Convergence

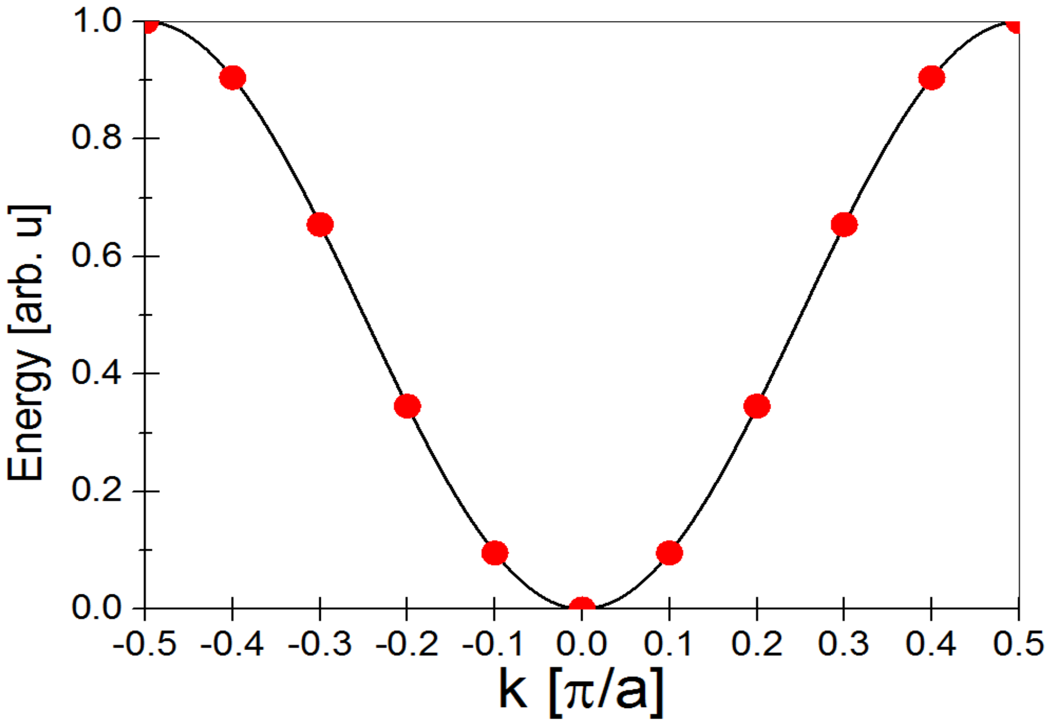
-

k-points

Converging the k-grid

For many properties, we must integrate over the Brillouin zone, e.g.:

$$n(\mathbf{r}) = \sum_{j}^{\mathrm{occ}} \int_{\Omega_{\mathrm{BZ}}} \left|\psi_{j\mathbf{k}}(\mathbf{r})\right|^2 \frac{d^3k}{\Omega_{\mathrm{BZ}}}$$



Target:

Get accurate values with as few k-points as possible

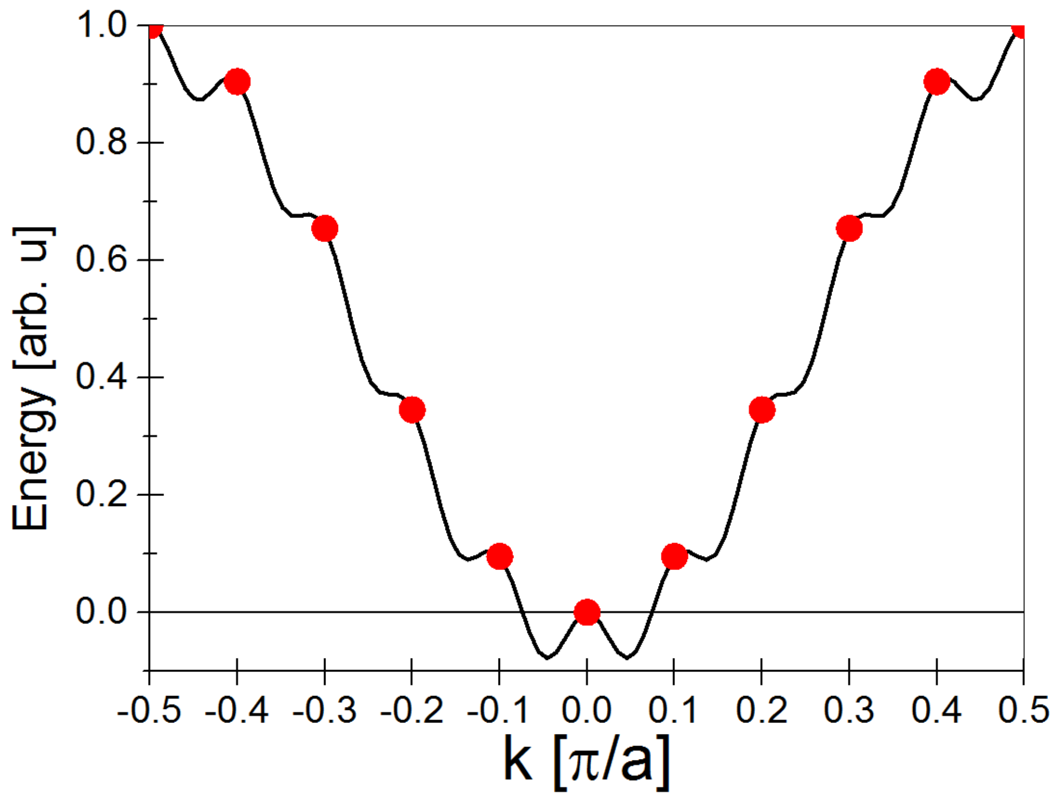
Challenge:

Function *a priori* unknown

Converging the k-grid

For many properties, we must integrate over the Brillouin zone, e.g.:

$$n(\mathbf{r}) = \sum_j^{\mathrm{occ}} \int_{\Omega_{\mathrm{BZ}}} \left|\psi_{j\mathbf{k}}(\mathbf{r})\right|^2 \frac{d^3k}{\Omega_{\mathrm{BZ}}}$$



