Localization

measurement of localization.

$\varphi \in L^2(\mathbb{R}^3)$

center $\langle \varphi | \vec{r} | \varphi \rangle = \int |\varphi(\vec{r})|^2 \vec{r} \, d\vec{r} := \langle \vec{r} \rangle.$

spread $\langle \varphi | (\vec{r} - \langle \vec{r} \rangle)^2 | \varphi \rangle$

$= \langle \varphi | \vec{r}^{\,2} | \varphi \rangle - \langle \varphi | \vec{r} | \varphi \rangle \cdot \langle \varphi | \vec{r} | \varphi \rangle.$

$$w_i = \sum_{j=1}^{N} \psi_j U_{ji}, \qquad U^* U = I_N. \quad \text{gauge.}$$

Find the best U to achieve smallest spread.

$$\inf_{\substack{U^*U = I \\ w_i = \sum_j \psi_j U_{ji}}} \sum_i \langle w_i | \vec{r}^2 | w_i \rangle - \langle w_i | \vec{r} | w_i \rangle^2$$

constrained optimization problem.

Boys orbital.

selected column of density matrix (SCDM).

$$P = \Psi \Psi^* = W W^*.$$

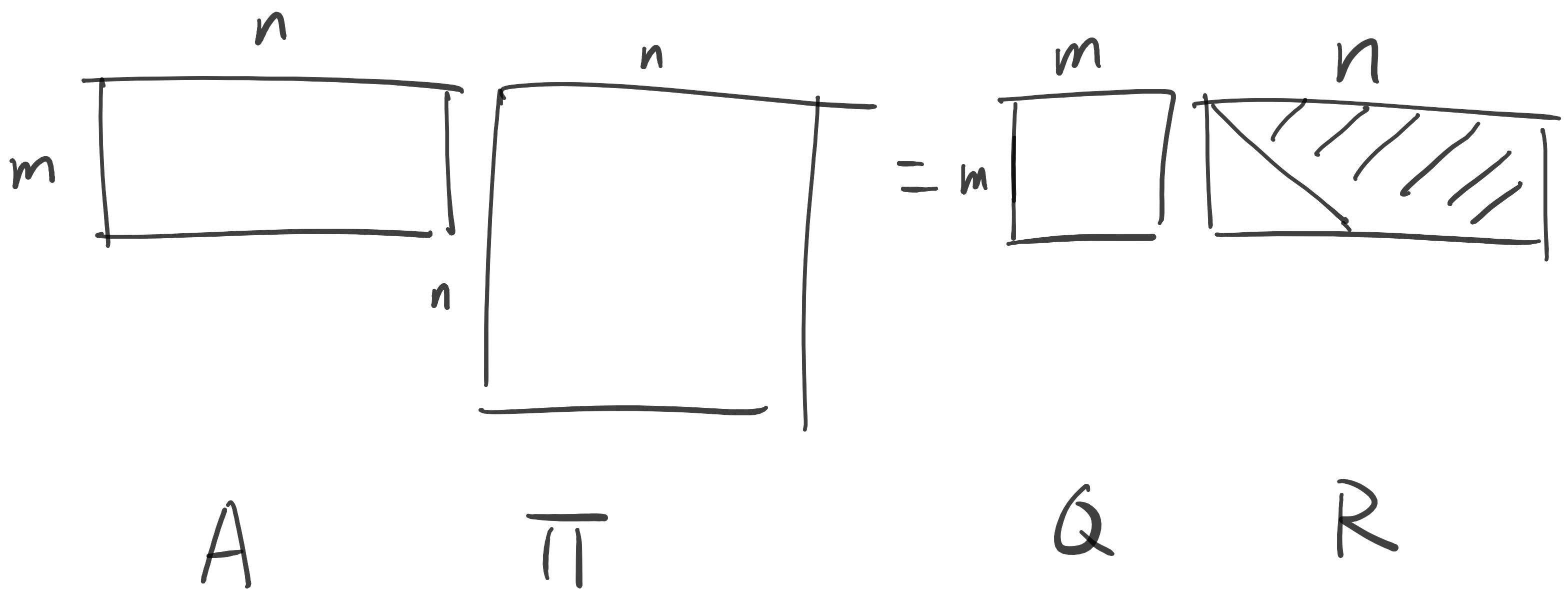
W localized $\Rightarrow$ P localized.

