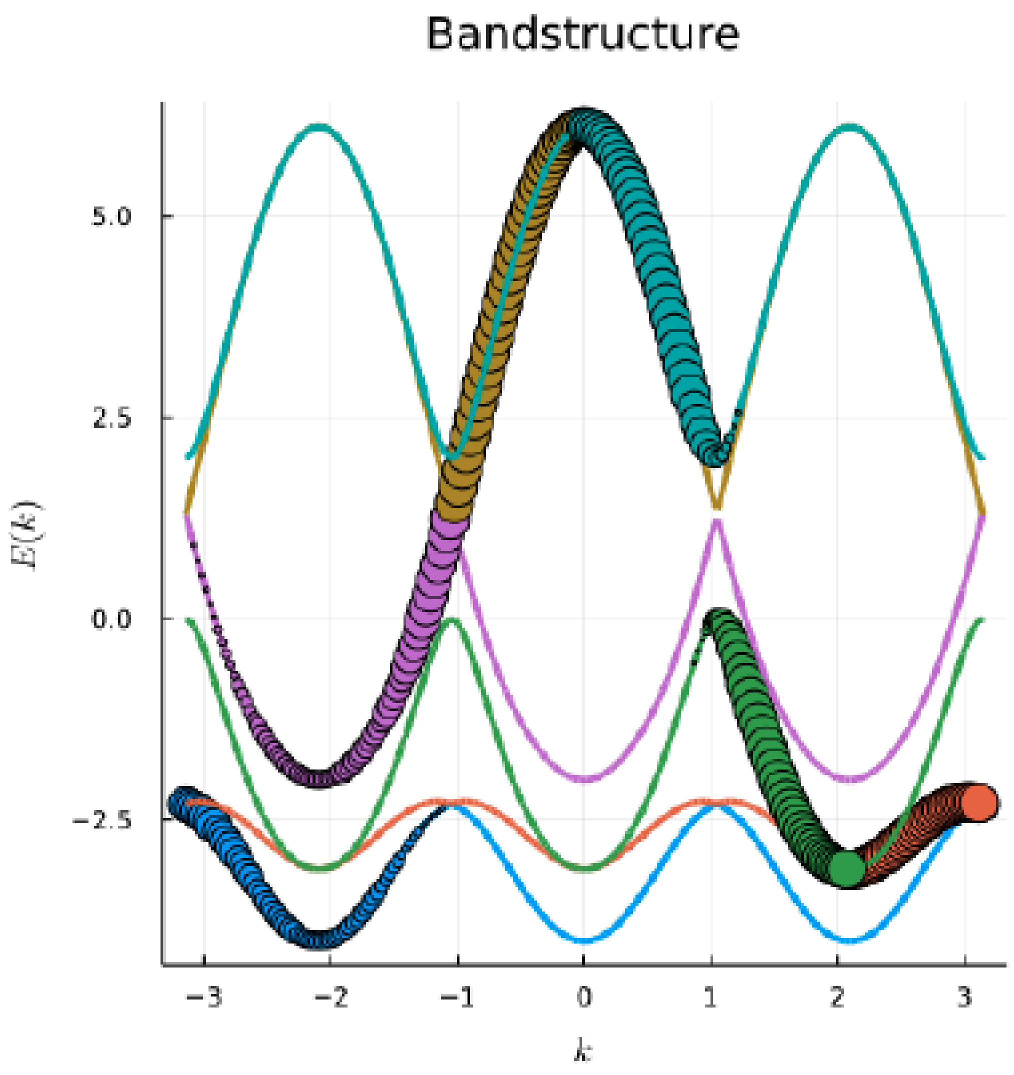
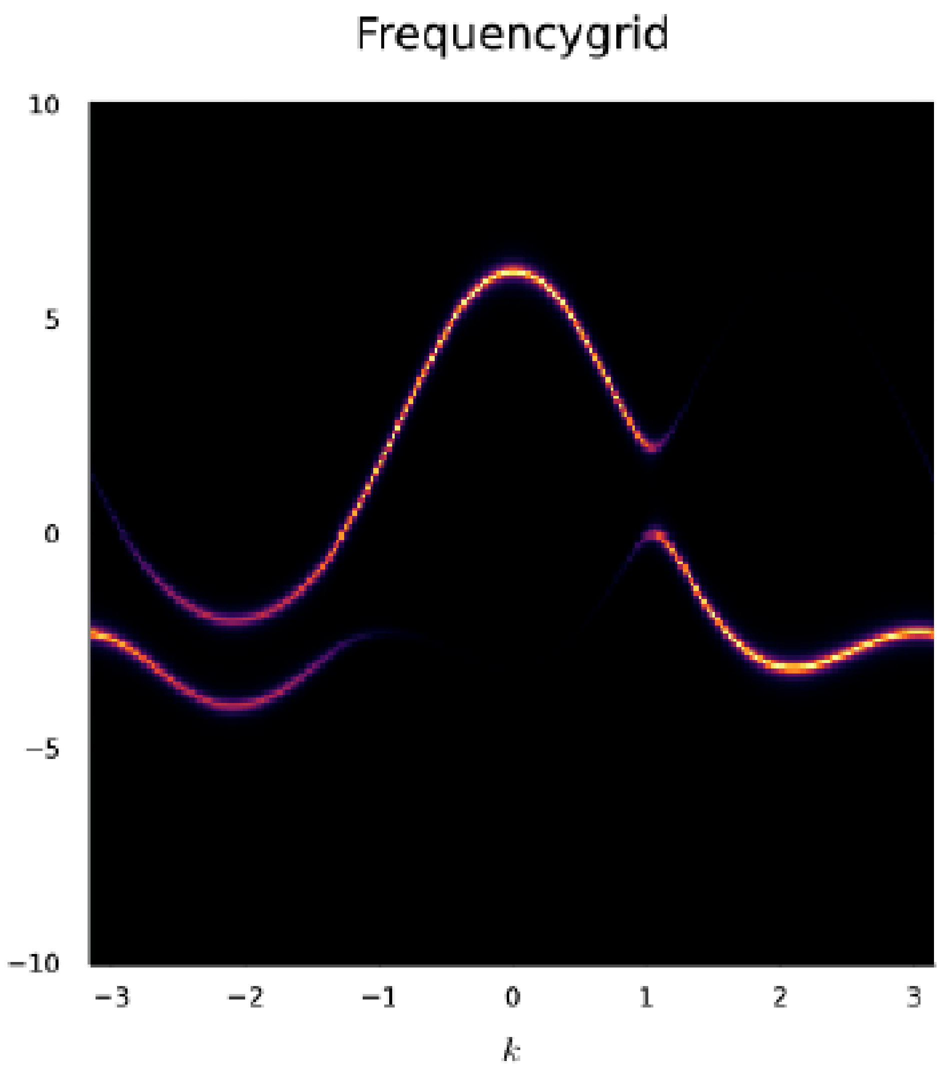
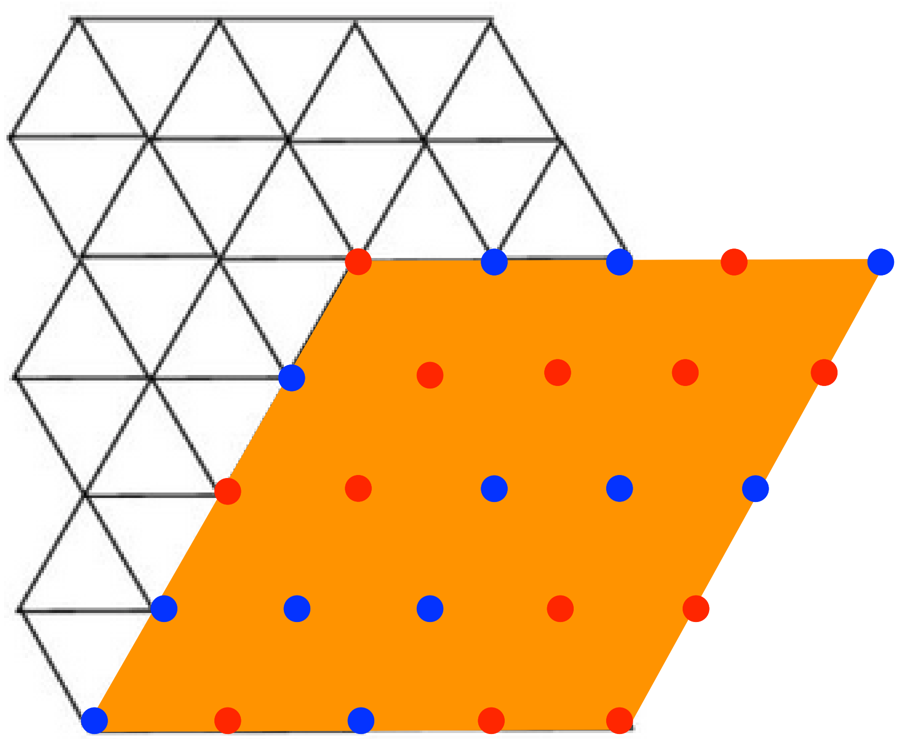
Unfolding of bandstructres





An alloy on triangular lattice

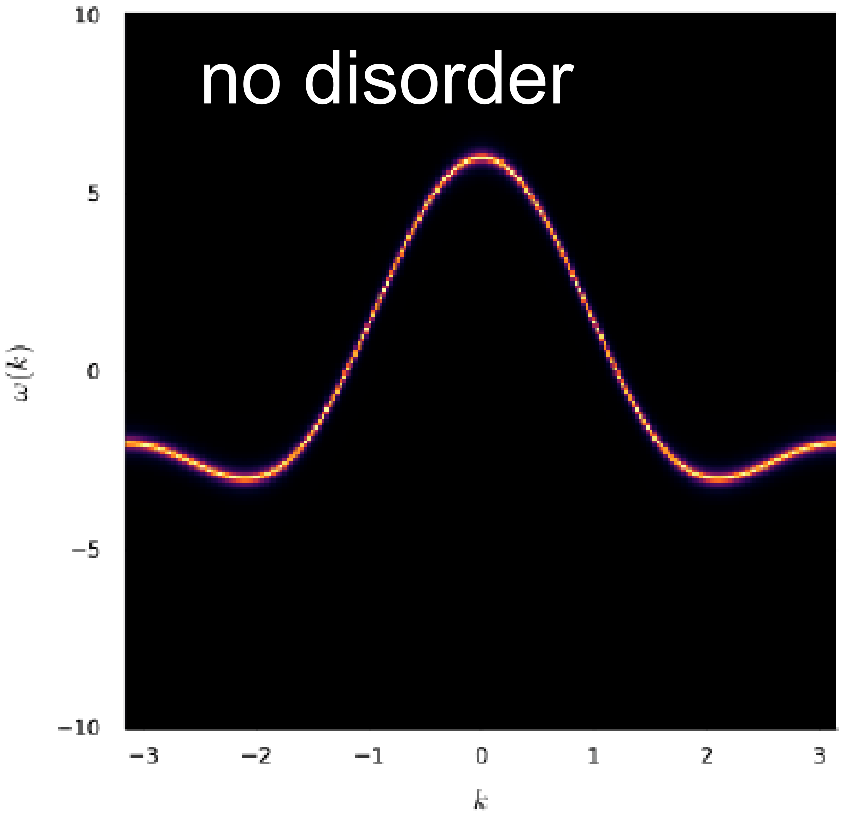
generate random binary potential
in the supercell

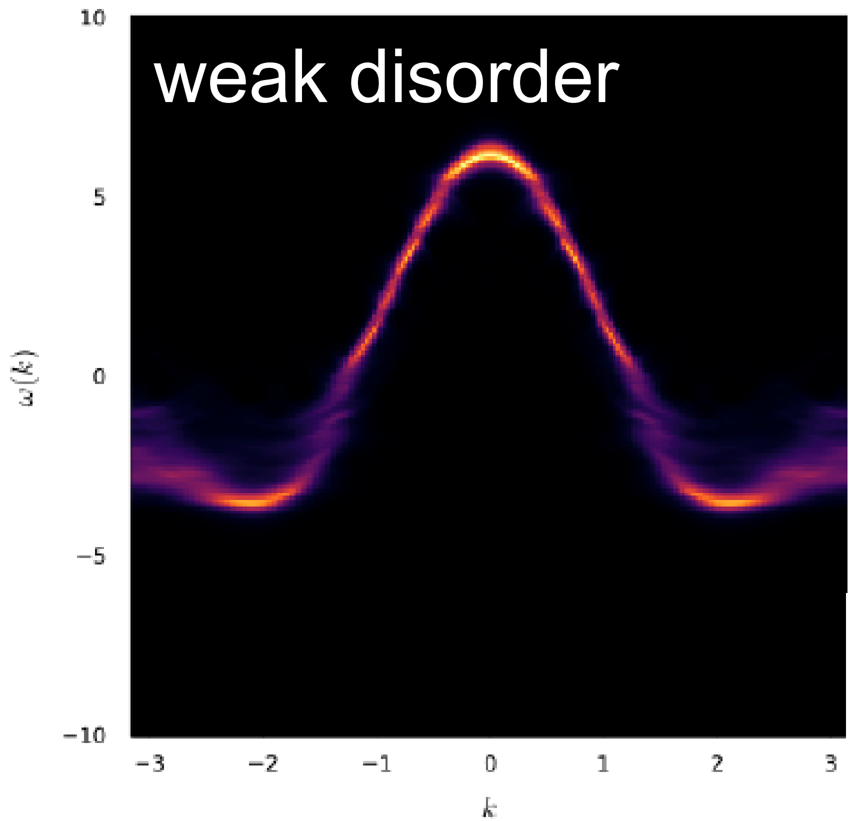


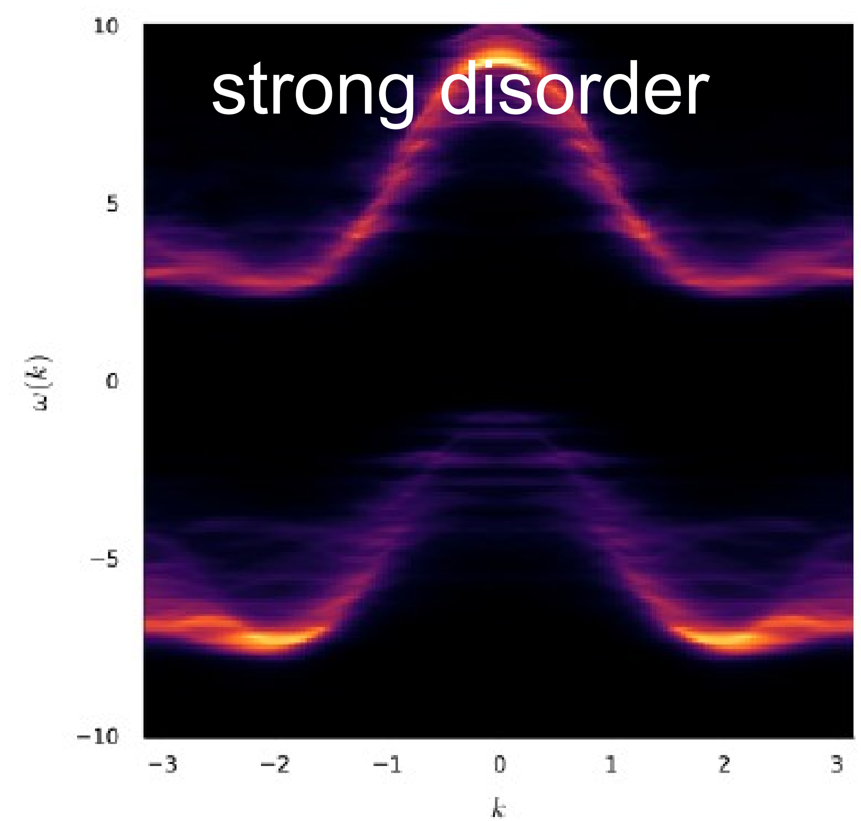
How to average over different realizations of the disorder?

How to get a 'bandstructure' in the elementary (1-atom) unit cell?

Brute force approach - many realizations of disorder







120 deg order on triangular lattice

Calculate the band dispersion and density of states for a triangular lattices with 120 def spin order. Consider non-interacting electrons on triangular lattice (calculate the band dispersion and density of states). Add a local exchange field which has a direction as indicated in the picture.