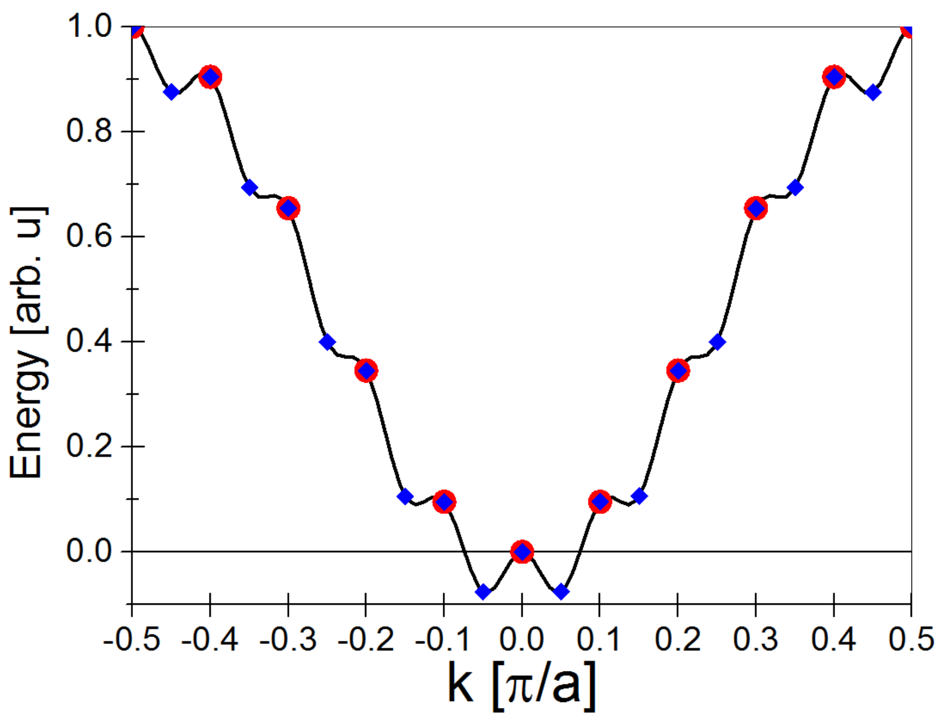
<u>Target:</u>

Get accurate values with as few k-points as possible

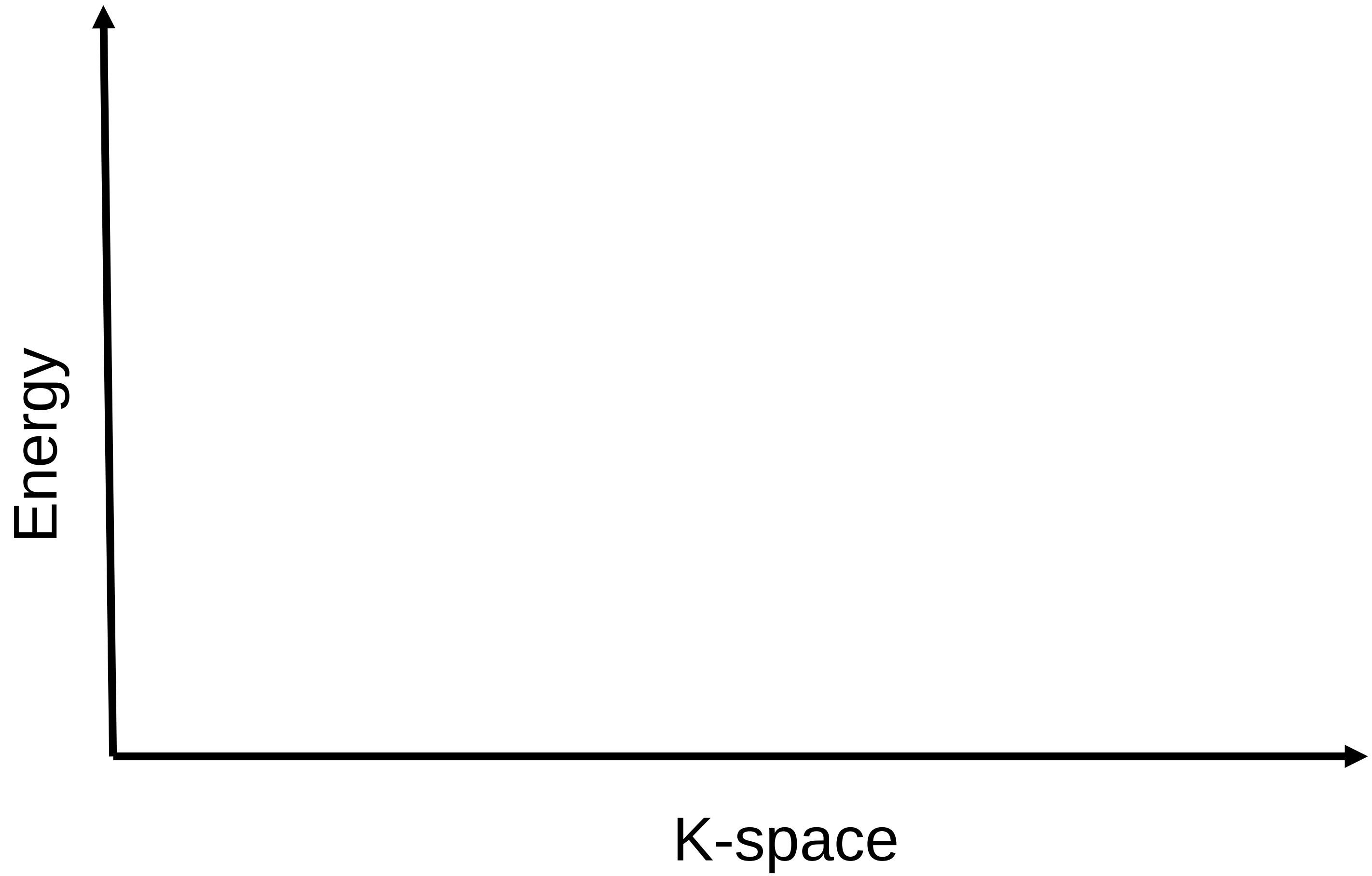
Converging the k-grid

Brute-Force Option:

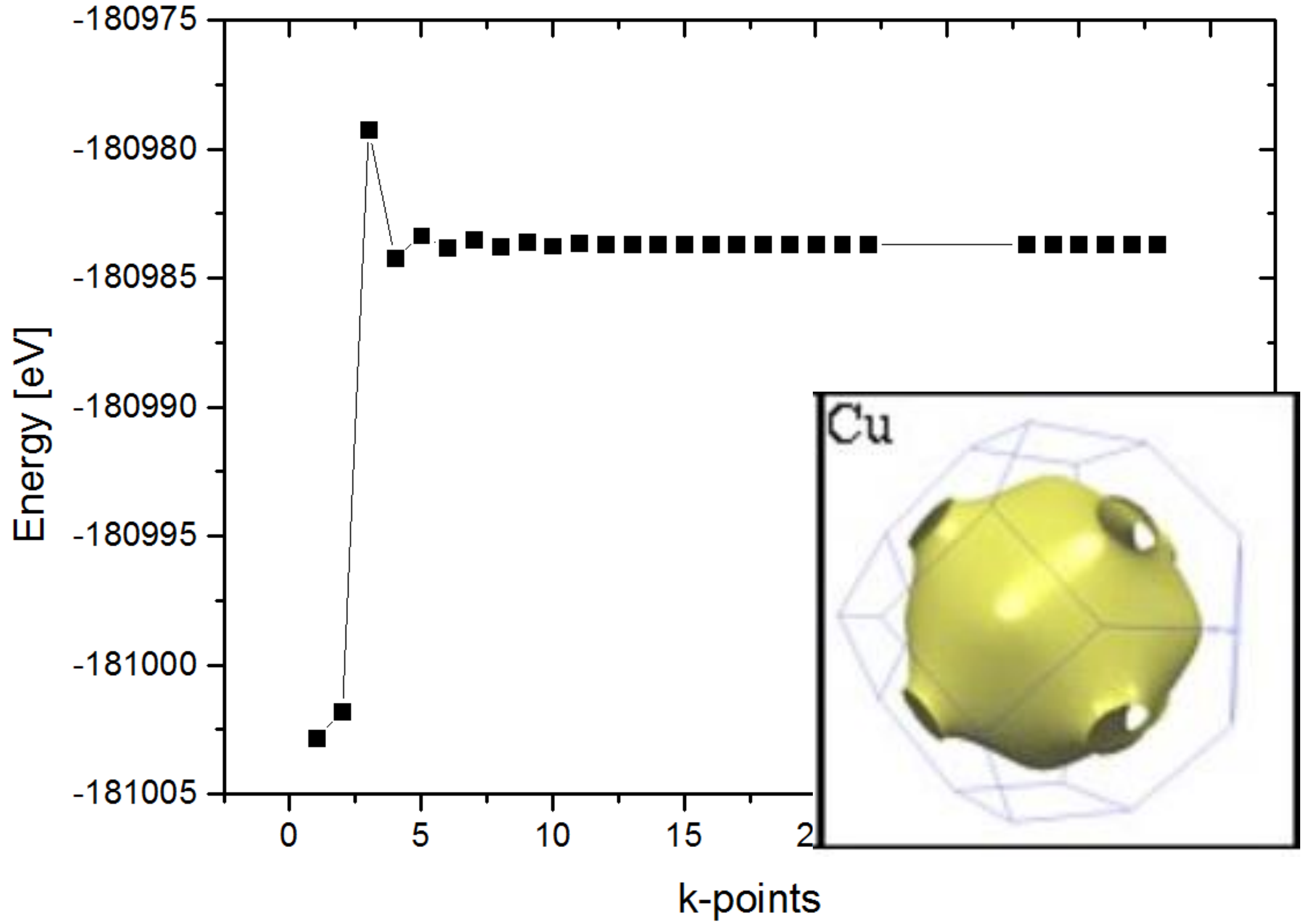
- Equally spaced grid
- Start at Γ-Point
- Increase k-point density until converged



K-points are not variational!



