SEMICONDUCTORS I

Dan Weatherill

BAND THEORY I

OUTLINE

- How bandstructure arises from basic QM
- Free Electron Gas
- Bloch's Theorem
- NFEM approach & Tight Binding Approach
- Important Properties of bandstructure
- Quasiparticles, crystal Momentum
- Density of States
- Electrons & Holes
- parabolic band approximation & effective mass
- Phonons
- Silicon & GaAs bandstructures

Hopefully, much of this is (perhaps not recent!) revision

INTRO

In this lecture we will look at the (very light touch) basics of how bandstructure appears from simple quantum mechanical considerations.

We will then discuss the parabolic band approximation which is relevant for >90% of semiconductor detector work (if you are working on the CDMS experiment you will need another lecture...)

Once we have bandstructure, we can then start doing actual "semiconductor physics" but we won't talk about that until lecture #2.

This is probably the "drier" part, stick around and it gets more relevant after we cover the background. Please feel free to put up hands throughout for questions.

There is a lot of detail we won't even touch on, but is important and relevant. The last slide gives a good selection of books to look into this further!

BLOCH'S THEOREM

A simple (but quite profound) result arising from the assumption of **translational symmetry** in the solid state. Bloch's theorem states:

> *Solutions to the Schrödinger equation in a periodic potential take the form:*
> $|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$
> *where* $u(\mathbf{r})$ *is a function with the same periodicity as the potential*

PROOF

We do the proof in 1D for clarity, but extension to 3D is pretty easy! Define a translation operator $\hat{T}_n$ such that:

$$\hat{T}_n\,|\psi(r)\rangle = |\psi(r+na)\rangle$$

where a is the lattice constant. Clearly $\hat{T}_n$ is a unitary operator.

Because the potential is periodic, this operator must commute with the Hamiltonian (and therefore energy eigenstates are also translation eigenstates).

Consider:

$$\hat{T}_n \hat{T}_m \left|\psi(r)\right\rangle = \left|\psi(r + na + ma)\right\rangle = \hat{T}_{n+m} \left|\psi(r)\right\rangle$$

If the eigenvalues of $\hat{T}_n$ are given by λ_n then the above implies:

$$\lambda_n \lambda_m = \lambda_{n+m}$$

which is satisfied, for example, by:

$$\lambda_n = Ae^{zna}; \quad z \in \mathbb{C}$$

Using normalization, we have:

$$\left\langle\psi\middle|\psi\right\rangle = \left\langle \psi \middle| \hat{T}_n^\dagger \, \hat{T}_n \psi \right\rangle = \lambda_n \lambda_n^* \left\langle\psi\middle|\psi\right\rangle; \quad \therefore \left\langle\psi\middle|\psi\right\rangle = \left|\lambda_n\right|^2$$

i.e. $\left|\lambda_n\right|$ = 1 and hence $\lambda_n = e^{ikna}$ for some $k \in \mathbb{R}$.

The above allows us to write:

$$\hat{T}_n \left|\psi(r)\right\rangle = e^{ikna} \left|\psi(r)\right\rangle$$

which can be satisfied for states $\left|\psi\right\rangle$ which can be written:

$$\left|\psi(r)\right\rangle = e^{ikr} u(r); \quad \text{iff} \quad u(r) = u(r + na)$$

since $\hat{T}_n$ commutes with the Hamiltonian, these states are clearly also the eigenstates of the Hamiltonian.

FREE ELECTRON MODEL

The Drude-Sommerfeld (free electron) model is a combination of the classical Drude conductivity model with fermi-dirac statistics. Electrons are assumed **independent**. Consider the equation of motion of each particle in a classical gas, acted on by an external Lorentz force (forget magnetic force for now), and which scatter back to zero momentum with a timescale τ.

$$\langle \mathbf{p}(t+\delta t)\rangle = \left(1-\frac{\delta t}{\tau}\right)\langle \mathbf{p}(t)\rangle - q\mathbf{E}$$

$$\frac{d\langle \mathbf{p}\rangle}{dt} = -q\mathbf{E} - \frac{\mathbf{p}}{\tau}$$

defining current density in terms of electron velocity as $\mathbf{J} = -qn\mathbf{v}$, we then find

$$\mathbf{J} = \frac{q^2\tau n}{m}\mathbf{E}$$

so the conductivity σ is :

$$\sigma = \frac{nq^2\tau}{m}$$

NOTE that in this model we have the (average) electron velocity $\mathbf{v}$ proportional to electric field $\mathbf{E}$. This is due to the diffusive nature of the transport: the scattering back to zero breaks the usual pattern of Force being proportional to field. We then can define another quantity μ called **mobility** by:

$$\mathbf{v} = \mu\mathbf{E}$$
$$\mu = \frac{q\tau}{m} \quad \therefore \quad \sigma = \mu q n$$

NEARLY FREE ELECTRON METHOD (NFEM)

- **Assume periodic potential is weak** then Bloch's theorem and insight from free electron gas imply that the electron wavefunctions are modified plane waves. The Hamiltonian is assumed to be that for a free electron plus a weak periodic perturbation representing the crystal lattice
- **Still Assume independent electrons** we are not dealing with superconductivity or spintronics here! For non-cryogenic semiconductors, assuming electrons don't directly interact with each other is fine. (Bandstructure as a concept doesn't really work if this doesn't apply)

Again we'll look in 1D but logic extends to 3D easily. Bloch's theorem tells us that the wavefunctions will be periodic, so we can write them as a Fourier series.

$$|\psi(x)\rangle = e^{ikx}u_k(x) = e^{ikx}\sum_p c_p(k)e^{\frac{2\pi ipx}{a}}$$

The potential $\hat{V}(r)$ is (by definition) also periodic, so that:

$$V(x) = \sum_p V_p e^{\frac{2\pi i p x}{a}}$$

Assuming nearly free electrons, we can consider single particle states $\psi_k(x)$ obeying the TISE:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}\right)|\psi_k\rangle = E_k|\psi_k\rangle$$

and noting that:

$$-\frac{\nabla^2}{2}|\psi\rangle = e^{ikx}\sum_p c_p(k)\frac{(k+\frac{2\pi p}{a})^2}{2}e^{\frac{2\pi i p x}{a}}$$

$$\hat{V}(x)|\psi\rangle = e^{ikx}\sum_p\sum_q c_p(k)V_q e^{\frac{2\pi i(p+q)x}{a}}$$

we simply substitute into the TISE to get:

$$\sum_p \left(\frac{\hbar^2 (k + \frac{2\pi p}{a})^2}{2m} - E_k \right) c_p(k) e^{\frac{2\pi i p x}{a}} + \sum_q \sum_p V_q c_p(k) e^{\frac{2\pi i (p+q) x}{a}} = 0$$

a simple re-labelling of variables then gets us:

$$\sum_p \left(\frac{\hbar^2 (k + \frac{2\pi p}{a})^2}{2m} - E_k \right) c_p(k) e^{\frac{2\pi i p x}{a}} + \sum_q \sum_p V_q c_{p-q}(k) e^{\frac{2\pi i p x}{a}} = 0$$

The only way to satisfy this equation for all values of x is if each of the p terms separately vanishes, and hence:

$$\left(\frac{\hbar^2 (k + \frac{2\pi p}{a})^2}{2m} - E_k \right) c_p(k) + \sum_q V_q c_{p-q}(k) = 0$$

THE CENTRAL EQUATION

$$\left(\frac{\hbar^2(k+\frac{2\pi p}{a})^2}{2m}-E_k\right)c_p(k)+\sum_q V_q c_{p-q}(k)=0$$

this is one of the most common ways to write what is called the **central equation** which gives us constraints between the allowed Fourier coefficients of the Bloch wavefunctions and the Fourier coefficients of the periodic potential.
As might seem obvious, analytic (or even simple numeric) solutions of this are all but impossible for realistic situations. There are whole fields of theoretical condensed matter physics devoted to solving this problem. Modern approaches are dominated by *Density Functional Theory*, or the *Hartree-Fock approximation* (way beyond the scope of today). However, there are two useful cases to look at now.

THE EMPTY LATTICE

If the lattice is empty, we have

$$V(x) = 0$$

and so all the V_m vanish and the central equation now reads:

$$\left(\frac{\hbar^2 (k + \frac{2\pi p}{a})^2}{2m} - E_k \right) c_p(k) = 0$$

To have non-trivial solutions for the electron wavefunction (i.e. for $c_p(k)$ not to all vanish) we then obtain the dispersion relationship

$$E_n(k) = \frac{\hbar^2 (k + \frac{2\pi p}{a})^2}{2m}$$

i.e. the free electron result but periodic in k-space.

THE KRONIG-PENNEY MODEL

Often, this model is solved via directly solving the TISE, which can be done in the case of an infinitely repeating narrow "top hat" potential. A very related solution using the machinery of the central equation can solve the problem in the case of an infinitely repeating delta function potential in 1D.