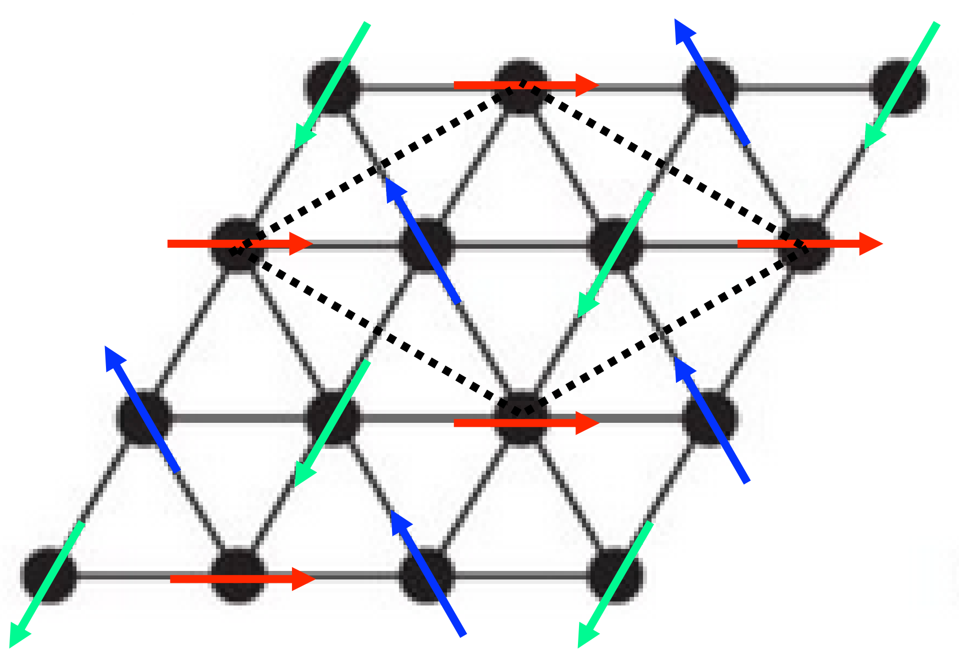
Hint: Use the enlarged unit cell indicated in the figure. Note that the local term depend on the lattice site (sublattice) and mixes the up and down spin directions (i.e. spin is not a good quantum number). Use t=1 and several different values of b (starting from 0).

$$H_0 = t \sum_{\langle ij \rangle} \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix}$$

$$H_i(b) = \begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$$

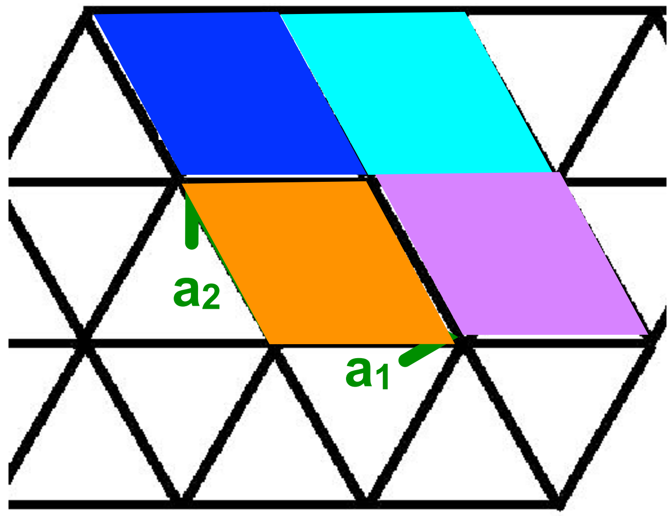
$$\begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} 0 & be^{-i2/3\pi} \\ be^{i2/3\pi} & 0 \end{pmatrix} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$$

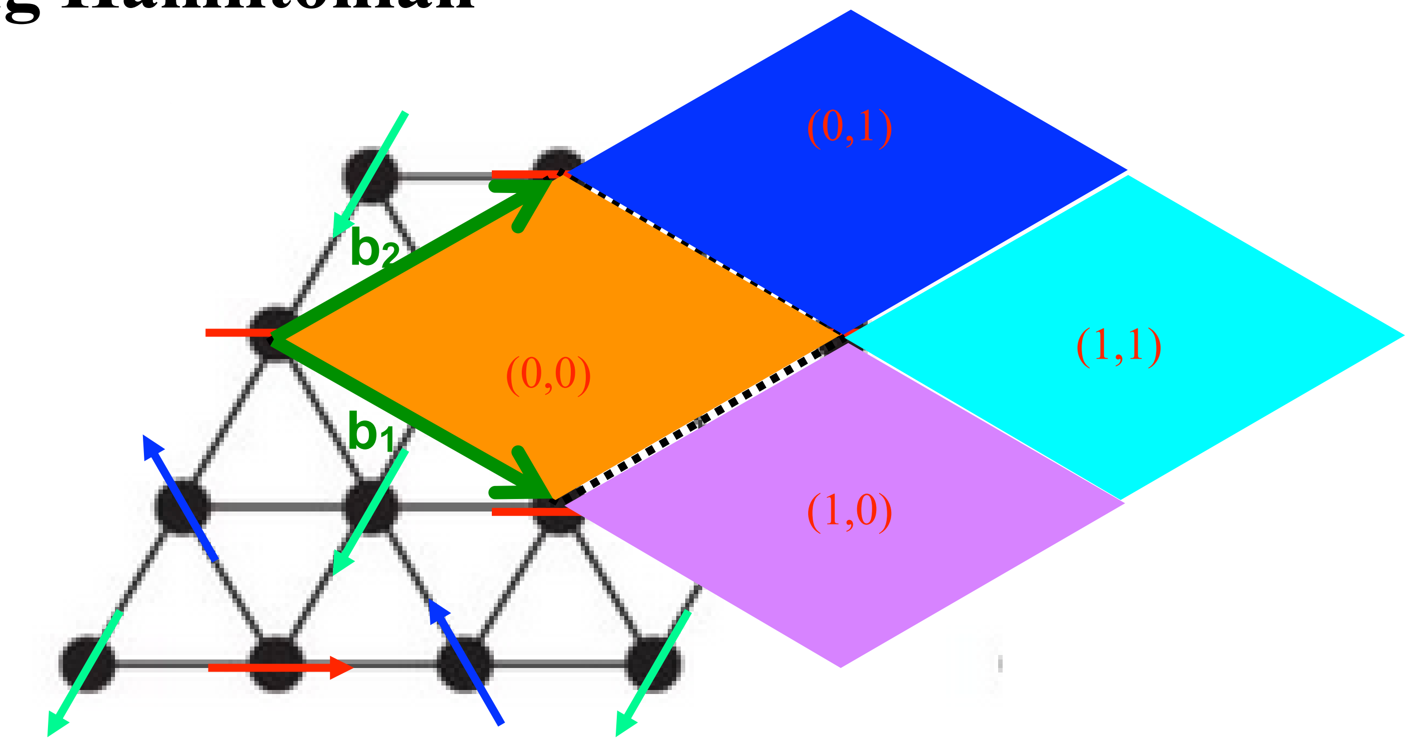
$$\begin{pmatrix} c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} 0 & be^{i2/3\pi} \\ be^{-i2/3\pi} & 0 \end{pmatrix} \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$$



Tight-binding Hamiltonian

$$H = t\sum_{\mathbf{R}}\left(c^\dagger_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$





hopping

$$T_{\mathbf{k}} = \begin{pmatrix} 0 & 1+e^{-ik_1}+e^{-ik_2} & e^{-ik_1}+e^{-ik_2}+e^{-i(k_1+k_2)} \\ 1+e^{ik_1}+e^{ik_2} & 0 & 1+e^{-ik_1}+e^{-ik_2} \\ e^{ik_1}+e^{ik_2}+e^{i(k_1+k_2)} & 1+e^{ik_1}+e^{ik_2} & 0 \end{pmatrix}$$

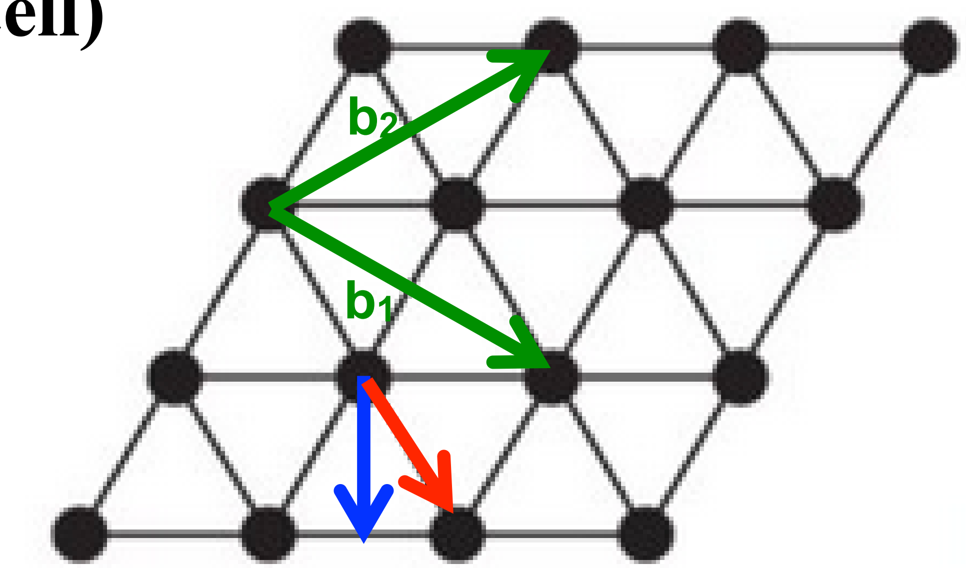
local fields in xy-plane

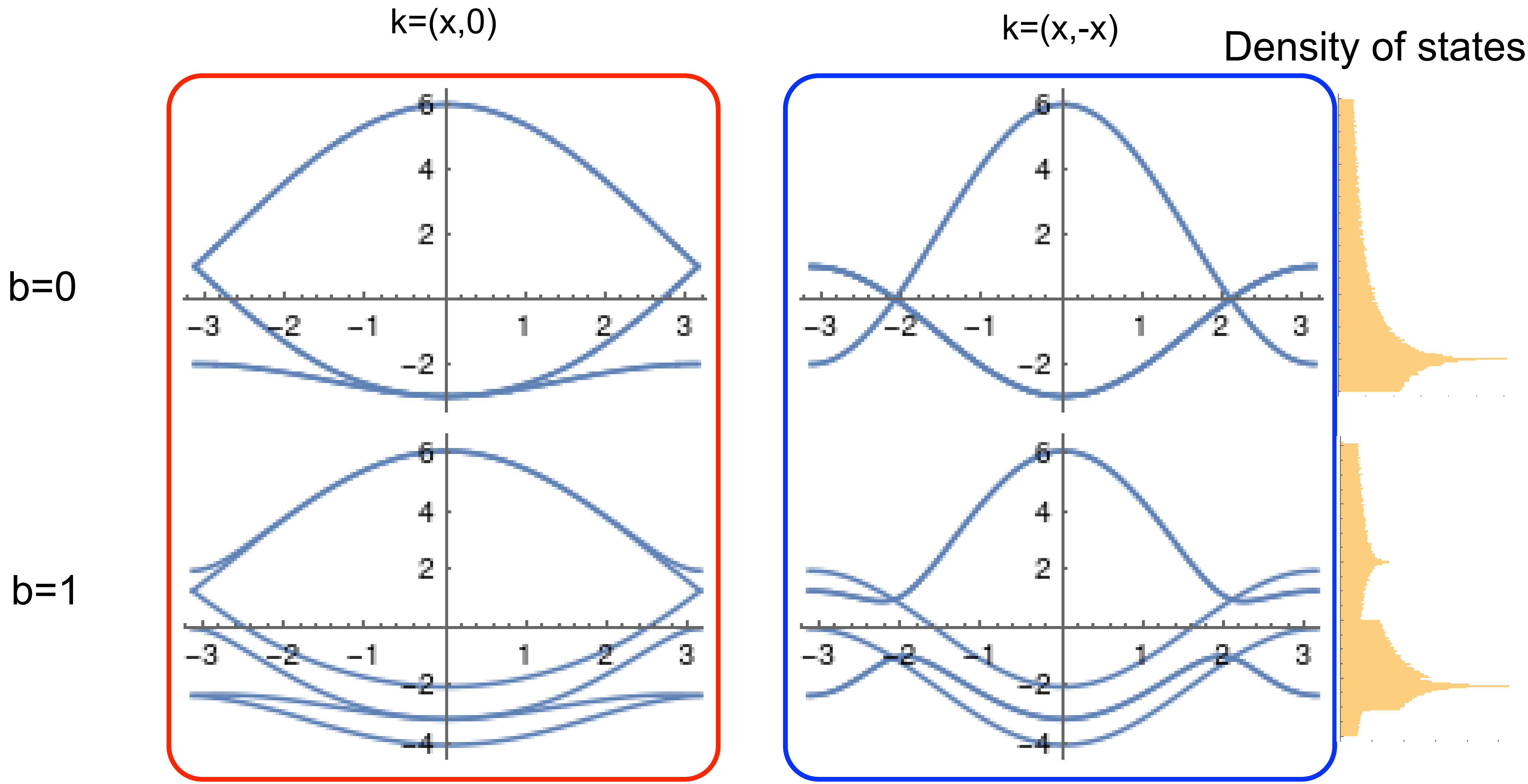
$$X = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \exp(-\frac{2}{3}i\pi) & 0 \\ 0 & 0 & \exp(\frac{2}{3}i\pi) \end{pmatrix}$$

total 6x6 structure

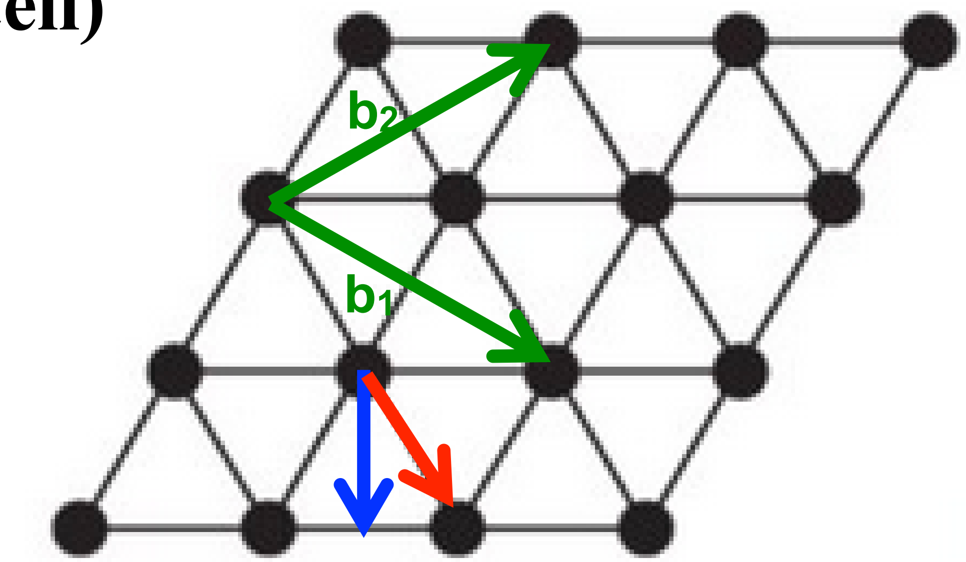
$$H_{\mathbf{k}}(b) = \begin{pmatrix} T_{\mathbf{k}} & bX \\ bX^\dagger & T_{\mathbf{k}} \end{pmatrix}$$

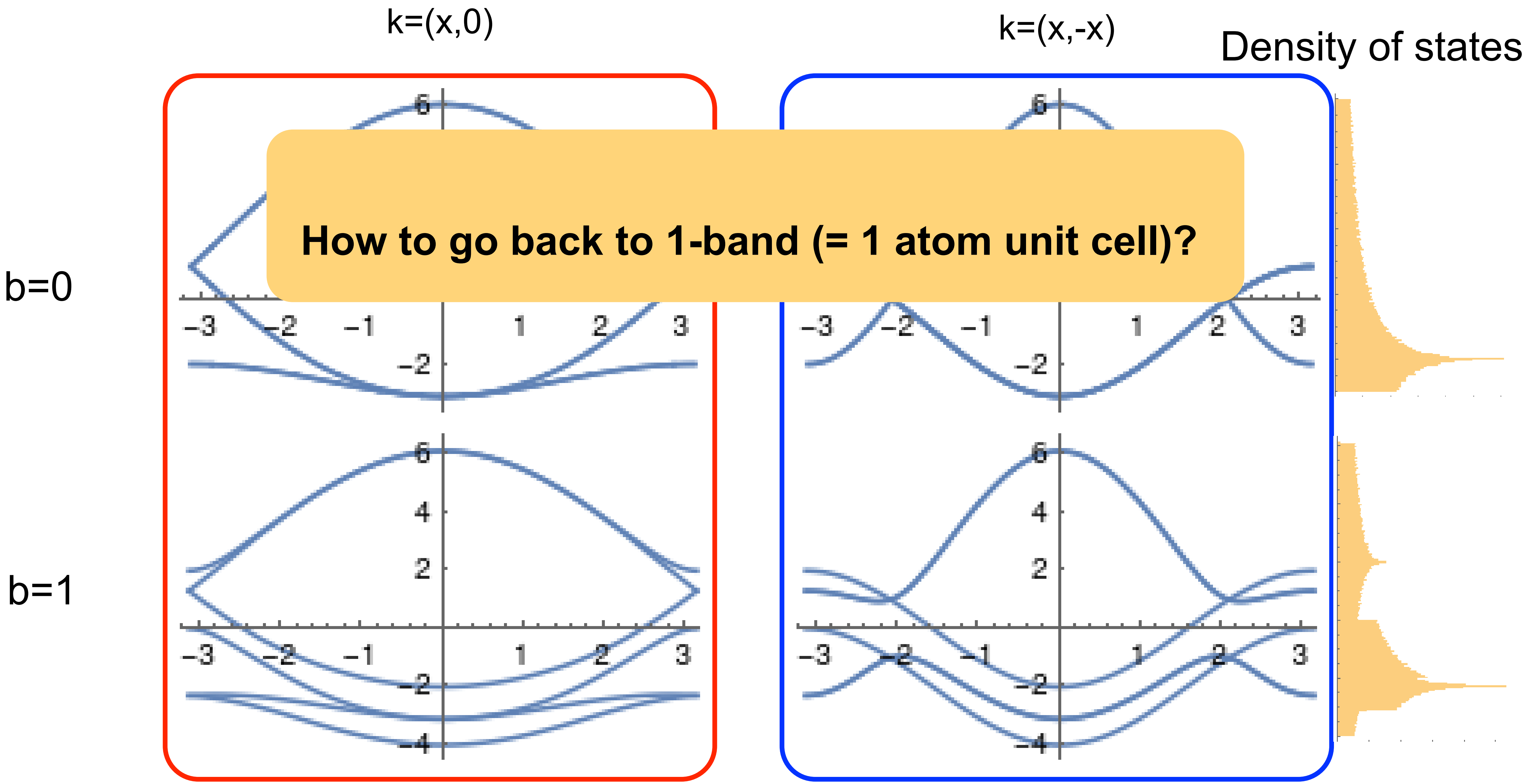
Bandstructure (3-site unit cell)





