Based on Eur. J. Phys. 35 (2014) 035023 – Claveau, Arnaud, Di Matteo

Mean field approximation

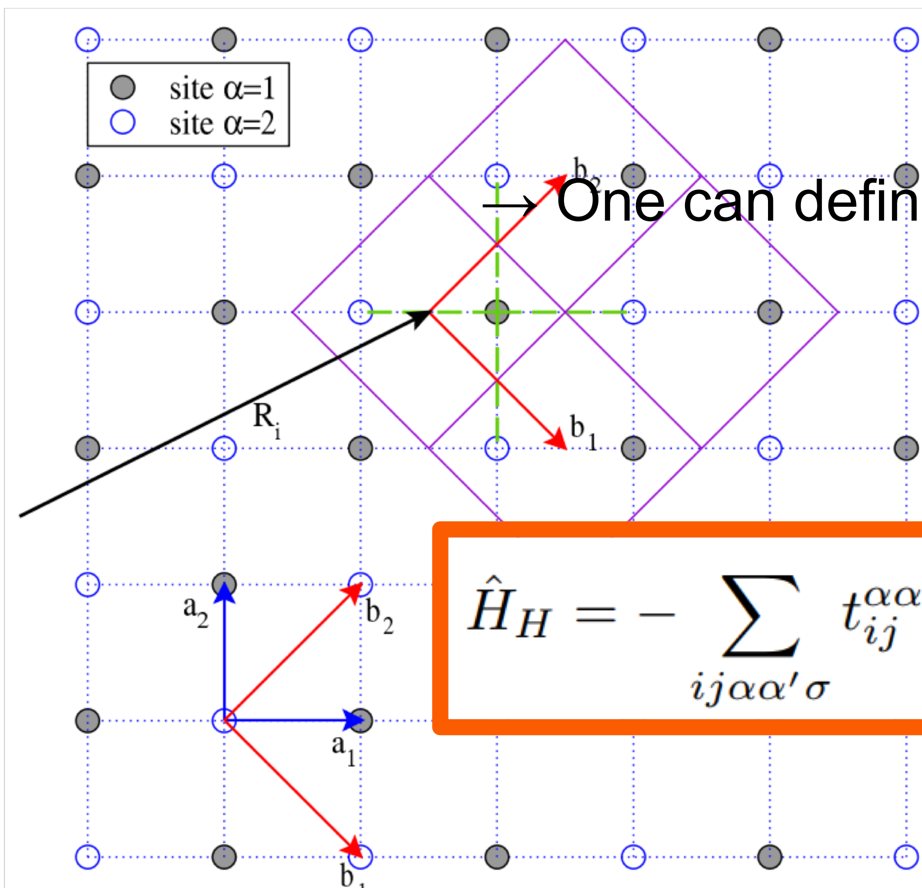
Rubem Mondaini

Beijing Computational Science Research Center

Hubbard model - definition

- Non-degenerate band (one orbital per site)

$$\hat{H}_H = -\sum_{ij\sigma} t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \equiv \hat{H}_t + \hat{H}_U$$



→ Bipartite lattice with NN hoppings

→ One can define unit cells with two sites instead (it will be

$$\boxed{\hat{H}_H = -\sum_{ij\alpha\alpha'\sigma} t^{\alpha\alpha'}_{ij}\hat{c}^\dagger_{i\alpha\sigma}\hat{c}_{j\alpha'\sigma} + U\sum_{i\alpha} \hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} \equiv \hat{H}_{\tilde{t}} + \hat{H}_{\tilde{U}}}$$

Tight-binding solution (U=0)

- Fourier transform of the fermionic operators

$$\hat{c}_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \mathrm{e}^{\imath \vec{k}\cdot\vec{R}_i} \hat{c}_{\vec{k}\alpha\sigma} \quad \text{and} \quad \hat{c}^{\dagger}_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \mathrm{e}^{-\imath \vec{k}\cdot\vec{R}_i} \hat{c}^{\dagger}_{\vec{k}\alpha\sigma}$$