We write the potential as:

$$V(x) = A \sum_{n=-\infty}^{\infty} \delta(x - na)$$

whose Fourier series representation is given by:

$$V(x) = \frac{A}{a} \sum_{n} e^{\frac{2\pi nix}{a}}$$

(i.e. all the V_q in the central equation are equal to a constant $\frac{A}{a}$)

The central equation then reduces to:

$$\left(\frac{\hbar^2(k+\frac{2\pi p}{a})^2}{2m}-E_k\right)c_m(k)+\frac{A}{a}\sum_n c_n(k)=0$$

From our original definition of the wavefunction, we note that:

$$\sum_n c_n(k)=\psi(x=0)=u(x=0)$$

where u is the periodic (Bloch) function part of the wavefunction. Substituting in and rearranging, we obtain:

$$c_p(k)=\frac{\frac{2m}{\hbar^2}\frac{A}{a}}{\frac{2mE_k}{\hbar^2}-(k+\frac{2\pi p}{a})^2}u(0)$$

If we use the "trick" of again summing both sides over all p, we can then see that:

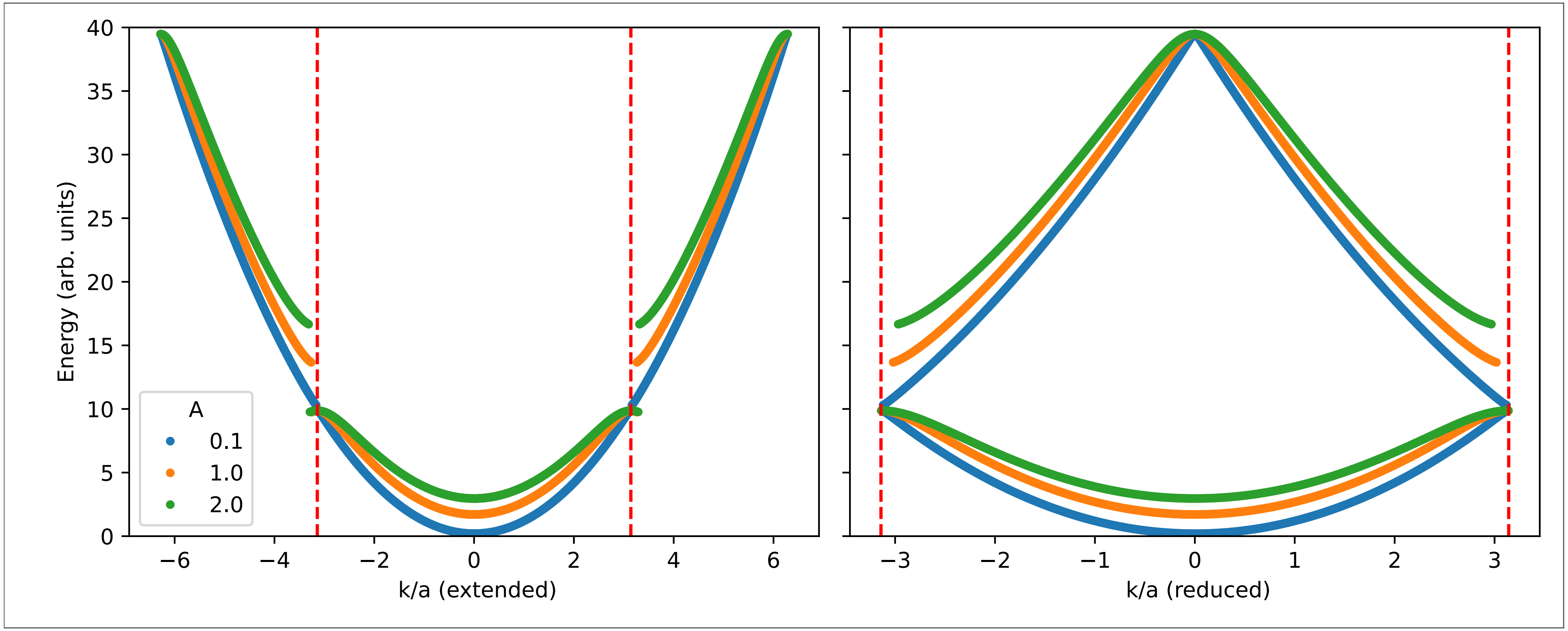
$$\frac{a}{A}u(0) = \sum_p \frac{\frac{2m}{\hbar^2}}{\frac{2mE_k}{\hbar^2} - (k + \frac{2\pi p}{a})^2}u(0)$$

from which we can now drop the $u(0)$ on both sides. Hopefully at this point you can see that this can be solved quite simply numerically. What is less obvious, is that it has an analytical solution. Using the definition of the infinite sum of the cotangent (and ~20 lines of algebra not shown here!) the above leads to:

$$\cos(ka) = \cos\left(\frac{\sqrt{2mE_k}}{\hbar}\right) + \frac{A}{\hbar}\sqrt{\frac{m}{2E_k}}\sin\left(\frac{\sqrt{2mE_k}}{\hbar}\right)$$

clearly, there are values of k for which no valid solution of E_k exists!
This solution can also be substituted back into the central equation to iteratively find the Fourier coefficients of the wavefunction $c_p(k)$ (for semiconductor physics work, we actually don't care too much about those!)

QUICK GRAPH OF NFEM BANDSTRUCTURE WITH δ POTENTIAL



CONSEQUENCES OF NFEM & BANDSTRUCTURE

> ***all*** *peturbative periodic potentials (except the empty lattice!) introduce band gaps! This can be thought of in terms of Bragg scattering of the electron wavefunctions off the Brillouin zones*

- (side note): analogous with X-ray diffraction, scattering amplitudes are proportional to the structure factor. Systematic absences and also 0 motif factors can allow band gaps to "close up" in 3D for some particular symmetry directions in particular structures (Silicon X-point is the quintissential example - see later).
- Because of the discrete translational symmetry, all states can be "folded" back into the 1st Brillouin zone. In 1D, this is the reciprocal space between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$. In higher dimensions, it is constructed as the Wigner-Seitz cell / Voronoi cell of the reciprocal lattice (ask if interested).

TIGHT BINDING APPROACH / LCAO

Start from the opposite picture to NFEM: electron states are tightly coupled to atom states and move around by "hopping" between sites.
Assume that the potential around a particular site can be approximated as a **Linear Combination of Atomic Orbitals (LCAO)**. Then the eigenfunctions of the Hamiltonian, similarly are a linear combination of the energy eigenstates of those orbitals (think of mixinfg the spherical harmonic eigenfunctions for the Hydrogenic model).
In reality, the best basis to use for this method in the solid state context are probably the **Wannier Functions** - way beyond our purposes today. For the purposes of simplicity we will also assume the orbitals are orthogonal, but this is not necessary for the model to work.
Again, we will look at a 1D chain of atoms and derive the band structure

SINGLE ORBITAL

We start by considering a single atomic orbital $|\phi_n\rangle$ where n labels the atom number associated with that orbital.
Clearly, atomic orbitals by themselves don't obey Bloch's theorem. But we can make a total linear combination of them obey it by using the ansatz:

$$|\psi\rangle = \sum_n e^{ikna} |\phi_n\rangle$$

(exercise for the reader: prove that this does satisfy Bloch's theorem!)
Using the variational method to find the ground state, we have:

$$\hat{H}|\psi\rangle = \sum_n e^{ikna} \hat{H} |\phi_n\rangle$$

$$\Rightarrow \left\langle \psi \middle| \hat{H} \middle| \psi \right\rangle = \sum_{n,m} e^{ik(n-m)a} \left\langle \phi_m \middle| \hat{H} \middle| \phi_n \right\rangle = E_{nk} \langle\psi|\psi\rangle$$

we then assume that electrons can only "hop" one orbital at a time, i.e. we need only consider nearest neighbours in the sum above. We label the matrix elements $\mathcal{H}_{n,m} = \left\langle \phi_n \middle| \hat{H} \middle| \phi_m \right\rangle$ such that we can write:

$$E_{nk} = \sum_{n,m} e^{ik(n-m)a} \mathcal{H}_{n,m} = \mathcal{H}_{n,n} + e^{ika}\mathcal{H}_{n,n+1} + e^{-ika}\mathcal{H}_{n,n-1}$$

It is reasonable (in 1D at least) to assume that the energy cost for hopping "left" is the same as for hopping "right", and we'll call this cost t. There is an onsite energy for the electron ϵ also. We then have:

$$E_{nk} = \epsilon - t\left(e^{ika} + e^{-ika}\right) = \epsilon - 2t\cos(ka)$$

NOTES FROM TIGHT BINDING

- For one orbital we only get one band, but it still has disallowed energies - i.e. everything outside the band!
- For each orbital we add to LCAO we will get another band in the dispersion.
- The band looks very much like free electrons for small $|\boldsymbol{k}|$

BUT WHAT IS k ?

In the dispersion of **free electrons**, we have:

$$E = \frac{\hbar^2}{2m}|\mathbf{k}|^2$$

So, by analogy with classical mechanics, $\hbar\mathbf{k}$ is the momentum:

$$E = \frac{|\mathbf{p}|^2}{2m} \therefore \mathbf{p} = \hbar\mathbf{k}$$

In solid state physics, we call $\hbar\mathbf{k}$ the **crystal momentum** because there is a subtlety.

