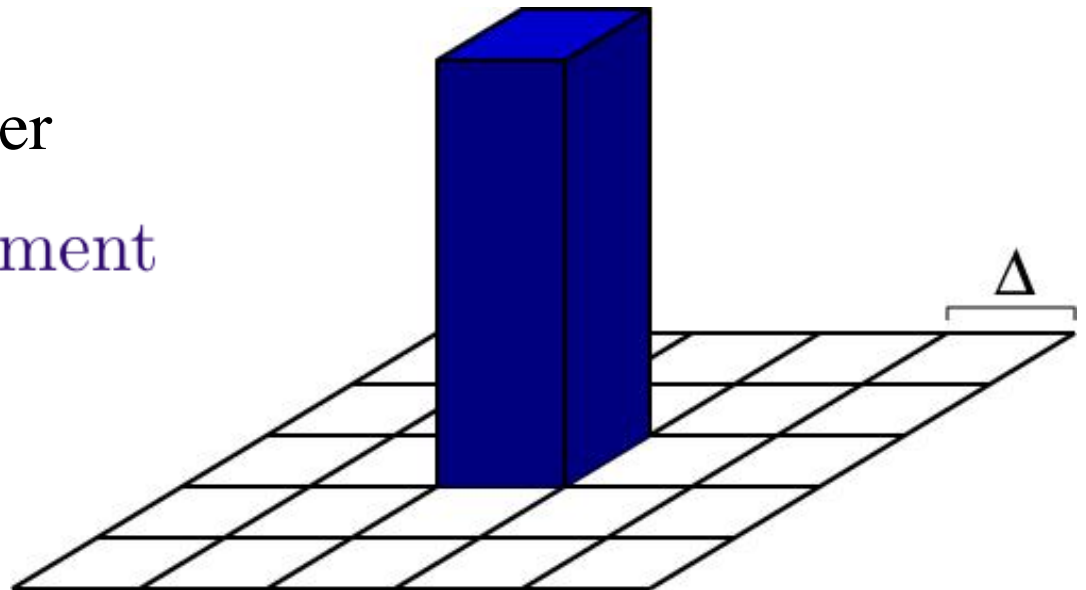
$$\text{volume} = \Delta^d$$

Label by coordinate or number

$$\phi_j(\vec{x}) = \frac{1}{\Delta^{d/2}} \quad \text{inside element}$$

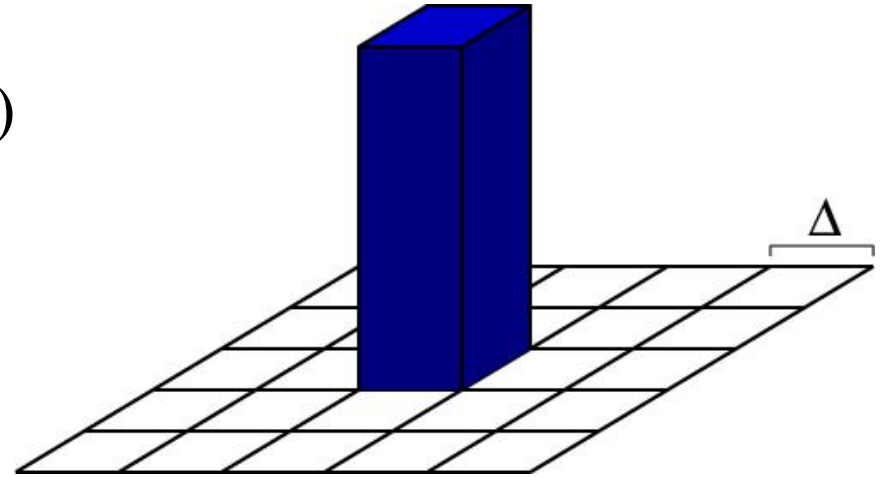
Coordinate of element \vec{r}_j

Non-overlapping $\langle j|l \rangle = \delta_{jl}$
(orthonormal basis)



Strictly speaking, these are not valid wave functions (discontinuous)

However, we will obtain a scheme that gives the correct physics in the limit $\Delta \rightarrow 0$ (we could also in principle use some continuous localized functions)



Size of the basis in a box with side L: $N = (L/\Delta)^d$

Matrix elements of Hamiltonian $H = K + V$

The potential energy is diagonal

$$V_{jl} = \langle j|V|l \rangle = \delta_{jl} \int dx^d |\phi_j(\vec{x})|^2 V(\vec{x}) \approx \delta_{jl} V(\vec{r}_j)$$

Kinetic energy

$$K_{jl} = \langle j|K|l \rangle = -\frac{1}{2} \int dx^d \phi_j^*(\vec{x}) \nabla^2 \phi_l(\vec{x})$$

How do we deal with the non-differentiability?