- Hamiltonian in momentum space:

$$\begin{aligned}
\hat{H}_{\tilde{t}} &= -\frac{1}{N} \sum_{ij\alpha\alpha'\sigma} t_{ij}^{\alpha\alpha'} \sum_{\vec{k}\vec{k}'} \mathrm{e}^{-\imath\vec{k}\cdot\vec{R}_i} \hat{c}^{\dagger}_{\vec{k}\alpha\sigma} \mathrm{e}^{\imath\vec{k}'\cdot\vec{R}_j} \hat{c}_{\vec{k}'\alpha'\sigma} \\
&= -\frac{1}{N} \sum_{\vec{k}\vec{k}'\alpha\alpha'\sigma} \hat{c}^{\dagger}_{\vec{k}\alpha\sigma} \hat{c}_{\vec{k}'\alpha'\sigma} \sum_{ij} t_{ij}^{\alpha\alpha'} \mathrm{e}^{-\imath\vec{k}\cdot\vec{R}_i} \mathrm{e}^{\imath\vec{k}'\cdot\vec{R}_j} \\
&= -\sum_{\vec{k}\vec{k}'\alpha\alpha'\sigma} \hat{c}^{\dagger}_{\vec{k}\alpha\sigma} \hat{c}_{\vec{k}'\alpha'\sigma} \sum_{j} t_{\vec{\eta}_j}^{\alpha\alpha'} \mathrm{e}^{\imath\vec{k}'\cdot\vec{\eta}_j} \underbrace{\frac{1}{N} \sum_{i} \mathrm{e}^{-\imath(\vec{k}-\vec{k}')\cdot\vec{R}_i}}_{\delta_{\vec{k},\vec{k}'}} \\
&= \sum_{\vec{k}\alpha\alpha'\sigma} \hat{c}^{\dagger}_{\vec{k}\alpha\sigma} \hat{c}_{\vec{k}\alpha'\sigma} \varepsilon_{\vec{k}}^{\alpha\alpha'}
\end{aligned}$$

where $\varepsilon_{\vec{k}}^{\alpha\alpha'} = -\sum_j t_{\vec{\eta}_j}^{\alpha\alpha'} \mathrm{e}^{\imath\vec{k}\cdot\vec{\eta}_j}$

Tight-binding solution (U=0)

➡ Two indices α, α', it defines a matrix: 2×2

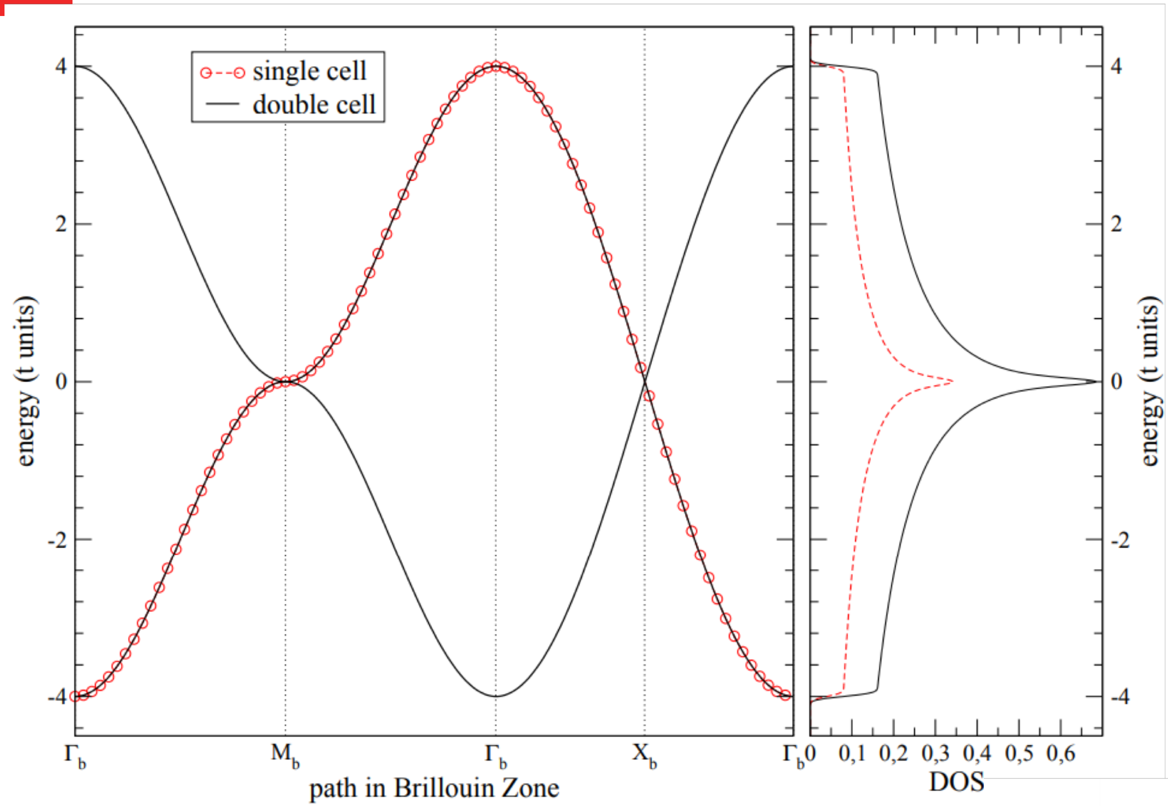
$$H_{\tilde{t}} = \begin{bmatrix} 0 & t\gamma_{\vec{k}} \\ t\gamma_{\vec{k}}^{*} & 0 \end{bmatrix}$$