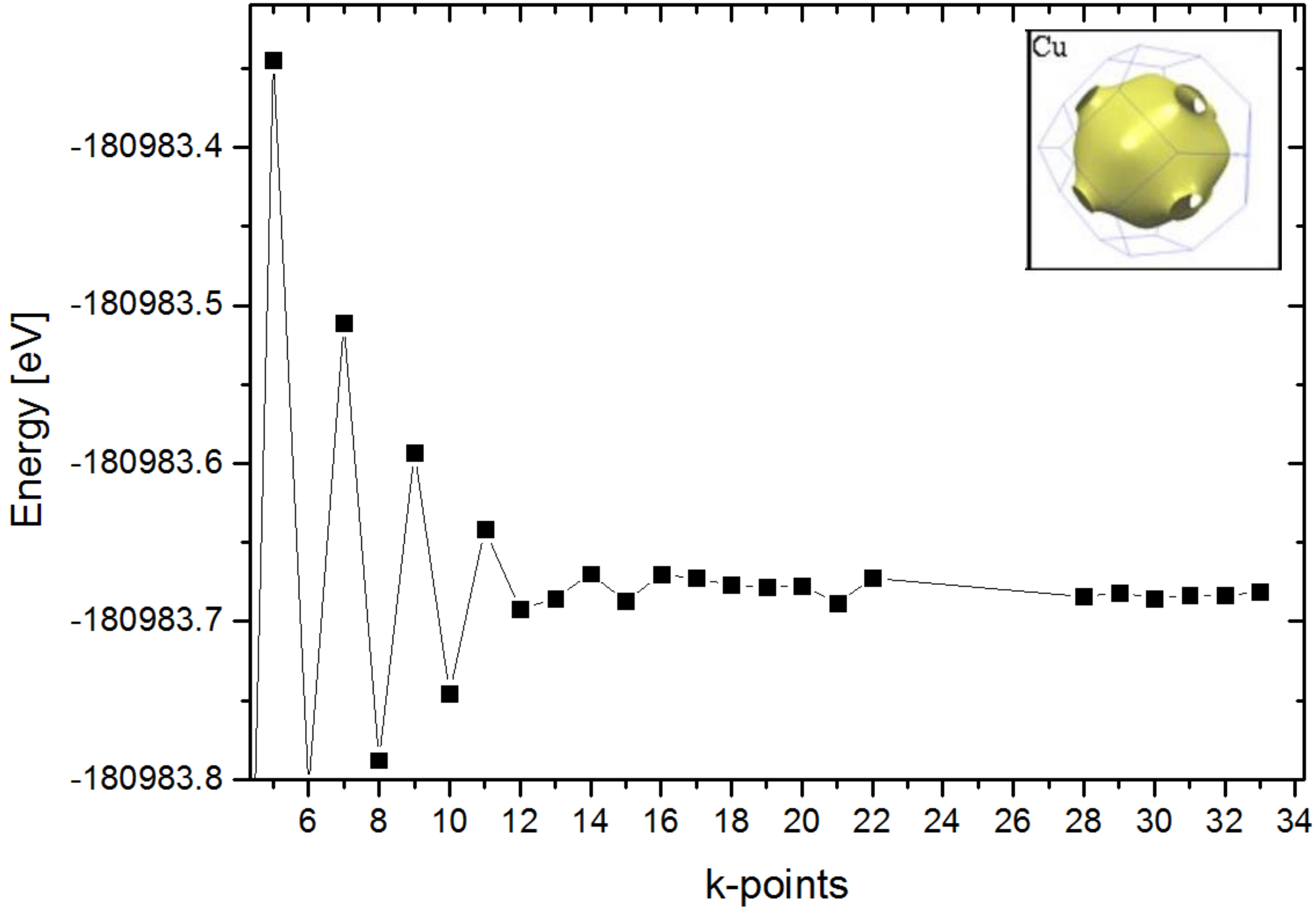
K-point convergence



Energy not variational

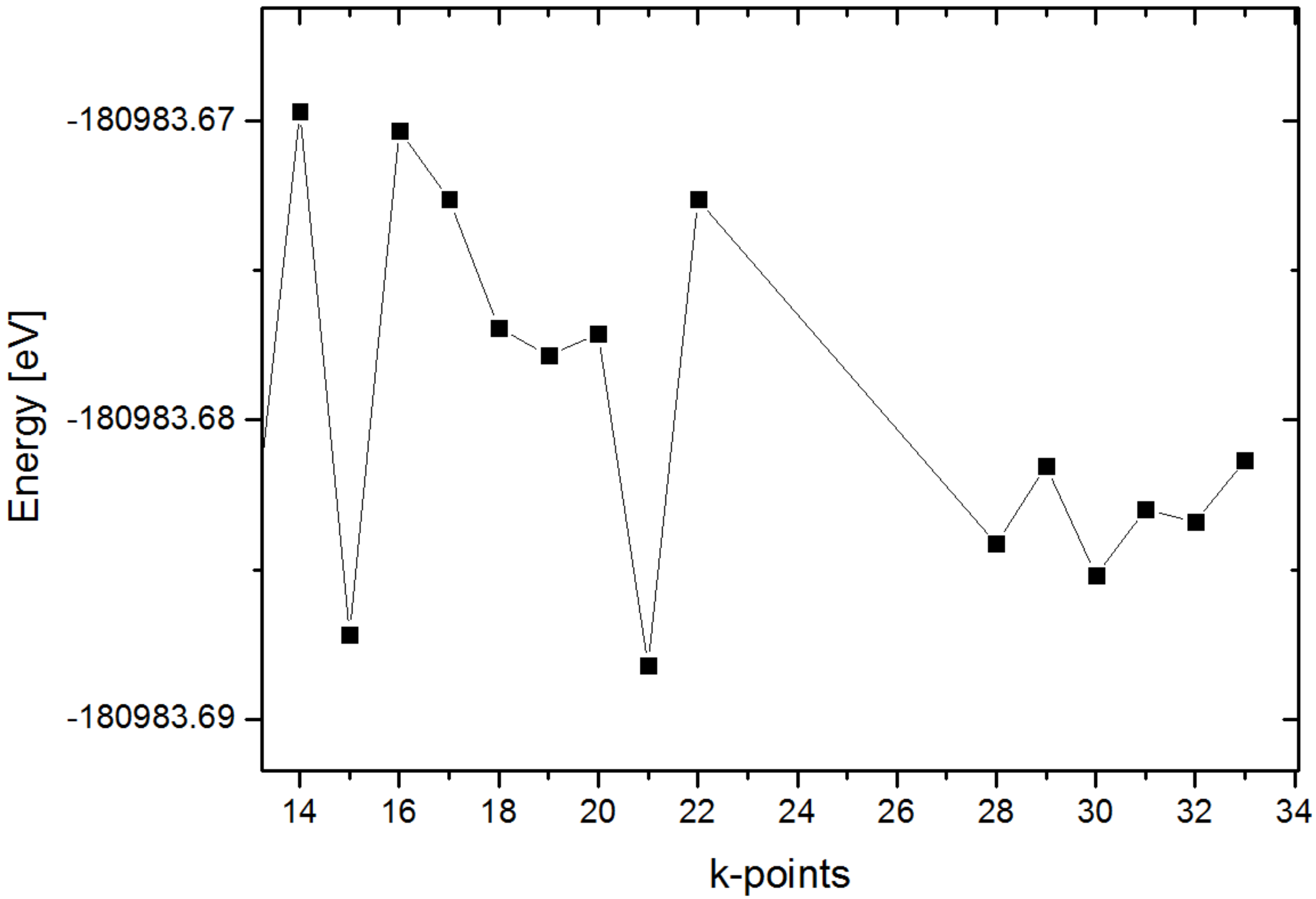
(seems to) converge quickly with k-pont density

K-point convergence



Zoom: Strong odd-even effect at moderate densities

K-point convergence



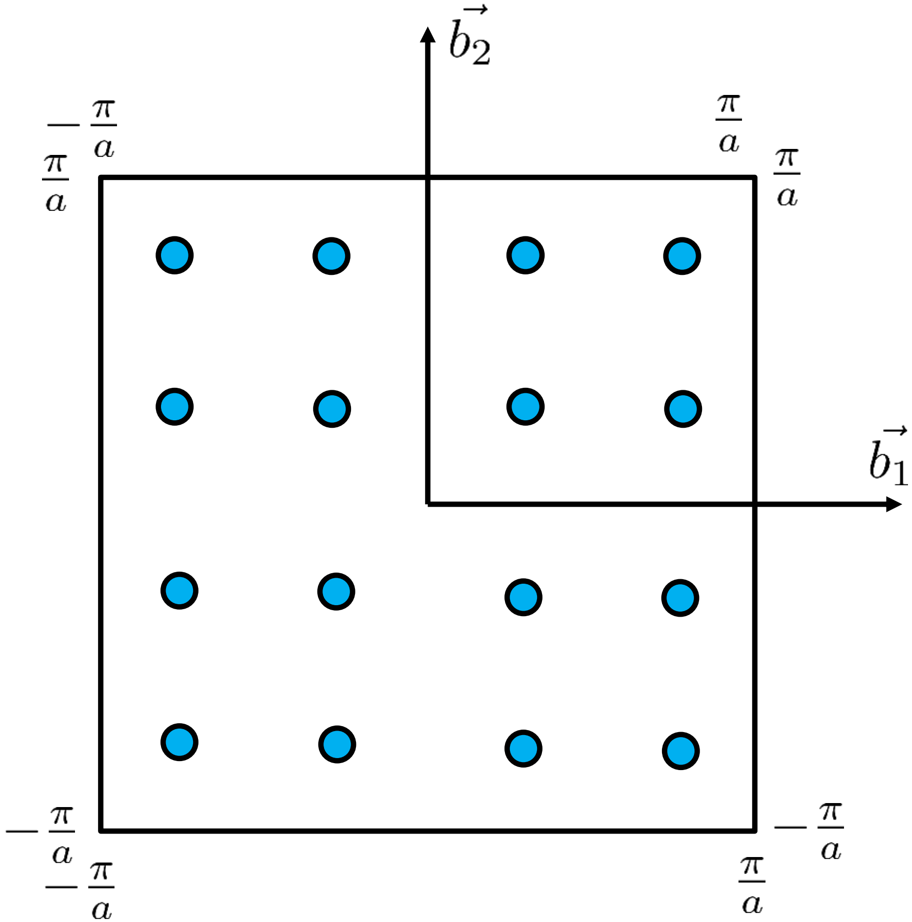
Zoom: Evem at (moderately) high densities, still seemingly erratic behaivor

Time-reversal symmetry

Brillouins theorem: $E(\vec{k}) = E(-\vec{k})$

Example:

- quadratic 2-dimensional lattice
- $q_1 = q_2 = 4 \Rightarrow$ 16 k-points



Time-reversal symmetry

Brillouins theorem: $E(\vec{k}) = E(-\vec{k})$

$$E(\vec{k_x}, \vec{k_y}) = E(-\vec{k_x}, \vec{k_y}) = E(\vec{k_x}, -\vec{k_y}) = E(-\vec{k_x}, -\vec{k_y})$$

Example:

- quadratic 2-dimensional lattice
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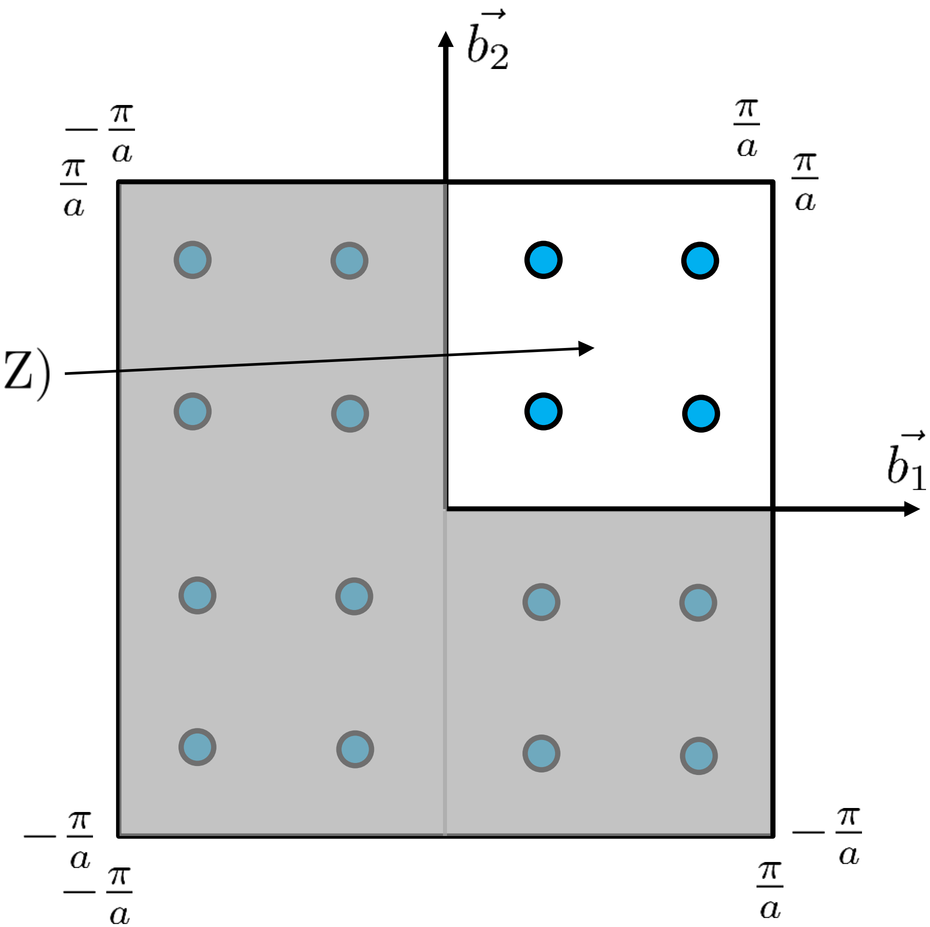
irreducible Brilloin zone (IBZ)



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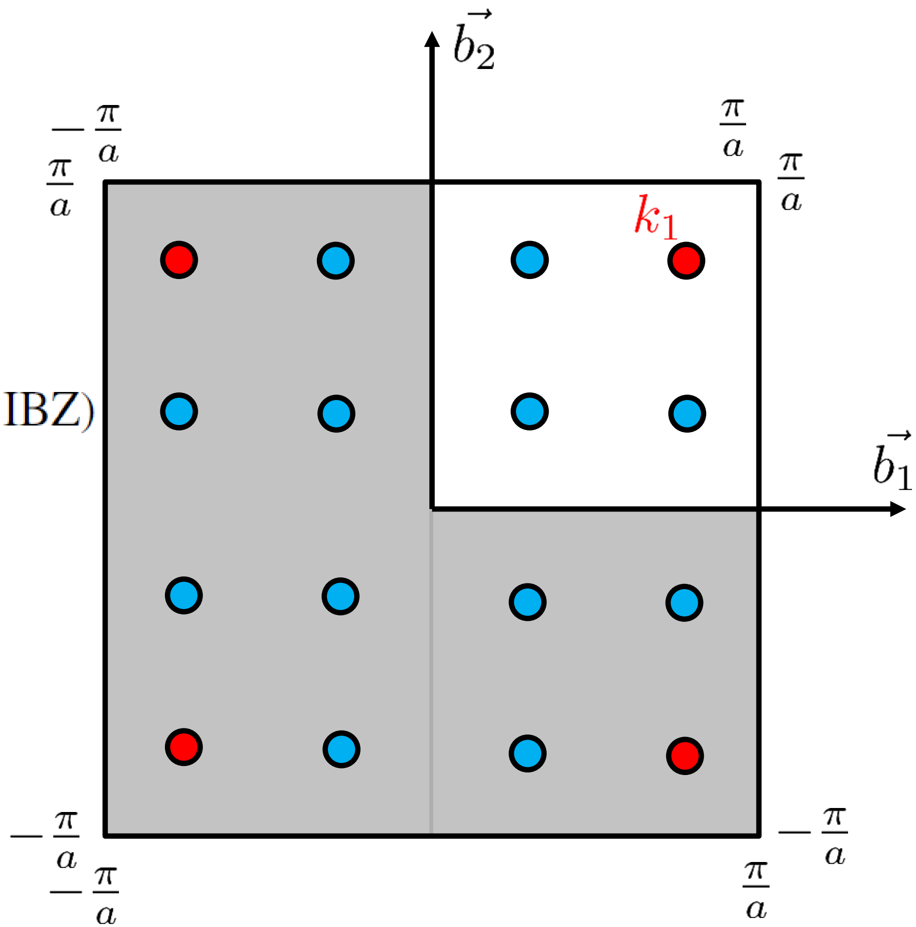
Example:

- quadratic 2-dimensional lattice
- $q_1 = q_2 = 4 \Rightarrow 16$ k-points
- only 3 inequivalent k-points ($\Rightarrow$ IBZ)
  - $4 \times \mathbf{k}_1 = (\frac{1}{8}, \frac{1}{8}) \Rightarrow \omega_1 = \frac{1}{4}$



