Review Questions 9

- What is the (semiclassical) equation of motion for a band electron?
  - A: dk/dt = F, $v = \mathrm{grad}_k \varepsilon / \hbar$
- What are electrons and holes in semiconductors, and what does their effective mass mean?
  - A: They are occupied or empty states at the bottom of the conduction or top of the valence band, respectively. The effective mass is the inverse of the band curvature at its minimum/maximum.
- Are effective masses in semiconductors smaller or larger than the electron mass, usually?
  - A: usually smaller.

Review Questions 10

- What are donors and acceptors?
  - A: They are impurity atoms in a semiconductor which tend to ionize, forming a charged ionic center and an oppositely charged "doped" electron or hole.
- How does the binding energy and Bohr radius of a donor depend on effective mass and dielectric constant?
  - A: The binding energy is $E = Ry\ (m^*/m)\ 1/(\varepsilon^2)$, and the radius is $a = a_B\ \varepsilon\ (m/m^*)$
- What measurements determine the sign and density of charge carriers?
  - A: Hall effect, and thermopower

Fermi surfaces

- Key result of band theory: electrons occupy quantum states described by continuous crystal momentum and discrete "band index" quantum numbers
- Energies of each band are smooth functions of quasi-momentum, $\varepsilon_n(k)$
- Fermi statistics: states below E_F are occupied, others empty
- Condition $\varepsilon_n(k)=E_F$ generally describes a surface (when it has solutions). This is the Fermi surface.

Why Fermi surfaces?

- Any time we weakly perturb a system, we excite mainly low energy excitations
  - in metals, the characteristic energy scale is E_F ~ eV, so most perturbations are weak
  - In a metal, the low energy excitations are adding or removing electrons near the Fermi energy (or moving them from below to above).
  - In some cases, one can think of the excitation as a deformation of the surface (c.f. displacement in E field)
- It is remarkable that this geometric object *in reciprocal space* becomes essential to the physics of something as simple as a piece of metal!
  - manifests both wavelike nature of electrons and quantum statistics!

Fermi surface shapes

- Surfaces can be complex, and many occur in nature
- Can try to understand via:
  - Nearly free electron theory
  - Tight binding
  - *ab initio* electronic structure
  - measurement