Consider the action of the quantum mechanical momentum operator on a Bloch state:

$$\hat{p}\,|\psi\rangle = -i\hbar\frac{\partial}{\partial x}|\psi\rangle = \hbar k e^{ikx}u - i\hbar e^{ikx}\frac{\partial u}{\partial x} = \hbar k\,|\psi\rangle - i\hbar e^{ikx}\frac{\partial u}{\partial x}$$

i.e. ***Bloch states are not momentum eigenstates****!*

WAIT, WHAT?

- The states we are dealing with are **not quite electrons**. More correctly we might call them "quasi-electrons". These states cannot and do not exist outside of the lattice.
- Crystal momentum is conserved, but only up to a factor of the reciprocal lattice vector. The translational symmetry of the lattice is a discrete (not continuous) symmetry. The quantity that is conserved is $\hbar k \bmod \frac{2\pi}{a}$
- *Technical note* because the symmetry which generates crystal momentum is discrete, its associated conservation law cannot be directly derived using Noether's theorem
- Luckily, **for most purposes in semiconductor physics**, you can think of crystal momentum as momentum (absorption, scattering, laws of motion etc)

DENSITY OF STATES

- If a system is well described by a bandstructure **(plenty of caveats there)**, then in principle the **dispersion relation** $E(\mathbf{k})$ contains all dynamical information about the electron (and hole, we'll get there!) states.
- The related quantity of **density of states per unit volume** $g(E)$ is also often needed. It is unambiguously defined by the combination of the dispersion relation and the geometry of the system.
- A corollory of Bloch's Theorem is that when it applies, we also have Born-von Karman boundary conditions (i.e. periodic boundary conditions). A consequence is that the Bloch waves have wavelengths which are integer multiples of the lattice periodicity. This, in turn, means that **states are evenly spaced in** k **space**

This gets quite messy in 3D, so we stick to 1D for now (and show some 3D pictures later). Because of the above condition, we can immediately write down the density of states in k space:

$$g(k) = 2\frac{L}{2\pi}$$

where L is the total size of the system. (In 3D we could write $g(\mathbf{k}) = 2\frac{V}{(2\pi)^3}$, but only if the system is isotropic in reciprocal space). The 2 in front comes from the fact that for each value of k, we can fit 2 electrons (via spin). This factor is different e.g. for phonons where typically we have 3 polarisation modes in 3D.

We obtain a very useful relationship by just considering counting the total number of states in the entire system:

$$\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} g(k)dk = \int_0^\infty g(E)dE$$

(This next bit is not rigorous, see Ashcroft & Mermin pp. 143-144 for chapter & verse)

Since $g(k)$ is a constant, the above suggests we can write:

$$g(E) = g(k)\left|\frac{dk}{dE}\right|$$

the extension to 3D is reasonable, if not obvious:

$$\boxed{g(E) = g(\mathbf{k})\int_{S(E)} \frac{1}{|\nabla_{\mathbf{k}} E|} dS}$$

where $S(E)$ is a contour of constant energy.

By analogy with classical optics, the quantity $\frac{\partial E}{\partial k}$ is called the **group velocity**.

The calculation and form of $g(E)$ is so important (more next time!) that we will look at several different "toy" examples in some detail

DENSITY OF STATES IN 1D CHAIN

Starting with the tight-binding dispersion for a 1D chain:

$$E = \epsilon - 2t\cos(ka)$$

we start by finding the group velocity:

$$v_g = \frac{\partial E}{\partial k} = -2t\sin(ka)$$

and then we use the previous expression for $g(E)$:

$$g(E) = \frac{L}{\pi}\frac{1}{|2t\sin(ka)|}$$

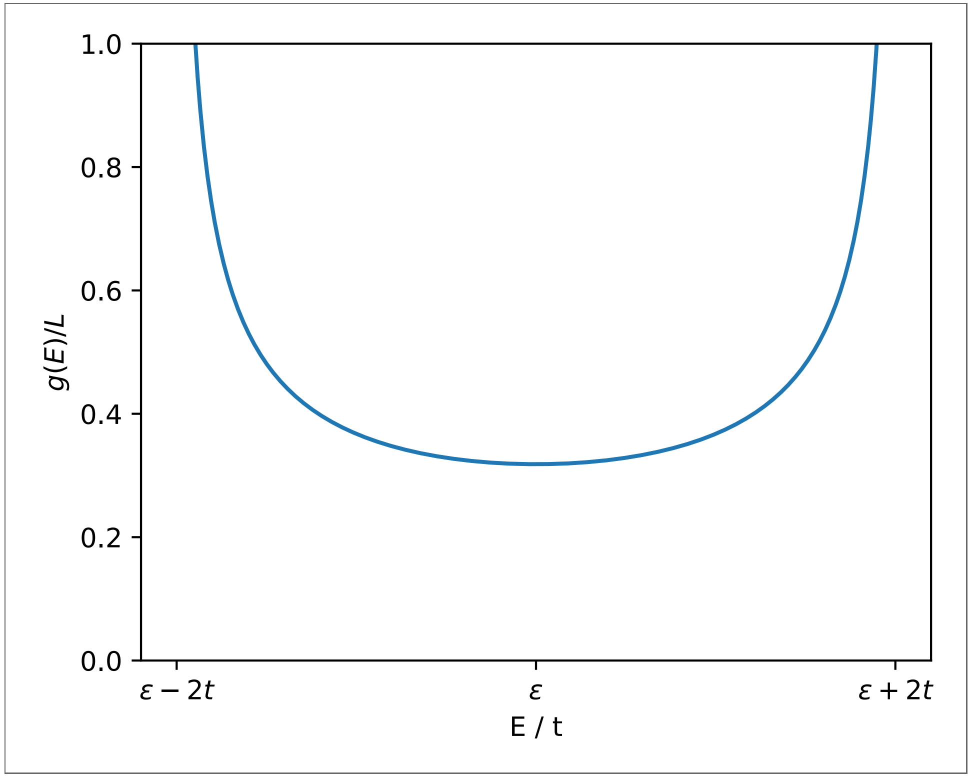
finally, we find an expression for $2t\sin(ka)$ in terms of E from the dispersion relationship

$$E = \epsilon - 2t\sqrt{1-\sin^2 ka}$$

$$\therefore \sqrt{1-\left(\frac{\epsilon - E}{2t}\right)^2} = \sin(ka)$$

and so the density of states is:

$$g(E) = \frac{L}{2t\pi}\frac{1}{\sqrt{1-\left(\frac{\epsilon-E}{2t}\right)^2}}$$


1.0
0.8
0.6
0.4
0.2
0.0
$g(E)/L$
$\varepsilon - 2t$
ε
$\varepsilon + 2t$
E / t

DENSITY OF STATES IN PARABOLIC BAND IN 1D, 2D, 3D

Assume a dispersion relationship of the form:

$$E = \frac{\hbar^2 k^2}{2m}$$

states are evenly spaced in k-space, so the "volume" of 1 k-state in dimension d is $\frac{L^d}{(2\pi)^d}$.

We can then consider the total volume of k-space filled up to energy E.

$$n = \frac{2}{(2\pi)^d} \int_0^{|k_{\max}|} \Omega_d k^{d-1} dk = \frac{2}{(2\pi)^d} \Omega_d \frac{|k|^d}{d}$$

Ω_d is the "spherical volume element" in d dimensions, $\Omega_1 = 2, \Omega_2 = 2\pi, \Omega_3 = 4\pi$.

The above implies:

$$\therefore |k| = \left(\frac{nd}{2} \frac{(2\pi)^d}{\Omega_d} \right)^{\frac{1}{d}}; \quad E = \frac{\hbar^2}{2m} \left(\frac{nd}{2} \frac{(2\pi)^d}{\Omega_d} \right)^{\frac{2}{d}}$$

This gives us, for 3D, the (hopefully!) familiar relationship:

$$k^3 = 3\pi^2 n$$

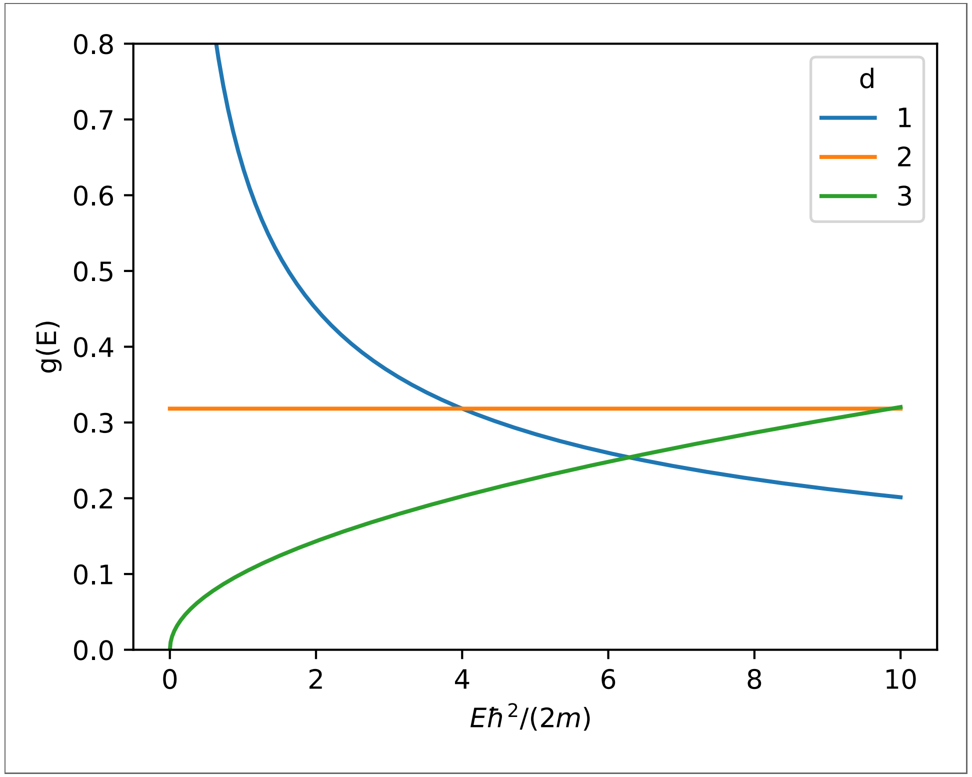
we can now find density of states $g(E)$ via:

