https://gitlab.com/gersonjferreira/computational-quantum-mechanics

Computational Quantum Mechanics

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Matrix representations for H

General expansion

$$\varphi_1(x), \varphi_2(x), \varphi_3(x), \ldots$$

General expansion

Consider a basis (plane-waves, polynomials, Hermite, …):

$$\varphi_1(x), \varphi_2(x), \varphi_3(x), \dots$$

$$|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \dots$$

Assuming orthonormal:

$$\langle\varphi_i|\varphi_j\rangle = \delta_{i,j}$$

Let’s write the matrix elements as $H_{j,i} = \langle\varphi_j| H |\varphi_i\rangle$

We want to solve $H|\psi\rangle = E|\psi\rangle$

expanding on the basis $|\psi\rangle = \sum_i c_i |\varphi_i\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle + \dots$

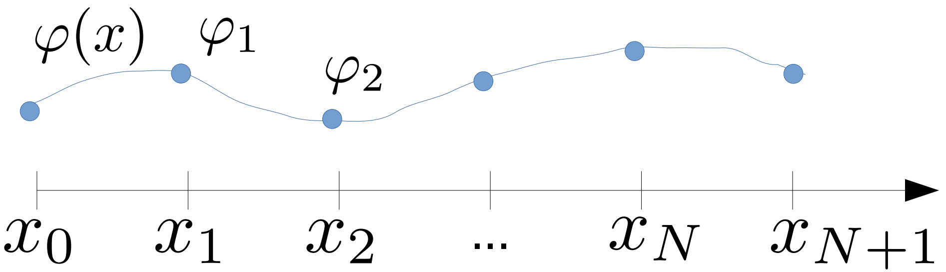
$$\sum_i c_i H |\varphi_i\rangle = \sum_i c_i E |\varphi_i\rangle$$

$$\sum_i c_i \langle\varphi_j| H |\varphi_i\rangle = \sum_i c_i E \langle\varphi_j|\varphi_i\rangle$$

$$\sum_i H_{j,i} c_i = E c_i$$

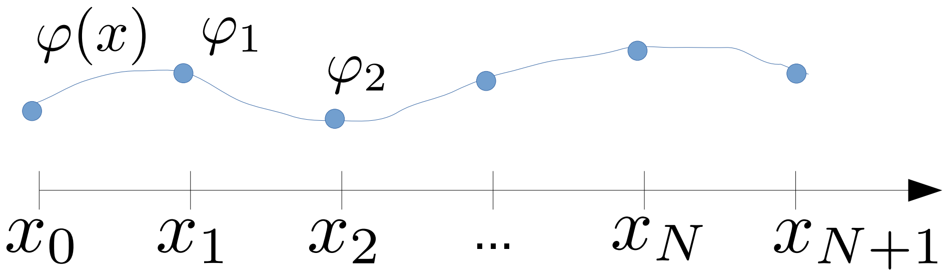
$$\boxed{\bar{\bar{H}}\vec{c} = E\vec{c}}$$

Finite differences



Finite differences: the second derivative

→ equivalent to a basis of discrete sites: $\varphi_1 = \varphi(x_1), \varphi_2 = \varphi(x_2), \ldots$



We have seen that the second derivative can be written as

$$\varphi_n'' = \frac{\varphi_{n-1} - 2\varphi_n + \varphi_{n+1}}{\Delta x^2}$$

Apply rule for n=1 .. N (inner points)

$$\varphi_1'' = \frac{\varphi_0 - 2\varphi_1 + \varphi_2}{\Delta x^2}$$

$$\varphi_2'' = \frac{\varphi_1 - 2\varphi_2 + \varphi_3}{\Delta x^2}$$

$$\varphi_3'' = \frac{\varphi_2 - 2\varphi_3 + \varphi_4}{\Delta x^2}$$

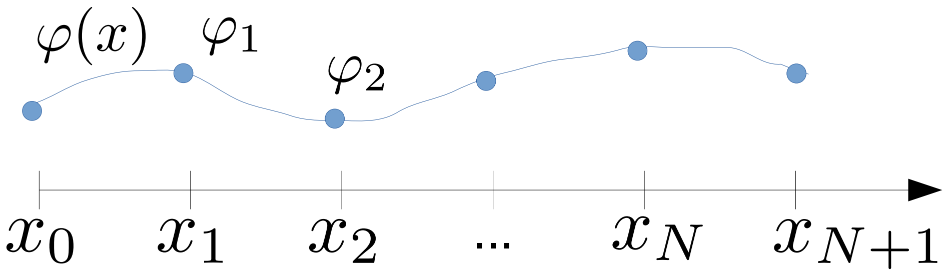
It takes a matrix form:

$$\frac{\partial^2}{\partial x^2}\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix} = \frac{1}{\Delta x^2}\begin{pmatrix}-2 & 1 & 0 & 0\\ 1 & -2 & 1 & 0\\ 0 & \ddots & \ddots & \ddots\\ 0 & 0 & 1 & -2\end{pmatrix}\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix} + \cancel{\frac{1}{\Delta x^2}\begin{pmatrix}\varphi_0\\ 0\\ \vdots\\ \varphi_{N+1}\end{pmatrix}}$$

vanishing boundary conditions: $\varphi_0 = \varphi_{N+1} = 0$

Finite differences: the potential term

→ equivalent to a basis of discrete sites: $\varphi_1 = \varphi(x_1), \varphi_2 = \varphi(x_2), \ldots$



Now let's consider the potential term as

$$V(x)\varphi(x) \to V_i\varphi_i$$

Apply rule for n=1 .. N (inner points)

$$V(x)\varphi(x)|_{x=x_1} = V_1\varphi_1$$

$$V(x)\varphi(x)|_{x=x_2} = V_2\varphi_2$$

$$V(x)\varphi(x)|_{x=x_3} = V_3\varphi_3$$

It takes a matrix form:

$$V(x)\varphi(x) \to \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & V_{N-1} & 0 \\ 0 & 0 & 0 & 0 & V_N \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-1} \\ \varphi_N \end{pmatrix}$$

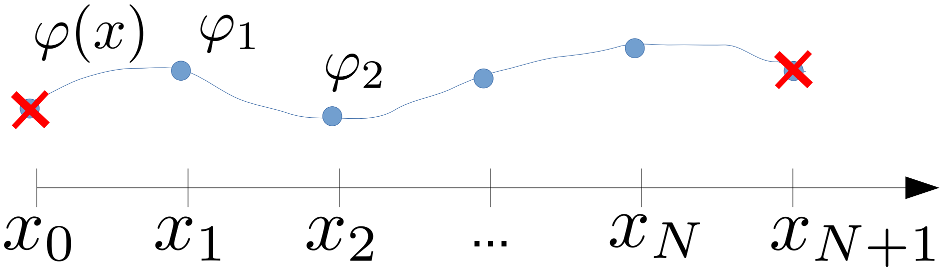
Finite differences

Therefore,

$$H\varphi(x) = E\varphi(x) \qquad\qquad H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$$

on a discrete lattice becomes

$$\bar{\bar{H}} = -\frac{1}{2}\frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & \ddots & \ddots & \ddots \\ 0 & 0 & 1 & -2 \end{pmatrix} + \begin{pmatrix} V_1 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & V_N \end{pmatrix}$$



Plane waves

$$\exp(ikx)$$

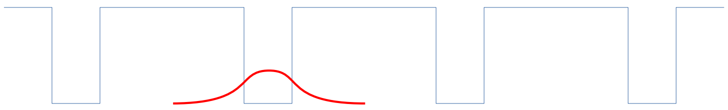
Plane waves

In this case, the basis is $\varphi_k(x) = e^{ikx}$

<u>How to choose the values of k?</u> There's a relation between k and x resolutions, which is due to the periodicity imposed by the plane-waves

It's easier if we start in x-space → let's assume that V(x+L) = V(x) is periodic

…but let's ignore Bloch's theorem for now...



Consequently, we want

$$\varphi_k(x+L) = \varphi_k(x)$$

which gives

$$e^{ikL} = 1 \rightarrow k_j = \frac{2\pi}{L} j$$

and j=0..N, **<u>but how to choose N?</u>**

The reciprocal k-space is also periodic

$$\varphi_{j+N}(x) = \varphi_j(x)$$

$$e^{i\frac{2\pi}{L}Nx_n} = 1 \rightarrow x_n = \frac{L}{N} n$$

Plane waves $\varphi_j(x_n) = e^{ik_j x_n}$

Summarizing:

Periodicity in x-space implies → $k_j = j\Delta k \qquad \Delta k = 2\pi/L \qquad j = 0...N$

Periodicity in k-space implies → $x_n = n\Delta x \qquad \Delta x = L/N \qquad n = 0...N$

Notice that the resolution in k and x spaces are related: $\Delta x \Delta k = \dfrac{2\pi}{N}$

For a fix N, if you increase the resolution in one space, you loose in the other
→ very **<u>similar</u>** to Heisenberg's uncertainty principle

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Implementation?

→ go back to the **<u>General expansion</u>** slide
→ calculate the matrix elements of each k either analytically or numerically if needed.
→ for many introductory problems it is possible to calculate H_{ij} analytically, and use the analytical expression to build the matrices in Python and diagonalize.