$$\text{where } \gamma_{\vec{k}} = -\left\{1 + e^{-i\vec{k}\cdot(\vec{b}_1+\vec{b}_2)} + e^{-i\vec{k}\cdot\vec{b}_1} + e^{-i\vec{k}\cdot\vec{b}_2}\right\}$$

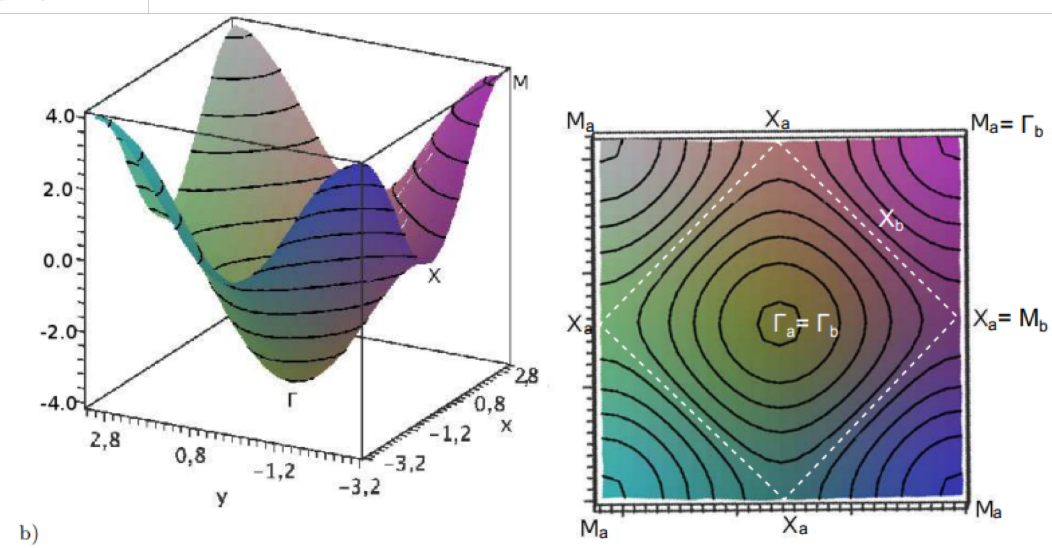
➡ After diagonalizing, it results in two bands:

$$\varepsilon_{0\vec{k}}^{\pm} = \pm t|\gamma_{\vec{k}}| = \pm t\left|2\cos\left(\vec{k}\cdot\frac{\vec{b}_1+\vec{b}_2}{2}\right) + 2\cos\left(\vec{k}\cdot\frac{\vec{b}_2-\vec{b}_1}{2}\right)\right|$$

Tight-binding solution (U=0)



- Comparison between the BZ of two different unit cells
- They are perfect equivalent
- after considering folding
- Note van Hove singularity



Introduction of interactions -Mean field

- mean-field approximation corresponds to neglecting the fluctuations around the mean density

- Fluctuations are defined as:

$$\Delta\hat{n}_{i\alpha\sigma} \equiv \hat{n}_{i\alpha\sigma} - \underbrace{\langle\hat{n}_{i\alpha\sigma}\rangle}_{\text{Mean occupation number}}$$

➡ $$\hat{n}_{i\alpha\sigma} \equiv \langle\hat{n}_{i\alpha\sigma}\rangle + \Delta\hat{n}_{i\alpha\sigma}$$

➡ Assuming homogeneity, the interaction term is written as

$$\begin{aligned}\hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} &= [\Delta\hat{n}_{i\alpha\uparrow} + \langle\hat{n}_{\alpha\uparrow}\rangle]\cdot[\Delta\hat{n}_{i\alpha\downarrow} + \langle\hat{n}_{\alpha\downarrow}\rangle] \\ &= \underbrace{\Delta\hat{n}_{i\alpha\uparrow}\Delta\hat{n}_{i\alpha\downarrow}}_{0} + \sum_{\sigma}\hat{n}_{i\alpha\sigma}\langle\hat{n}_{\alpha\bar{\sigma}}\rangle - \langle\hat{n}_{\alpha\uparrow}\rangle\langle\hat{n}_{\alpha\downarrow}\rangle\end{aligned}$$