$$g_d(E) = \frac{dn}{dE} = \frac{dn}{dk}\frac{dk}{dE} = \frac{2}{(2\pi)^d}\Omega_d|k|^{d-1} \times \frac{m}{\hbar^2 k}$$

$$\therefore g_d(E) = \frac{2m}{\hbar^2(2\pi)^d}\Omega_d\left(\frac{2mE}{\hbar^2}\right)^{\frac{d-2}{2}}$$

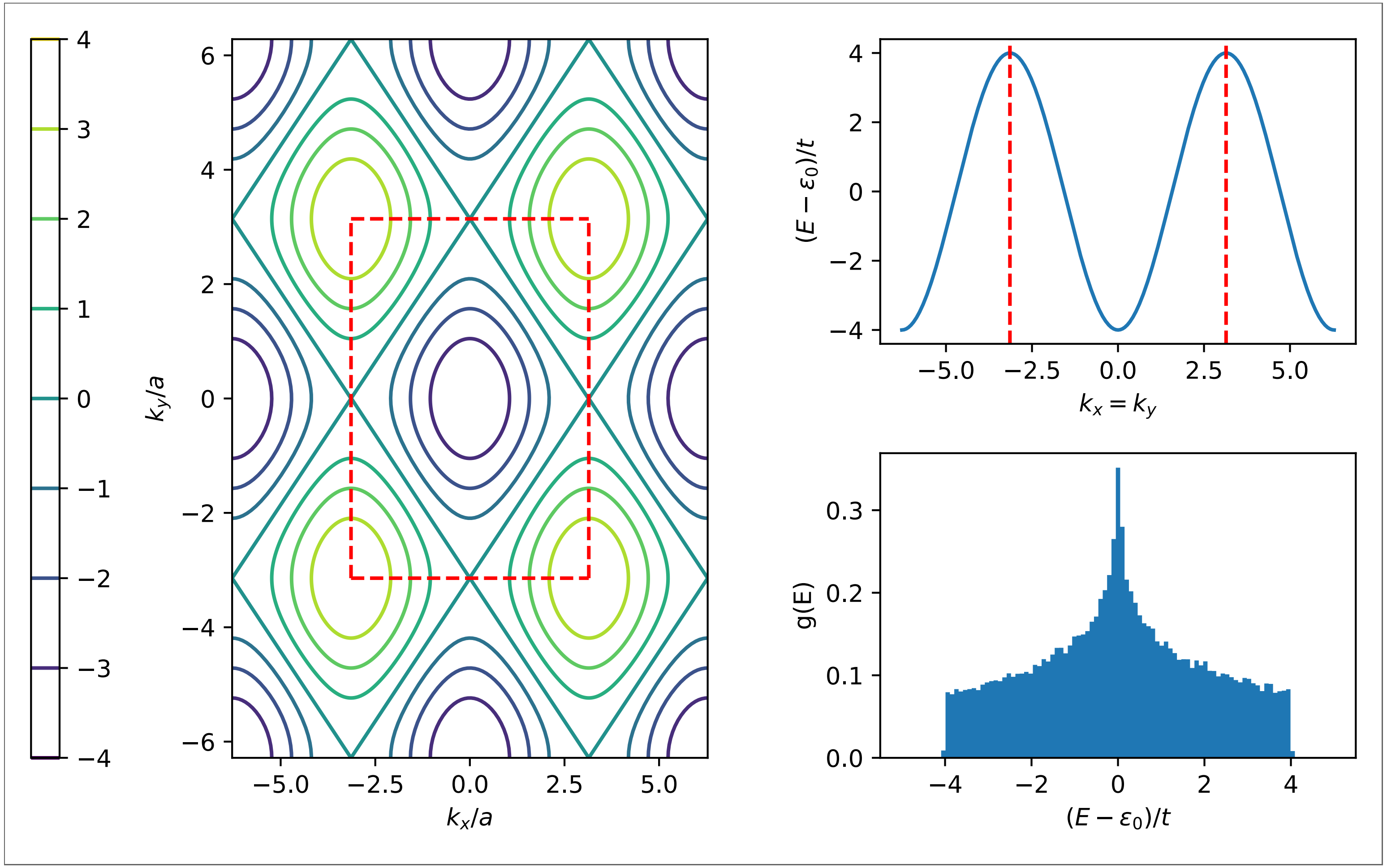
takeaway message (important!!):

$$g_1(E) \propto \frac{1}{\sqrt{E}}; \quad g_2(E) \propto E^0; \quad g_3(E) \propto \sqrt{E}$$


0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
g(E)
0
2
4
6
8
10
$E\hbar^2/(2m)$
d
1
2
3

DENSITY OF STATES IN 2D TIGHT BINDING

We now consider a dispersion relationship of the form:
$E = \epsilon_0 - 2t(\cos(k_x a) + \cos(k_y a))$
as in 1D, at small $|\mathbf{k}|$ this looks exactly like the parabolic case due to cos small angle formula.
The density of states must be calculated using the full integral over contours, though, and is more interesting.
It is based on the 2D case for parabolic bands, i.e. E^0
The DoS integral is impossible analytically. Numerically it is also very difficult. We estimate the DoS by randomly choosing $|\mathbf{k}|$ points, working out the energy, and plotting histograms

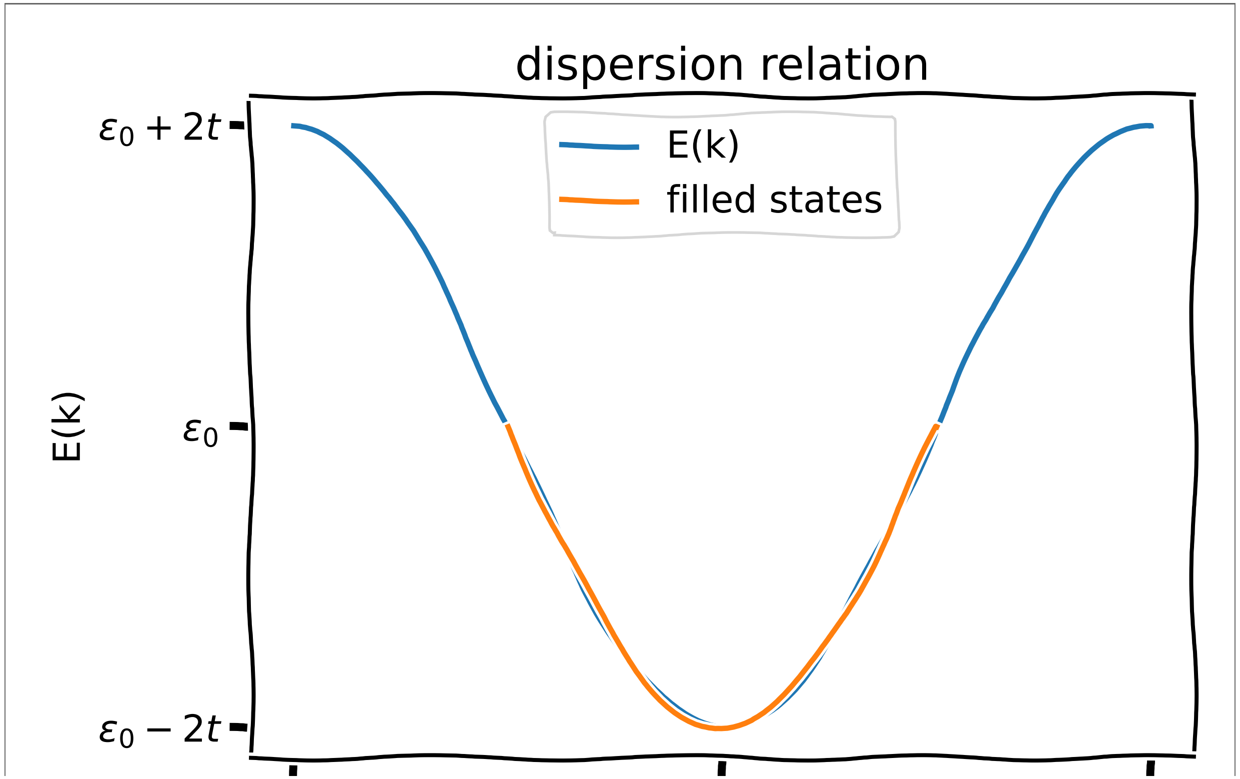

4
3
2
1
0
−1
−2
−3
−4
k_y/a
k_x/a
6
4
2
0
−2
−4
−6
−5.0
−2.5
0.0
2.5
5.0
$(E-\varepsilon_0)/t$
$k_x = k_y$
g(E)
$(E-\varepsilon_0)/t$
0.3
0.2
0.1
0.0

SIDE

- As a consequence of the periodicity of bandstructure, **the dispersion relation must cross the Brillouin Zone boundary at right angles**. This may lead to divergences in the density of states. Divergences may also occur (in 2D & higher) due to saddle points in the dispersion.
- A divergence in density of states is usually not a problem, because in calculations we generally integrate over it, and the nature of these divergences is logarithmic.
- These van-Hove singularities have important consequences on physical properties though, in particular on the optical absorption of the material.

