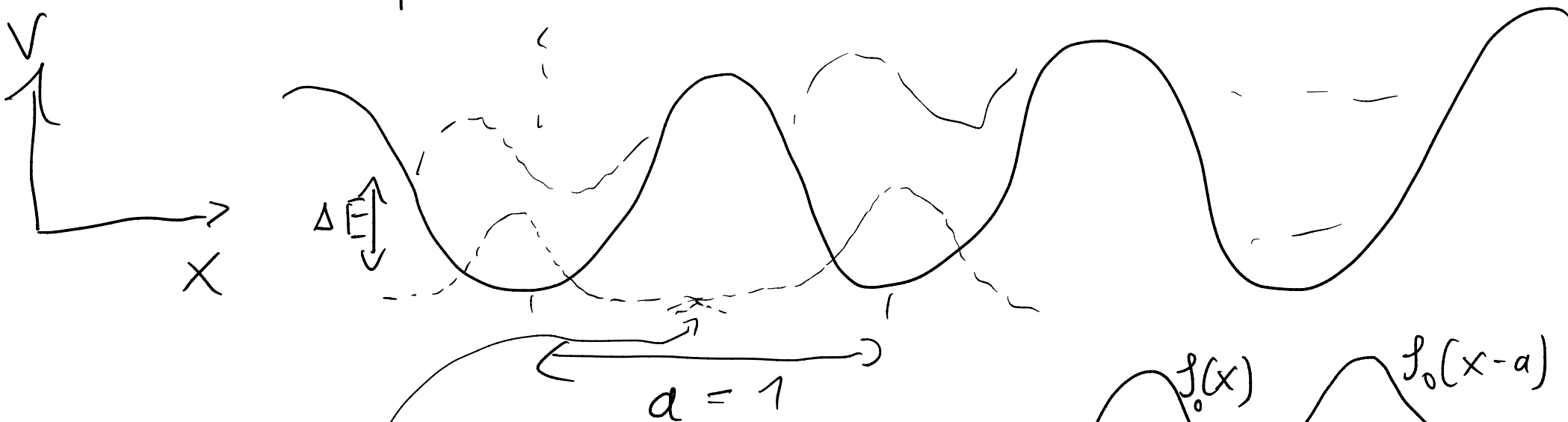
A.2 Tight-Binding, Hubbard-, and Spin Models

- Consider particles in a periodic potential



small but finite overlap:

$\rightsquigarrow$ hopping integral $t = \int dx\, \varphi_0^*(x-a)\, \Delta V(x)\, \varphi_0(x)$

with $\Delta V(x) = \sum_{l \in \mathbb{Z} \setminus \{0\}} V_2(x - l \cdot a)$

V_2: atomic potential of atom at position $l \cdot a$

- Neglect the influence of higher excited states (well justified ΔE is large).

- Resulting single band tight-binding model ($a = t = 1$):

$$H = -t \sum_{j,\sigma} \psi^{+}_{j,\sigma} \psi_{j+1,\sigma} + h.c. + \sum_{j,\sigma} (-\mu)\, \psi^{+}_{j,\sigma} \psi_{j,\sigma}$$

j: sites, σ: spin, $-\mu$: chemical potential

Solution by Fourier transform:

$$c_{k,\sigma} = \frac{1}{\sqrt{L}} \sum_{j} e^{-ikj} \psi_{j,\sigma}, \quad \psi_{j,\sigma} = \frac{1}{\sqrt{L}} \sum_{k} e^{ikj} c_{k,\sigma}, \quad k = \frac{2\pi}{L} n,$$