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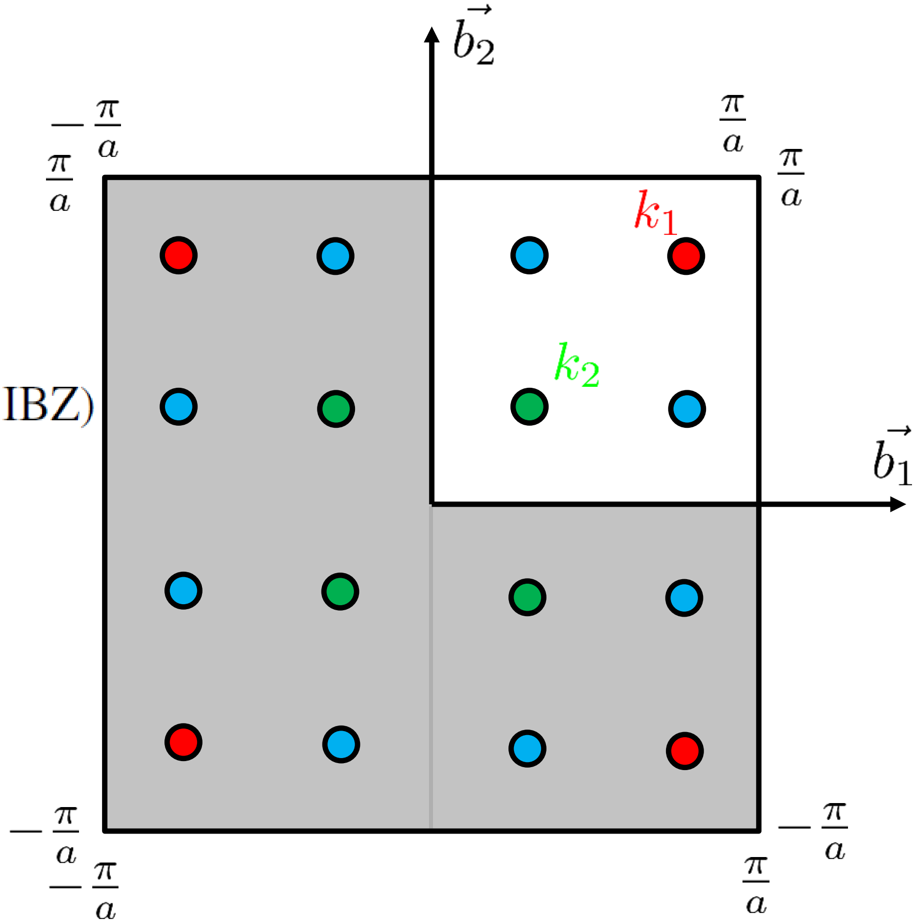
  - $4 \times \mathbf{k}_2 = (\frac{3}{8}, \frac{3}{8}) \Rightarrow \omega_2 = \frac{1}{4}$



Time-reversal symmetry

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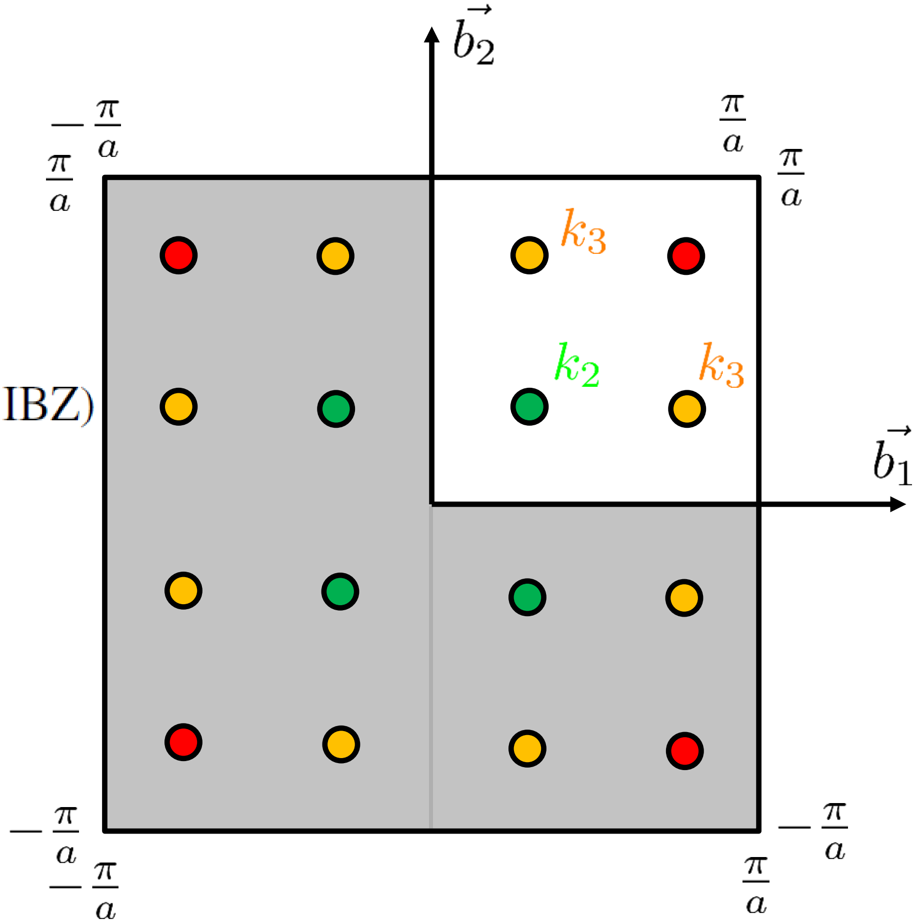
  - $8 \times \mathbf{k}_3 = (\frac{3}{8}, \frac{1}{8}) \Rightarrow \omega_3 = \frac{1}{2}$



Time-reversal symmetry

Brillouins theorem: $E(\vec{k}) = E(-\vec{k})$

$$\boxed{\frac{1}{\Omega_{\mathrm{BZ}}} \int\limits_{BZ} F(\mathbf{k}) d\mathbf{k} \Rightarrow \tfrac{1}{4} F(\mathbf{k}_1) + \tfrac{1}{4} F(\mathbf{k}_2) + \tfrac{1}{2} F(\mathbf{k}_3)}$$

Example:

- quadratic 2-dimensional lattice
- $q_1 = q_2 = 4 \Rightarrow$ 16 k-points
- only 3 inequivalent k-points ($\Rightarrow$ IBZ)
  - $4 \times \mathbf{k}_1 = (\frac{1}{8}, \frac{1}{8}) \Rightarrow \omega_1 = \frac{1}{4}$
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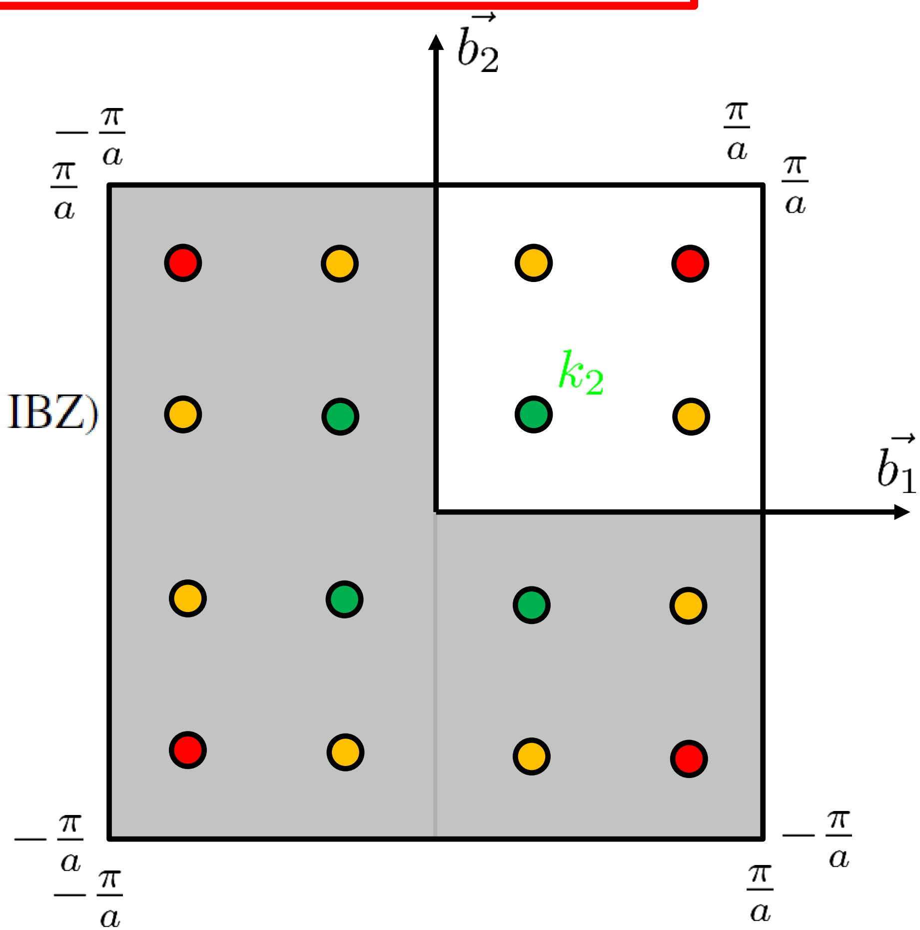