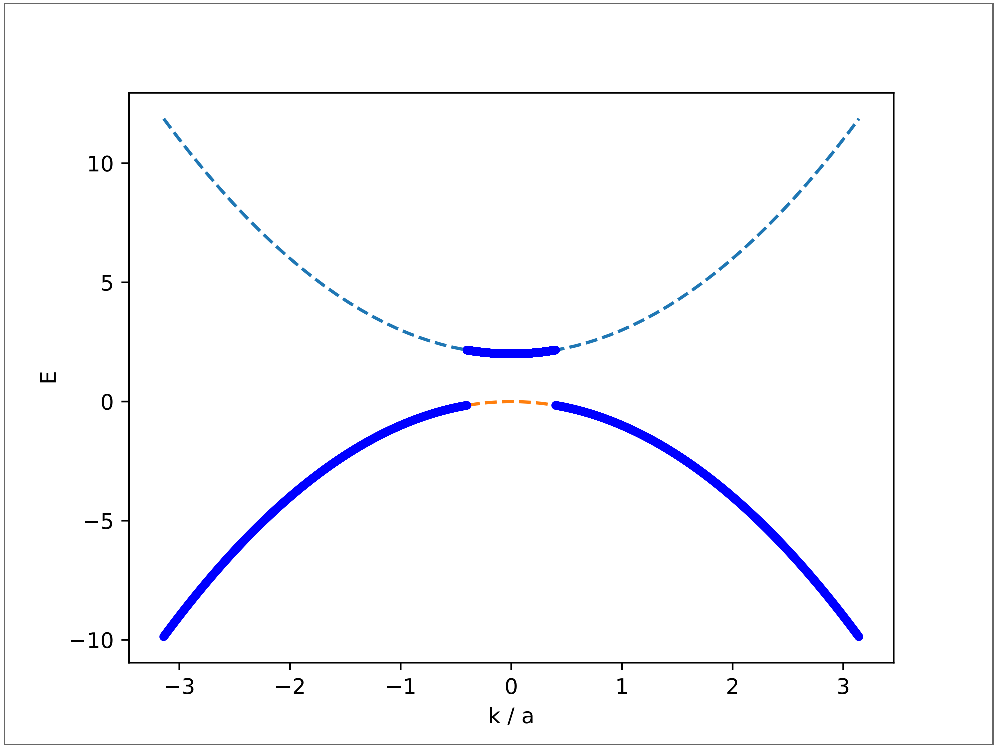
FILLING OF BANDS & FERMI LEVEL

Electrons are fermions, and as such they "fill up" from lower energies to higher ones. Due to spin, every available state in k space allows for 2 electrons. For example, a monovalent material which has 1 atom per unit cell in its structure has a half full band. The level at which the probability of occupation is 1/2 is called the "Fermi Level" (more on this next time)




$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
k

- At finite temperature, the occupation probability "smears" out around the Fermi level.
- If the Femi level is in a region without any density of states (i.e. in a "band gap"), then this smearing results in a small number of electrons being in the upper ("conduction") band, and almost all of the lower ("valence") band being filled.
- The empty electron states in the valence band can move around **as though they were themselves charge carriers**. We call these "holes".



PARABOLIC BAND APPROXIMATION

Recall that when we looked at the simple tight-binding model, we obtained a dispersion relation that looked like

$$E(k) = \epsilon - 2t\cos(ka)$$

If we consider values of $k \approx 0$ (i.e. near the bottom of the band), we can use the small angle approximation $\cos(\theta) \approx 1 - \frac{\theta^2}{2}$:

$$E(k) \approx \epsilon - 2t + t(ka)^2$$

Recall the dispersion relation for a free electron is:

$$E_{free}(k) = \frac{\hbar^2 k^2}{2m}$$

If we measure the energies with respect to the band edge, we can by analogy write

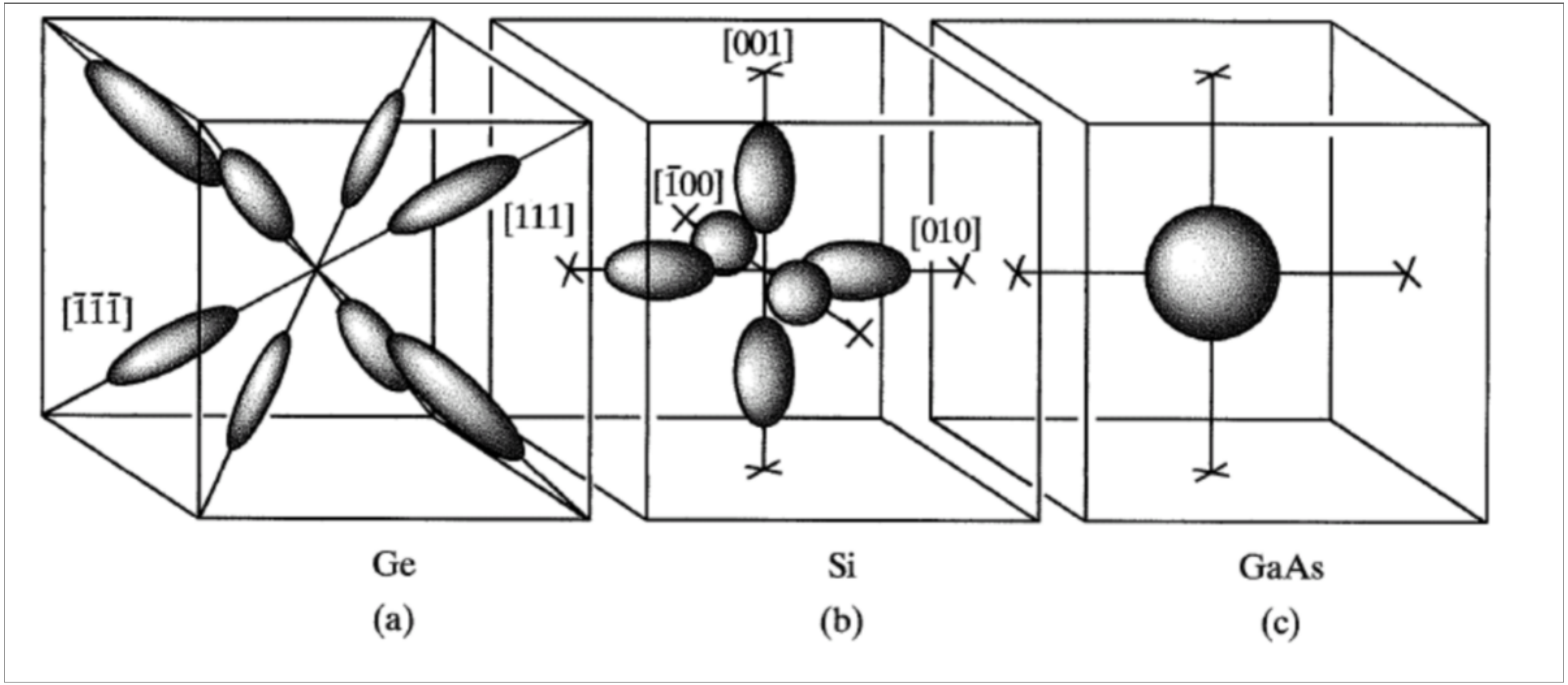
$$E(k) \approx \frac{\hbar^2 k^2}{2m^*}; \quad \text{where} \quad m^* = \frac{\hbar^2}{2ta^2}$$

The quantity m^* is called the **effective mass** and more generally is defined as:

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$$

for a particular dispersion relationship. The parabolic band approximation works the same way as a Taylor series - anything with a minimum or maximum looks quadratic if you zoom in enough.
This approximation turns out to be so convenient and useful that even though it is quite rough in many cases, in semiconductor physics we often go to quite extravagent lengths to preserve its validity (by patching up other bits of physics - we will talk about this next time). In particular, this is the basis of the "semi-classical" transport model - treating the particles as though they were free, with the details of the actual quantum mechanical physics encapsulated inside m^* (and a couple of other quantities).