$$n = 0, 1, \ldots, L-1$$

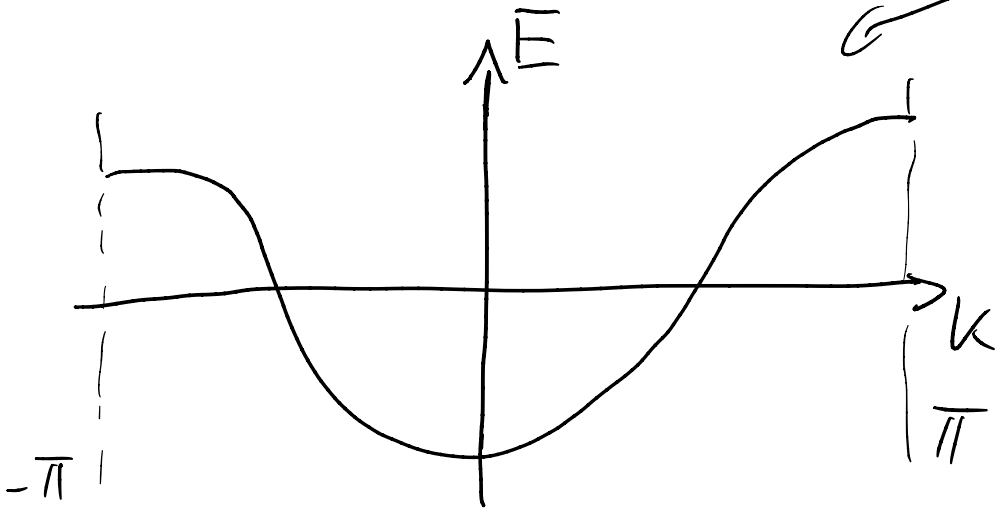
$$H = \frac{1}{L} \sum_{\substack{j,\sigma \\ k,q}} \left(-t e^{-iqj} e^{ik(j+1)} c^{+}_{q,\sigma} c_{k,\sigma} + h.c. - \mu e^{i(k-q)j} c^{+}_{q,\sigma} c_{k,\sigma} \right)$$

$$= \sum_{k,\sigma} -t e^{ik} c^{+}_{k,\sigma} c_{k,\sigma} + h.c. - \mu c^{+}_{k,\sigma} c_{k,\sigma} =$$

$\sum_j e^{ipj} = L \delta_{p,0}$

$$= \sum_{k,\sigma} c^{+}_{k,\sigma} \left(-2t \cos k - \mu \right) c_{k,\sigma}$$

band structure



- Generalization to nearest neighbor (NN) tight-binding model in 1D with n orbitals (including spin)

$$H = \sum_j \left(\Psi_j^\dagger \, h_t \, \Psi_{j+1} + \text{h.c.} + \Psi_j^\dagger \, h_{on} \, \Psi_j \right) =$$

(h_t: $n \times n$ matrix)

($\Psi_j^\dagger$: n-spinor $(\Psi_{j,1}^\dagger, \cdots, \Psi_{j,n}^\dagger)$)

(h_{on}: $n \times n$ onsite potential matrix (Hermitian))

F.T. →

$$= \sum_k c_k^\dagger \underbrace{\left(h_t e^{ik} + h_t^\dagger e^{-ik} + h_{on} \right)}_{h_k \text{ (Bloch Hamiltonian)}} c_k$$

(h_k: $(n \times n)$)

- Generalization to higher spatial dimension and hopping displacements $\vec{\delta}$ beyond NN hopping:

$$H = \sum_{\vec{j},\vec{\delta}} \Psi^{+}_{\vec{j}} h_{t,\vec{\delta}} \Psi_{\vec{j}+\vec{\delta}} + h.c. + \sum_{\vec{j}} \Psi^{+}_{\vec{j}} h_{on} \Psi_{\vec{j}} =$$

$\uparrow$ no double counting $\vec{\delta}$ and $-\vec{\delta}$

$$= \sum_{\vec{k}} c^{+}_{\vec{k}} \underbrace{\left(\left[\sum_{\vec{\delta}} \left(h_{t,\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}} + h^{+}_{t,\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}} \right) \right] + h_{on} \right)}_{h_{\vec{k}}} c_{\vec{k}}$$

$\uparrow$ F.T.

$h_{\vec{k}}$ (Bloch Hamiltonian)

- Practical implementation in real space (relevant for open boundary conditions or disordered systems, i.e. $h_{on} \to h_{on,j}$)

- Start with $n = 1$ and $H = \sum_j \left(-t\,\psi_j^\dagger \psi_{j+1} + \text{h.c.} - \mu \psi_j^\dagger \psi_j\right)$