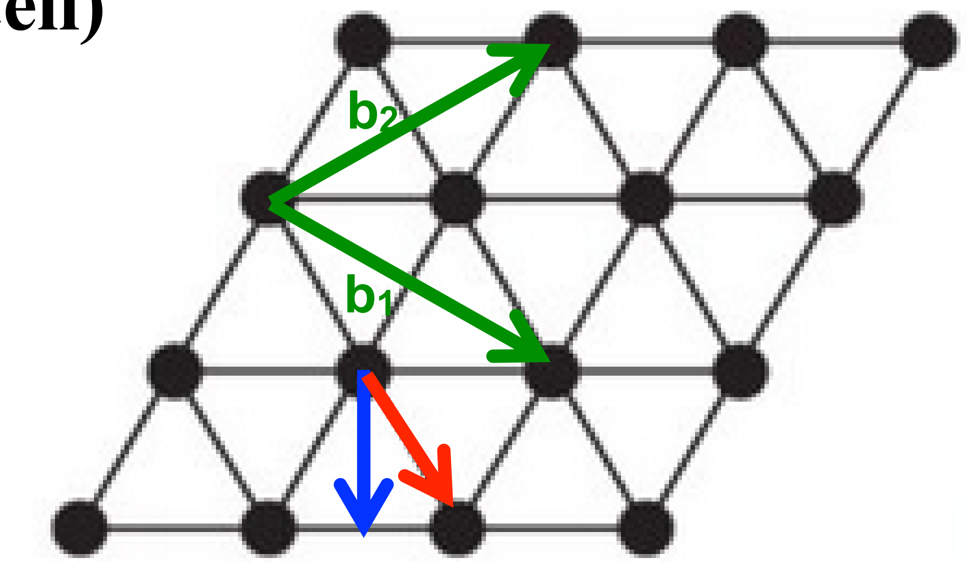
Bandstructure (3-site unit cell)

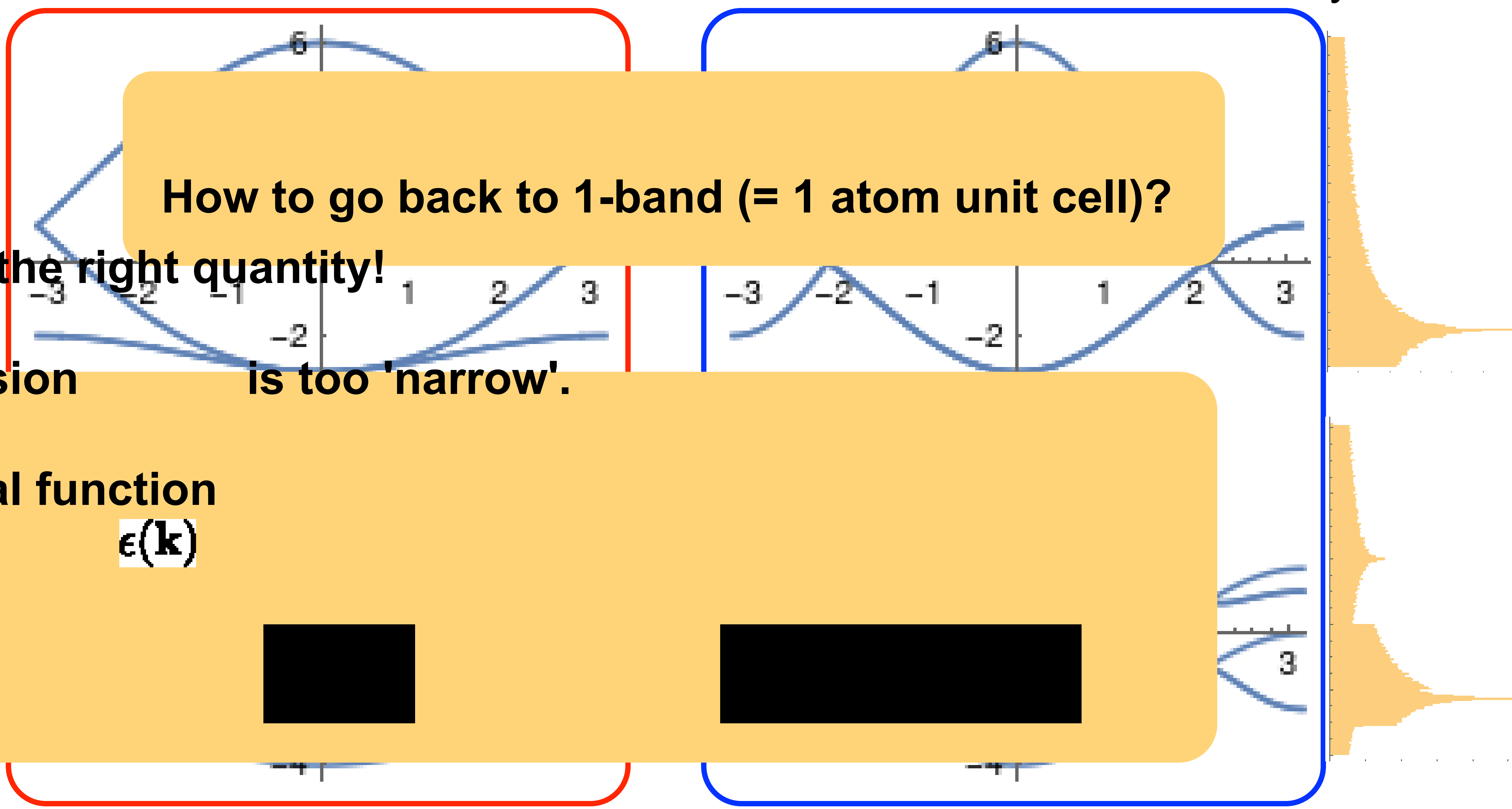




How to go back to 1-band (= 1 atom unit cell)?

Bandstructure (3-site unit cell)





How to go back to 1-band (= 1 atom unit cell)?

Chose the right quantity!

Dispersion is too 'narrow'.

Spectral function

$\epsilon(\mathbf{k})$

[redacted] [redacted]

Spectral function

$$\langle b; a^\dagger\rangle_\omega \equiv A_{ba}(\omega) = \sum_m \langle 0|b|m\rangle\langle m|a^\dagger|0\rangle\delta(\omega - E_m + E_0)$$
$$+ \sum_{m'} \langle 0|a^\dagger|m'\rangle\langle m'|b|0\rangle\delta(\omega + E_{m'} - E_0)$$

many-body (general) formalism

$$= \sum_{n,k} \langle\varphi_b|n,k\rangle\langle n,k|\varphi_a\rangle\delta(\omega - \epsilon_{n,k})$$

non-interacting electrons (1p functions)

$$\langle c_{\mathbf{k}}; c^\dagger_{\mathbf{k}}\rangle_\omega = ?$$

$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{3}}\left(r^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{ik_1} b^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{2ik_1} g^\dagger_{\bar{\mathbf{k}}(\mathbf{k})}\right)$$

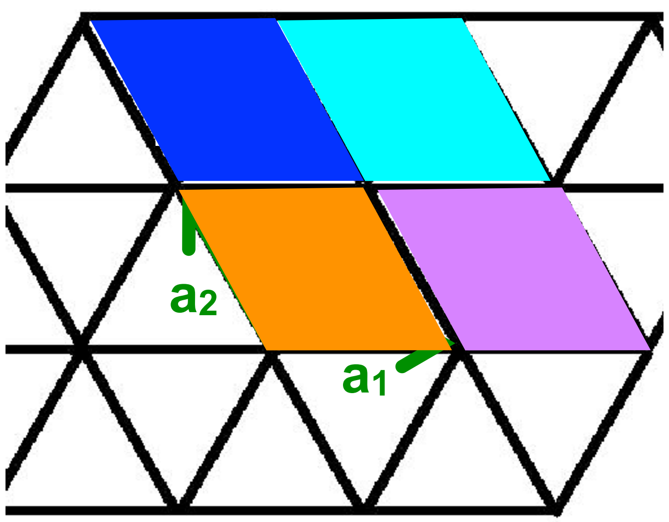
$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

$$\langle c_{\mathbf{k}}; c^\dagger_{\mathbf{k}}\rangle_\omega = \frac{1}{3}\Big(\langle r_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle r_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{2ik_1}\langle r_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+ e^{-ik_1}\langle b_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle b_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle b_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+ e^{-2ik_1}\langle g_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{-ik_1}\langle g_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle g_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega\Big)$$

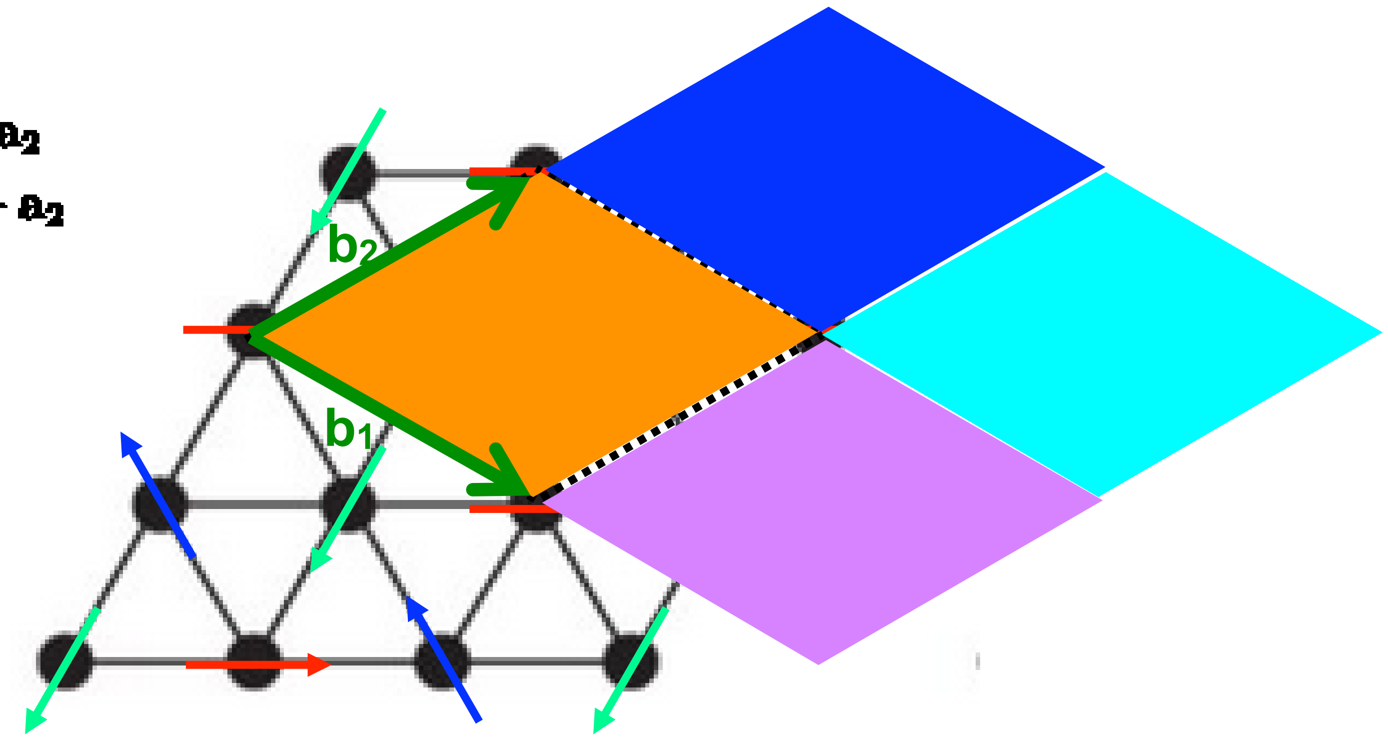
k-diagonal elements of object, which has also off-diagonal (kk') elements

Going between different cells

$$H = t\sum_{\mathbf{R}}\left(c^{\dagger}_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$



$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$



$$\tilde{\mathbf{R}} \equiv \tilde{m}\mathbf{b}_1 + \tilde{n}\mathbf{b}_2$$
$$= (2\tilde{n} + \tilde{m})\mathbf{a}_1 + (\tilde{n} - \tilde{m})\mathbf{a}_2$$

$$\begin{pmatrix} m \\ n \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix}$$

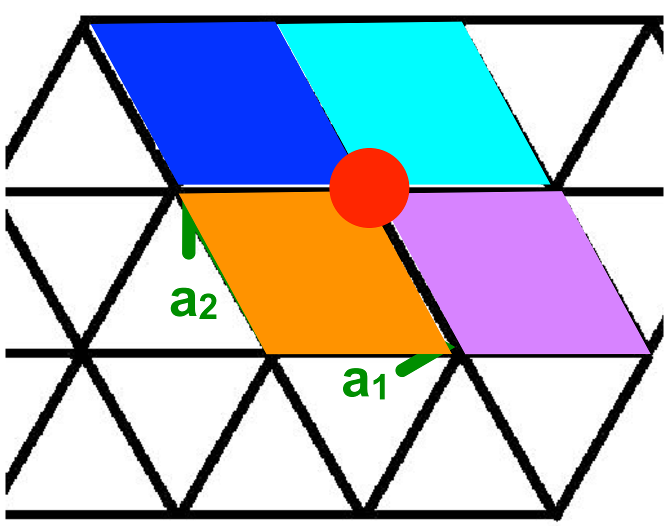
$$\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}$$

$$\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix} = \mathrm{Div}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}, 3\right]$$

$$\mathrm{Flavor} = \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}, 3\right]$$

Going between different cells

$$H = t\sum_{\mathbf{R}}\left(c^{\dagger}_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$



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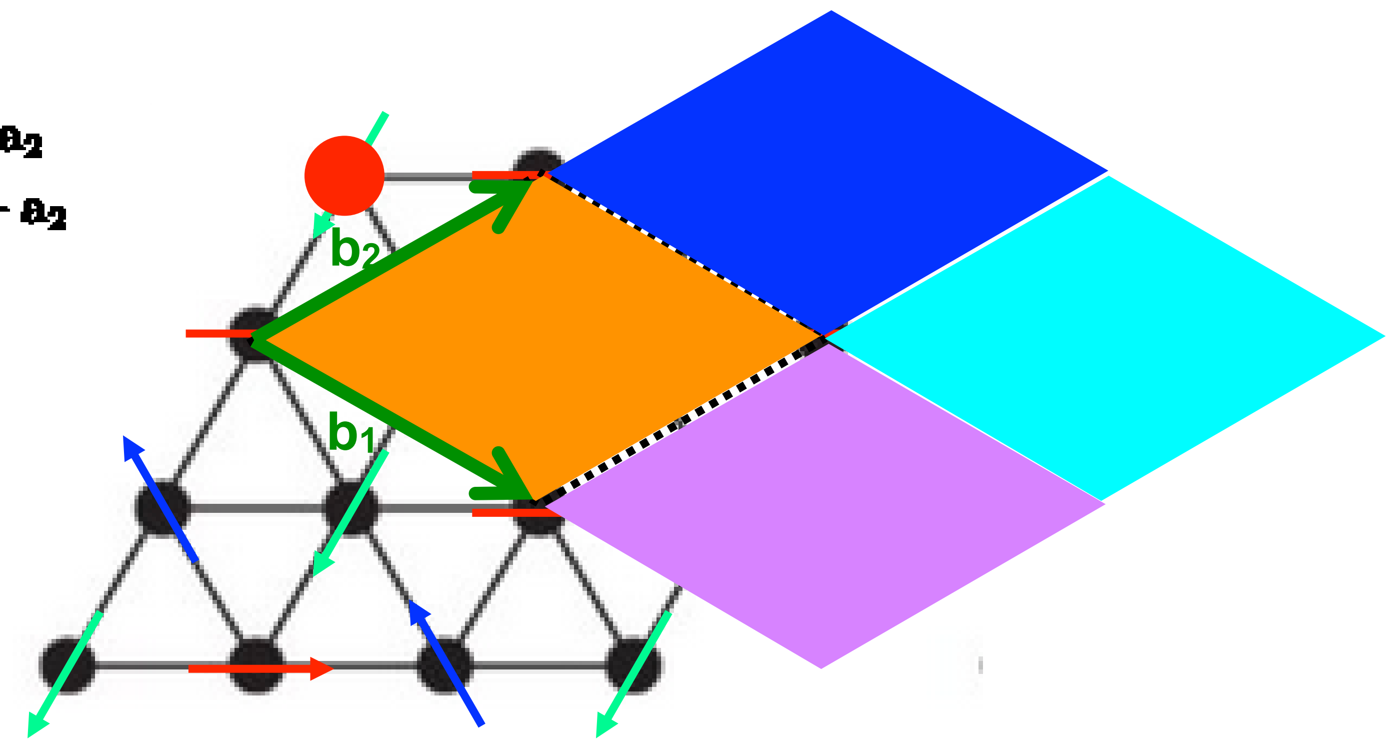

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$$\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}$$

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$$\mathrm{Flavor} = \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}, 3\right] \qquad \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, 3\right] = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \text{ (green)}$$

Going between different cells

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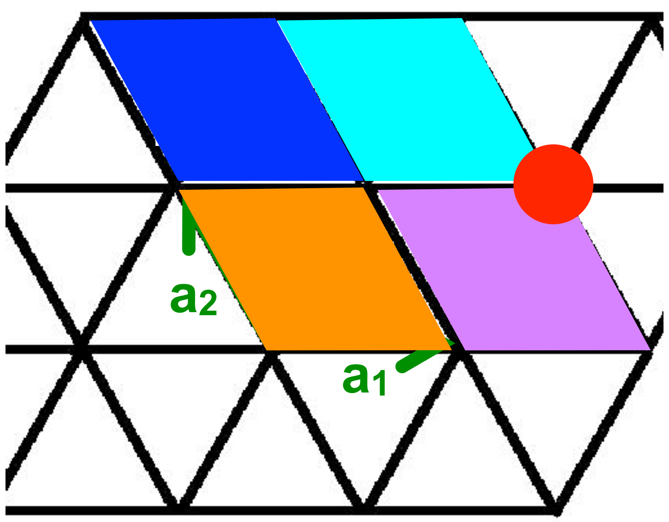