EFFECTIVE MASS IN 3D

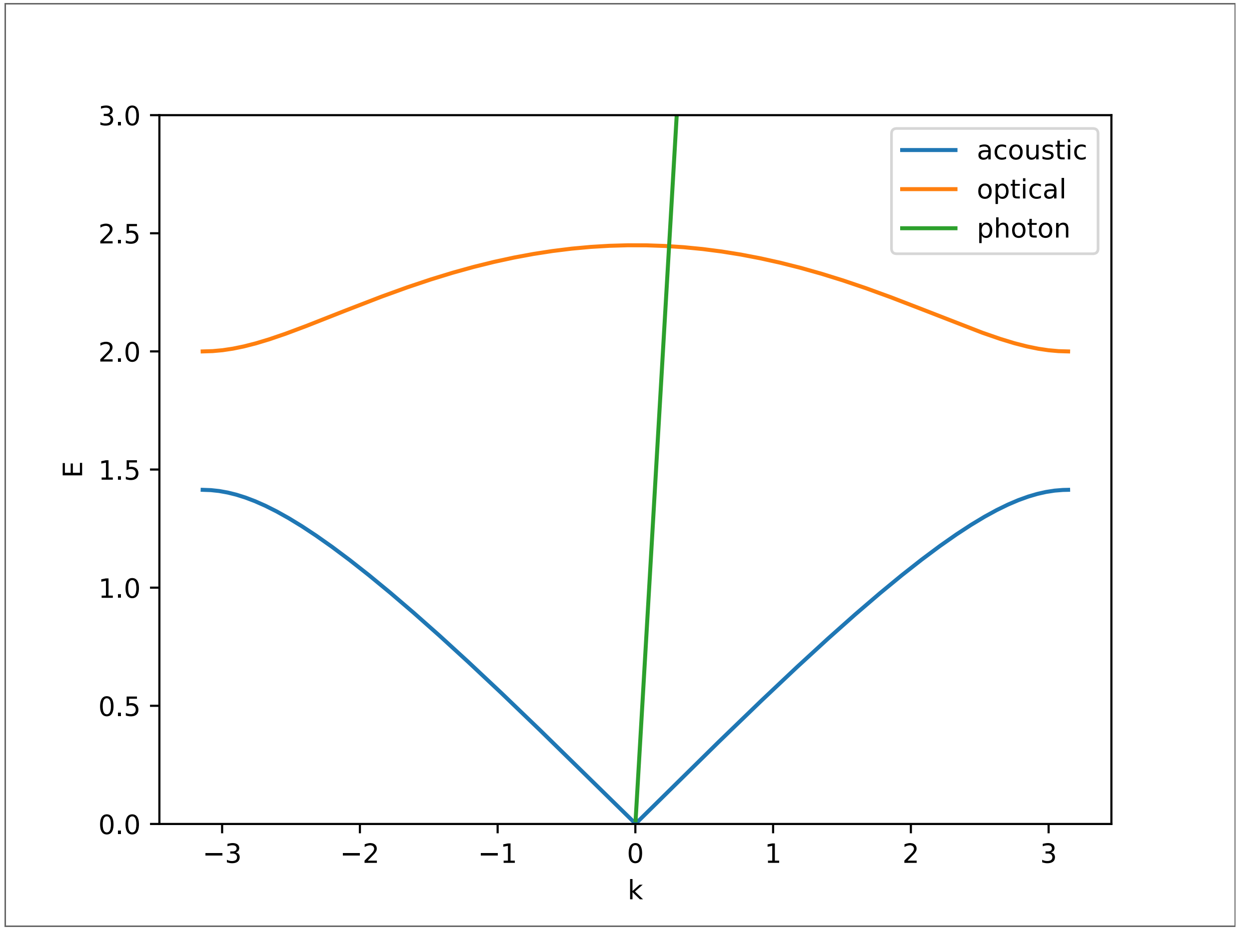


- Because k is a vector, in fact the effective mass is technically a tensor quantity.
- image above (from nanohub.org) shows constant energy ellipsoid shapes in k-space for Ge, Si and GaAs.

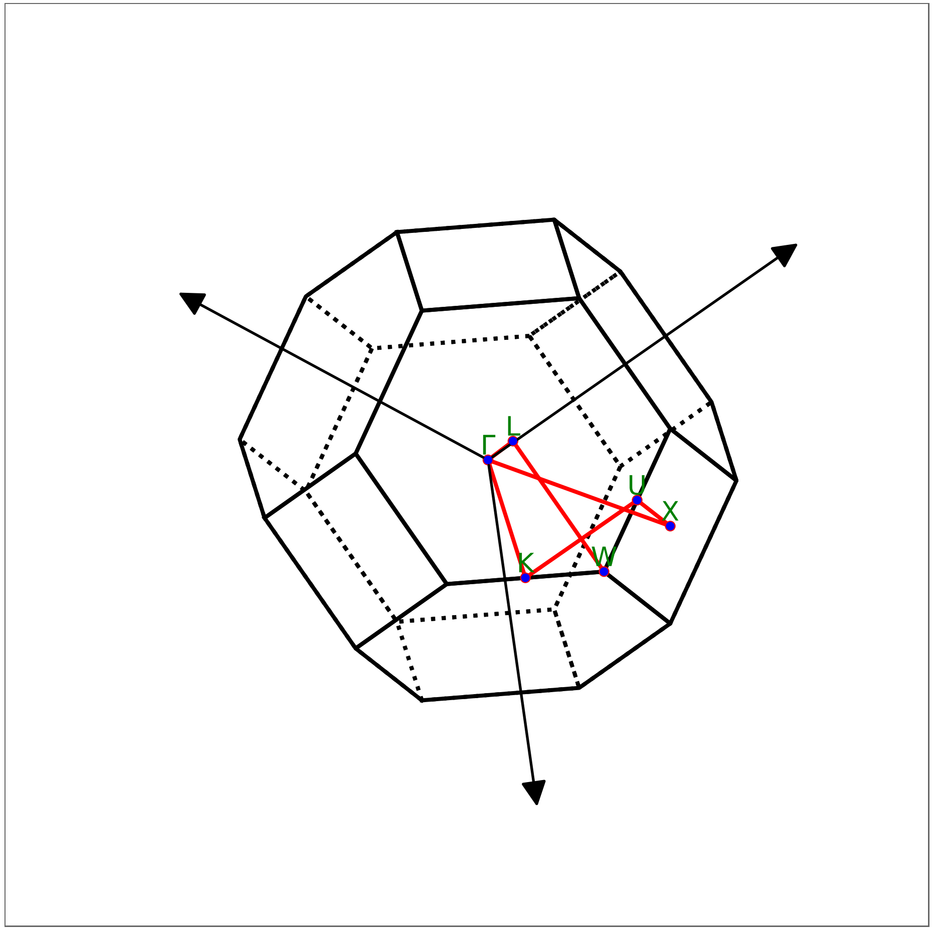
- In some situations, need to consider the directions separately (the details of this would be a whole hour talk on its own).
- In GaAs, due to its direct band gap and high symmetry, typically can use a scalar approximation
- In Si, typically we need **two** effective masses, depending on what calculation we are doing:
    - **density of states** we use the geometric mean of the principal components of the effective mass tensor. This is called m^*_{dos}
    - **Conductivity** we use the harmonic mean of the principal components. This is called m^*_{cond}

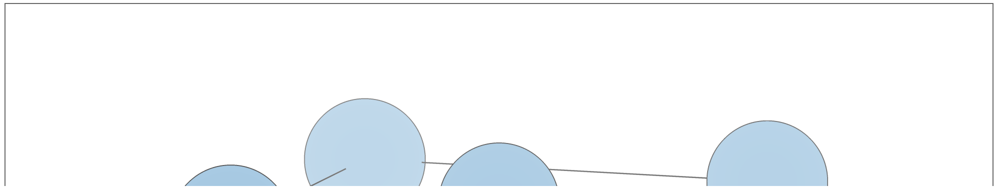
PHONONS

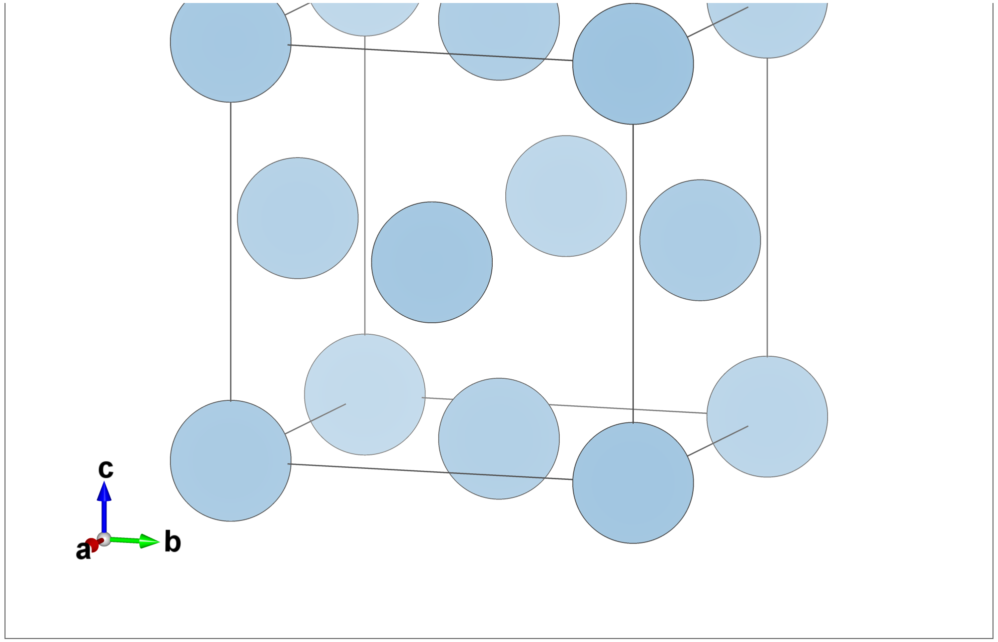
Lattice vibrations are also quantised. These bosonic quasi-particle excitations are called phonons. They carry energy, and crystal momentum.
For semiconductors, relevant as: - one of the principle energy loss mechanisms in electron transport - providing crystal momentum during absorption and emission to make sure crystal momentum conserved in indirect transitions
Responsible for most of the heat conductivity of the material, and also for sound transmission.
Can interact with photons (but only on the optical branch, for energy/momentum conservation reasons)