$$= \psi^\dagger h \psi$$

L-vector $j = 1, \dots, L$

$L \times L$ matrix

with $h =$

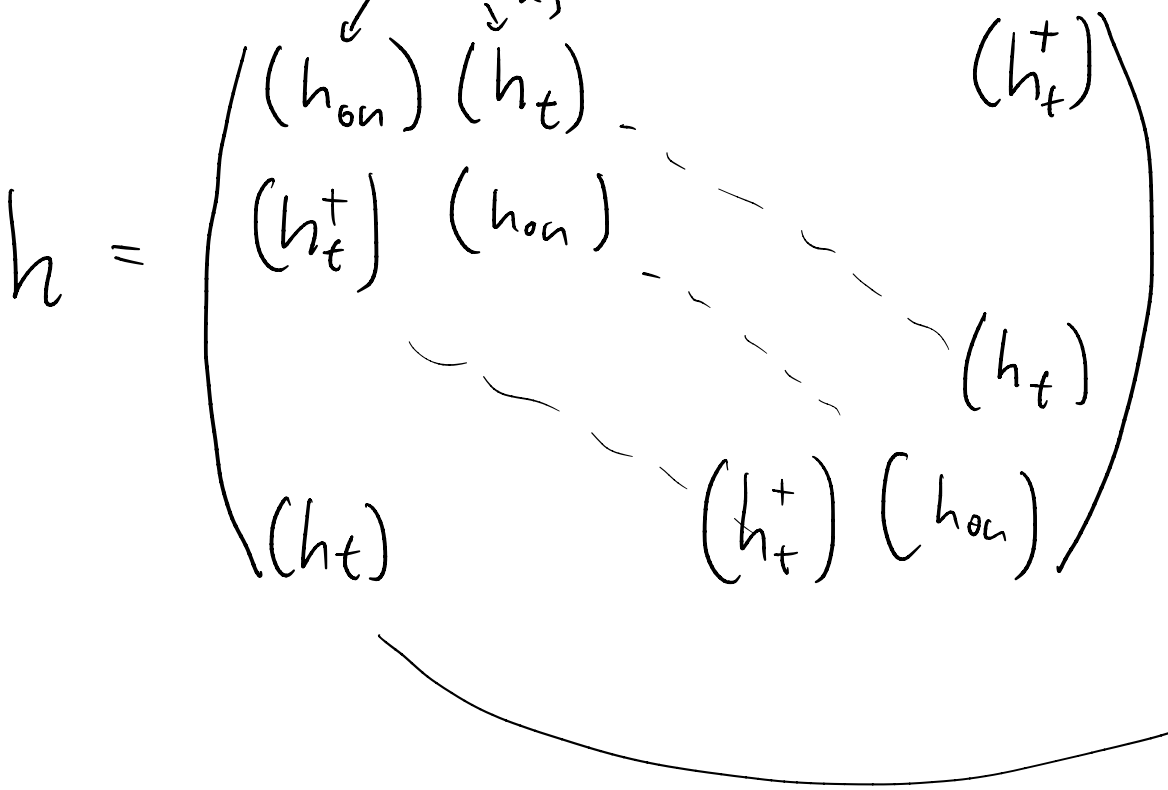
$$\begin{pmatrix} -\mu & -t & & & -t \\ -t & -\mu & -t & & \\ & -t & \ddots & \ddots & \\ & & \ddots & \ddots & -t \\ -t & & & -t & -\mu \end{pmatrix}$$

periodic boundaries

- Generalization to n orbitals with NN coupling $H = \Psi^\dagger h \Psi$

Ψ: $n \cdot L$-vectors

with



$$h = \begin{pmatrix} (h_{on}) & (h_t) & & (h_t^\dagger) \\ (h_t^\dagger) & (h_{on}) & \ddots & \\ & \ddots & \ddots & (h_t) \\ (h_t) & & (h_t^\dagger) & (h_{on}) \end{pmatrix}$$

- Generalization to dimension d and hopping displacements $\vec{\delta}$:

$$H = \Psi^\dagger h \Psi \quad \text{with} \quad N = n \cdot L_1 L_2 \cdots L_d$$

Ψ: N-vector

Implementation of h:

(i) Define h as a $n \times n$-matrix valued tensor with indices

$h_{\vec{i}\vec{j}}$;

$\vec{i} = (i_1, i_2, \ldots, i_d)$

(ii) Initialize $h_{\vec{i}\vec{j}} = 0_{n \times n} \quad \forall_{\vec{i},\vec{j}}$