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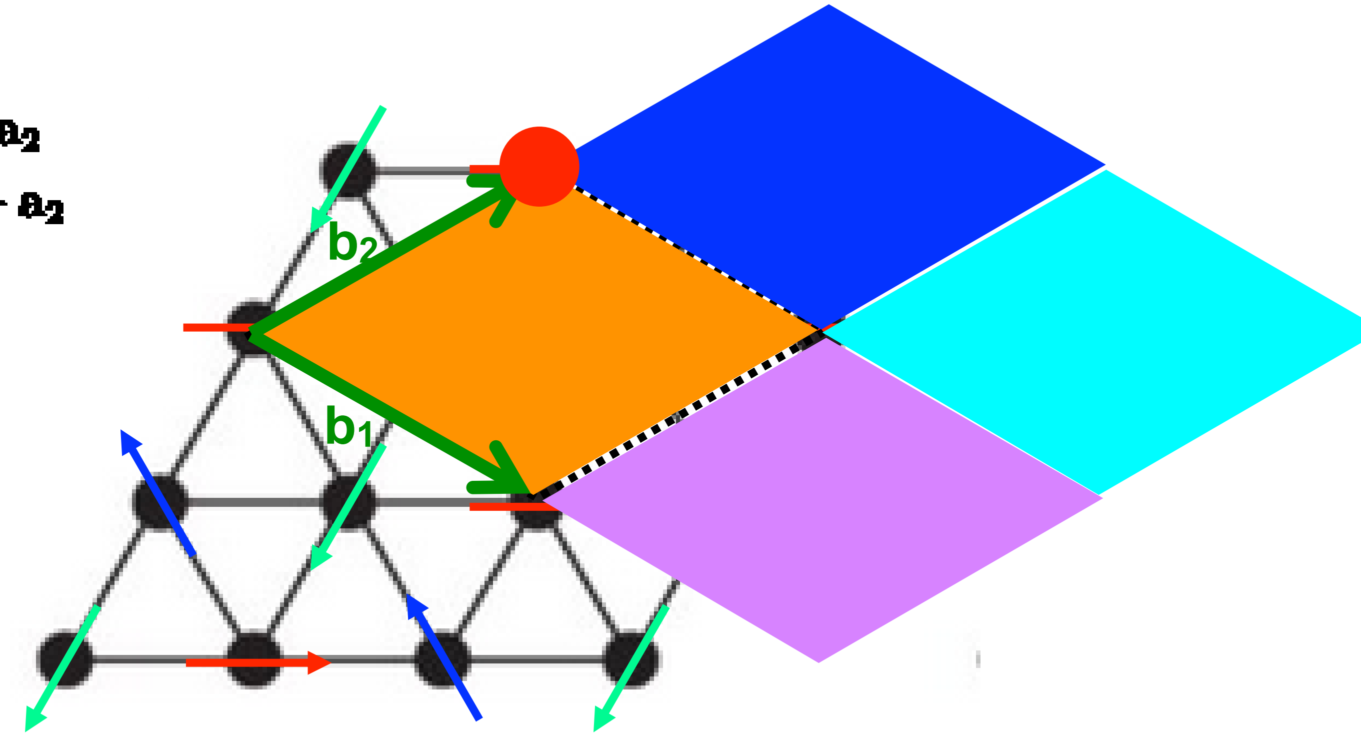

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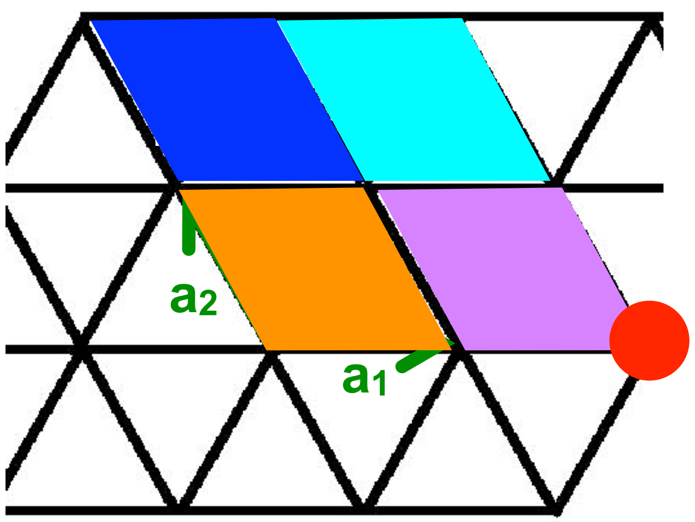
$$\mathrm{Flavor} = \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} m \\ n \end{pmatrix}, 3\right]$$

$$\mathrm{Div}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 2 \\ 1 \end{pmatrix}, 3\right] = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 2 \\ 1 \end{pmatrix}, 3\right] = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ (red)}$$

Going between different cells

$$H = t \sum_{\mathbf{R}} \left(c^\dagger_{\mathbf{R}+(1,0)} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)} c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,1)} c_{\mathbf{R}} + H.c. \right)$$



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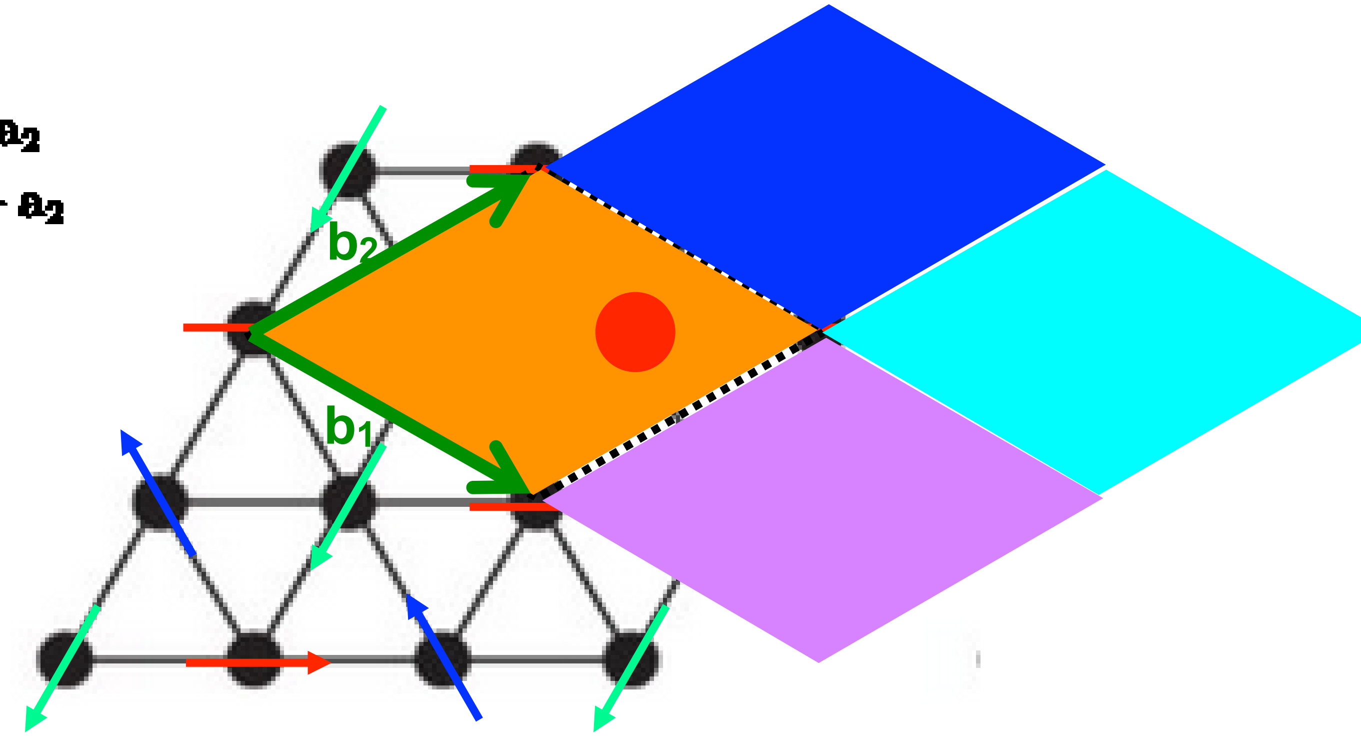

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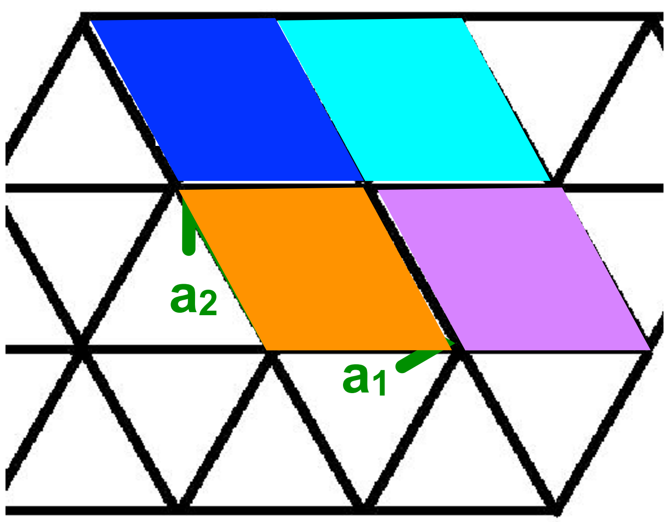
$$\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} m \\ n \end{pmatrix}$$

$$\begin{pmatrix} \tilde{m} \\ \tilde{n} \end{pmatrix} = \mathrm{Div}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} m \\ n \end{pmatrix}, 3 \right] \qquad \mathrm{Div}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \end{pmatrix}, 3 \right] = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\mathrm{Flavor} = \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} m \\ n \end{pmatrix}, 3 \right] \qquad \mathrm{Mod}\left[\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 0 \end{pmatrix}, 3 \right] = \begin{pmatrix} 2 \\ 2 \end{pmatrix} \text{(green)}$$

Going between different cells

$$H = t\sum_{\mathbf{R}}\left(c^\dagger_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$



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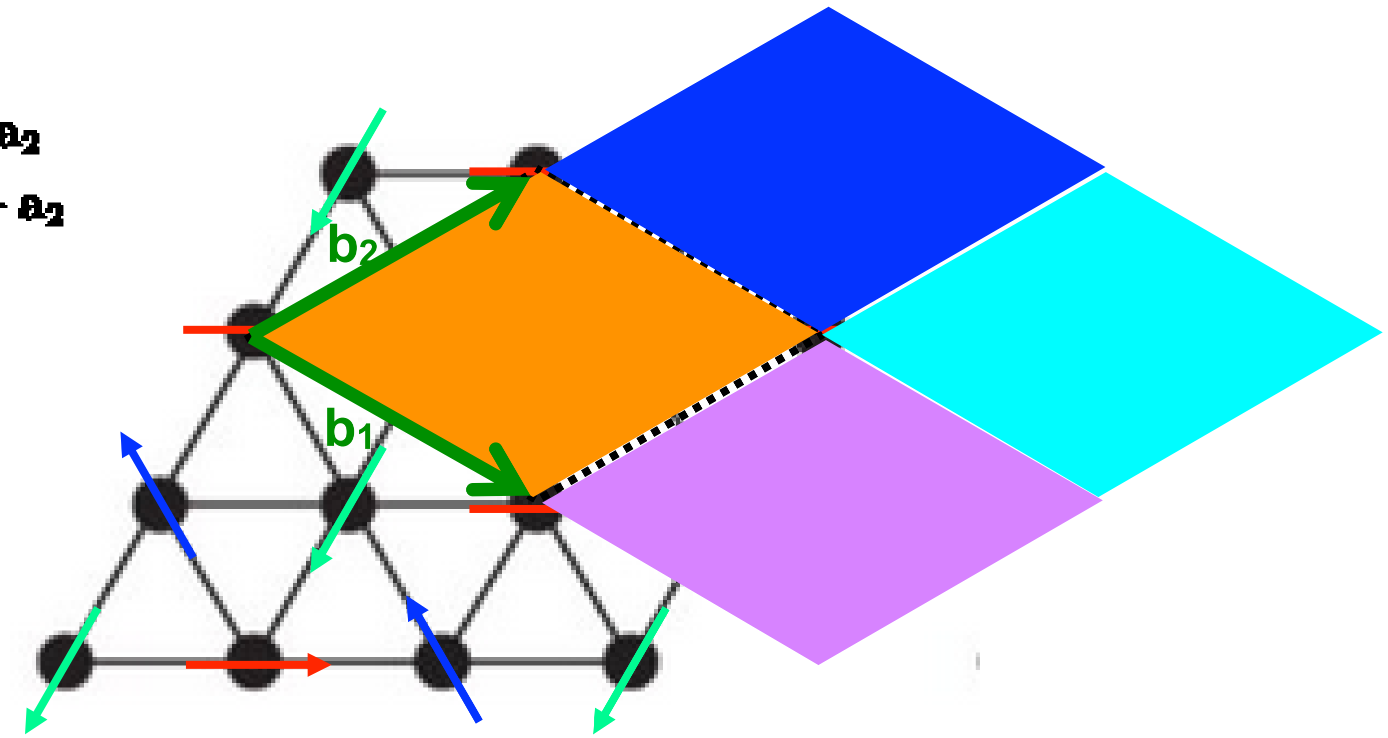


$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{R}}$$

$$c^\dagger_{\mathbf{R}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{k}}$$

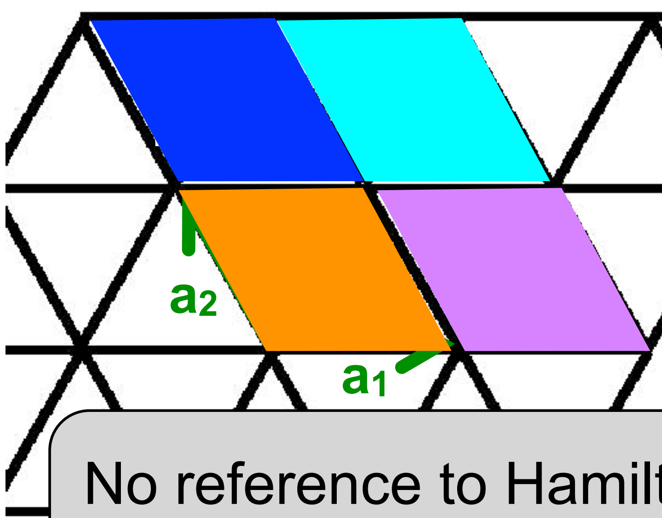
$$r^\dagger_{\bar{\mathbf{k}}} = \sqrt{\frac{3}{N}}\sum_{\bar{\mathbf{R}}} e^{i\bar{\mathbf{k}}\cdot\bar{\mathbf{R}}} r^\dagger_{\bar{\mathbf{R}}}$$

$$r^\dagger_{\bar{\mathbf{R}}} = \sqrt{\frac{3}{N}}\sum_{\bar{\mathbf{k}}} e^{-i\bar{\mathbf{k}}\cdot\bar{\mathbf{R}}} r^\dagger_{\bar{\mathbf{k}}}$$

$$\sum_{\mathbf{R}} f(\mathbf{R})c^\dagger_{\mathbf{R}} = \sum_{\bar{\mathbf{R}}}\left(f[\mathbf{R}(\bar{\mathbf{R}})]r^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\bar{\mathbf{R}}) + \mathbf{a}_1]b^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\bar{\mathbf{R}}) + 2\mathbf{a}_1]g^\dagger_{\bar{\mathbf{R}}}\right)$$

Going between different cells

$$H = t\sum_{\mathbf{R}}\left(c^\dagger_{\mathbf{R}+(1,0)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(0,1)}c_{\mathbf{R}} + c^\dagger_{\mathbf{R}+(1,1)}c_{\mathbf{R}} + H.c.\right)$$



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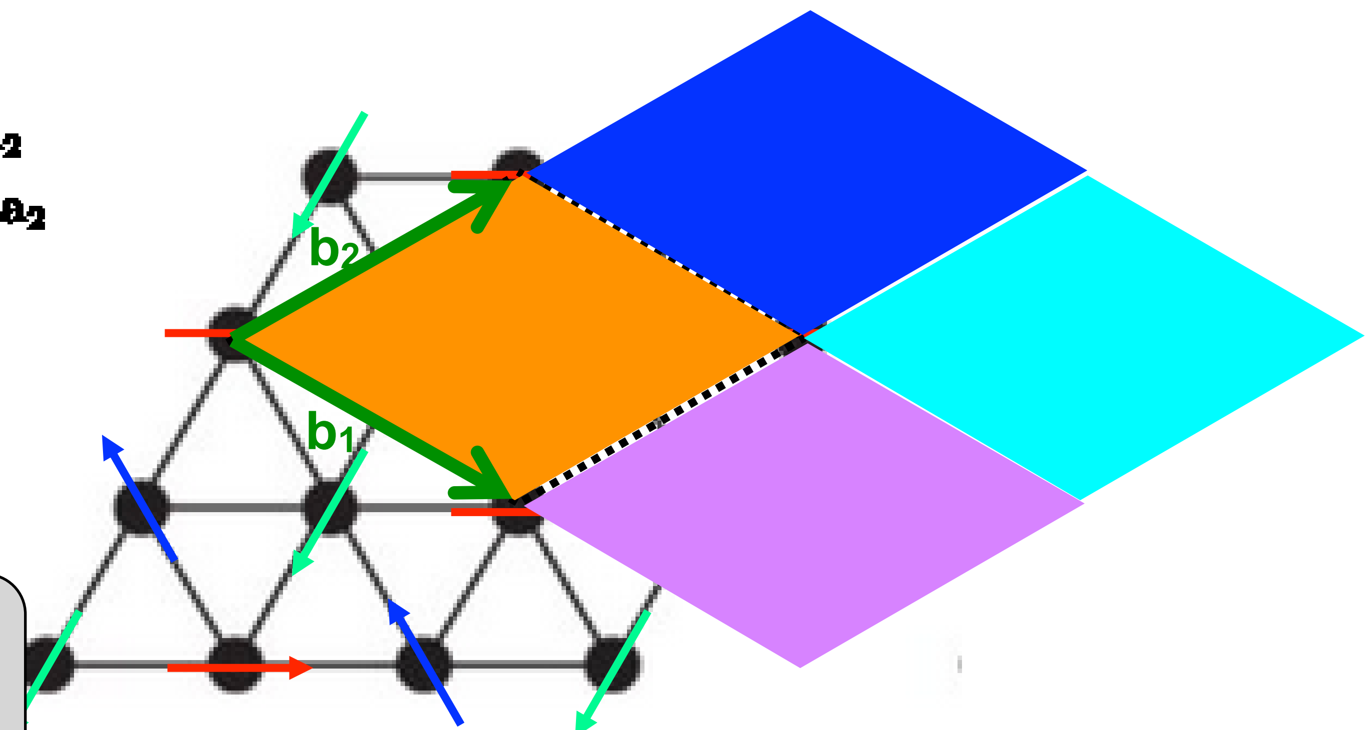