3.0
2.5
2.0
1.5
1.0
0.5
0.0
E
−3
−2
−1
0
1
2
3
k
acoustic
optical
photon

FCC STRUCTURE

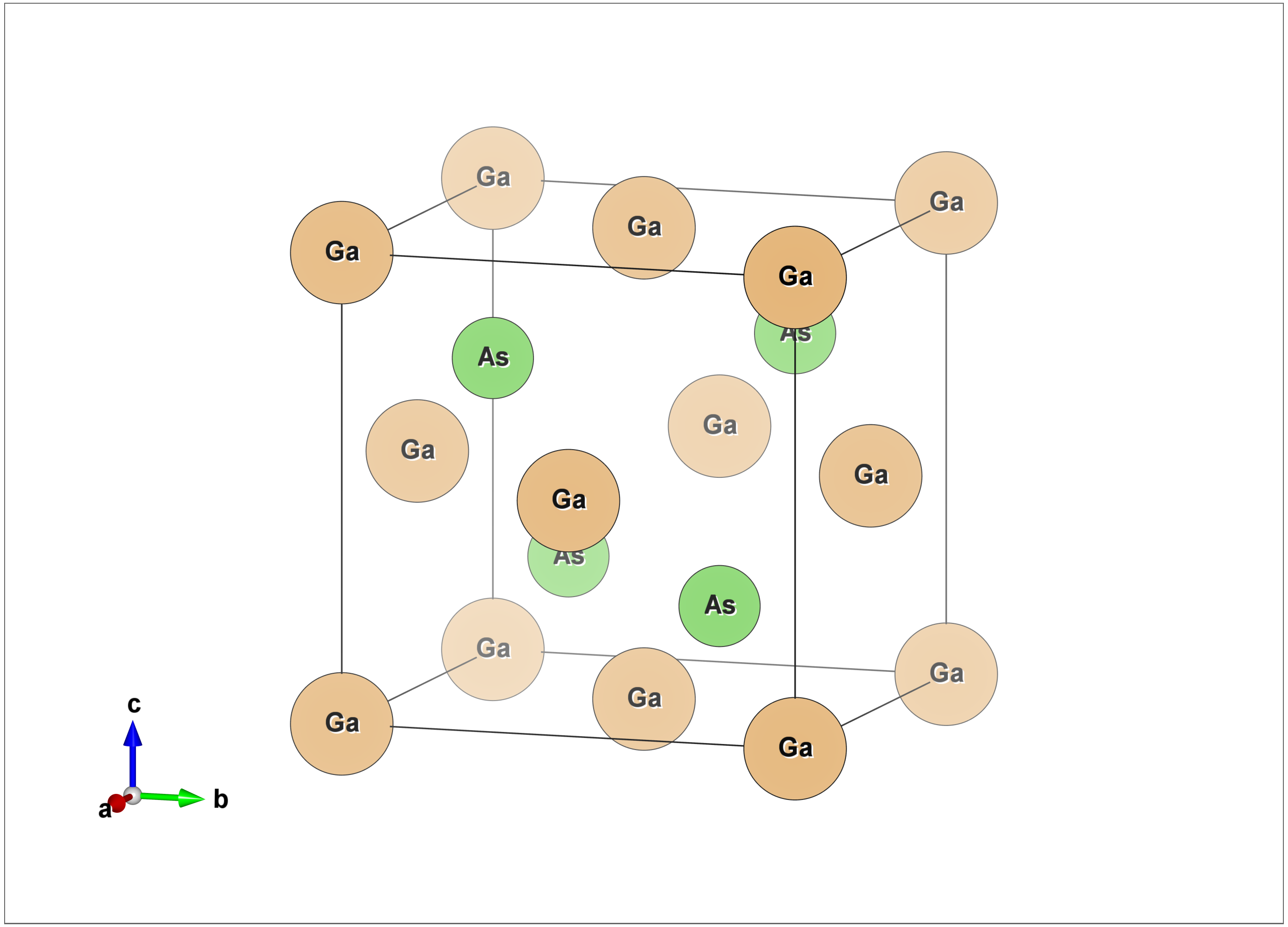


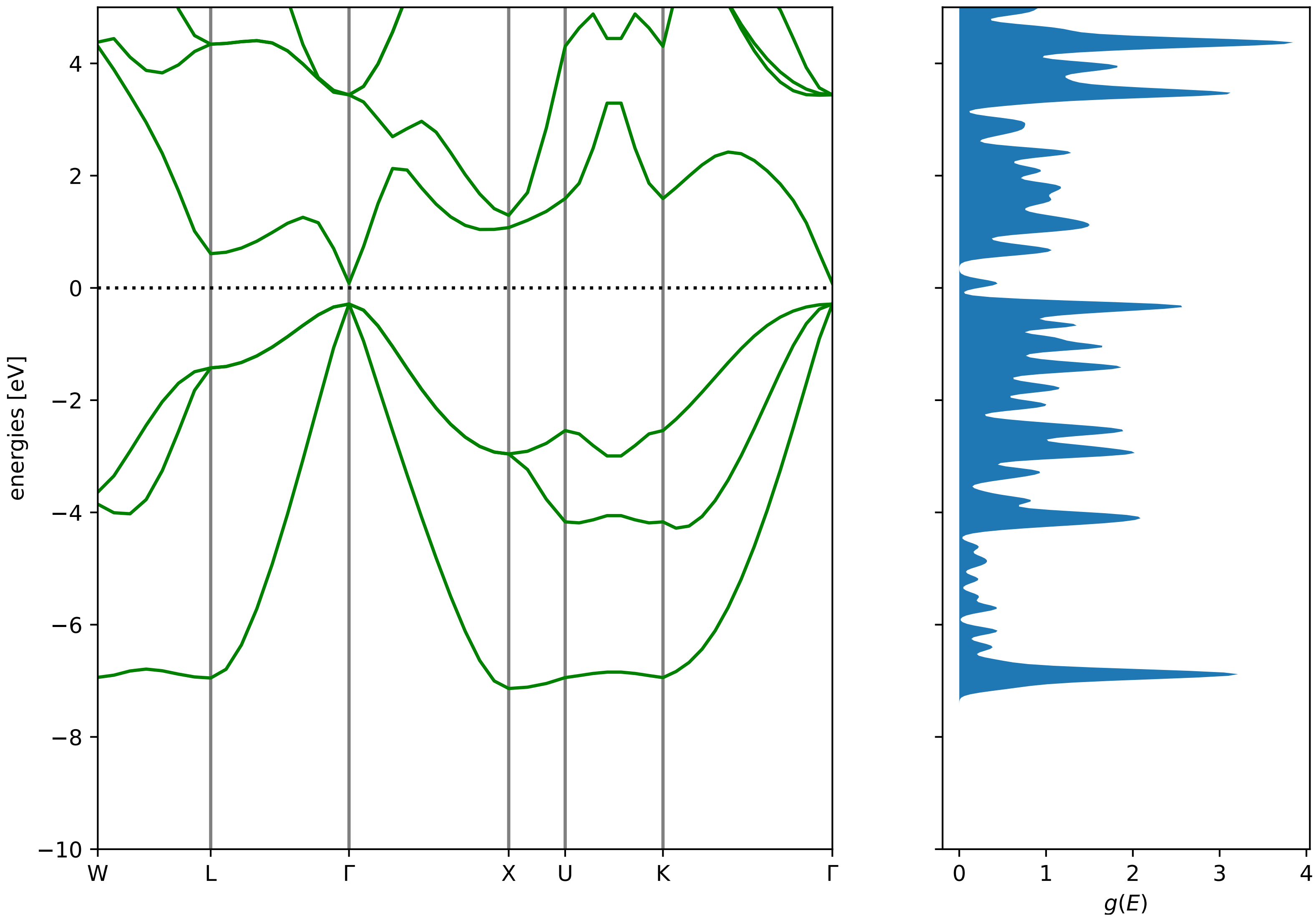



c
a
b

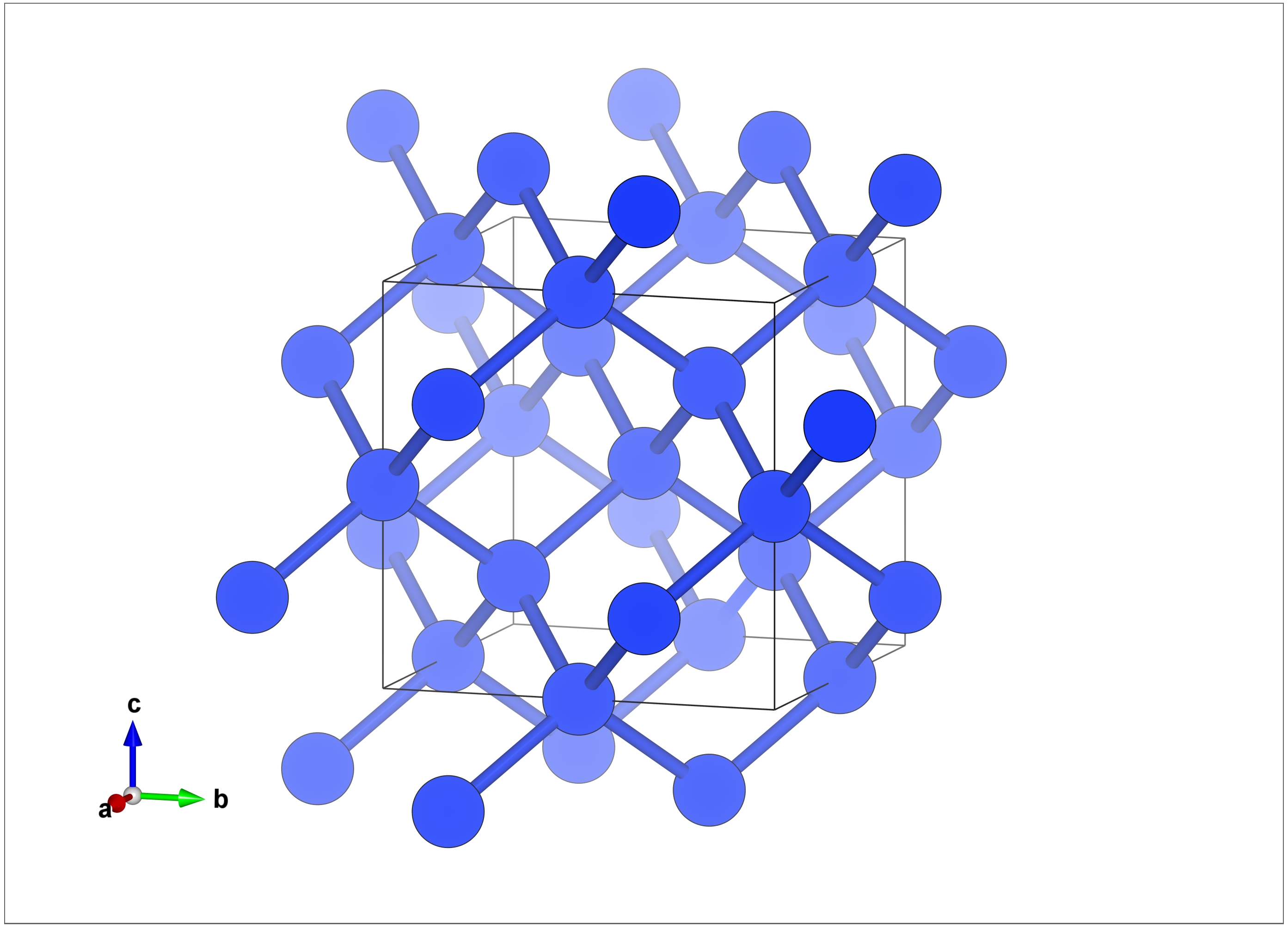
- 4 lattice points per (conventional) unit cell
- FCC equivalent to hexagonal close packing (demo if time!)
- reciprocal lattice of FCC is a BCC lattice
- Wigner-seitz cell in reciprocal space is a truncated octahedron (good visualisation at **http://lampx.tugraz.at/~hadley/ss1/bzones/fcc.php**)

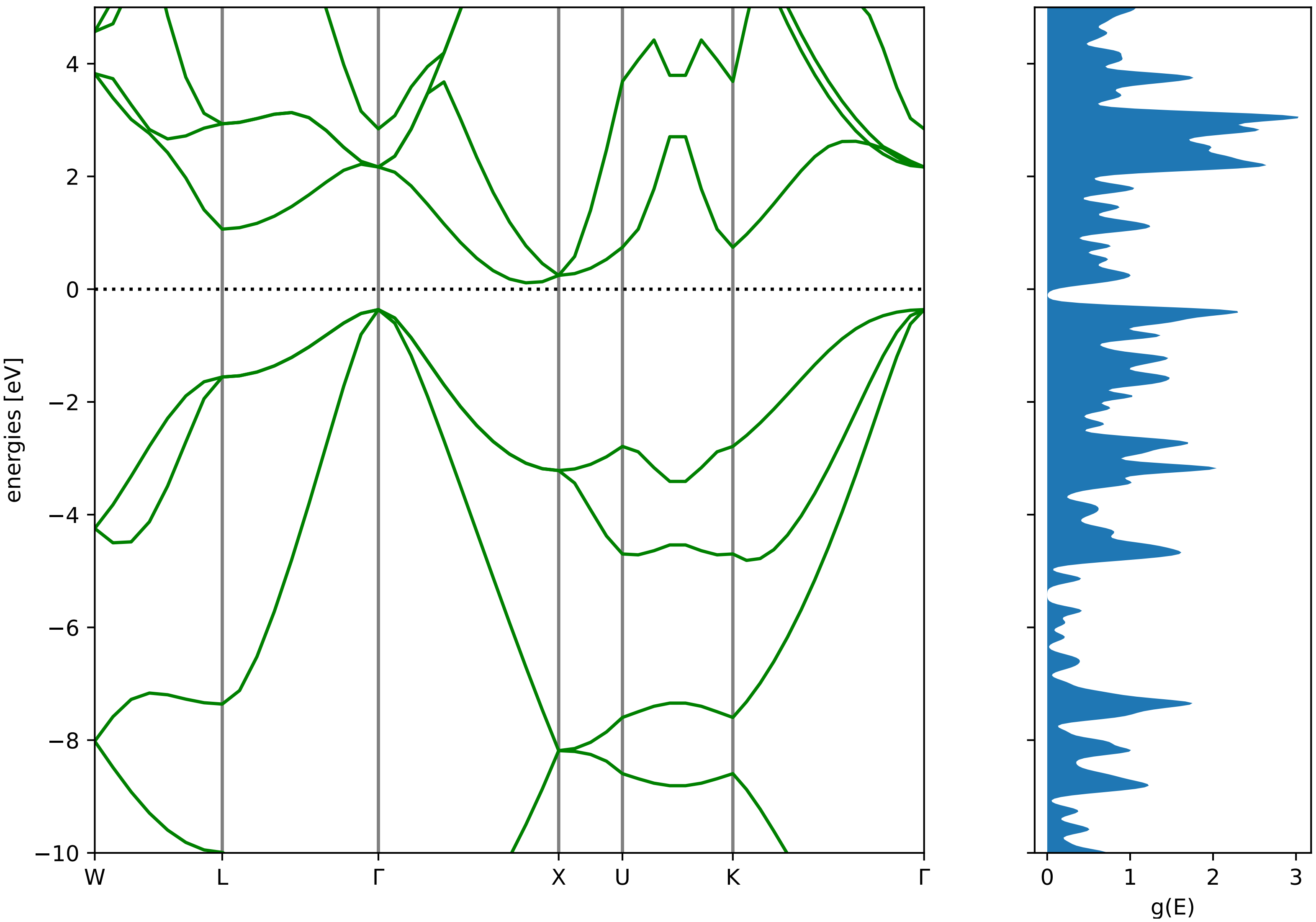
THE BANDSTRUCTURE OF GAAS




energies [eV]
4
2
0
−2
−4
−6
−8
−10
W
L
Γ
X
U
K
Γ
0
1
2
3
4
g(E)

THE BANDSTRUCTURE OF SILICON




4
2
0
−2
−4
−6
−8
−10
energies [eV]
W
L
Γ
X
U
K
Γ
0
1
2
3
g(E)

IMPORTANT THINGS WE MISSED OUT

- How to **measure** bandstructure: most common method is Angularly Resolved Photoelectron Emission Spectroscopy (ARPES)
- optical absorption & Joint Density of States & Fermi's Golden Rule
- other quantised phenomena & energy loss mechanisms relevant to semiconductors - surface plasmons, polaritons, excitons

RECOMMENDED READING

Band Theory and Electronic Properties of Solids - John Singleton great introductory level discussion on bandstructure
Solid State Physics - Ashcroft & Mermin - absolutely comprehensive presentation of solid state physics including band structure
Computational Electronics: Semiclassical and Quantum Device Modeling and Simulation - Vasileska & Goodnick - the absolute best text to follow on how to model & treat semiconductors
Physics of Semiconductor Devices - Simon Sze - reference text on operations of various types of semiconductor devices
Understanding Semiconductor Devices - Sima Dimitrijev - alternative and comprehensive presentation of semiconductor physics from a devices perspective

THANKS

This is only the 2nd year of AITL so there may still be many errors and problems with the slides, sorry about that!
Any comments, questions & corrections greatly received:
daniel.weatherill@physics.ox.ac.uk

Speaker notes