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 neded in 2D and 3D
- the resulting N*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;

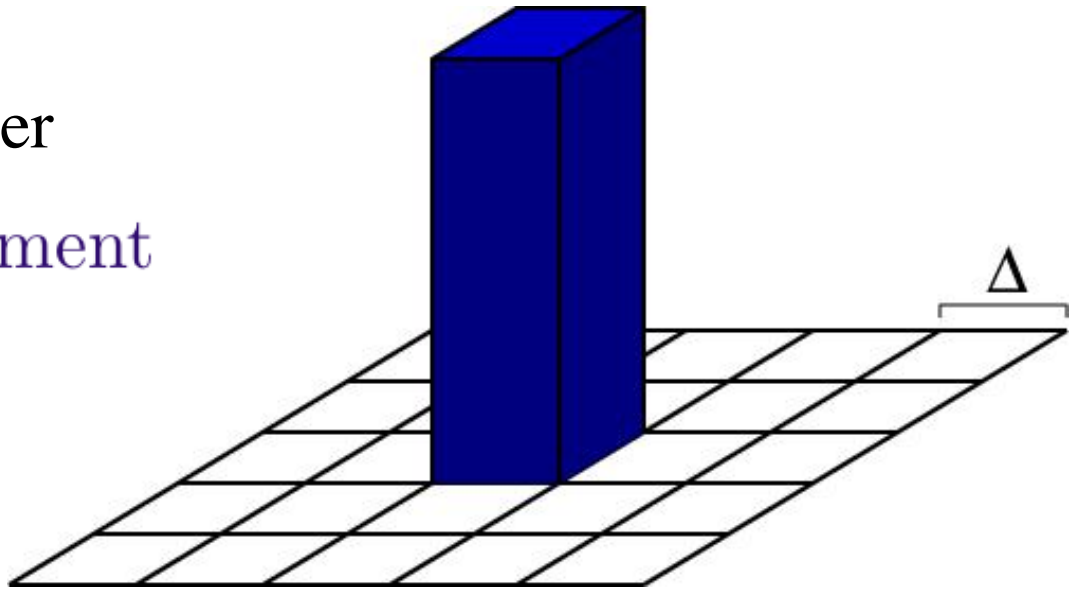
$$\text{volume} = \Delta^d$$

Label by coordinate or number

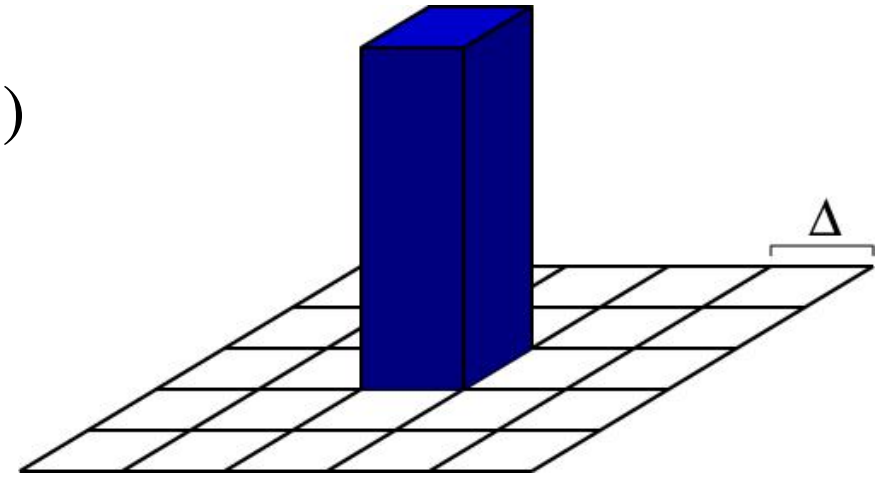
$$\phi_j(\vec{x}) = \frac{1}{\Delta^{d/2}} \quad \text{inside element}$$

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 $\Delta \to 0$

(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

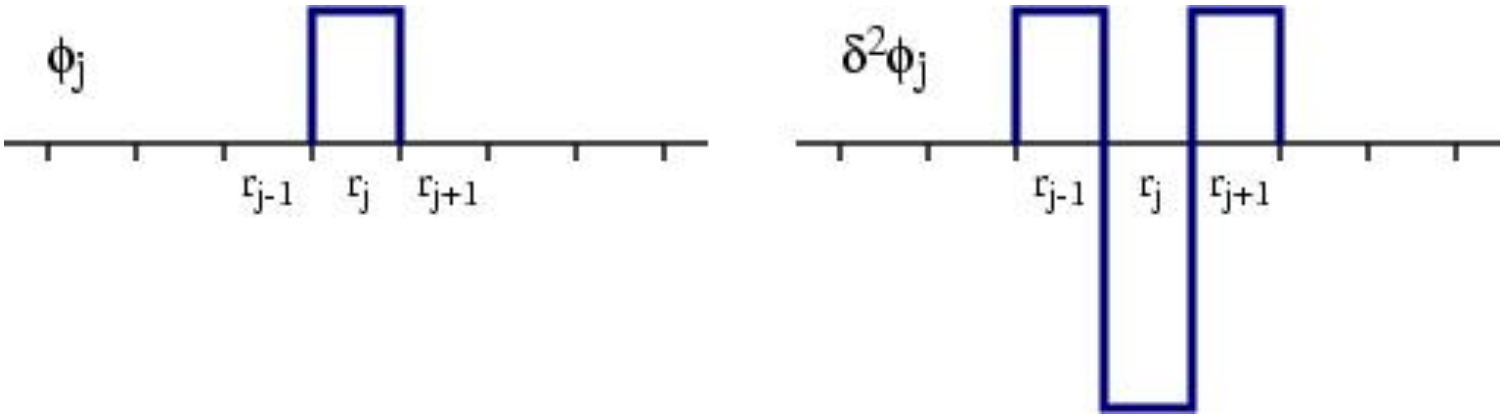
- Can be directly generalized to higher dimensionality

Replace second derivatives of the basis functions by

$$\frac{1}{\Delta^2}\delta^2\phi_j(x) = \frac{1}{\Delta^2}[\phi_j(x-\Delta) - 2\phi_j(x) + \phi_j(x+\Delta)]$$

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

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

$$H_{j,j} = V(r_j) + \frac{1}{\Delta^2} \qquad H_{j\pm1,j} = -\frac{1}{2}\frac{1}{\Delta^2}$$

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

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

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