- In the MF approx. we neglect terms which are quadratic in the fluctuations

Introduction of interactions -Mean field

- The interaction term becomes:

$$\hat{H}^{\mathrm{MF}}_{\tilde{U}} = \underbrace{U\sum_{i\alpha\sigma}\hat{n}_{i\alpha\sigma}\langle n_{\alpha\bar{\sigma}}\rangle}_{\tilde{H}_U} - \underbrace{UN\sum_{\alpha}\langle n_{\alpha\uparrow}\rangle\langle n_{\alpha\downarrow}\rangle}_{E_U}$$

It is a number but
It needs to be taken
Into account → regulates
The appearance of different
Magnetic phases

- Fourier transform (again!):

$$\tilde{H}_U = U\sum\nolimits_{i\alpha\sigma}\langle n_{\alpha\bar{\sigma}}\rangle\hat{c}^{\dagger}_{i\alpha\sigma}\hat{c}_{i\alpha\sigma} = U\sum\nolimits_{\vec{k}\alpha\sigma}\langle n_{\alpha\bar{\sigma}}\rangle\hat{c}^{\dagger}_{\vec{k}\alpha\sigma}\hat{c}_{\vec{k}\alpha\sigma}$$

(diagonal in momentum)

Introduction of interactions -Mean field

- The final Hamiltonian (incorporating both kinetic and MF term):

$$\hat{H}_H \equiv \hat{H}_{\tilde{t}} + \hat{H}_{\tilde{U}} = \begin{bmatrix} U\langle n_{1\bar{\sigma}}\rangle & t\gamma_{\vec{k}} \\ t\gamma^*_{\vec{k}} & U\langle n_{2\bar{\sigma}}\rangle \end{bmatrix}$$

- Diagonalizing:

$$\varepsilon^2_{\vec{k}} - \varepsilon_{\vec{k}}\left(U\langle n_{1\bar{\sigma}}\rangle + U\langle n_{2\bar{\sigma}}\rangle\right) + U^2\langle n_{1\bar{\sigma}}\rangle\langle n_{2\bar{\sigma}}\rangle - t^2|\gamma_{\vec{k}}|^2 = 0$$