No reference to Hamiltonian
(lattice dimension) needed in principle

$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{R}}$$

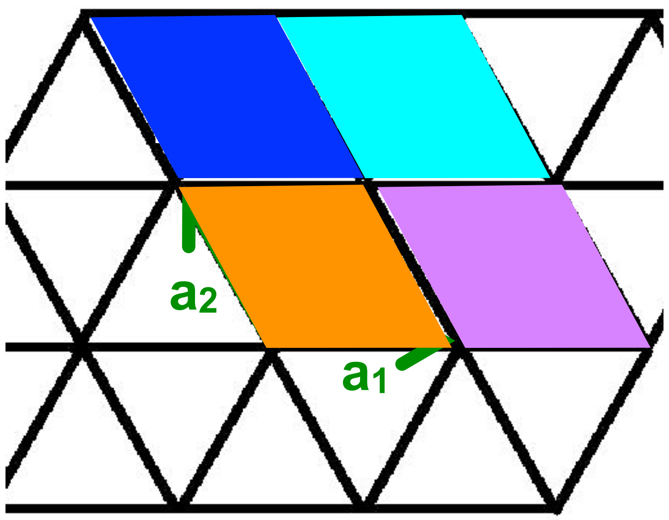
$$c^\dagger_{\mathbf{R}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{k}}$$

$$r^\dagger_{\bar{\mathbf{k}}} = \sqrt{\frac{3}{N}}\sum_{\bar{\mathbf{R}}} e^{i\bar{\mathbf{k}}\cdot\bar{\mathbf{R}}} r^\dagger_{\bar{\mathbf{R}}}$$

$$r^\dagger_{\bar{\mathbf{R}}} = \sqrt{\frac{3}{N}}\sum_{\bar{\mathbf{k}}} e^{-i\bar{\mathbf{k}}\cdot\bar{\mathbf{R}}} r^\dagger_{\bar{\mathbf{k}}}$$

$$\sum_{\mathbf{R}} f(\mathbf{R})c^\dagger_{\mathbf{R}} = \sum_{\bar{\mathbf{R}}}\left(f[\mathbf{R}(\bar{\mathbf{R}})]r^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\bar{\mathbf{R}}) + \mathbf{a}_1]b^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\bar{\mathbf{R}}) + 2\mathbf{a}_1]g^\dagger_{\bar{\mathbf{R}}}\right)$$

Going between different cells



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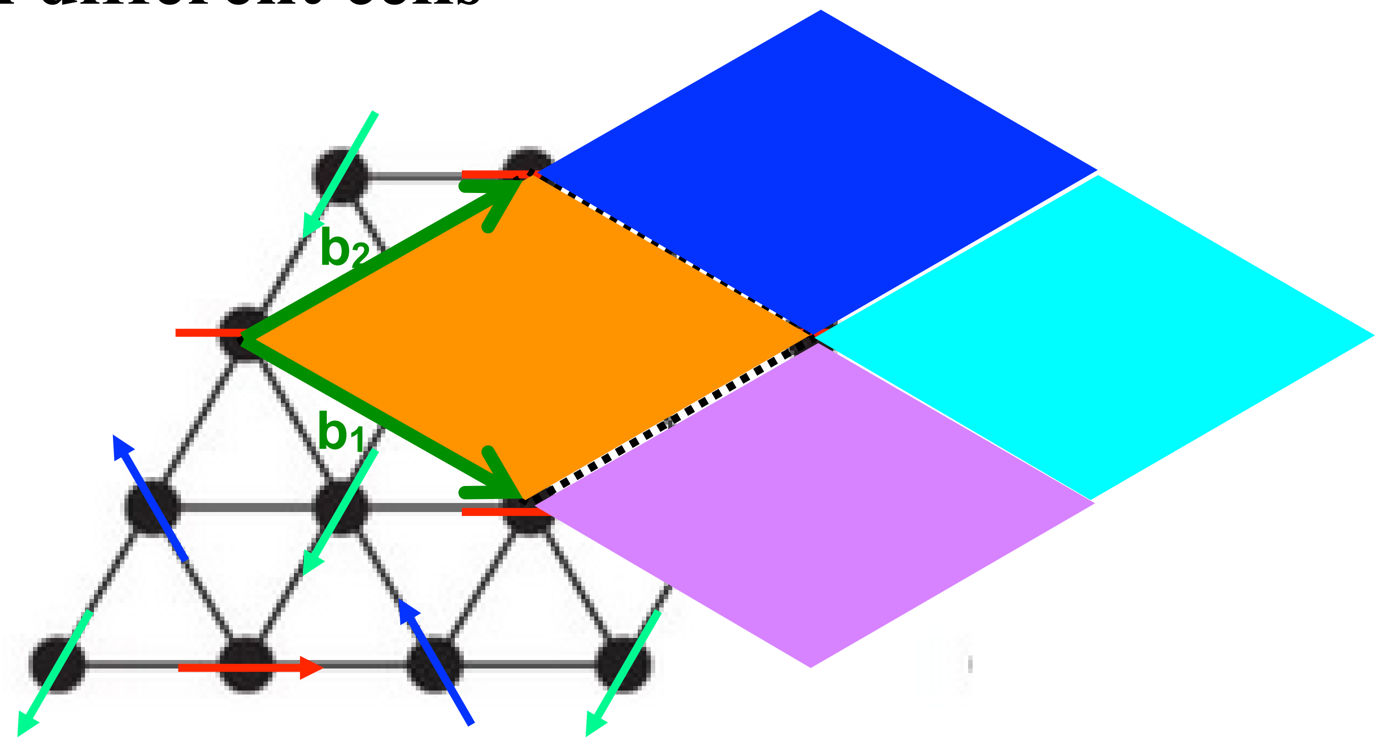


$$c_{\mathbf{k}}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{R}}^{\dagger}$$
$$c_{\mathbf{R}}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{k}}^{\dagger}$$

$$r_{\tilde{\mathbf{k}}}^{\dagger} = \sqrt{\frac{3}{N}} \sum_{\tilde{\mathbf{R}}} e^{i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{R}}} r_{\tilde{\mathbf{R}}}^{\dagger}$$
$$r_{\tilde{\mathbf{R}}}^{\dagger} = \sqrt{\frac{3}{N}} \sum_{\tilde{\mathbf{k}}} e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{R}}} r_{\tilde{\mathbf{k}}}^{\dagger}$$

$$\sum_{\mathbf{R}} f(\mathbf{R}) c_{\mathbf{R}}^{\dagger} = \sum_{\tilde{\mathbf{R}}} \left(f[\mathbf{R}(\tilde{\mathbf{R}})] r_{\tilde{\mathbf{R}}}^{\dagger} + f[\mathbf{R}(\tilde{\mathbf{R}}) + \mathbf{a}_1] b_{\tilde{\mathbf{R}}}^{\dagger} + f[\mathbf{R}(\tilde{\mathbf{R}}) + 2\mathbf{a}_1] g_{\tilde{\mathbf{R}}}^{\dagger} \right)$$

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{R}}^{\dagger} = \sum_{\tilde{\mathbf{R}}} e^{i\mathbf{k}\cdot\mathbf{R}(\tilde{\mathbf{R}})} \left(r_{\tilde{\mathbf{R}}}^{\dagger} + e^{i\mathbf{k}\cdot\mathbf{a}_1} b_{\tilde{\mathbf{R}}}^{\dagger} + e^{2i\mathbf{k}\cdot\mathbf{a}_1} g_{\tilde{\mathbf{R}}}^{\dagger} \right)$$

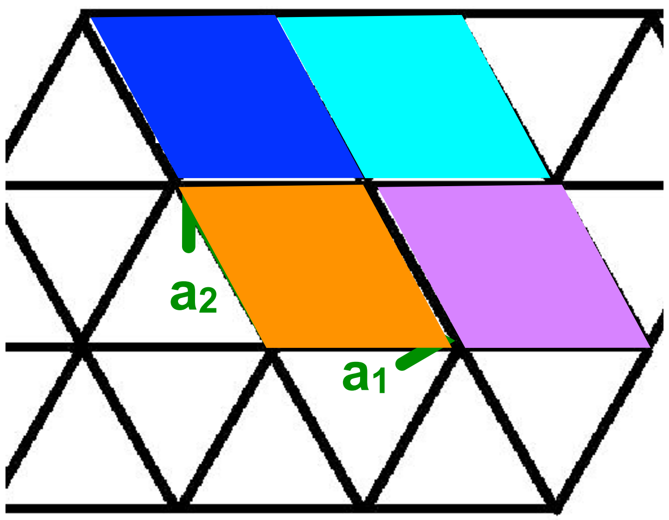
$$\tilde{\mathbf{R}} \equiv m\mathbf{b}_1 + n\mathbf{b}_2$$
$$= (2n+m)\mathbf{a}_1 + (n-m)\mathbf{a}_2 \equiv \mathbf{R}(\tilde{\mathbf{R}})$$

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{R}}^{\dagger} = \sum_{\tilde{\mathbf{R}}} e^{i\tilde{\mathbf{k}}(\mathbf{k})\cdot\tilde{\mathbf{R}}} \left(r_{\tilde{\mathbf{R}}}^{\dagger} + e^{ik_1} b_{\tilde{\mathbf{R}}}^{\dagger} + e^{2ik_1} g_{\tilde{\mathbf{R}}}^{\dagger} \right)$$

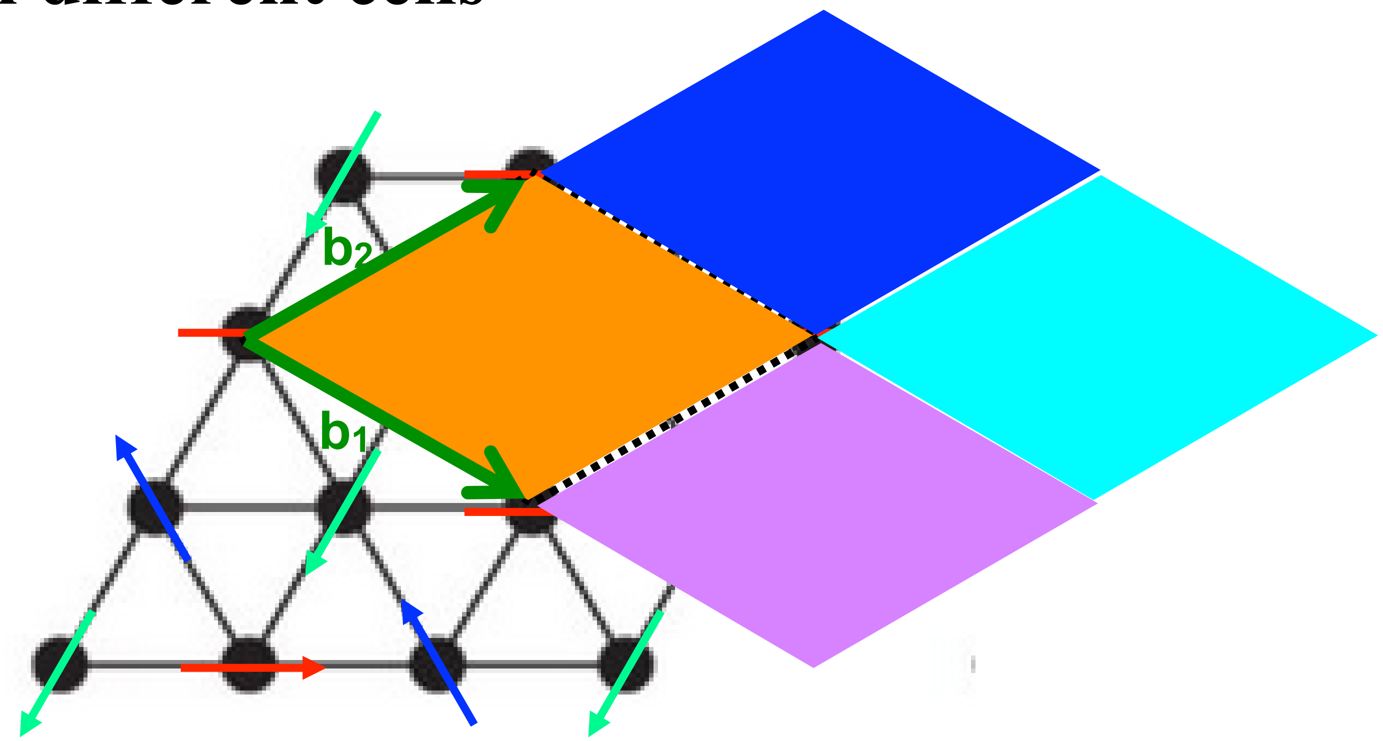
$$\tilde{k}_1 = k_1 - k_2$$
$$\tilde{k}_2 = 2k_1 + k_2$$

$$\mathbf{k}\cdot\mathbf{R}(\tilde{\mathbf{R}}) \equiv (2n+m)k_1 + (n-m)k_2$$
$$= m(k_1 - k_2) + n(2k_1 + k_2) \equiv m\tilde{k}_1 + n\tilde{k}_2$$

Going between different cells



$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$



$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{R}}$$
$$c^\dagger_{\mathbf{R}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{k}}$$

$$r^\dagger_{\bar{\mathbf{k}}} = \sqrt{\frac{3}{N}} \sum_{\bar{\mathbf{R}}} e^{i\bar{\mathbf{k}}\cdot\bar{\mathbf{R}}} r^\dagger_{\bar{\mathbf{R}}}$$

Strictly speaking we are working with covariant and contravariant tensors: $k^\alpha R_\alpha$

$$\sum_{\mathbf{R}} f(\mathbf{R}) c^\dagger_{\mathbf{R}} = \sum_{\bar{\mathbf{R}}} \left(f[\mathbf{R}(\bar{\mathbf{R}})] r^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\mathbf{R}) + \mathbf{a}_1] b^\dagger_{\bar{\mathbf{R}}} + f[\mathbf{R}(\mathbf{R}) + 2\mathbf{a}_1] g^\dagger_{\bar{\mathbf{R}}} \right)$$

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{R}} = \sum_{\bar{\mathbf{R}}} e^{i\mathbf{k}\cdot\mathbf{R}(\bar{\mathbf{R}})} \left(r^\dagger_{\bar{\mathbf{R}}} + e^{i\mathbf{k}\cdot\mathbf{a}_1} b^\dagger_{\bar{\mathbf{R}}} + e^{2i\mathbf{k}\cdot\mathbf{a}_1} g^\dagger_{\bar{\mathbf{R}}} \right)$$

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c^\dagger_{\mathbf{R}} = \sum_{\bar{\mathbf{R}}} e^{i\bar{\mathbf{k}}(\mathbf{k})\cdot\bar{\mathbf{R}}} \left(r^\dagger_{\bar{\mathbf{R}}} + e^{ik_1} b^\dagger_{\bar{\mathbf{R}}} + e^{2ik_1} g^\dagger_{\bar{\mathbf{R}}} \right)$$

$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{3}} \left(r^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{ik_1} b^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{2ik_1} g^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} \right)$$

$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

$$\bar{\mathbf{R}} \equiv m\mathbf{b}_1 + n\mathbf{b}_2 = (2n+m)\mathbf{a}_1 + (n-m)\mathbf{a}_2 \equiv \mathbf{R}(\bar{\mathbf{R}})$$

$$\mathbf{k}\cdot\mathbf{R}(\bar{\mathbf{R}}) \equiv (2n+m)k_1 + (n-m)k_2 = m(k_1 - k_2) + n(2k_1 + k_2) \equiv m\bar{k}_1 + n\bar{k}_2$$

Spectral function

$$\langle b; a^\dagger\rangle_\omega \equiv A_{ba}(\omega) = \sum_m \langle 0|b|m\rangle\langle m|a^\dagger|0\rangle\delta(\omega - E_m + E_0)$$
$$+ \sum_{m'} \langle 0|a^\dagger|m'\rangle\langle m'|b|0\rangle\delta(\omega + E_{m'} - E_0)$$

many-body (general) formalism

$$= \sum_{n,k} \langle \varphi_b|n,k\rangle\langle n,k|\varphi_a\rangle\delta(\omega - \epsilon_{n,k})$$

non-interacting electrons (1p functions)

$$\langle c_{\mathbf{k}}; c_{\mathbf{k}}^\dagger\rangle_\omega = ?$$

$$c_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{3}}\left(r^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{ik_1} b^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{2ik_1} g^\dagger_{\bar{\mathbf{k}}(\mathbf{k})}\right)$$

$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

$$\langle c_{\mathbf{k}}; c_{\mathbf{k}}^\dagger\rangle_\omega = \frac{1}{3}\Big(\langle r_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle r_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{2ik_1}\langle r_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+e^{-ik_1}\langle b_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle b_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle b_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+e^{-2ik_1}\langle g_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{-ik_1}\langle g_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle g_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega\Big)$$

k-diagonal elements of object, which has also off-diagonal (kk') elements

Spectral function

$$\langle b; a^\dagger\rangle_\omega \equiv A_{ba}(\omega) = \sum_m \langle 0|b|m\rangle\langle m|a^\dagger|0\rangle\delta(\omega - E_m + E_0)$$
$$+ \sum_{m'} \langle 0|a^\dagger|m'\rangle\langle m'|b|0\rangle\delta(\omega + E_{m'} - E_0)$$
$$= \sum_{n,k} \langle \varphi_b|n,k\rangle\langle n,k|\varphi_a\rangle\delta(\omega - \epsilon_{n,k})$$

many-body (general) formalism

non-interacting electrons (1p functions)

$$\langle c_{\mathbf{k}}; c^\dagger_{\mathbf{k}}\rangle_\omega = ?$$

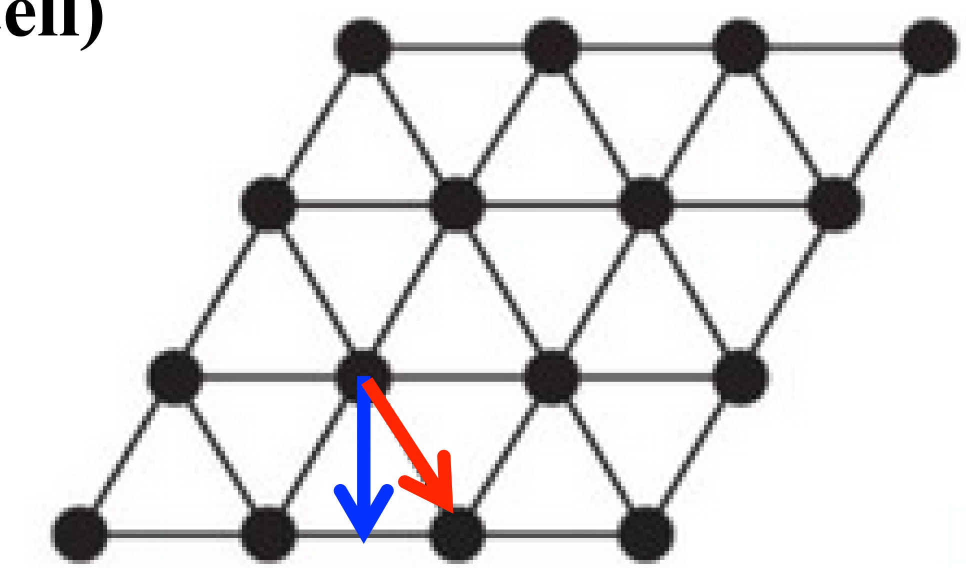
$$c^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{3}}\left(r^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{ik_1} b^\dagger_{\bar{\mathbf{k}}(\mathbf{k})} + e^{2ik_1} g^\dagger_{\bar{\mathbf{k}}(\mathbf{k})}\right)$$

