DISCRETIZATION

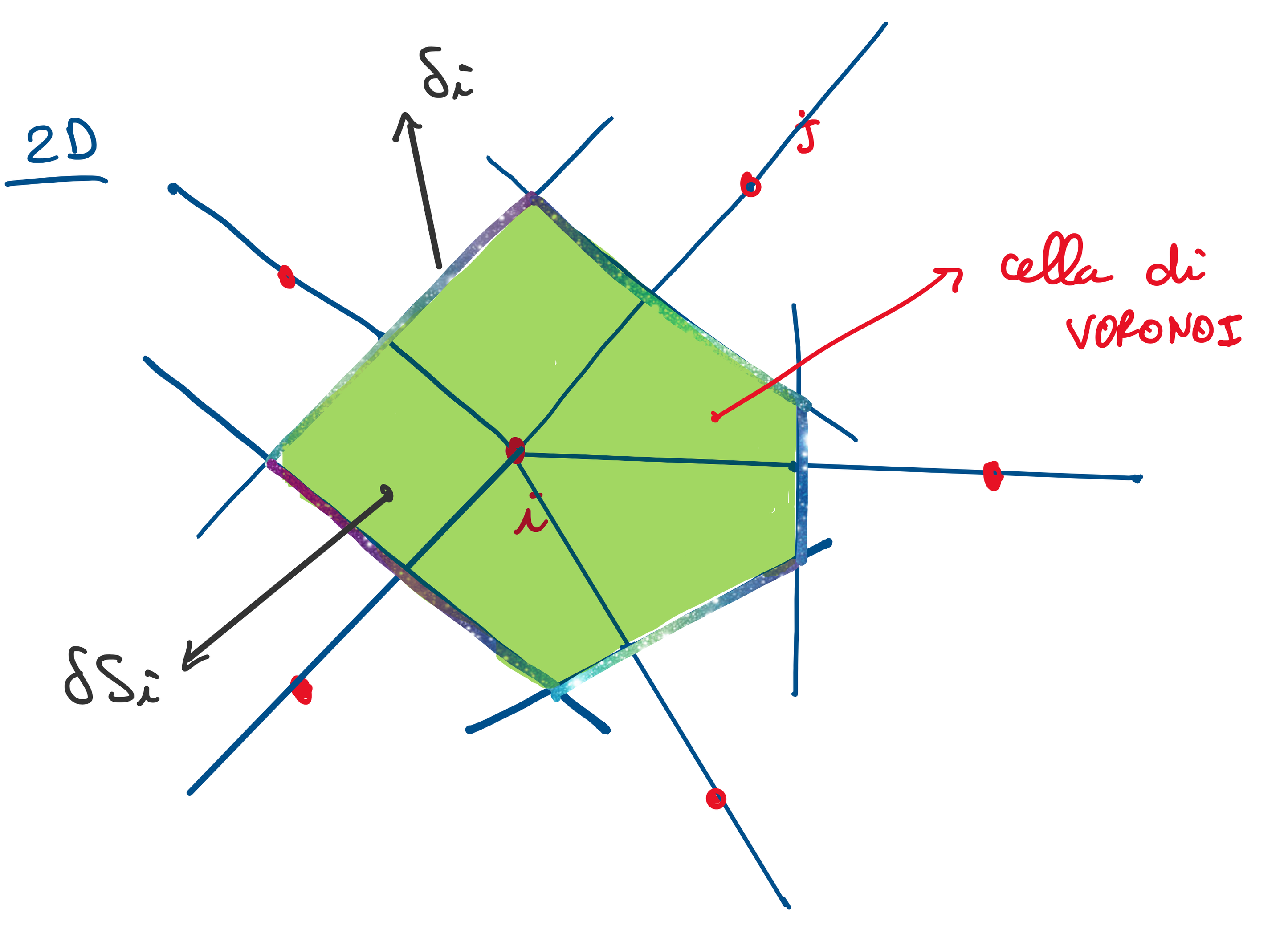
Friday, 4 October 2019 09:06

$$\begin{cases} eq_1(\vec{r},t) = 0 \\ \vdots \\ eq_n(\vec{r},t) = 0 \end{cases}$$

$$-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m(\vec{r})}\nabla\varphi(\vec{r})\right) + V(\vec{r})\,\varphi(\vec{r}) = E\,\varphi(\vec{r})$$