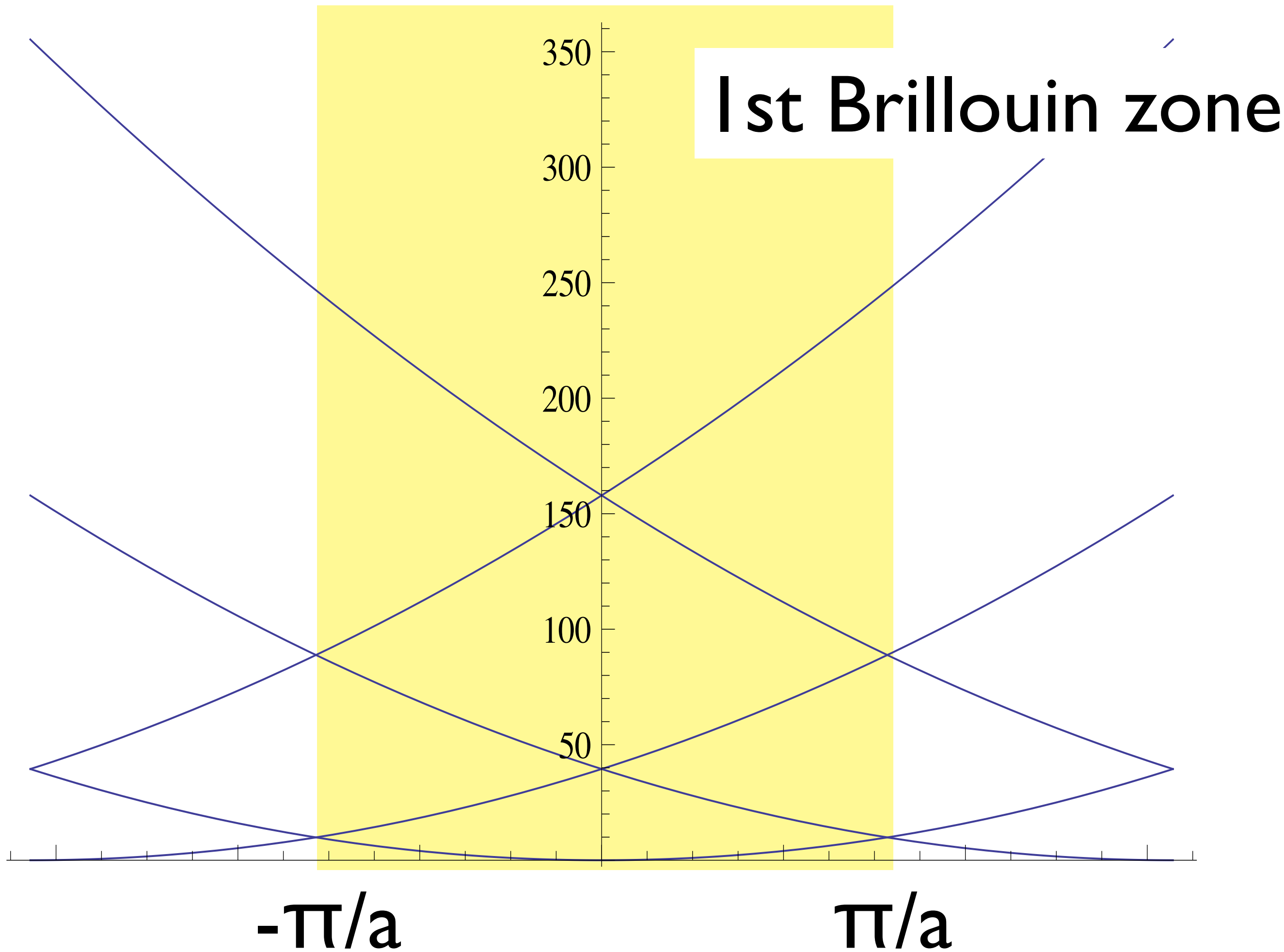
Nearly free electrons

- Sometimes can regard the ionic potential as a small perturbation to the free electron states
- We can start by interpreting the free electron states as bands

$$\psi = e^{i\mathbf{p}\cdot\mathbf{r}} = e^{i(\mathbf{p}-\mathbf{G})\cdot\mathbf{r}} \times \left(e^{i\mathbf{G}\cdot\mathbf{r}}\right)$$

