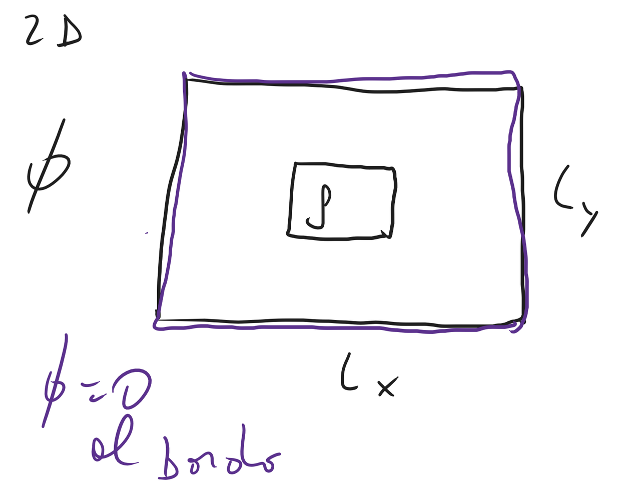
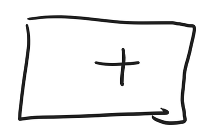
ESEMPIO

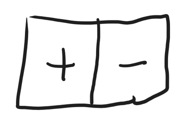


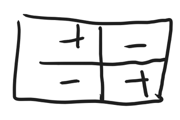

tre casi

monopolo



dipolo





quadrupolo

ALGORITMO DI RICHARDSON

Vogliamo risolvere $\hat{M} \cdot \vec{\phi} = \vec{f}$

Prendiamo $\vec{\phi}^{(0)}$ in maniera casuale

$$\vec{\phi}^{(i+1)} = \vec{\phi}^{(i)} + \alpha(\vec{f} - \hat{M} \cdot \vec{\phi}^{(i)})$$

con $\alpha \in \mathbb{R}$ e 'piccolo'

es $\alpha = 0.1$

Se abbiamo convergenza

$$\vec{\phi}^{(i+1)} = \vec{\phi}^{(i)}$$

$$0 = \alpha \underbrace{(\vec{f} - \hat{M} \cdot \vec{\phi}^{(i)})}_{=0} \Rightarrow \hat{M} \cdot \vec{\phi} = \vec{f}$$

Possiamo definire il funzionale

$$E(|\phi\rangle) = \langle\phi|M|\phi\rangle - (\langle f|\phi\rangle + \langle\phi|f\rangle)$$

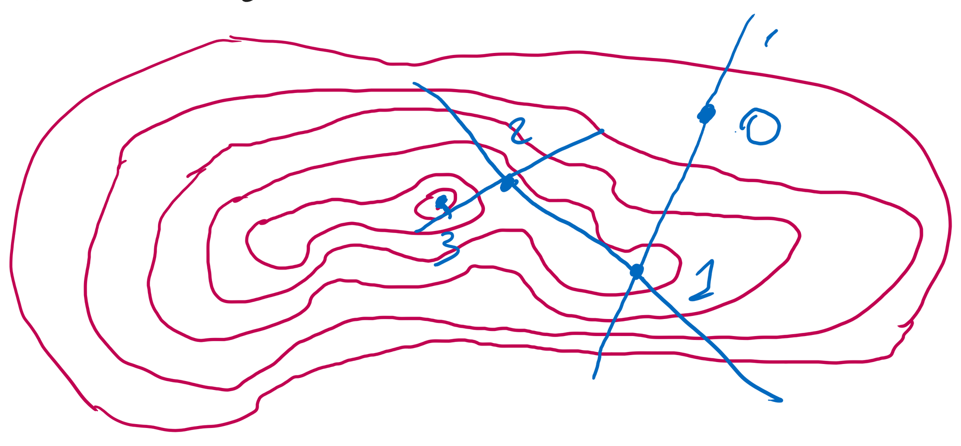
cerchiamo il minimo di $E$ rispetto a $|\phi\rangle$

al minimo

$$\frac{\partial E(|\phi\rangle)}{\partial \langle\phi|} = 0$$

$$M|\phi\rangle - |f\rangle = 0$$

Metodo STEEPEST DESCENT




sia la funzione da minimizzare $e(\vec{x})$

1) Prendo $\vec{x}^{(0)}$ in maniera 'casuale'

2) Calcolo $\vec{y}^{(i)} = -\frac{\partial e}{\partial \vec{x}}(\vec{x}^{(i)})$

3) Trovo $\lambda_{min}$ che minimizza $f(\lambda) = e(\vec{x}^{(i)} + \lambda \vec{y}^{(i)})$

4) Pongo $\vec{x}^{(i+1)} = \vec{x}^{(i)} + \lambda_{min} \vec{y}^{(i)}$

5) Se $\|\vec{x}^{(i+1)} - \vec{x}^{(i)}\|^2 < \epsilon_{soglia}$ allora la soluzione è $\vec{x}^{(i+1)}$

altrimenti torno al punto 2

EQ. DI SCHRÖDINGER 3D

$$\nabla^2 \psi(\vec{r}) + c(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

con $\vec{r} \in \Omega$ $\quad \Omega = [a_x, b_x] \times [a_y, b_y] \times [a_z, b_z]$

$\psi(\vec{r}) = 0$ per $\vec{r} \in \partial\Omega$

$$\sum_m H_{lm} \psi_m = E \psi_l$$

$l \Leftrightarrow (i, j, k) \qquad m \Leftrightarrow (i', j', k')$

$$H_{lm} = \begin{cases} \frac{1}{h_x^2} & \text{se } (i',j',k') = (i+1,j,k) \text{ o } (i',j',k') = (i-1,j,k) \\ \frac{1}{h_y^2} & \text{se } (i',j',k') = (i,j+1,k) \text{ o } '' = (i,j-1,k) \\ \frac{1}{h_z^2} & \text{se } (i',j',k') = (i,j,k+1) \text{ o } '' = (i,j,k-1) \\ -2\left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}\right) + c_{ijk} & \text{se } (i',j',k') = (i,j,k) \end{cases}$$

con
$i$ e $i'$ $\quad 2, \ldots N_x - 1$
$j, j'$ $\quad 2, \ldots, N_y - 1$
$k, k'$ $\quad 2, \ldots, N_z - 1$