BOX INTEGRATION METHOD

i

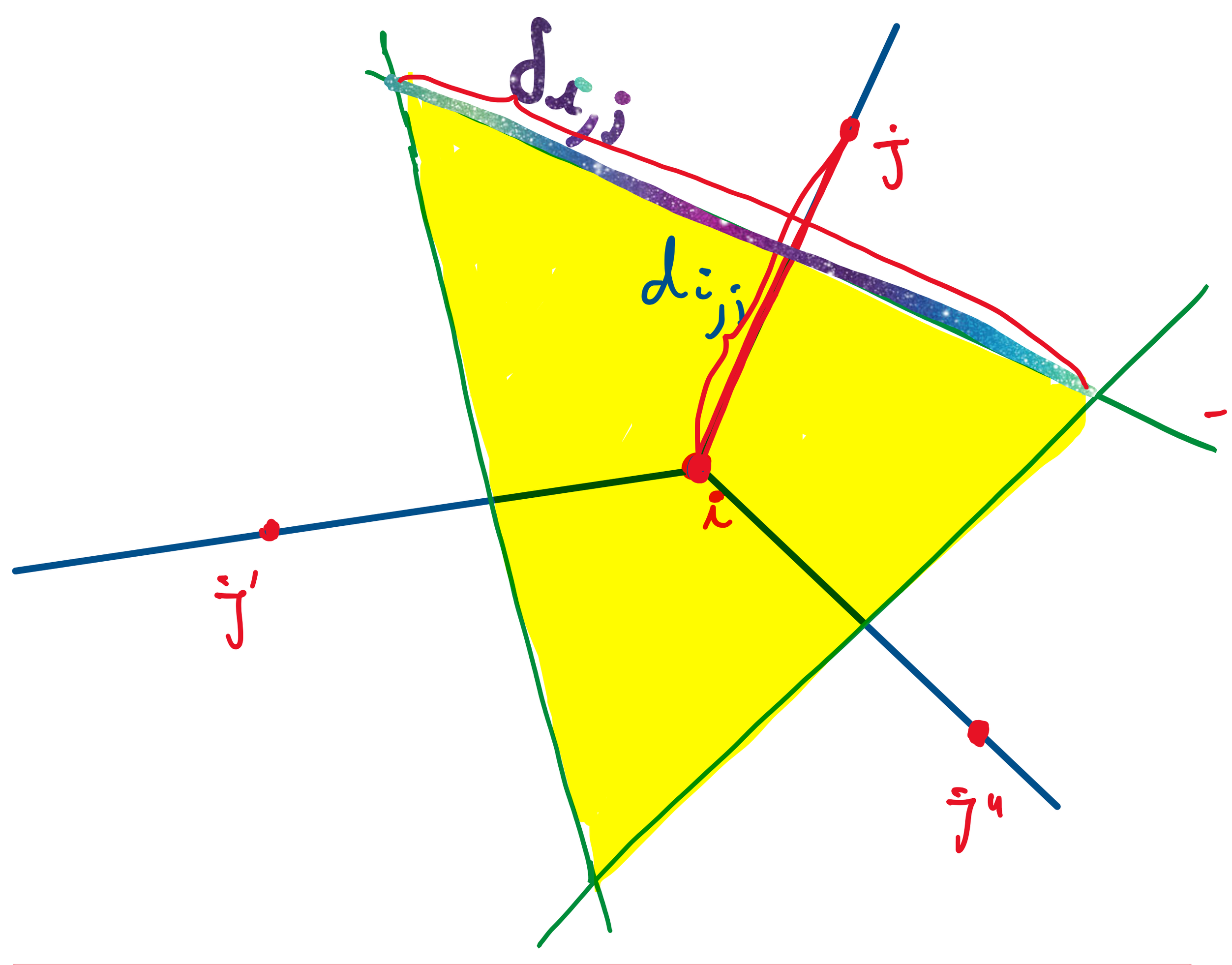


$$\underbrace{\int_{\delta S_i} -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m}\nabla\varphi\right)ds}\ + \underbrace{\int_{\delta S_i} V\varphi\, ds} = \underbrace{\int_{\delta S_i} E\varphi\, ds}$$

$$\underbrace{\int_{\delta S_i} -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m}\nabla\varphi\right)ds}_{\text{GAUSS-GREEN}} + V_i\varphi_i\,\delta S_i = E\varphi_i\,\delta S_i$$

$$\int_{\delta S}\nabla\cdot\underline{F}\, ds = \oint_{\delta e}\underline{F}\cdot d\underline{e}$$