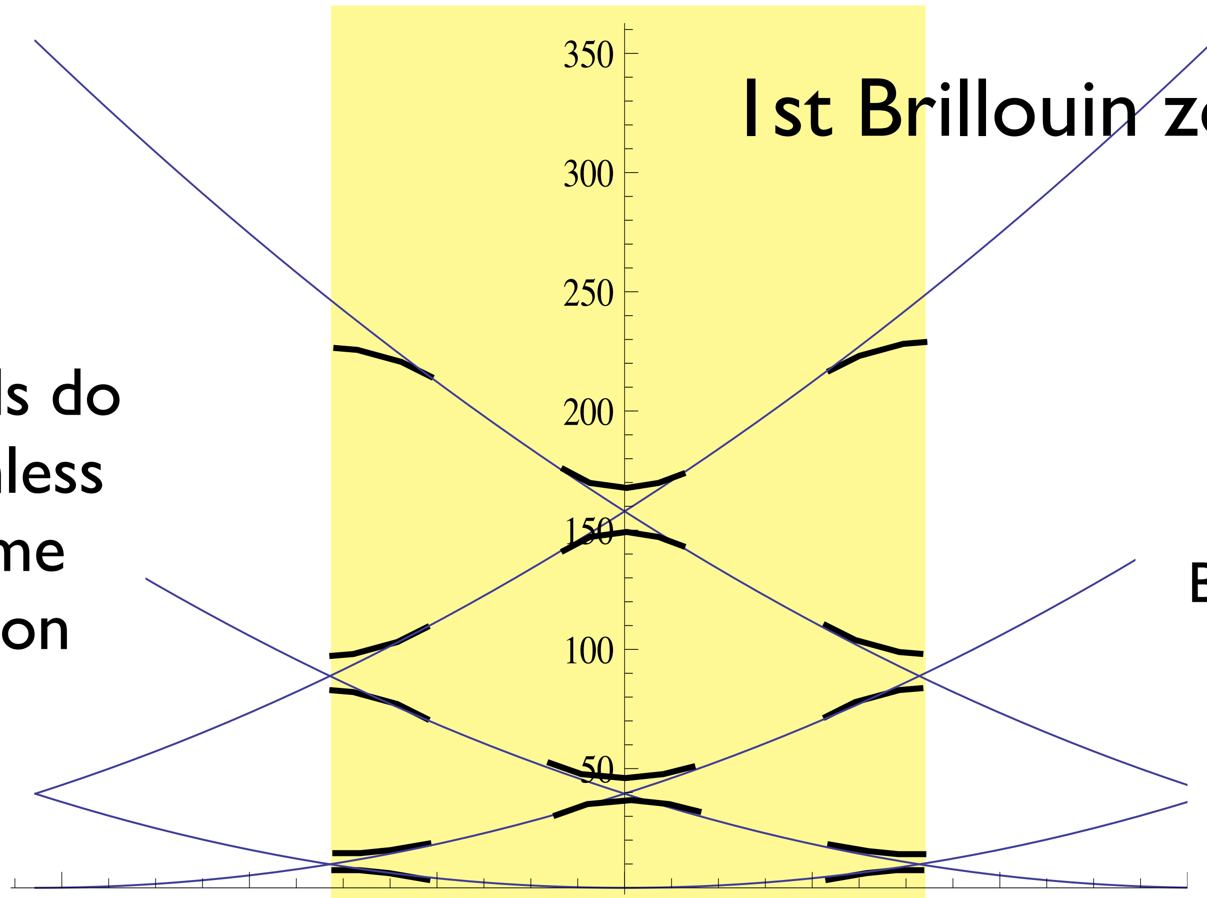
- Then we interpret plane wave states with “large” p instead as Bloch states of higher bands with crystal momentum k=p-G, with G chosen to make k small
- Then we can always choose k inside the “smallest” unit cell of the reciprocal lattice = the first Brillouin zone