$0_{n \times n}$ ↑ zero-matrix

(iii) Loop over $\vec{i}$ ε

Loop over $\vec{\delta}$ { (no double counting)

set $h_{\vec{i},\vec{i}+\vec{\delta}} = h_{t,\vec{\delta}}$

set $h_{\vec{i}+\vec{\delta},\vec{i}} = h^{+}_{t,\vec{\delta}}$

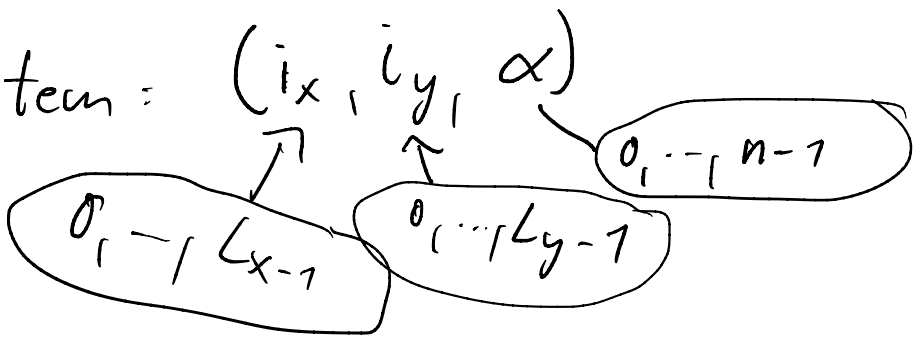
}

set $h_{\vec{i},\vec{i}} = h_{on}$ ← { for disorder: $h_{on,\vec{i}}$

}

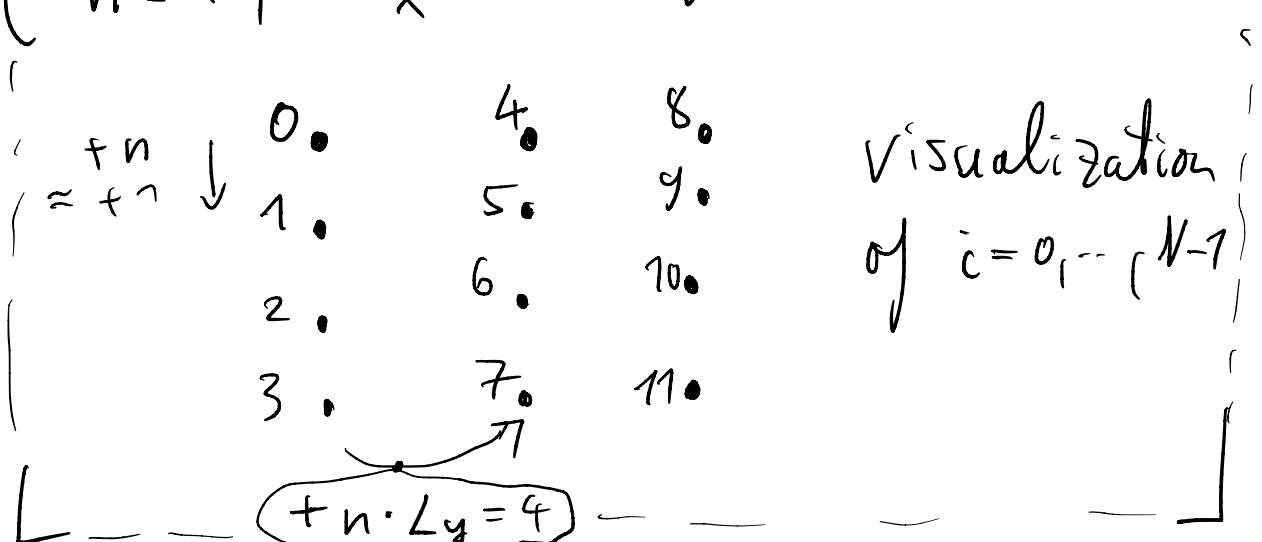
(iv) Flatten h to ordinary $N \times N$ matrix by combining indices

↳ Example for 2D system: (i_x, i_y, α)



$\rightarrow i = i_x L_y n + i_y n + \alpha$.

$n = 1, \; L_x = 3, \; L_y = 4 \rightarrow N = 12$



- Full diagonalization of $N \times N$ matrix h as

$h = U \tilde{h} U^\dagger$ at computational cost $\sim N^3$

$U = (\vec{v}_1, \dots, \vec{v}_N)$

$\tilde{h} = \mathrm{diag}(\varepsilon_1, \dots, \varepsilon_N)$

gives full spectrum of eigenvalues ε_i and eigenvectors $\vec{v}_i$ of single-particle states

$\rightsquigarrow$ As we will see in A.3, this is all we need to efficiently calculate all many-body properties of non-interacting systems.