Using central difference operator in place of derivatives

- Can we do this when the functions are not smooth?
- We will show that it in fact produces correct results

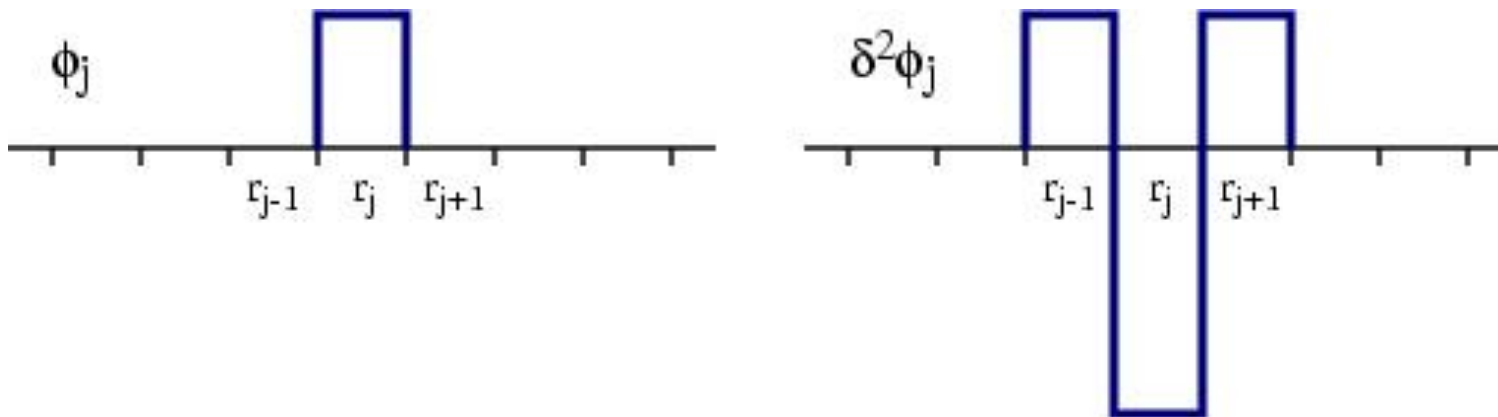
Work in one dimension for simplicity

- Can be directly generalized to higher dimensionality

Replace second derivatives of the basis functions by

$$\begin{aligned}\frac{1}{\Delta^2} \delta^2 \phi_j(x) &= \frac{1}{\Delta^2} [\phi_j(x - \Delta) - 2\phi_j(x) + \phi_j(x + \Delta)] \\ &= \frac{1}{\Delta^2} [\phi_{j-1}(x) - 2\phi_j(x) + \phi_{j+1}(x)]\end{aligned}$$

Produces non-zero values in the neighboring elements



The kinetic energy matrix elements are

$$K_{jl} = -\frac{1}{2} \int dx^d \phi_j^*(\vec{x}) \frac{1}{\Delta^2} \delta^2 \phi_l(\vec{x}) = \begin{cases} -\Delta^{-2}/2, & \text{for } j = l \pm 1 \\ \Delta^{-2}, & \text{for } j = l \end{cases}.$$

This means that when K acts on a state

$$K|j\rangle = -\frac{1}{\Delta^2} \left[\frac{1}{2}|j-1\rangle - |j\rangle + \frac{1}{2}|j+1\rangle \right]$$

Non-zero matrix elements of the full Hamiltonian

$$H_{j,j} = V(r_j) + \frac{1}{\Delta^2} \quad H_{j\pm 1,j} = -\frac{1}{2} \frac{1}{\Delta^2}$$

Generalizes to 2D and 3D; kinetic energy “hops” localized particle between nearest-neighbor volume elements

$$H_{j,j} = V(\vec{r}_j) + \frac{d}{\Delta^2} \quad H_{\delta[j],j} = -\frac{1}{2} \frac{1}{\Delta^2}$$

$\delta[j]$ denotes a neighbor of j (2,4,6 neighbors in 1D, 2D, 3D)

Proof of correct continuum limit for free particle in a box

1D for simplicity (generalizes easily)

Periodic box of length L ; energy eigenstates

$$\phi_k(x) = e^{-ikx}, \quad \text{with } k = n2\pi/L, \quad n = 0, 1, \dots$$

$$\text{Energy: } E_k = \frac{1}{2}k^2 \quad (\hbar = m = 1)$$

Discretized space, N cells; we will prove that the eigenstates are

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-ikr_j} |j\rangle, \quad k = n2\pi/L \quad \text{with } n = 0, 1, \dots, N-1$$

Discrete coordinate $r_j = j\Delta = jL/N$ limits momentum;

$$e^{-i(n+N)2(\pi/L)r_j} = e^{-in2(\pi/L)r_j}$$

so only N different momenta

Acting with kinetic energy on proposed state:

$$K|k\rangle = -\frac{1}{\Delta^2} \frac{1}{\sqrt{N}} \sum_{j=0}^N e^{-ikr_j} \left[\frac{1}{2}|j-1\rangle - |j\rangle + \frac{1}{2}|j+1\rangle \right]$$

Shifting the indexes in the $j \pm 1$ terms by ± 1

$$\begin{aligned} K|k\rangle &= -\frac{1}{\Delta^2} \frac{1}{\sqrt{N}} \sum_{j=0}^N e^{-ikr_j} \left[\frac{1}{2}(e^{ik\Delta} + e^{-ik\Delta}) - 1 \right] |j\rangle \\ &= \frac{1}{\Delta^2} [\cos(k\Delta) - 1] |k\rangle \end{aligned}$$

Energy eigenvalues are $E_k = \frac{1}{\Delta^2} [1 - \cos(k\Delta)]$

Taylor expand for small $k\Delta$

$$E_k = \frac{1}{2}k^2 - \frac{1}{24}\Delta^2 k^4 + \dots$$

Agrees with continuum result to leading order, i.e., the way we treated the kinetic energy in the discretized space was ok.

Note that the discretized energy is lower than the true energy

$$\text{3D: } E_k = \frac{1}{\Delta^2} [3 - \cos(k_x\Delta) - \cos(k_y\Delta) - \cos(k_z\Delta)]$$