Nearly free electrons



reduced zone scheme

Nearly free electrons



-π/a π/a

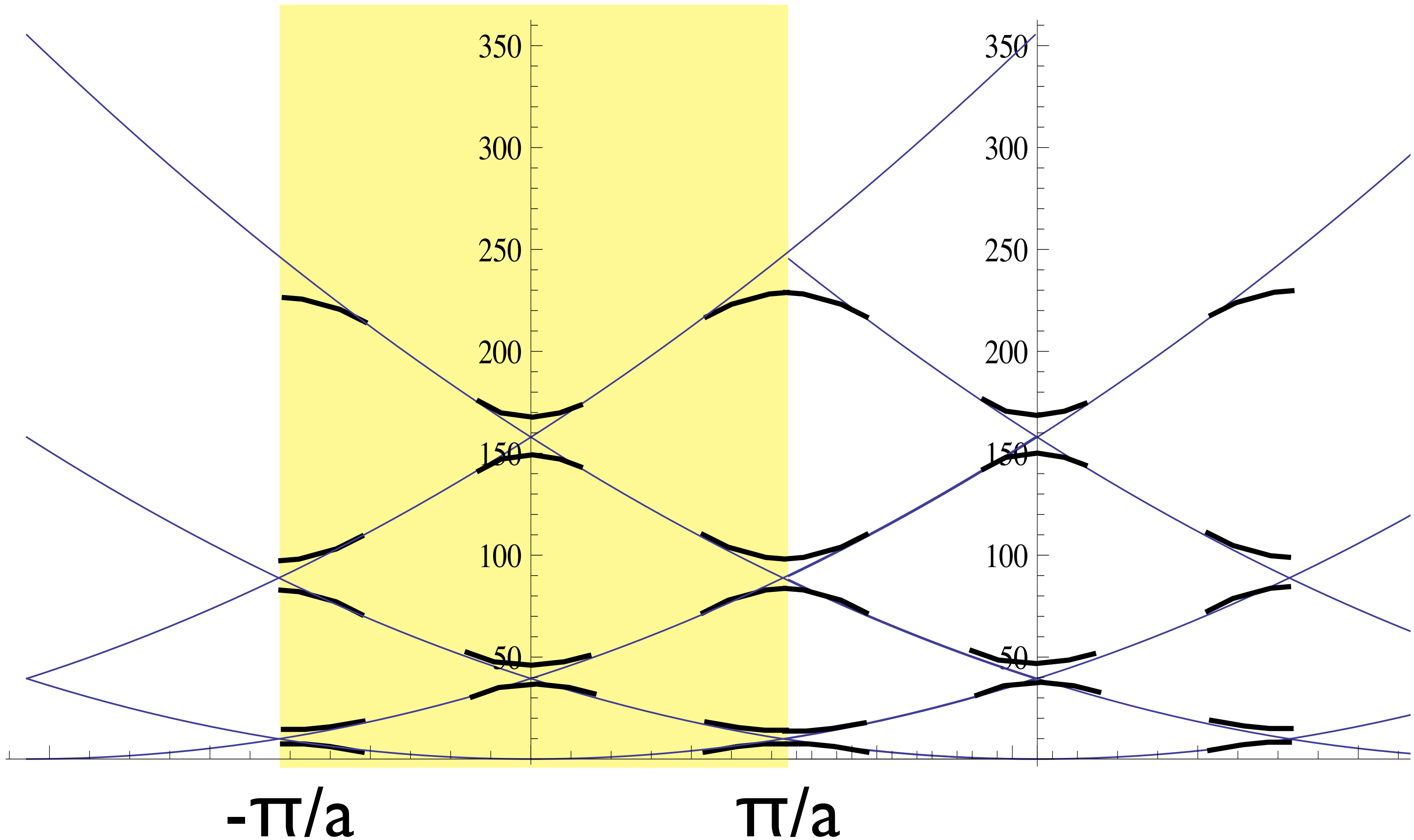
reduced zone scheme

typically bands do not cross, unless there is some special reason

the avoided crossings correspond to Bragg reflections

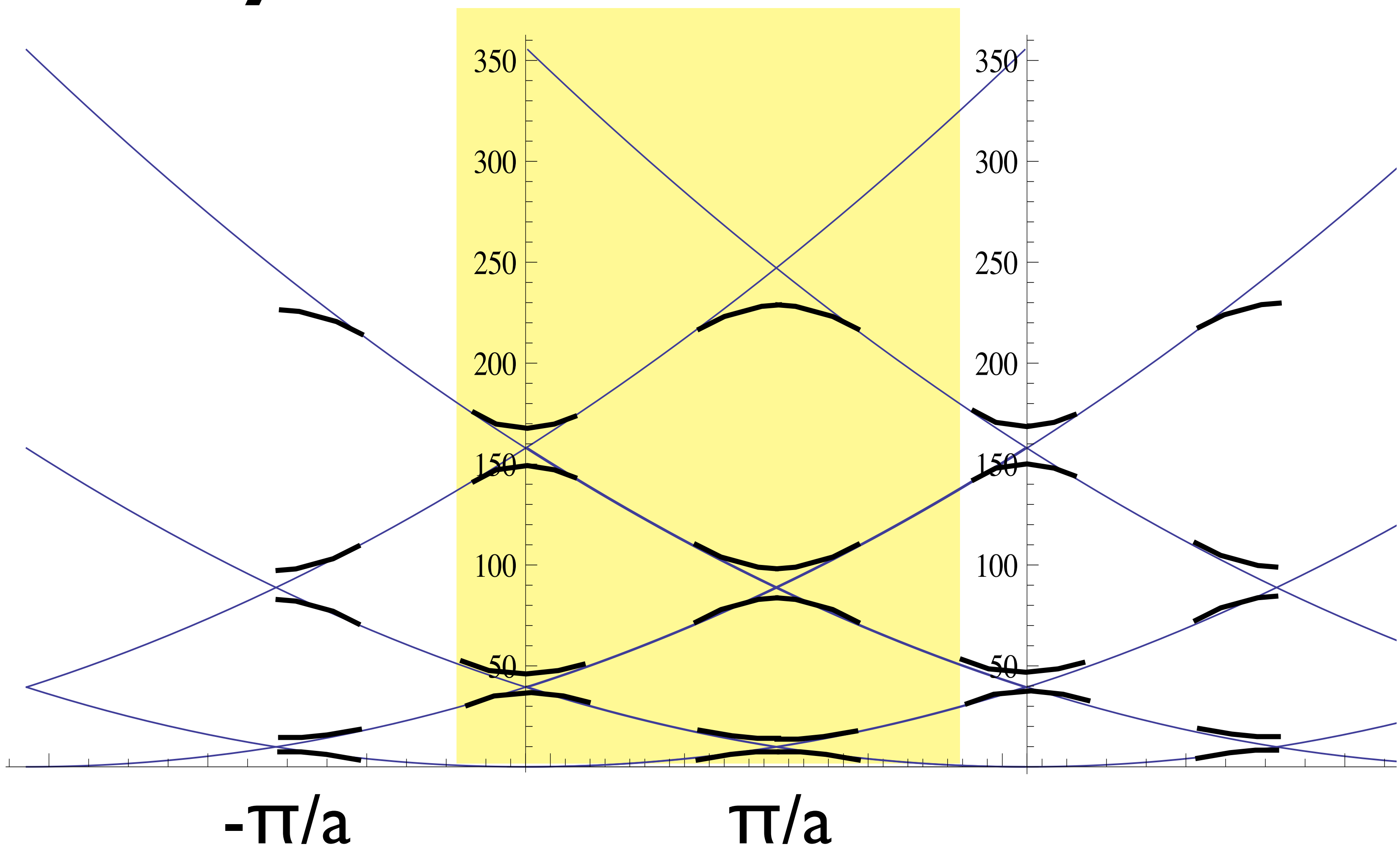
"bonding" state/ valence band is lowered in energy