$$\int_{\delta S_i} -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m}\nabla\varphi\right)ds = \boxed{-\frac{\hbar^2}{2}\oint_{\delta_i}\frac{1}{m}\nabla\varphi\cdot d\hat{n}}$$



$$-\frac{\hbar^2}{2}\,\frac{1}{\frac{m_i+m_j}{2}}\,\frac{\varphi_j-\varphi_i}{d_{i,j}}\cdot\delta_{i,j}$$

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

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

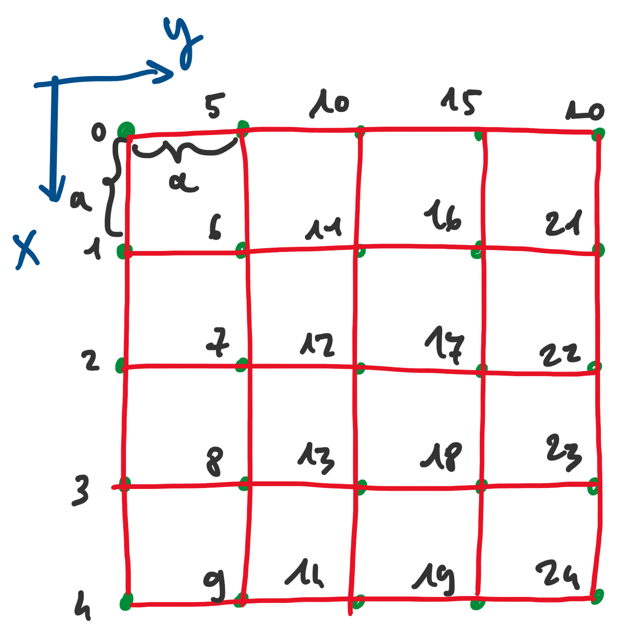
$$\nabla\cdot(\varepsilon\nabla\phi) = -q\rho$$