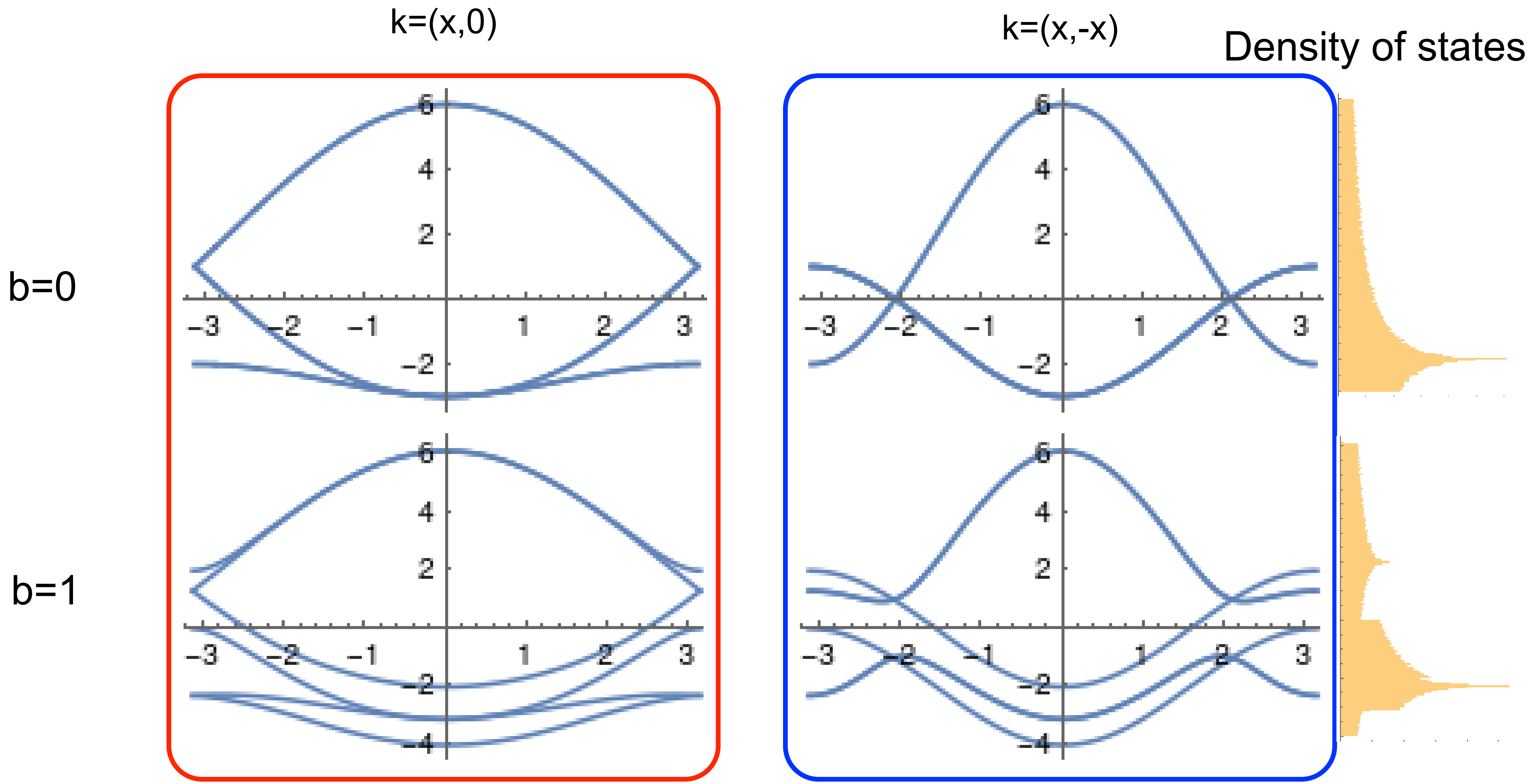
$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

$$\langle c_{\mathbf{k}}; c^\dagger_{\mathbf{k}}\rangle_\omega = \frac{1}{3}\Big(\langle r_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle r_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{2ik_1}\langle r_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+ e^{-ik_1}\langle b_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle b_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{ik_1}\langle b_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega$$
$$+ e^{-2ik_1}\langle g_{\bar{\mathbf{k}}}; r^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + e^{-ik_1}\langle g_{\bar{\mathbf{k}}}; b^\dagger_{\bar{\mathbf{k}}}\rangle_\omega + \langle g_{\bar{\mathbf{k}}}; g^\dagger_{\bar{\mathbf{k}}}\rangle_\omega\Big)$$

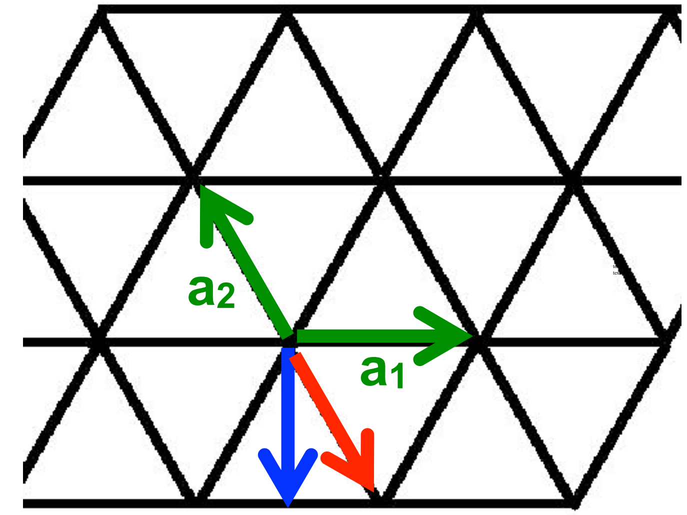
k-diagonal elements of object, which has also off-diagonal (kk') elements

Bandstructure (3-site unit cell)





Bandstructure (1-site unit cell)



b=0

[redacted]

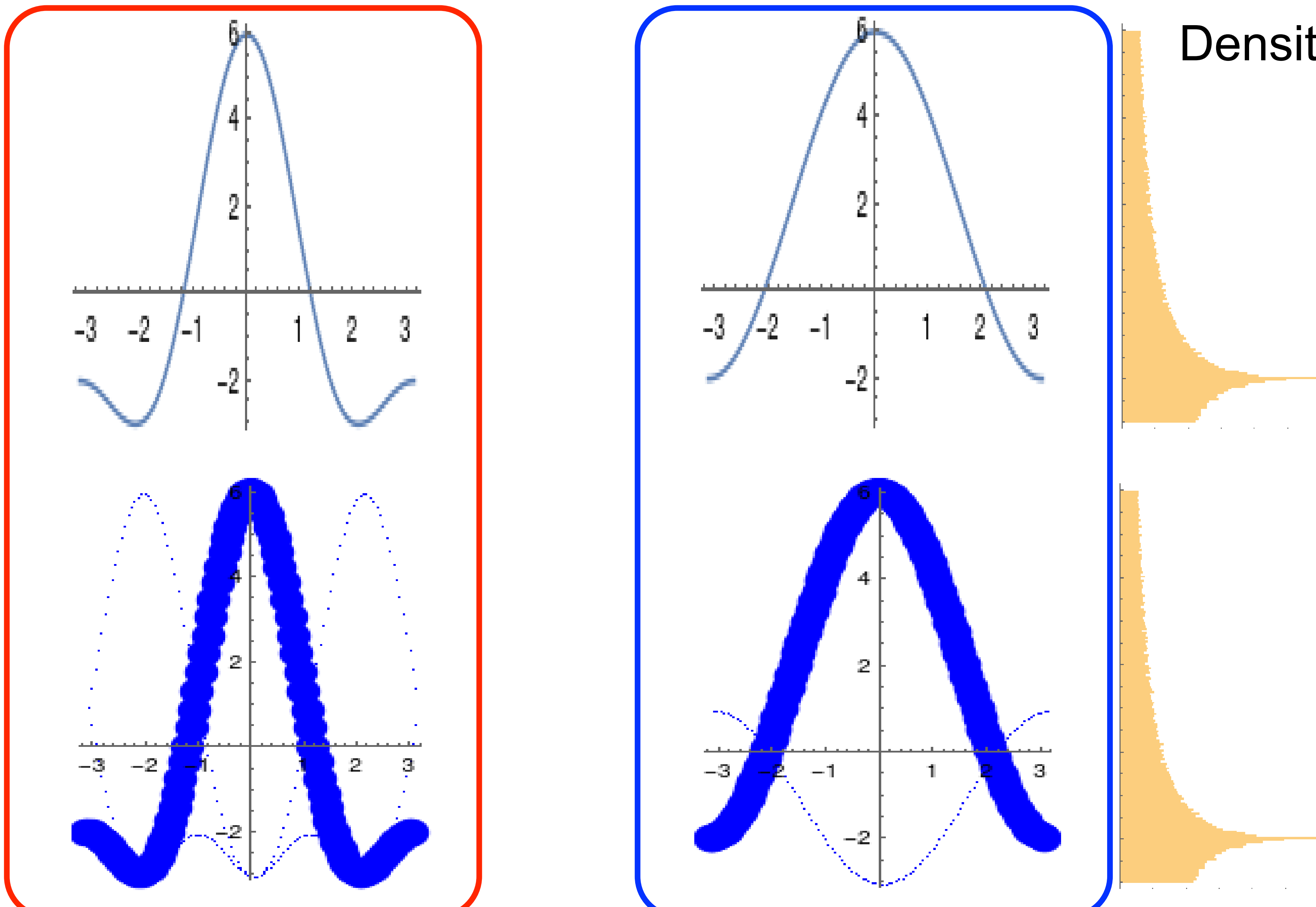
k=(x,x)

k=(x,0)

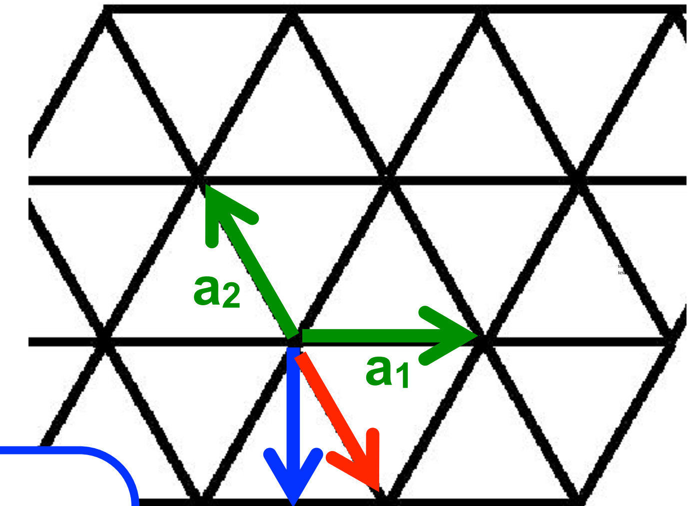
Density of states

1-site cell

3-site cell
unfolded



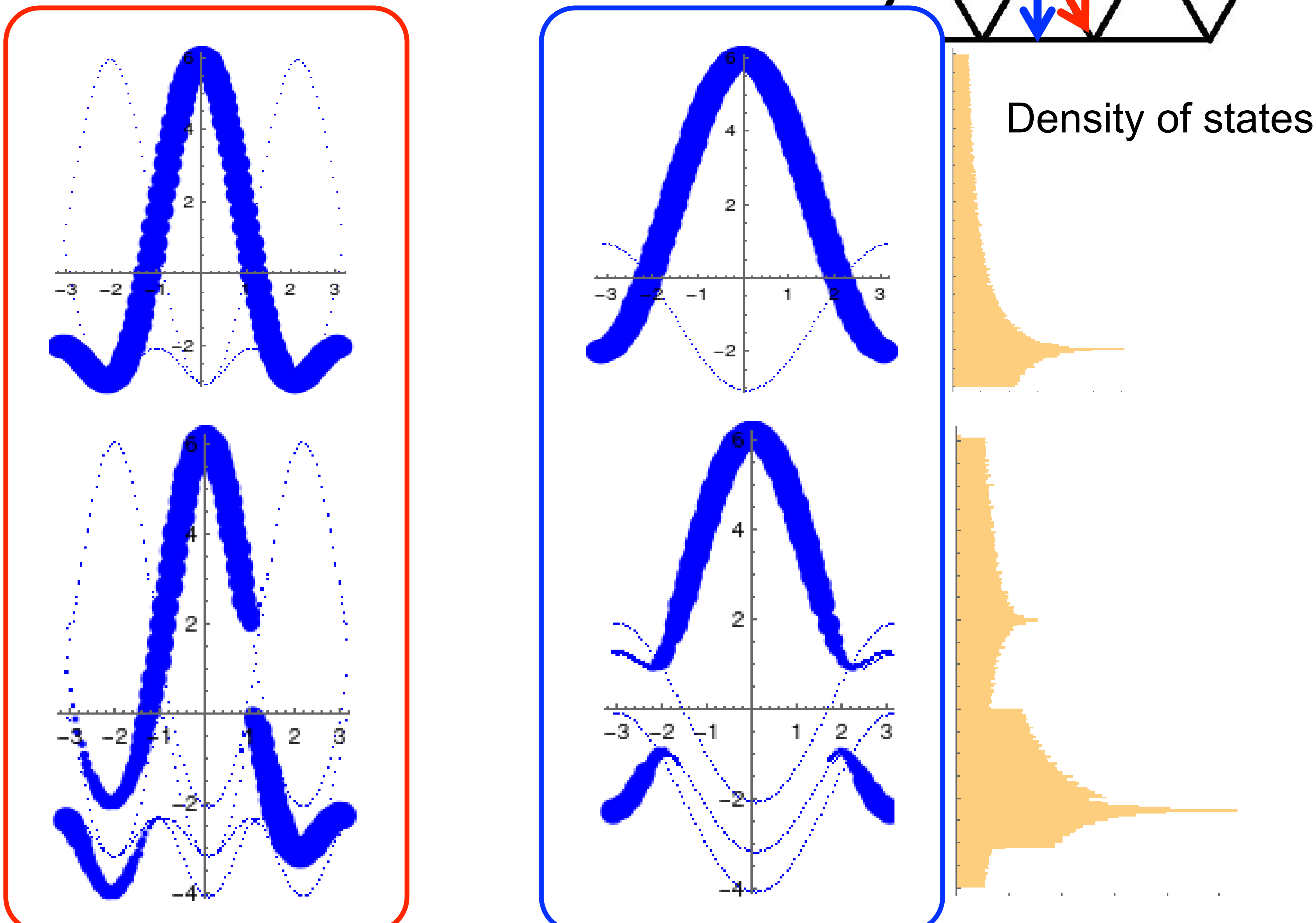
Bandstructure (1-site unit cell)



[redacted]

