DISCRETIZATION

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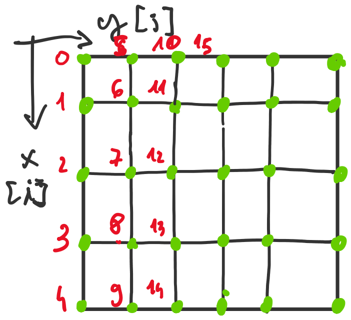
$$\boxed{i:\ -\frac{\hbar^2}{2}\sum_{j=1}^{N_i}\frac{1}{\frac{m_i+m_j}{2}}\frac{\varphi_j-\varphi_i}{d_{ij}}\,\delta_{ij}+V_i\varphi_i=E\varphi_i\,\delta S_i}$$

2D grid



Let's take a 2D grid and order the points as on the left

n_x is the number of points along x and n_y along y-axis, i is the index x and j the y-index

N_p (total number of points) $= n_x \cdot n_y$

Let's call ix the generic point over the 2D grid.

$$\boxed{ix = i + j \cdot n_x}$$

If I order in this way, φ becomes a vector

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For N_p points, I will have N_p equations to solve.

Or in other words I am solving a system of equations

I have N_p variables (the number of grid points)

The problem I am solving is:

$$\boxed{H\varphi = E\varphi}$$

Hamiltonian of the system

From a numerical point of view φ is a vector $[N_p \times 1]$

and H is a $[N_p \times N_p]$ matrix

SCHRÖDINGER EQUATION IN 1D

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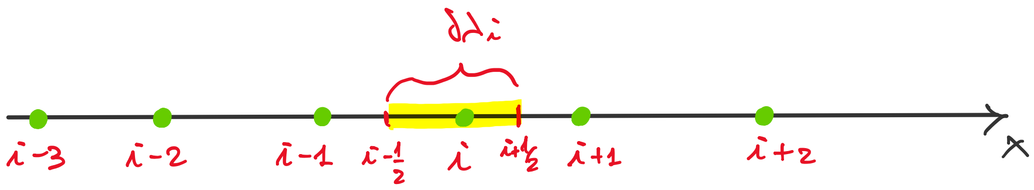

$$-\frac{\hbar^2}{2}\frac{\delta}{\delta x}\frac{1}{m}\frac{\delta}{\delta x}\varphi(x)+V(x)\varphi(x)=E\varphi(x)$$

Let's integrate the 1D equation in the segment $\delta\lambda_i$

$$-\frac{\hbar^2}{2}\int_{\delta\lambda_i}\frac{\delta}{\delta x}\frac{1}{m}\frac{\delta}{\delta x}\varphi(x)\,dx+\int_{\delta\lambda_i}V(x)\varphi(x)\,dx=E\int_{\delta\lambda_i}\varphi(x)\,dx$$

If we again assume that $\varphi(x)$ and $V(x)$ are ~ constant in $\delta\lambda_i$, then

$$-\frac{\hbar^2}{2}\int_{\delta\lambda_i}\frac{\delta}{\delta x}\frac{1}{m}\frac{\delta}{\delta x}\varphi(x)\,dx+V_i\varphi_i\,\delta\lambda_i=E\,\varphi_i\,\delta\lambda_i$$

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Let's solve the term

$$-\frac{\hbar^2}{2}\int_{\delta\lambda_i} \frac{\delta}{\delta x}\underbrace{\frac{1}{m}\frac{\delta}{\delta x}\varphi(x)dx} = -\frac{\hbar^2}{2}\frac{1}{m}\frac{\delta}{\delta x}\varphi(x)\Big|_{i-\frac{1}{2}}^{i+\frac{1}{2}} =$$

$$= -\frac{\hbar^2}{2}\left[\frac{1}{m_{i+\frac{1}{2}}}\frac{\varphi_{i+1}-\varphi_i}{d_{i,i+1}} - \frac{1}{m_{i-\frac{1}{2}}}\frac{\varphi_i-\varphi_{i-1}}{d_{i,i-1}}\right]$$

So in 1D we obtain

$$\boxed{-\frac{\hbar^2}{2}\left[\frac{1}{m_{i+\frac{1}{2}}}\frac{\varphi_{i+1}-\varphi_i}{d_{i,i+1}} - \frac{1}{m_{i-\frac{1}{2}}}\frac{\varphi_i-\varphi_{i-1}}{d_{i,i-1}}\right] + V_i\varphi_i\,\delta\lambda_i = E\varphi_i\,d\lambda_i}$$

UNIFORM GRID

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If the grid is uniform $\Rightarrow$ $d_{i,j} = a \quad \forall i,j$

Let's also suppose that m is constant

Then we obtain

$$-\frac{\hbar^2}{2}\frac{1}{m}\underbrace{\frac{\varphi_{i+1}+\varphi_{i-1}-2\varphi_i}{a^2}}_{\text{This is the discretized } \frac{\delta^2\varphi}{\delta x^2}} + V_i\varphi_i = E\varphi_i$$

The first derivative $\frac{\delta\varphi}{\delta x} \simeq \frac{\varphi_{i+1}-\varphi_i}{a} \simeq \frac{\varphi_i-\varphi_{i-1}}{a} \simeq \frac{\varphi_{i+1}-\varphi_{i-1}}{2a}$

We can define $t \triangleq \underbrace{-\frac{\hbar^2}{2ma^2}}_{\text{Energy}}$, $\boxed{\text{called hopping parameter}}$

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For the generic i-th point we have:

$$i: \quad \boxed{t\varphi_{i+1} + (V_i - 2t)\varphi_i + t\varphi_{i-1} = E\varphi_i}$$

In the matrix form:

$$H\varphi = E\varphi$$

The Hamiltonian is:

$$H = \begin{bmatrix} V_i-2t & t & & \emptyset \\ t & \ddots & \ddots & \\ & \ddots & \ddots & t \\ \emptyset & & t & V_i-2t \end{bmatrix}$$

H is a tridiagonal matrix