Nearly free electrons



repeated zone scheme (sorry bad drawing)

Nearly free electrons



note: any translation of the 1BZ is just as good, really.

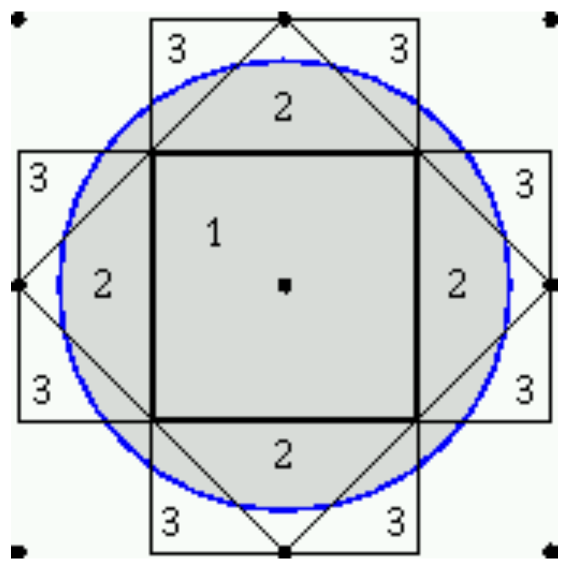
Nearly free electrons

- Generally, we expect non-degenerate (non-crossing) bands to be smooth, analytic functions $\varepsilon_n(k)$ of k.
- They are periodic by construction, so $\varepsilon_n(k+G) = \varepsilon_n(k)$
- If we don't mind redundancy, we can regard them all as functions of all k, not just in 1BZ
    - this is called the repeated zone scheme
    - but we need to remember that k and k+G represent the same state in this scheme!

NFE Fermi surfaces

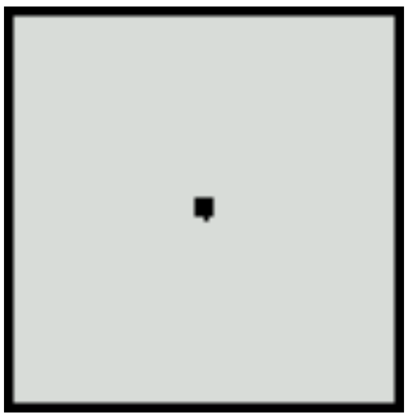
- in 2d or 3d, it becomes hard to draw $\varepsilon_n(k)$
- Instead we draw the Fermi surface

2,3... represent "higher Brillouin zones" = independent regions that map back to the 1BZ. All the states associated to one BZ form one band. Higher BZ's give higher energy bands.