QR factorization w. column pivoting (QRCP).

$$A \in \mathbb{C}^{m \times n}.$$

$$A \Pi = Q R. \qquad |R_{11}| \geq |R_{22}| \geq \cdots$$

$Q^* Q = I$. R: upper triangular. Π: permutation.



$(m<n)$.

$$R = \begin{array}{cc} & \begin{array}{cc} n & (n-m) \end{array} \\ m & \begin{bmatrix} R_1 & R_2 \end{bmatrix} \end{array} \qquad \Pi = \begin{array}{cc} & \begin{array}{cc} m & n-m \end{array} \\ n & \begin{bmatrix} \Pi_1 & \Pi_2 \end{bmatrix} \end{array}$$

$$A[\Pi_1, \Pi_2] = [A\Pi_1 \quad A\Pi_2] = QR_1 [I \quad R_1^{-1} R_2]$$

$$:= A\Pi_1 [I \quad T]$$

$A\Pi_2$ are represented by lin. comb. of $A\Pi_1$.

Alg. SCDM.

(1) $\Psi^* \Pi = QR$.

$W = \Psi Q$.

(2) $\Psi^* \Pi = QR$. $\Pi = [\Pi_1, \Pi_2]$

$R = [R_1, R_2]$

$\Psi^* \Pi_1 = U S V^*$

$W = \Psi U$.

i.e. $Q = U$.

Cholesky QR

Löwdin orthogonalization.

require explanation.

$P \in \mathbb{C}^{d\times d}$. rank N.

$P\Pi = \tilde{Q} R$. $\qquad \Pi = \begin{array}{cc} & \begin{array}{cc} N & d-N \end{array} \\ d & \begin{bmatrix} \Pi_1 & \Pi_2 \end{bmatrix} \end{array}$

$\tilde{Q} \in \mathbb{C}^{d\times N}$. $R \in \mathbb{C}^{N\times d} = \begin{array}{cc} & \begin{array}{cc} N & \end{array} \\ N & \begin{bmatrix} R_1 & R_2 \end{bmatrix} \end{array}$

$$P\left[\Pi_1, \Pi_2\right] = \tilde{Q} R_1 \left[I \quad R_1^{-1} R_2 \right]$$

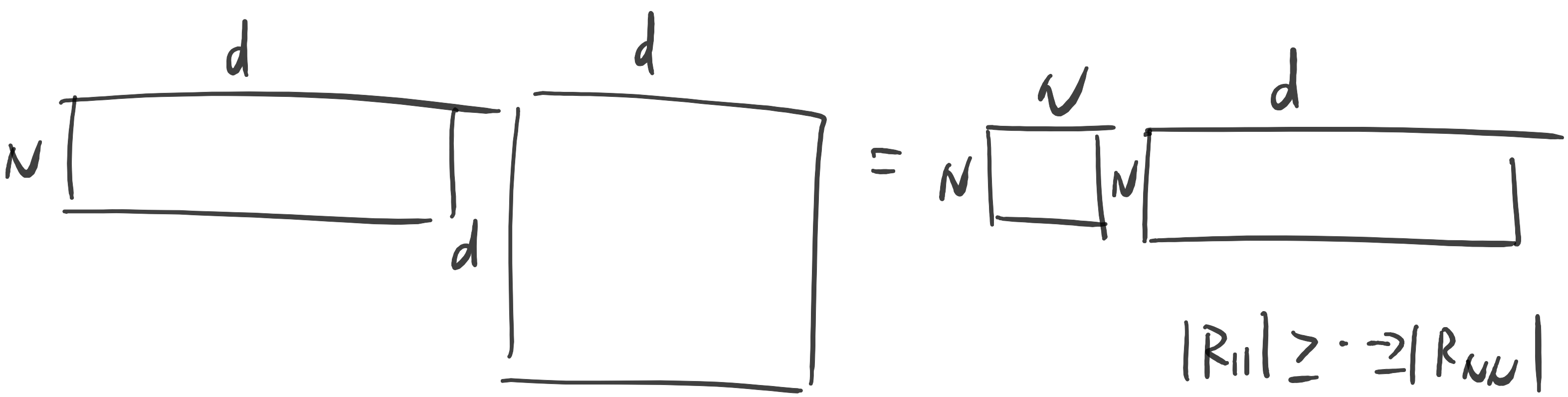
$P\Pi_1$: important columns of P. localized.