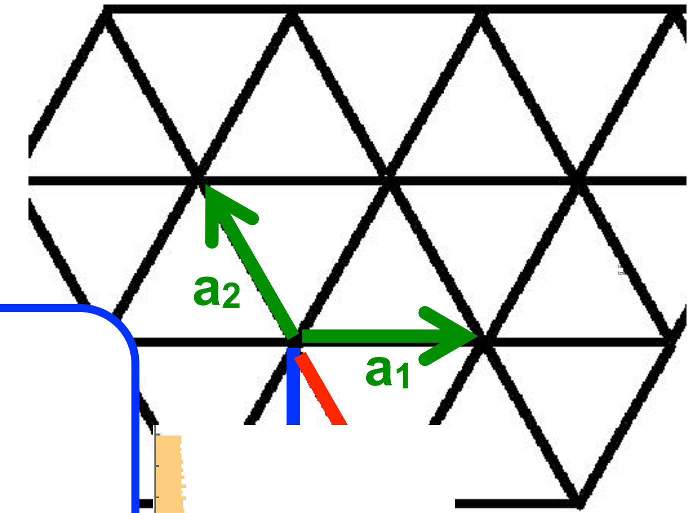
b=0

b=1



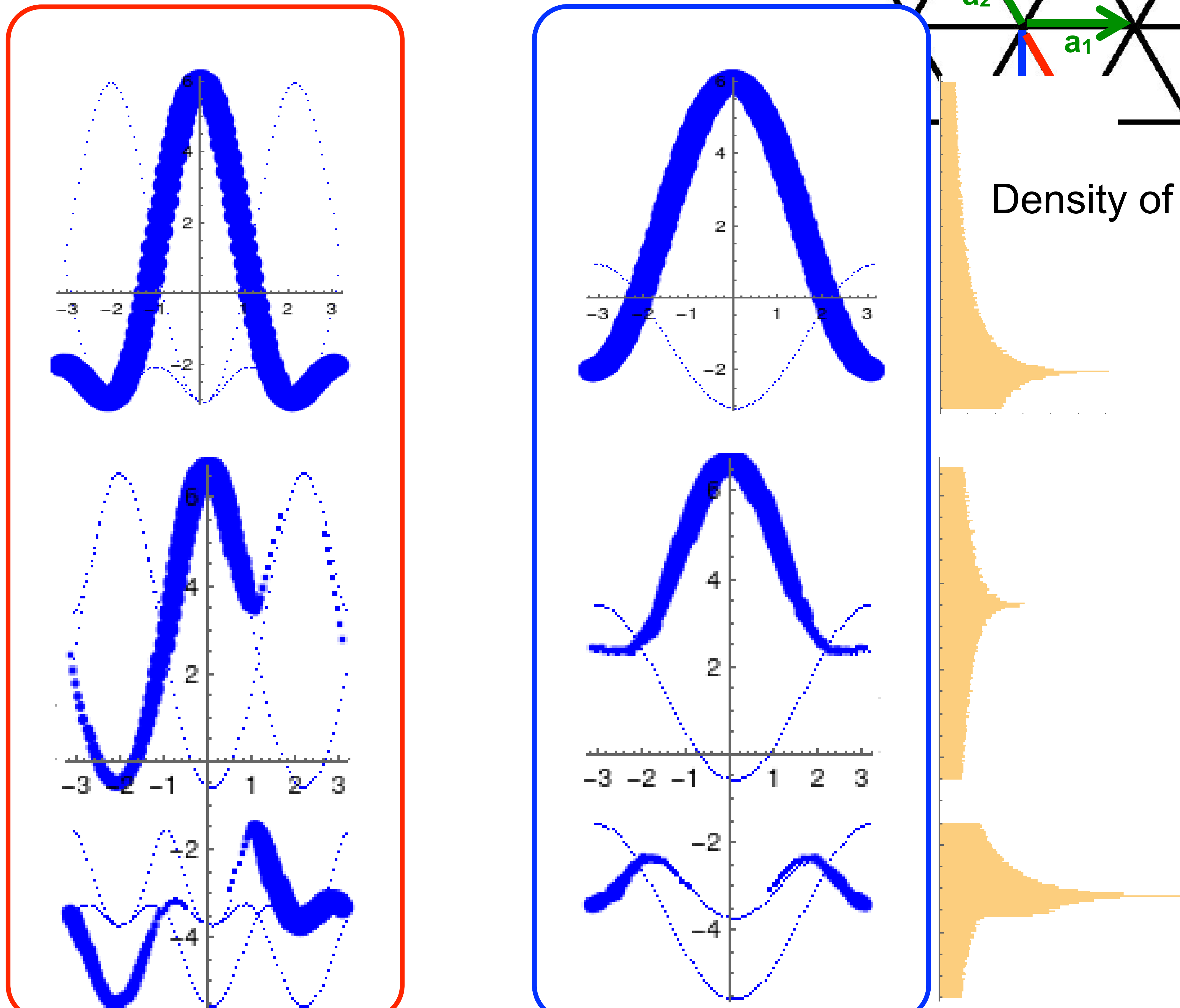
Bandstructure (1-site unit cell)

[redacted]



b=0

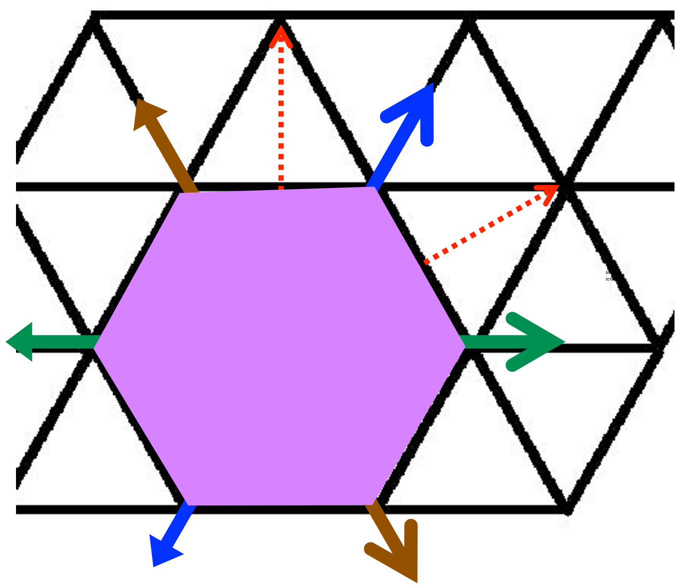
b=2.5

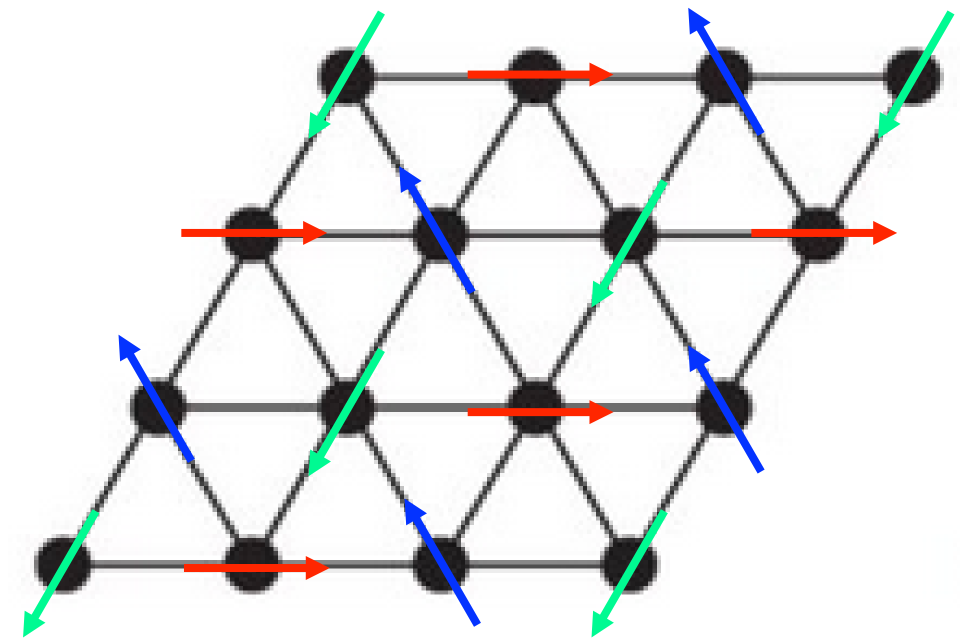


Symmetry and asymmetry (1-site unit cell)

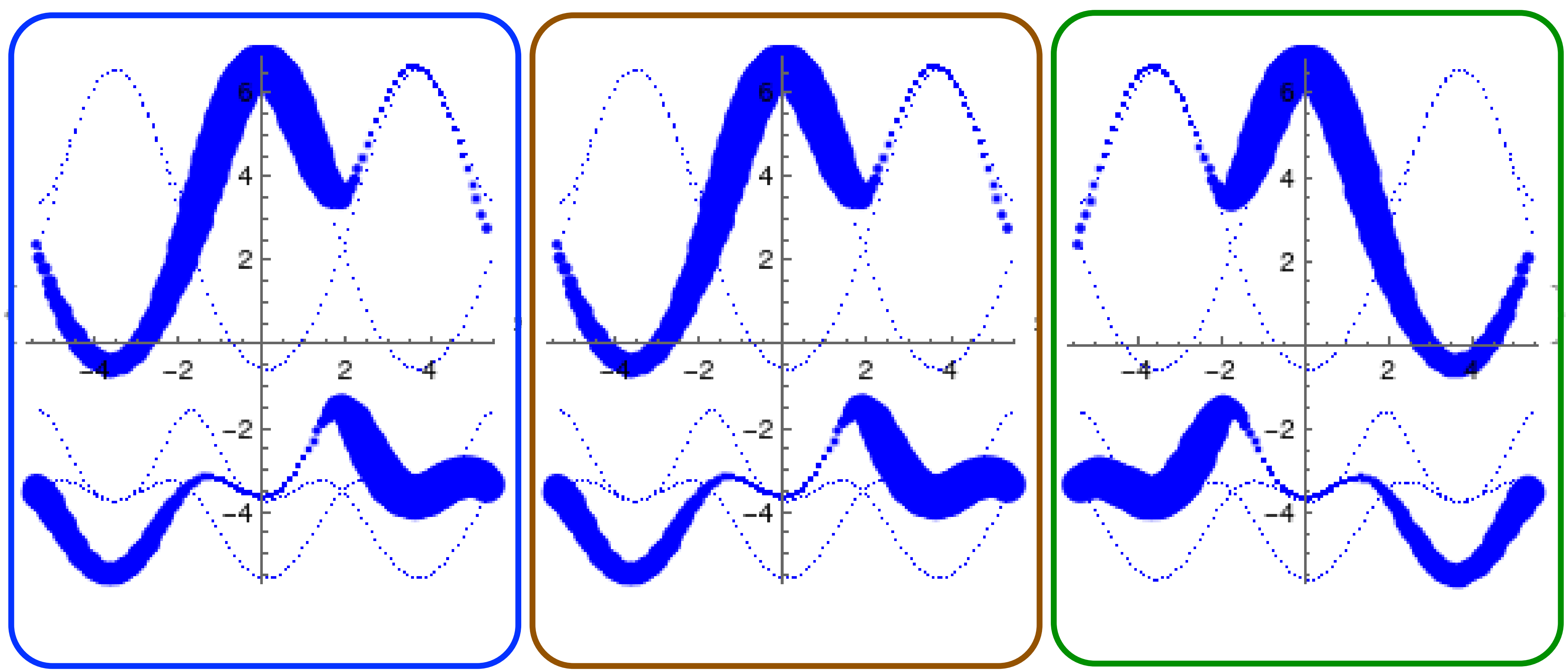
[redacted]

k-space:





b=2.5



Brillouin zone folding

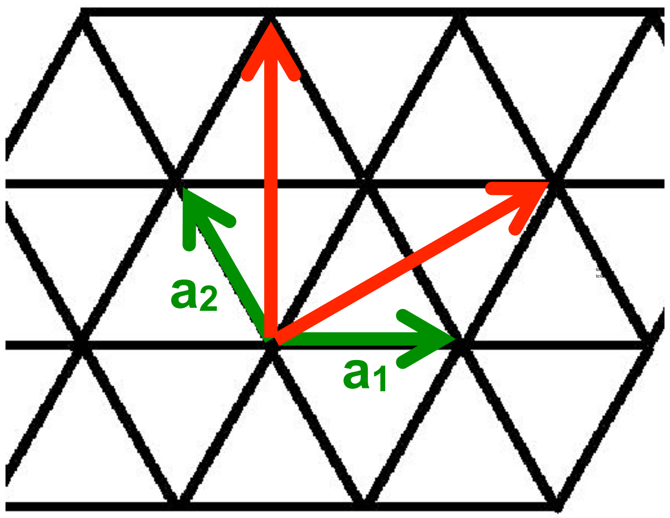
basis vectors:

$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$

k-vectors coordinates:

$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

1-atom unit cell:



The reciprocal lattice is also triangular

Brillouin zone folding

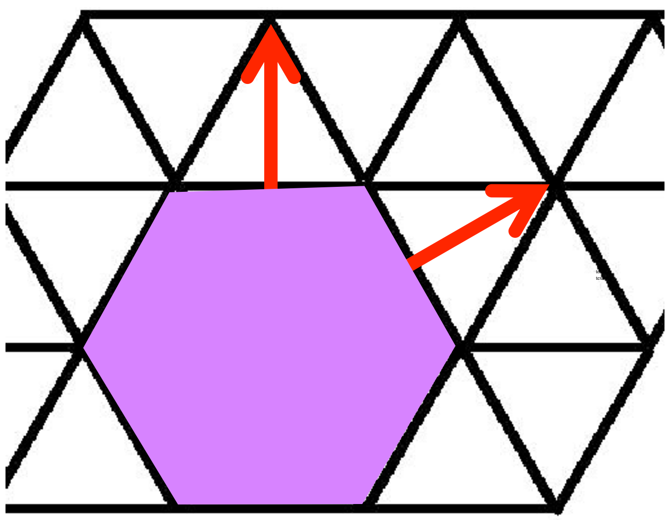
basis vectors:

$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$

k-vectors coordinates:

$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

1-atom unit cell:
(k-space)



Brillouin zone

Brillouin zone folding

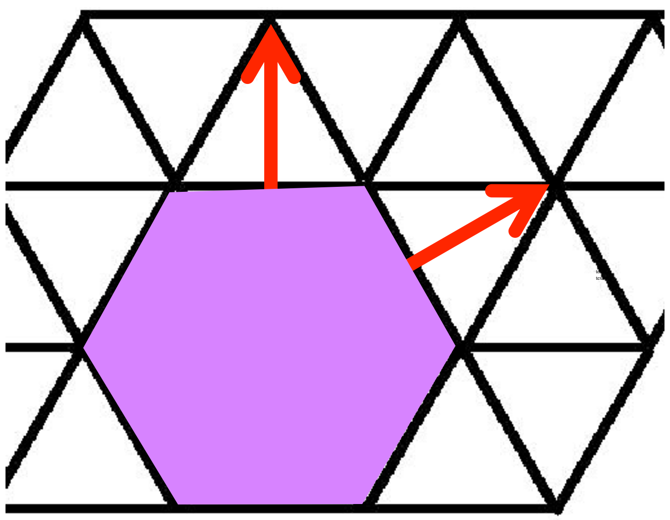
basis vectors:

$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$

k-vectors coordinates:

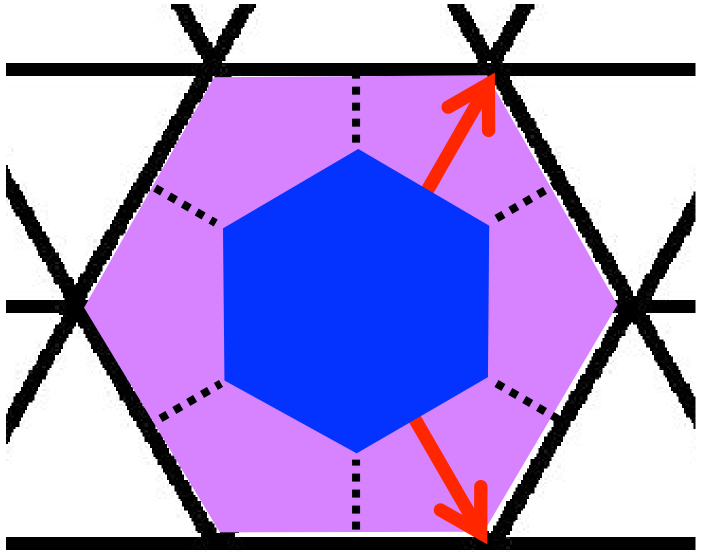
$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

1-atom unit cell:
(k-space)



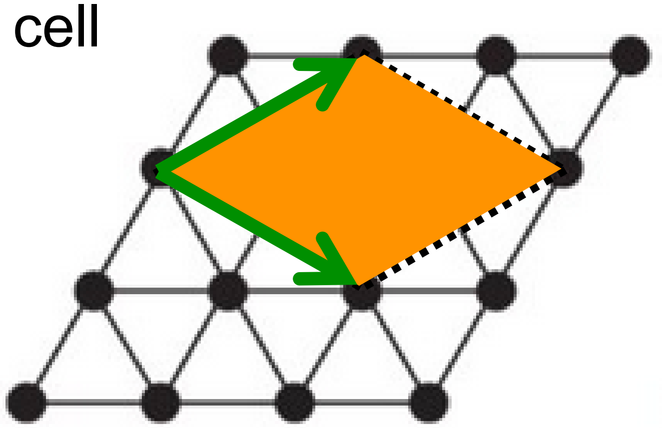
Brillouin zone

3-atom unit cell
(k-space):



The small BZ is 1/3 of the large BZ.

3-atom unit cell
(lattice):



Brillouin zone folding

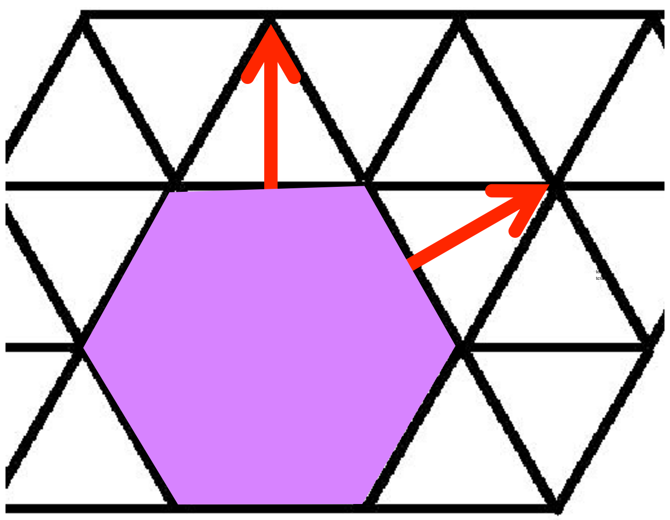
basis vectors:

$$\mathbf{b}_1 = \mathbf{a}_1 - \mathbf{a}_2$$
$$\mathbf{b}_2 = 2\mathbf{a}_1 + \mathbf{a}_2$$

k-vectors coordinates:

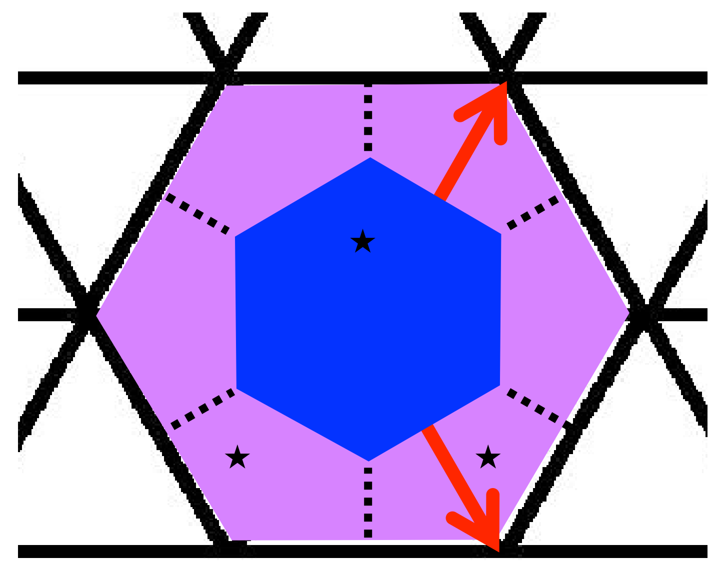
$$\bar{k}_1 = k_1 - k_2$$
$$\bar{k}_2 = 2k_1 + k_2$$

1-atom unit cell:
(k-space)



Brillouin zone

3-atom unit cell
(k-space):



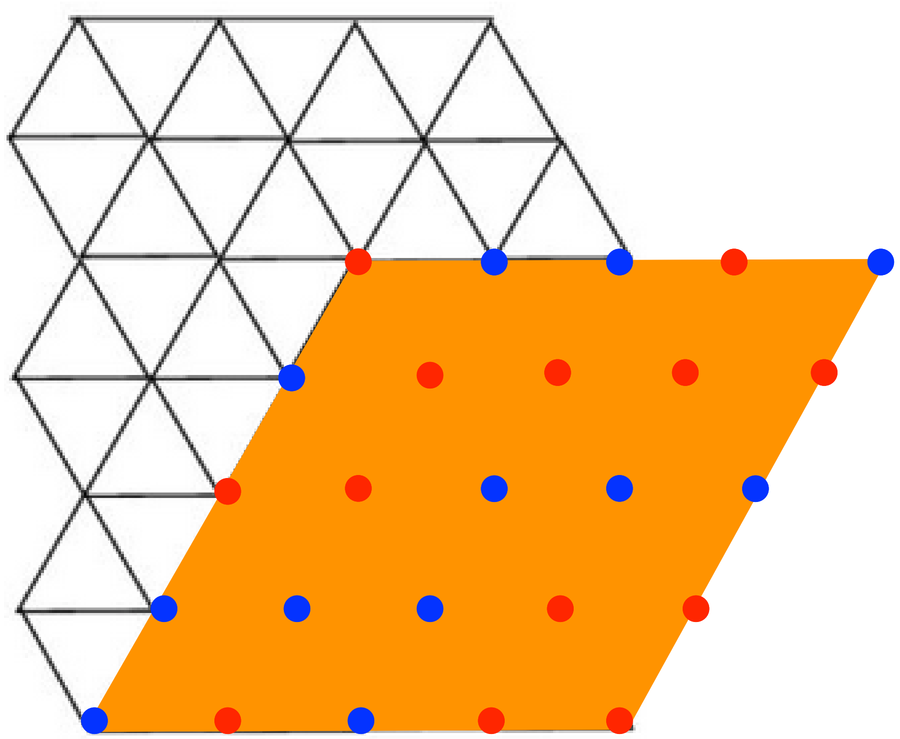
For each point in the small (blue) BZ there are 3 points in the large BZ.