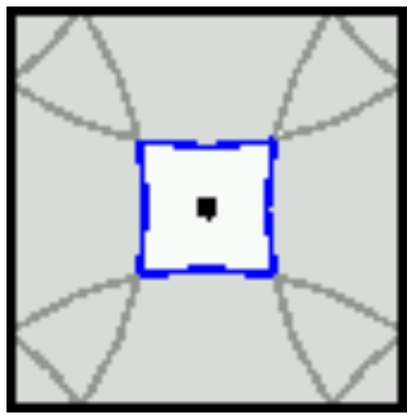


it should all be translated back into the 1BZ

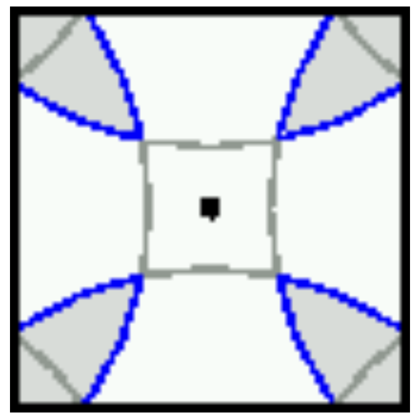
Folded back



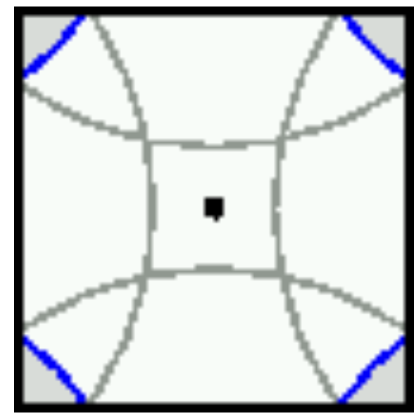
1BZ



2BZ



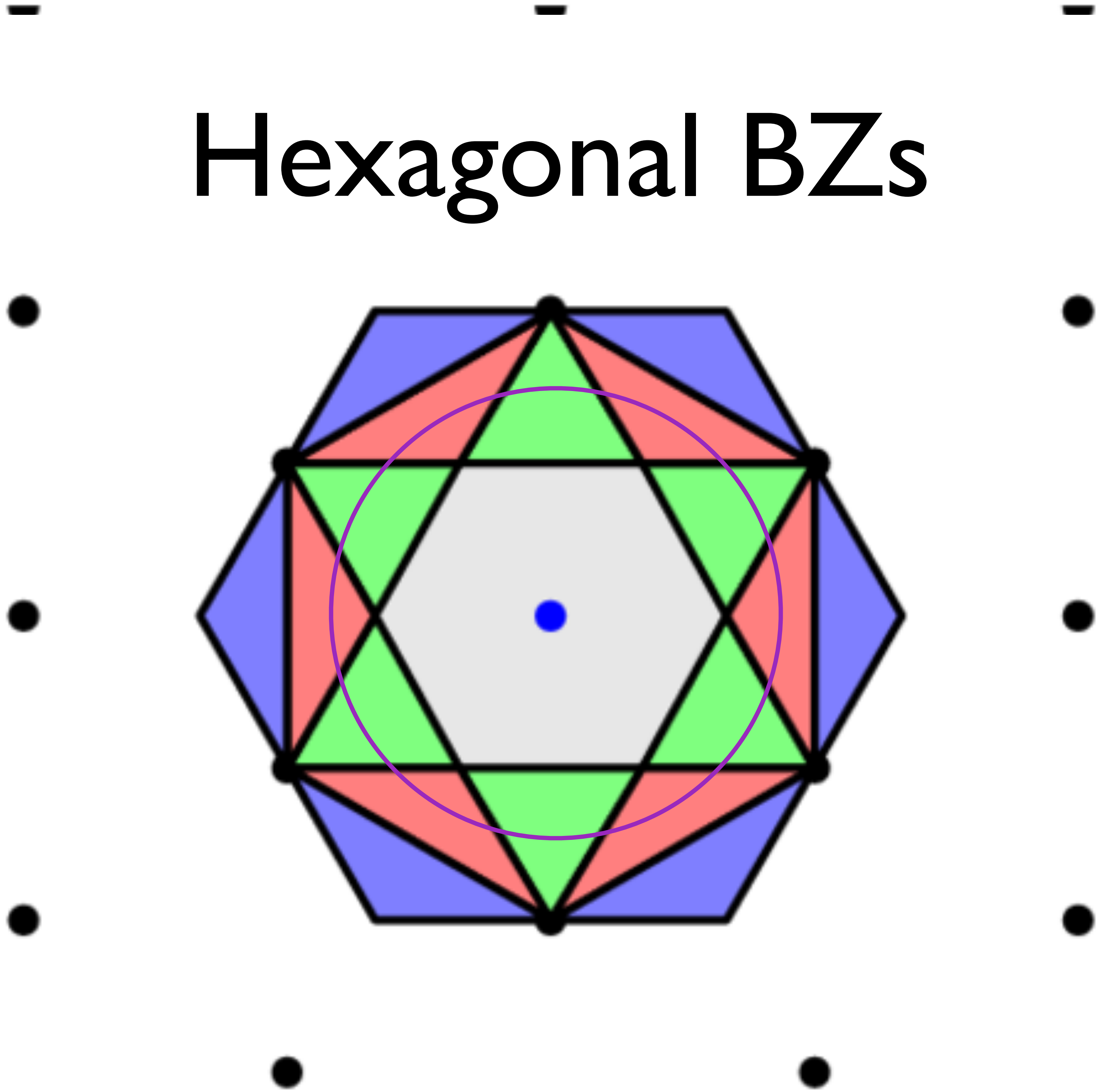
3BZ



4BZ

I could draw the rest, but see Kittel for more pictures

Hexagonal BZs



Fermi surface pockets