$P\Pi_1$ not orthogonal $\Rightarrow$ project to orthogonal representation.

$P\Pi_1 = \tilde{Q} R_1$. $R_1 \approx I$. $W = \tilde{Q}$!

Problem: $P \in \mathbb{C}^{d\times}$. $d >> N$.

$$\Psi^* \Pi = Q R$$



$|R_{11}| \geq \cdots \geq |R_{NN}|$

$\Psi \Psi^* \Pi = (\Psi Q) R$. $(\Psi Q)^* (\Psi Q) = I_N$.

implicitly a QRCP for P! $W = \Psi Q$

Another possibility.

$$A \in \mathbb{C}^{m \times n}.$$

$$\inf_{\substack{U \in \mathbb{C}^{m\times n} \\ U^*U = I_n}} \frac{1}{2}\| U - A \|_F^2$$

$$\mathcal{L} = \frac{1}{2}\operatorname{Tr}\left[U^*U - U^*A - A^*U + A^TA\right] + \frac{1}{2}\operatorname{Tr}\left[(U^*U - I)\Lambda\right]$$

$$\frac{\delta \mathcal{L}}{\delta U^*} = U - A + U\Lambda = 0 .$$

$$\Rightarrow \quad U\tilde{\Lambda} = A , \qquad \tilde{\Lambda} = I + \Lambda$$

$$A^*A = \tilde{\Lambda}^* U^* U \tilde{\Lambda}$$

a choice

$$A = \tilde{U}\tilde{S}\tilde{V}^* \Rightarrow \tilde{\Lambda}^2 = V\tilde{S}^2 V^* \Rightarrow \tilde{\Lambda} = \tilde{V}\tilde{S}\tilde{V}^*$$

$$\Rightarrow U = A\tilde{\Lambda}^{-1} = \tilde{U}\tilde{S}\tilde{V}^*\tilde{V}\tilde{S}^{-1}\tilde{V}^* = \tilde{U}\tilde{V}^*$$

Alg. $A = \tilde{U}\tilde{S}\tilde{V}^*$.

$U = \tilde{U}\tilde{V}^*$.

Cr. $U = A(A^*A)^{-\frac{1}{2}}$ Löwdin orthogonalization.

$$W = (P\Pi_1)(\Pi_1^* P^2 \Pi_1)^{-\frac{1}{2}} = (P\Pi_1)(\Pi_1^* P \Pi_1)^{-\frac{1}{2}}$$

SCDM orbital.

Use $\quad P\Pi_1 = \Psi(\Psi^*\Pi_1) = \Psi Q R_1$

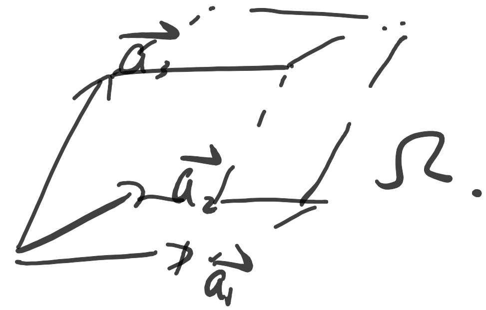
$$W = (P\Pi_1)(\Pi_1^* P \Pi_1)^{-\frac{1}{2}} = \Psi\, Q R_1 \,(\Pi_1^* \Psi_1 \Psi_1^* \Pi_1)^{-\frac{1}{2}}$$

$$= \Psi\, Q\, \underbrace{R_1 (R_1^* R_1)^{-\frac{1}{2}}}_{\text{difference}}$$

. or replace $(R_1^2)^{-\frac{1}{2}}$ by $(R_1^* R_1)^{-\frac{1}{2}}$

check this from SVD of $\Psi^*\Pi_1$.