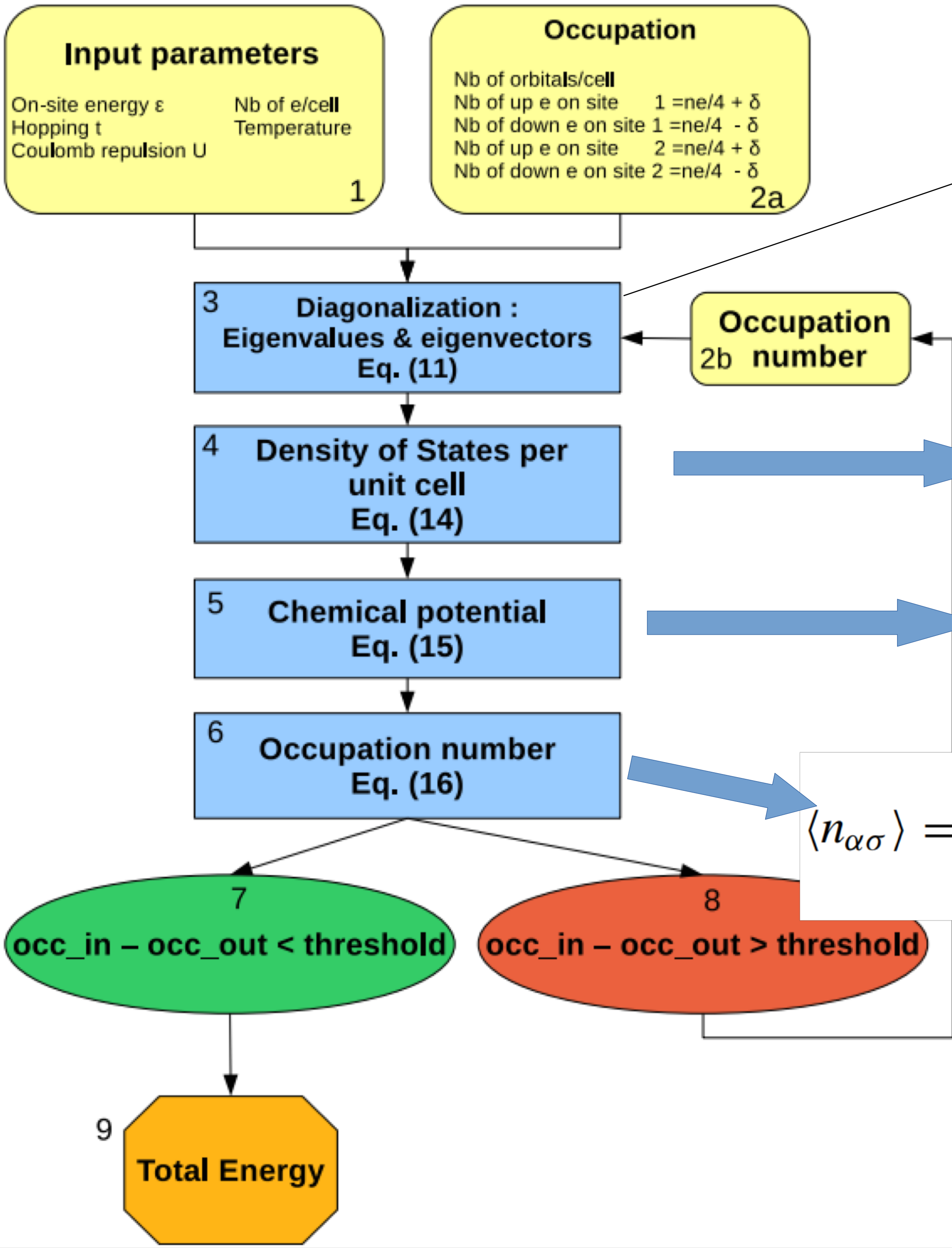
$$\varepsilon^{\pm}_{\vec{k}\sigma} = U\left(\frac{\langle n_{1\bar{\sigma}}\rangle + \langle n_{2\bar{\sigma}}\rangle}{2}\right) - \underbrace{\boxed{U\left(\langle n_{1\uparrow}\rangle\langle n_{1\downarrow}\rangle + \langle n_{2\uparrow}\rangle\langle n_{2\downarrow}\rangle\right)}}_{\to E_U}$$

$$\pm\frac{1}{2}\sqrt{U^2(\langle n_{1\bar{\sigma}}\rangle - \langle n_{2\bar{\sigma}}\rangle)^2 + 16t^2\left(\cos\left[\vec{k}\cdot\frac{\vec{b}_1+\vec{b}_2}{2}\right] + \cos\left[\vec{k}\cdot\frac{\vec{b}_1-\vec{b}_2}{2}\right]\right)^2}$$

$$= U\left(\frac{\langle n_{1\bar{\sigma}}\rangle + \langle n_{2\bar{\sigma}}\rangle}{2}\right) - \underbrace{\boxed{U\left(\langle n_{1\uparrow}\rangle\langle n_{1\downarrow}\rangle + \langle n_{2\uparrow}\rangle\langle n_{2\downarrow}\rangle\right)}}_{\to E_U}$$

$$\pm\frac{1}{2}\sqrt{U^2(\langle n_{1\bar{\sigma}}\rangle - \langle n_{2\bar{\sigma}}\rangle)^2 + 4(\varepsilon^{\pm}_{0\vec{k}})^2}$$

Computational protocol - self-consistency



$$\varepsilon_{j\sigma}(\vec{k}) \qquad |\Psi^{j}_{\vec{k}\sigma}\rangle = \sum_\alpha A^{j}_{\alpha,\sigma}(\vec{k})|\alpha\vec{k}\rangle$$

$$\rho(\varepsilon) = \frac{1}{N}\sum_{\vec{k},j,\sigma}\delta[\varepsilon - \varepsilon_{j\sigma}(\vec{k})]$$

$$\int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, \rho(\varepsilon)\frac{1}{\exp[\beta(\varepsilon-\mu)]+1} = n_e$$

$$\langle n_{\alpha\sigma}\rangle = \frac{1}{N}\sum_{\vec{k},j=1,2}|A^{j}_{\alpha,\sigma}(\vec{k})|^2\frac{1}{\exp[\beta(\varepsilon_{j\sigma}(\vec{k})-\mu)]+1}$$

Phase diagram – square lattice