Shifting points

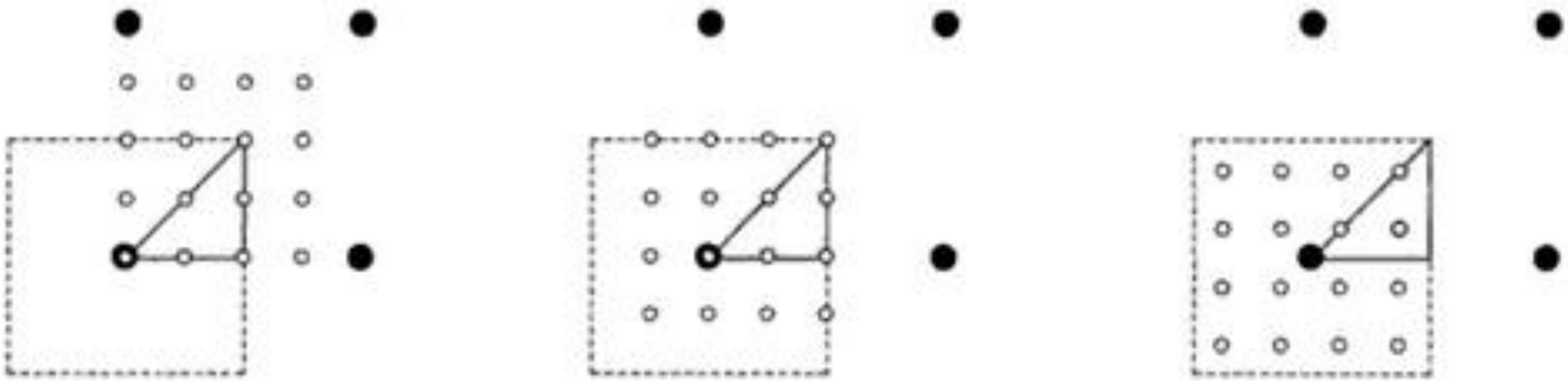


Figure 4.12. Grids for integration for a 2d square lattice, each with four times the density of the reciprocal lattice in each dimension. The left and center figures are equivalent with one point at the origin, and six inequivalent points in the irreducible BZ shown in grey. Right: A shifted special point grid of the same density but with only three inequivalent points. Additional possibilities have been given by Moreno and Soler [277], who also pointed out that different shifts and symmetrization can lead to finer grids.

Electronic Structure: Basic Theory and Practical Methods
von Richard M. Martin,Richard Milton Martin

Theory of Special Points

<u>Chadi/Cohen</u>: Define special points in the Brillouin zone. From that converge fast to the average.

<u>Concept:</u>

Lattice-periodic function expanded in Fourier series

$$f(k) = f_0 + \sum_{m=1}^{\infty} f_m A_m(k)$$

$$A_m(k) = \sum_{|R|=C_m} e^{ikR}$$

Coefficients A_m are “shells“ of lattice vectors, chosen such that

$$\sum_i \omega_{k_i} A_m(k_i) = 0$$

$$\rightarrow \bar{f} = f_0$$

Chadi, Cohen, PRB 8 (1973) 5747.

Theory of Special Points

Monkhorst/Pack:

➢ **Realization with equally-spaced mesh**

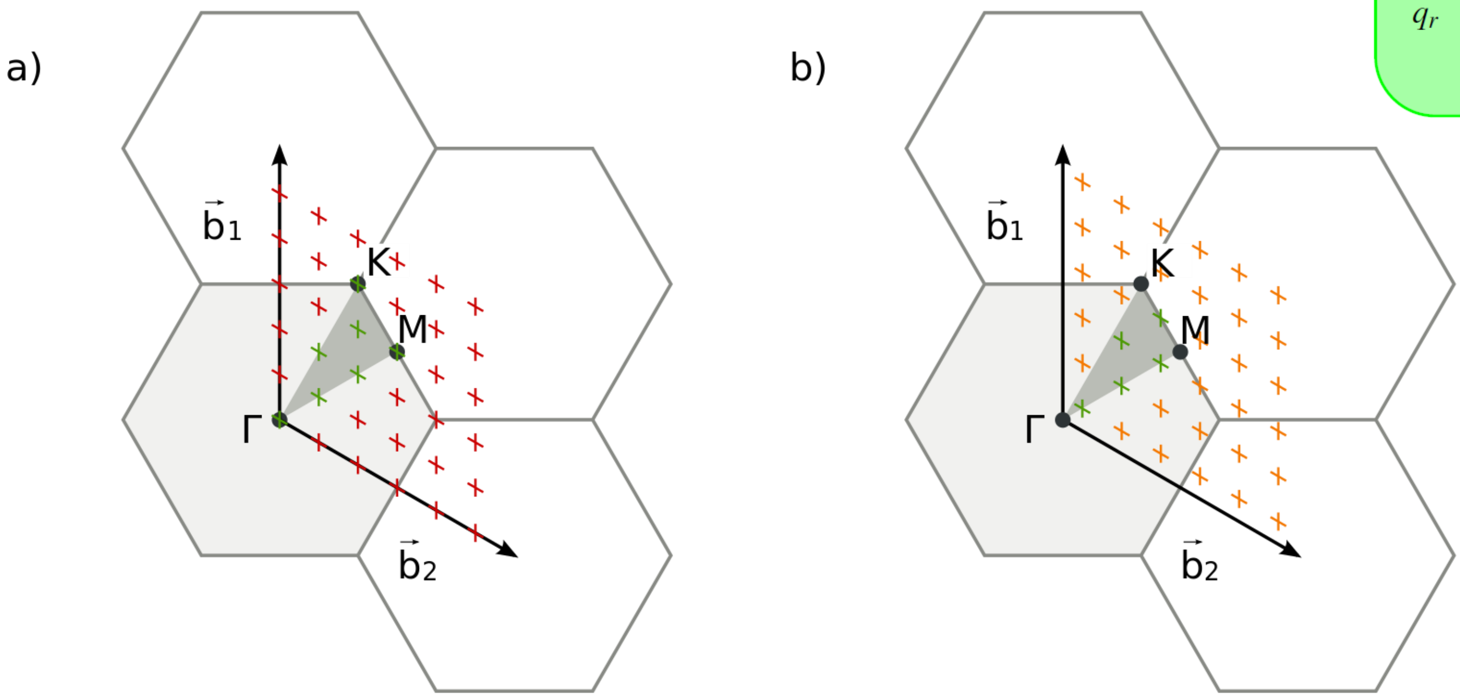
$$\mathbf{k}_{prs} = u_p \mathbf{b}_1 + u_r \mathbf{b}_2 + u_s \mathbf{b}_3$$