Periodic system.



$$H = -\frac{1}{2}\Delta + V(\vec{r}).$$

$$V(\vec{r}+\vec{R}) = V(\vec{r}), \quad \vec{R} \in \mathbb{L}.$$

$$(T_{\vec{R}}\psi)(\vec{r}) = \psi(\vec{r}+\vec{R}).$$

$$[T_{\vec{R}}, H] = 0.$$

Note. $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r}), \quad u(\vec{r}+\vec{R}) = u(\vec{r})$

$$(T_{\vec{R}}\psi)(\vec{r}) = e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r})$$

$$H\psi(\vec{r}) = \left(-\frac{1}{2}\Delta + V(\vec{r})\right) e^{i\vec{k}\cdot\vec{r}} u(\vec{r})$$

$$= e^{i\vec{k}\cdot\vec{r}}\left[-\frac{1}{2}(\nabla + i\vec{k})^2 + V(\vec{r})\right] u(\vec{r}) = E e^{i\vec{k}\cdot\vec{r}} u(\vec{r})$$

$$\Rightarrow \quad H(\vec{k})\, u(\vec{r}) = E\, u(\vec{r})$$

$\vec{a}_i \cdot \vec{b}_j = 2\pi\,\delta_{ij}$, $\quad \vec{b}_1, \vec{b}_2, \vec{b}_3$

$\mathbb{L}^*$ reciprocal lattice.

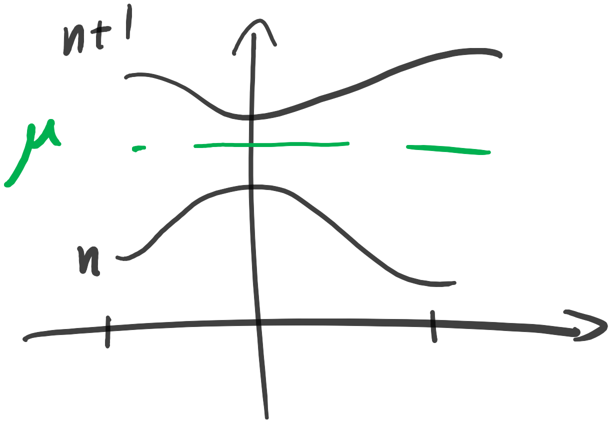
$$\Omega^* = \left\{ \vec{k} \;\middle|\; \vec{k} = \sum_{\alpha=1}^{3} k_\alpha \vec{b}_\alpha, \; -\frac{1}{2} \le k_\alpha \le \frac{1}{2} \right\}.$$

(first) Brillouin zone.

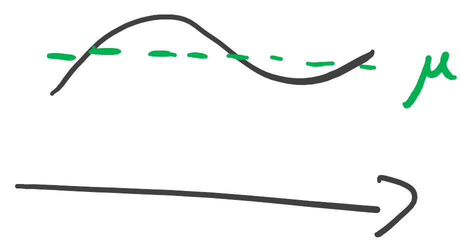
Kohn-Sham DFT.

$$H(\vec{k})\, u_{n,\vec{k}}(\vec{r}) = \varepsilon_{n,\vec{k}}\, u_{n,\vec{k}}(\vec{r})$$

Choose $\varepsilon_{n,\vec{k}} \leq \mu$.



insulator



metal

discretization : read notes

Wannier function (insulator)

$$\psi_{n,k}(\vec{r}) = \sum_{n'=1}^{N} \psi_{n,\vec{k}}(\vec{r})\, U_{n',n}(\vec{k})$$

$$w_{n,\vec{R}}(\vec{r}) = \frac{1}{|\Omega^*|} \int_{\Omega^*} \tilde{\psi}_{n,\vec{k}}(\vec{r})\, e^{-i\vec{k}\cdot\vec{R}}\, d\vec{k}$$

(exer). $\displaystyle\int_{\mathbb{R}^3} w^*_{n',\vec{R}'}(\vec{r})\, w_{n,\vec{R}}(\vec{r})\, d\vec{r} = \delta_{n'n}\, \delta_{\vec{R}',\vec{R}}$

$$w_{n,\vec{R}}(\vec{r}) = w_{n,0}(\vec{r}-\vec{R})$$

exponential decay property.

topological obstruction.

optimization. SCDM.