2D grid

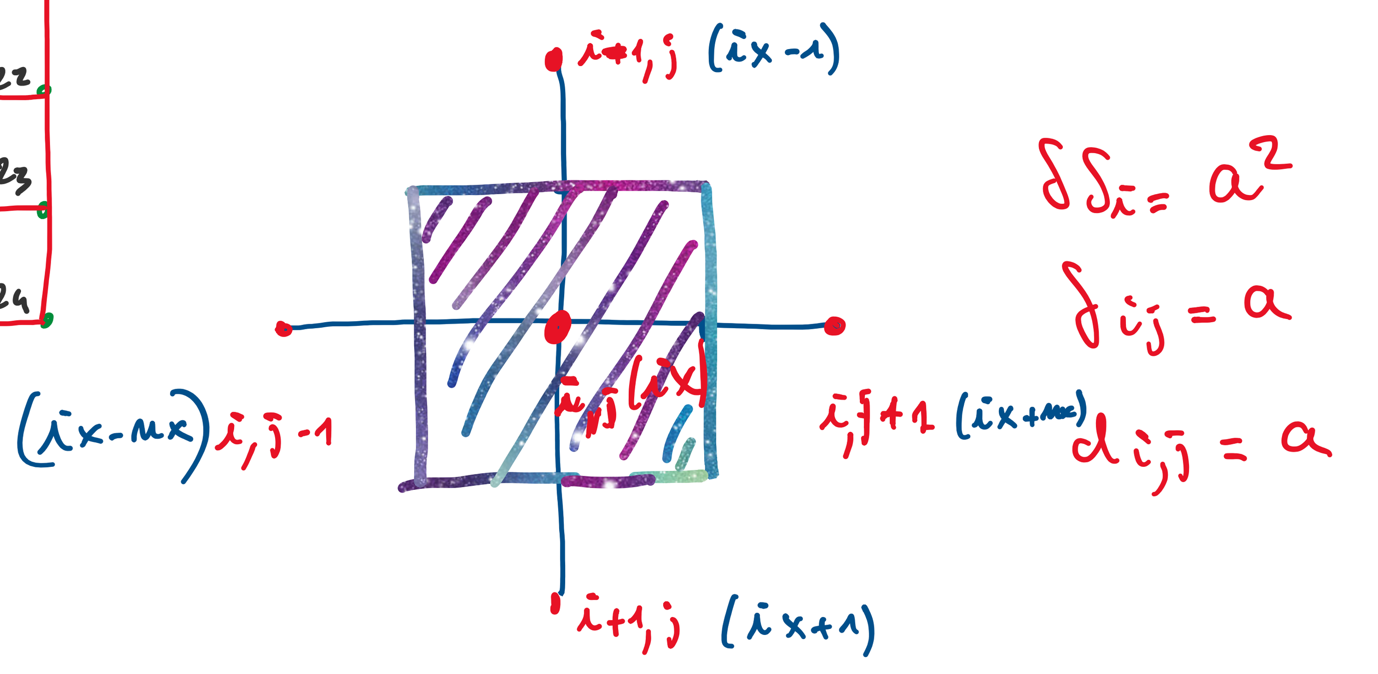
$i = 0..n_x-1$

$j = 0..n_y-1$

$i_x = i + j\cdot n_x$



$\Delta x = \Delta y = a$



$\delta S_i = a^2$

$\delta_{ij} = a$

$d_{ij} = a$

$i_x \quad -\frac{\hbar^2}{2}\sum_{j=1}^{4}\frac{1}{m}\frac{\varphi_j-\varphi_{i_x}}{\cancel{a}}\cdot\cancel{a} + V_{i_x}\varphi_{i_x}a^2 = E\varphi_{i_x}\cdot a^2$

$$\underbrace{-\frac{\hbar^2}{2ma^2}}\sum_{j=1}^{4}\varphi_j-\varphi_{i_x} + V_{i_x}\varphi_{i_x} = E\varphi_{i_x}$$

$$-\frac{\hbar^2}{2ma^2} = t \quad [J]\ [eV]$$

<u>hopping parameter</u>

$N_p = n_x\cdot n_y$

$i_x:\quad t\varphi_{i_x-n_x} + t\varphi_{i_x+n_x} + t\varphi_{i_x+1} + t\varphi_{i_x-1} - 4t\varphi_{i_x} + V_{i_x}\varphi_{i_x} = E\varphi_{i_x}$

$$H:\ i_x \rightarrow \begin{bmatrix} V_1-4t & t & & t & & \\ t & \ddots & \ddots & & \ddots & \\ & t & \ddots & \ddots & & \\ t \xleftrightarrow{n_x} t & & V_{i_x}-4t & t \xleftrightarrow{n_x} t & & \\ & \ddots & & \ddots & \ddots & t \\ & & t & & t & V_{N_p}-4t \end{bmatrix}\begin{bmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \vdots\\ \varphi_{N_p}\end{bmatrix} = E\begin{bmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \vdots\\ \varphi_{N_p}\end{bmatrix}$$