Band folding: 1 -> 3 bands

Band unfolding: 3 bands (+ off diagonal elements) @ k-point in small BZ
-> 3 k-points in large BZ

An alloy on triangular lattice

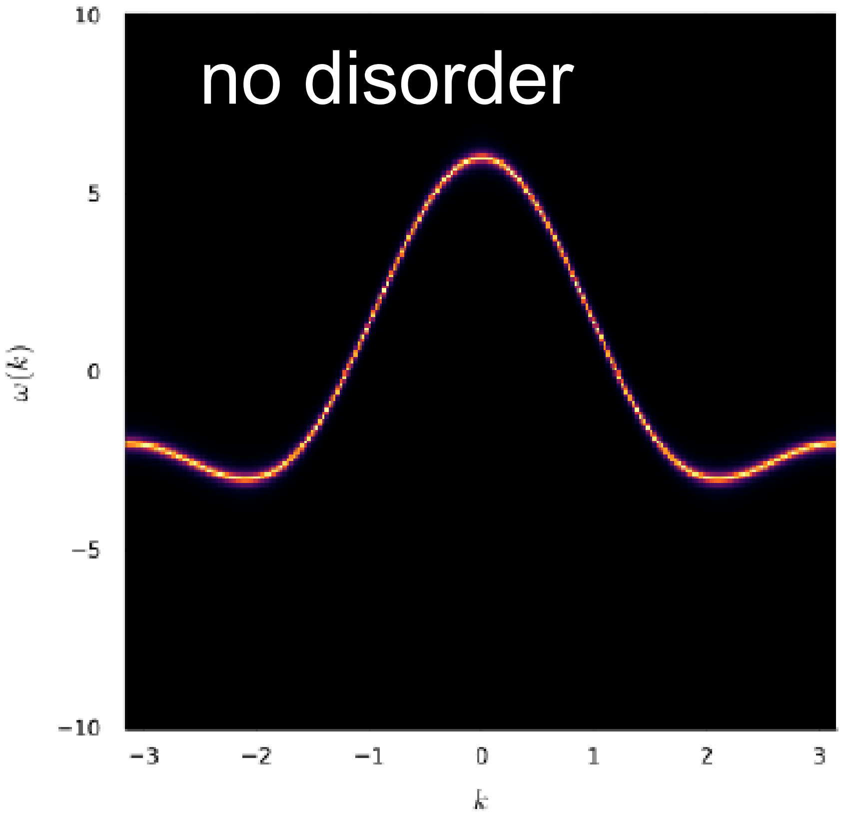
generate random binary potential
in the supercell

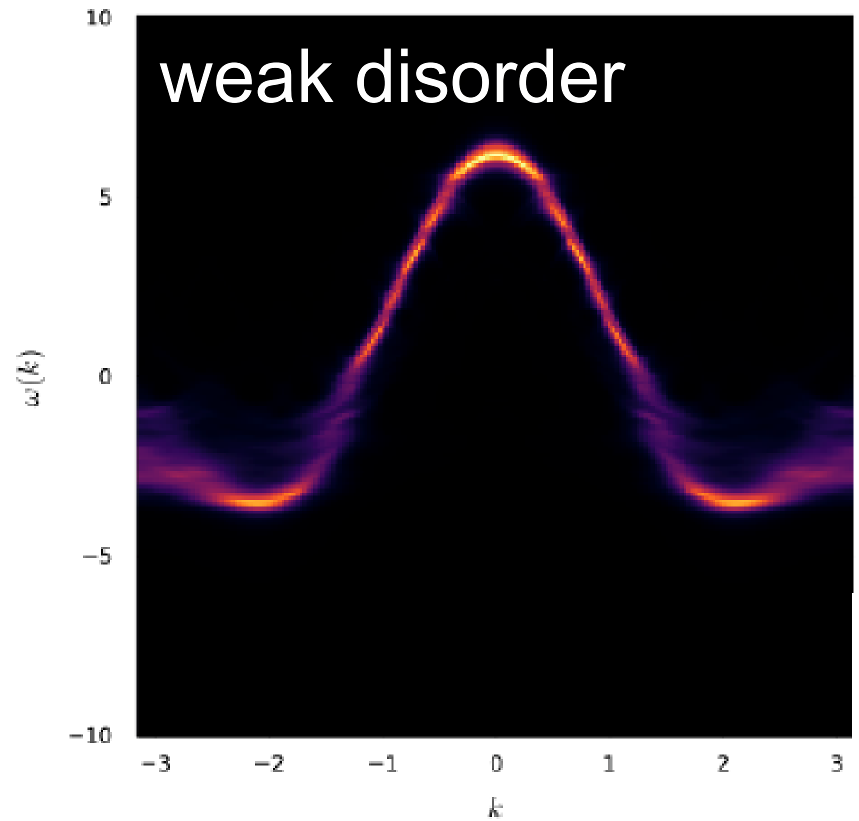


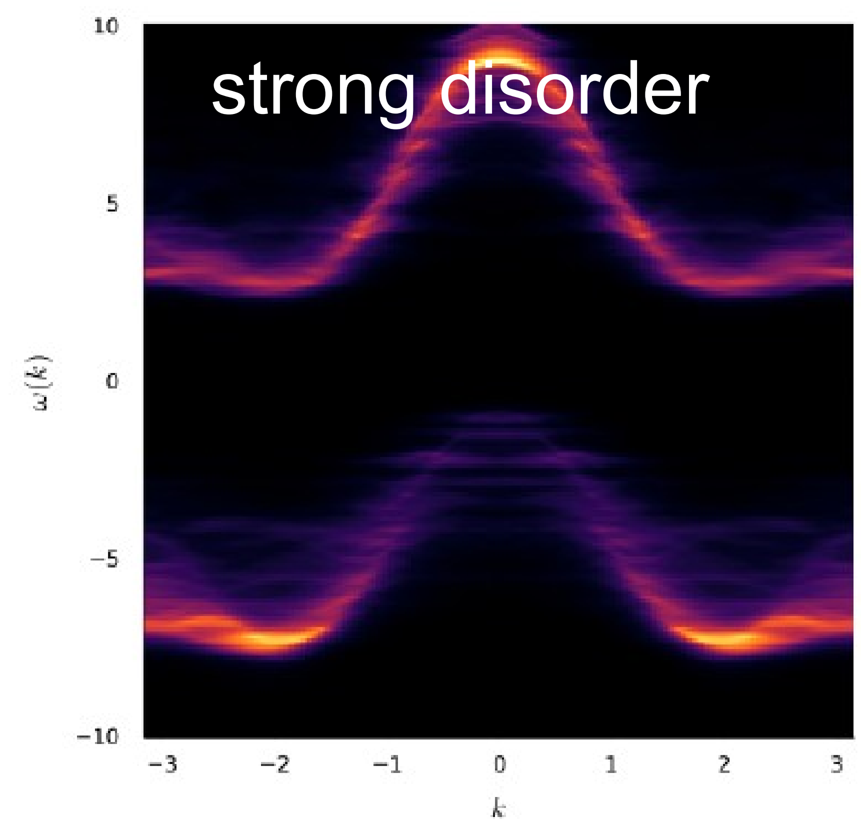
How to average over different realizations of the disorder?

How to get a 'bandstructure' in the elementary (1-atom) unit cell?

Brute force approach - many realizations of disorder







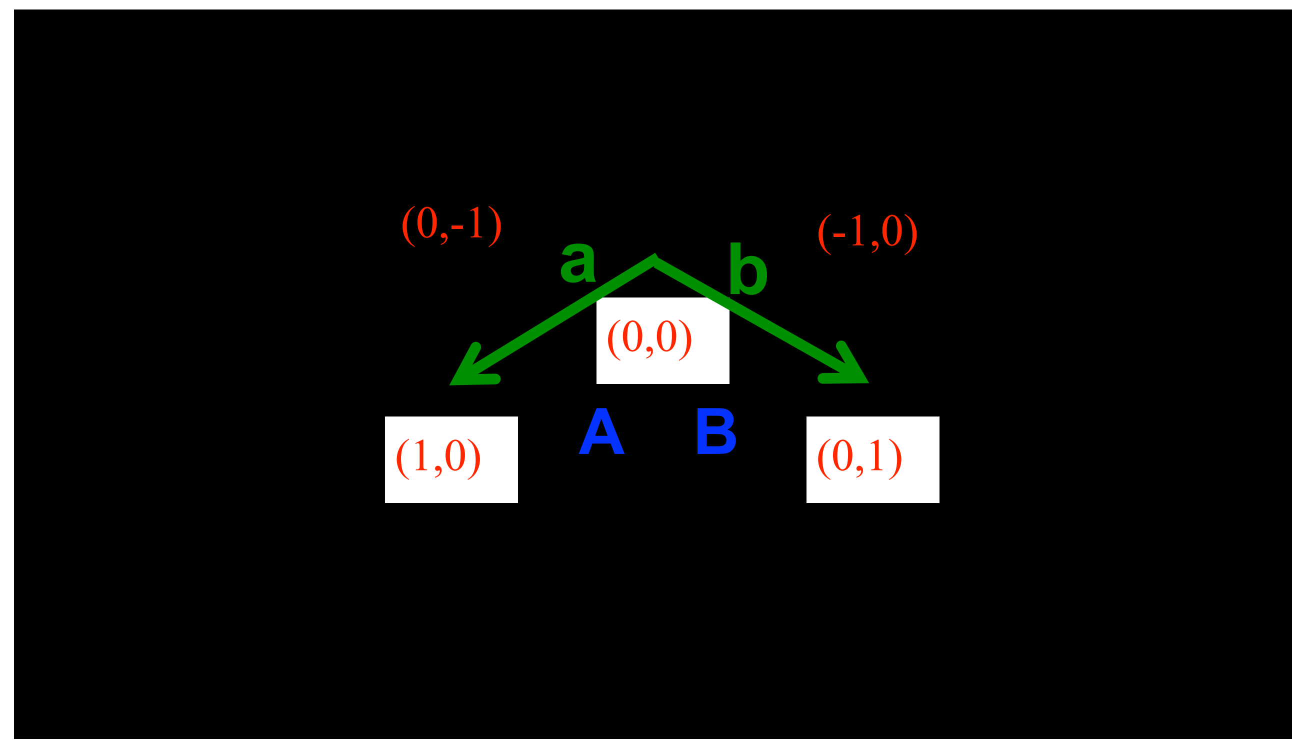
Lattice <-> continuum (theo <-> exp)

Lattice models 'live' on k-space torus <-> materials live in non-compact k-space ?

Bring in the structure of the underlying orbitals.

A: s=(2/3,1/3)
B: s=(1/3,2/3)

$$
\begin{aligned}
m(r) &= \sum_{R,s} S_{R,s}\,\rho(r - R - s) \\
m(k) &= \int dr\, e^{-ik\cdot r} m(r) \\
&= \sum_{R,s} e^{-ik\cdot R} e^{-ik\cdot s} S_{R,s} \int dr\, e^{ik\cdot r} \rho(r) \\
&\equiv f(k) \sum_{s} e^{-ik\cdot s} S_s(k)
\end{aligned}
$$



$$
\langle m(k); m(-k)\rangle = f(k)^2 \sum_{s,s'} \langle S_s(k); S'_s(-k)\rangle e^{ik\cdot(s'-s)}
$$

$$
= \langle S_A(k); S_A(-k)\rangle + \langle S_B(k); S_B(-k)\rangle + \langle S_A(k); S_B(-k)\rangle e^{i\frac{k_b - k_a}{3}} + \langle S_B(k); S_A(-k)\rangle e^{-i\frac{k_b - k_a}{3}}
$$

Lattice <-> continuum (theo <-> exp)

Lattice models 'live' on k-space torus <-> materials live in non-compact k-space ?

The model ***correlation functions*** capture long wavelength behavior (k inside the 1st BZ).
The ***matrix elements*** encode the short wavelength behavior (variation between BZs).

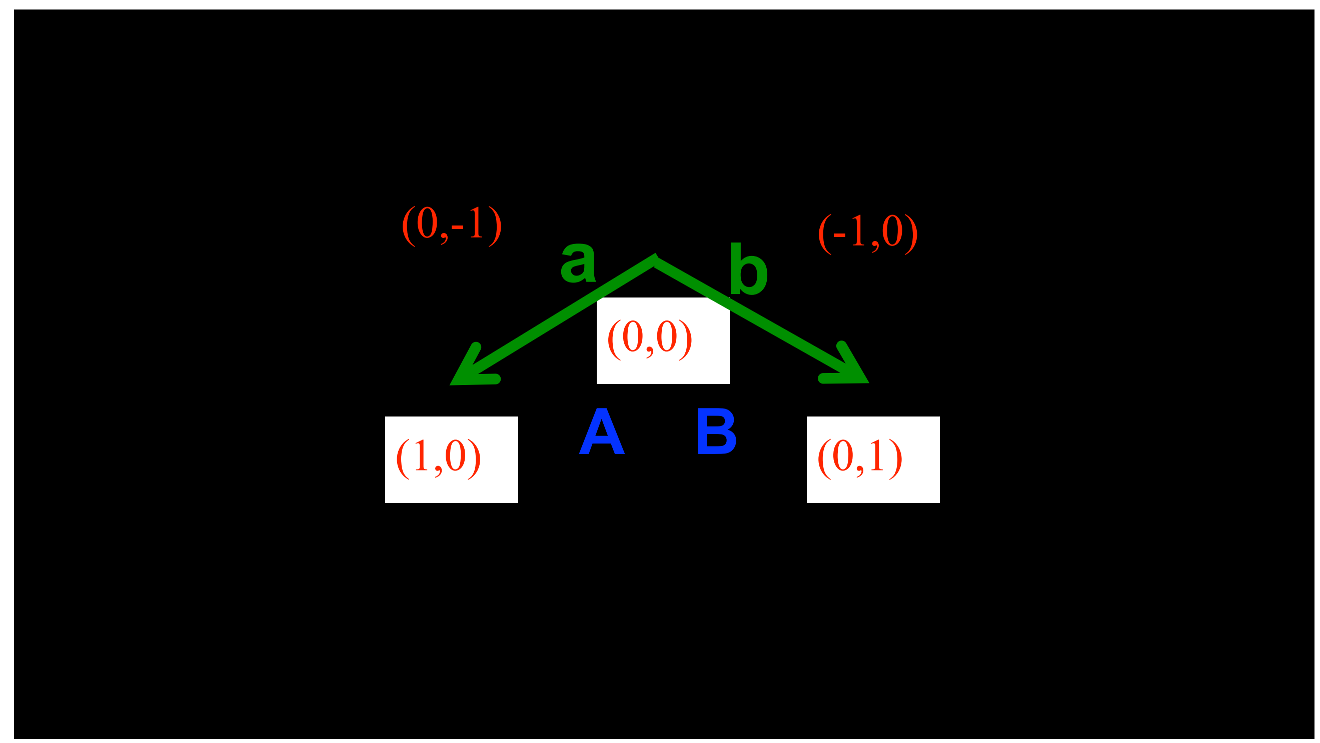
A: s=(2/3,1/3)
B: s=(1/3,2/3)

$$m(r) = \sum_{R,s} S_{R,s}\,\rho(r - R - s)$$

$$m(k) = \int dr e^{-ik\cdot r} m(r)$$

$$= \sum_{R,s} e^{-ik\cdot R} e^{-ik\cdot s} S_{R,s} \int dr e^{ik\cdot r} \rho(r)$$

$$\equiv f(k) \sum_{s} e^{-ik\cdot s} S_s(k)$$



$$\langle m(k); m(-k)\rangle = f(k)^2 \sum_{s,s'} \langle S_s(k); S'_s(-k)\rangle e^{ik\cdot(s'-s)}$$

$$= \langle S_A(k); S_A(-k)\rangle + \langle S_B(k); S_B(-k)\rangle + \langle S_A(k); S_B(-k)\rangle e^{i\frac{k_b - k_a}{3}} + \langle S_B(k); S_A(-k)\rangle e^{-i\frac{k_b - k_a}{3}}$$