Center for Molecular Modeling

Computational Materials Physics

Department of Materials Science and Engineering

conversion to matrix algebra

Stefaan.Cottenier@ugent.be
Technologiepark 903, Zwijnaarde

http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

$$\hat{\mathcal{H}}\,\Psi\left(\vec{x}_1,\ldots,\vec{x}_N\right) = E\,\Psi\left(\vec{x}_1,\ldots,\vec{x}_N\right)$$

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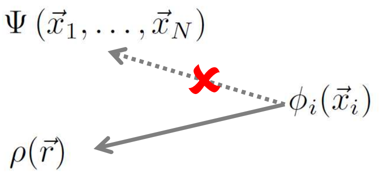
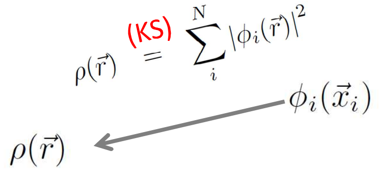
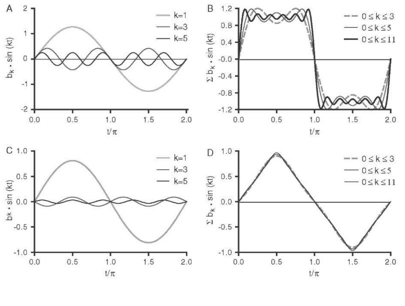




$$\hat{\mathcal{H}}_{KS}\,\phi_i = \epsilon_i\,\phi_i \qquad \text{(i = 1 – N)}$$

$$\phi = \sum_{k=1}^{\infty} c_k \chi_k$$



$$\phi = \sum_{k=1}^{\infty} c_k \chi_k$$

$$\phi \approx \sum_{k=1}^{M} c_k \chi_k$$

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$$\phi_i \approx \sum_{k=1}^{M} c_k^i \chi_k$$

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$$\phi_i \approx c_1^i \chi_1 + c_2^i \chi_2$$

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$$\hat{\mathcal{H}}_{KS}\,\left(c_1^i\,|\chi_1\rangle + c_2^i\,|\chi_2\rangle\right) = \epsilon_i\,\left(c_1^i\,|\chi_1\rangle + c_2^i\,|\chi_2\rangle\right)$$

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left-"multiply" with $\langle\chi_1|$:

$$c_1^i\underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{11}} + c_2^i\underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{12}} = \epsilon_i c_1^i\underbrace{\langle\chi_1|\chi_1\rangle}_{s_{11}} + \epsilon_i c_2^i\underbrace{\langle\chi_1|\chi_2\rangle}_{s_{12}}$$

$$c_1^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{11}} + c_2^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{12}} = \epsilon_i c_1^i \underbrace{\langle\chi_1|\chi_1\rangle}_{s_{11}} + \epsilon_i c_2^i \underbrace{\langle\chi_1|\chi_2\rangle}_{s_{12}}$$

$$c_1^i \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{21}} + c_2^i \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{22}} = \epsilon_i c_1^i \underbrace{\langle\chi_2|\chi_1\rangle}_{s_{21}} + \epsilon_i c_2^i \underbrace{\langle\chi_2|\chi_2\rangle}_{s_{22}}$$

$$c_1^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{11}} + c_2^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{12}} = \epsilon_i c_1^i \underbrace{\langle\chi_1|\chi_1\rangle}_{s_{11}} + \epsilon_i c_2^i \underbrace{\langle\chi_1|\chi_2\rangle}_{s_{12}}$$

$$c_1^i \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{21}} + c_2^i \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{22}} = \epsilon_i c_1^i \underbrace{\langle\chi_2|\chi_1\rangle}_{s_{21}} + \epsilon_i c_2^i \underbrace{\langle\chi_2|\chi_2\rangle}_{s_{22}}$$

$$|c_1^i|^2 + |c_2^i|^2 = 1$$

$$c_1^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{11}} + c_2^i \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{12}} = \epsilon_i c_1^i \underbrace{\langle\chi_1|\chi_1\rangle}_{s_{11}} + \epsilon_i c_2^i \underbrace{\langle\chi_1|\chi_2\rangle}_{s_{12}}$$

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$$c_1^j \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{11}} + c_2^j \underbrace{\langle\chi_1|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{12}} = \epsilon_j c_1^j \underbrace{\langle\chi_1|\chi_1\rangle}_{s_{11}} + \epsilon_j c_2^j \underbrace{\langle\chi_1|\chi_2\rangle}_{s_{12}}$$

$$c_1^j \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_1\rangle}_{h_{21}} + c_2^j \underbrace{\langle\chi_2|\hat{\mathcal{H}}_{KS}|\chi_2\rangle}_{h_{22}} = \epsilon_j c_1^j \underbrace{\langle\chi_2|\chi_1\rangle}_{s_{21}} + \epsilon_j c_2^j \underbrace{\langle\chi_2|\chi_2\rangle}_{s_{22}}$$

$$\left|c_1^j\right|^2 + \left|c_2^j\right|^2 = 1$$

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

H

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

H S

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

H C S C

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

H C = S C E

$$\begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} \begin{bmatrix} c_1^i & c_1^j \\ c_2^i & c_2^j \end{bmatrix} \begin{bmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{bmatrix}$$

H C = S C E

M x M $\quad \phi_i \approx \sum_{k=1}^{M} c_k^i \chi_k$

M > N $\quad \rho(\vec{r}) = \sum_{i}^{N} |\phi_i(\vec{r})|^2$