$$u_r = \frac{2r - q_r - 1}{2q_r} \qquad r = 1, 2, \ldots, q_r$$

$\mathbf{b}_i$ reciprocal lattice-vectors

q_r determines number of k-points in r-direction

Γ-centered (7 points in IBZ) **Off-Γ (5 points in IBZ)**



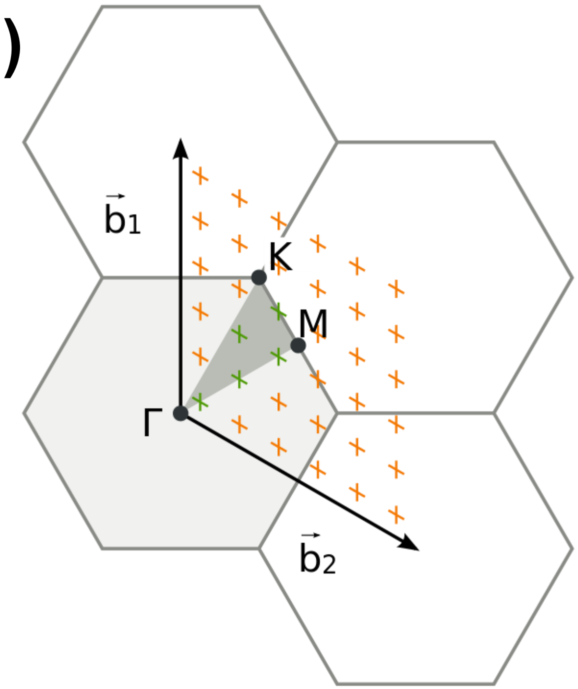
https://commons.wikimedia.org/wiki/File:Example_Brillouin_zone_sampling_of_hexagonal_lattice_with_Monkhorst-Pack_grid.svg

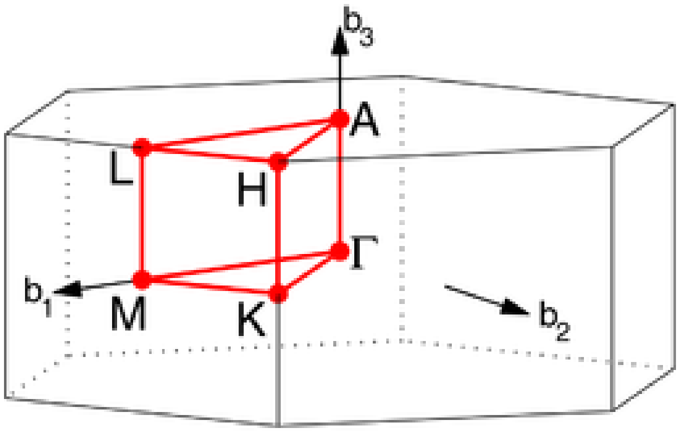
Monkhorst and Pack (1976):

Monkhorst-Pack grids

Intentionally avoids high-symmetry points

(Γ, K, M,…)





HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Designed to be good for averages

(electron density, energy, dielectric function)

.. not for k-dependent quantities

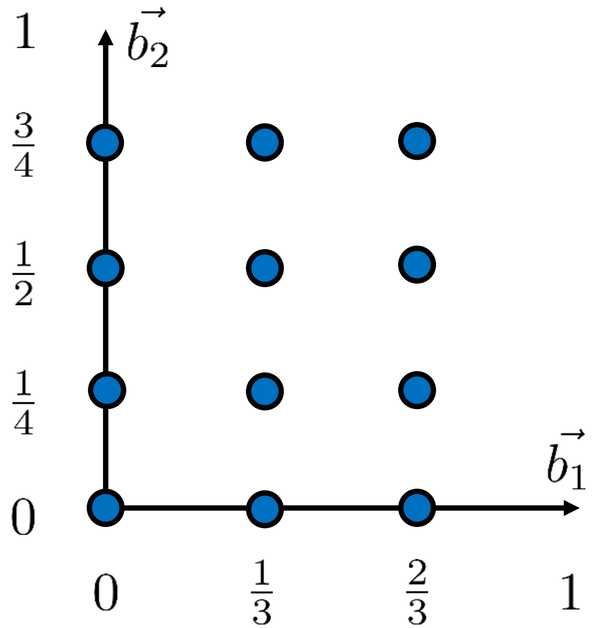
(DOS, band structure, work function)

K-point mesh in practise

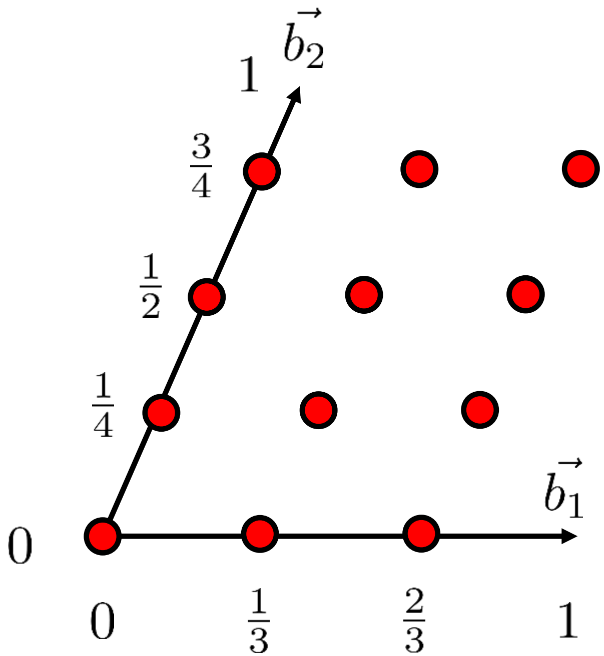
```
xc pbe

k_grid 4 3 1
k_offset 0 0.5 0
```

Number of segments in b_1, b_2, b_3
offset in b_1, b_2, b_3

3x4 k-grid, no offset



3x4 k-grid, no offset



K-Point Summary

- Used to integrate functions in reciprocal space

- Not variational

- Quality is determined by
  - Grid Density
  - Cell Size
  - Cell Shape

- Always use consistent k-grids

Self-Assessment / Q&A

https://fbr.io/join/lzape