

HW5 solution

MTLE-6120: Spring 2018

Due: Feb 26, 2018

1. Effective mass

For the simplest tight-binding model in 1D, the band structure consists of a single band $E(k) = E_0 - 2t \cos ka$, where E_0 is the isolated energy and t is the coupling strength.

- (a) Calculate the effective mass $m^*(k)$ at any point in the band structure.

The effective mass is defined by

$$(m^*(k))^{-1} \equiv \frac{\partial^2 E}{\hbar^2 \partial k^2} = \frac{2a^2 t}{\hbar^2} \cos ka,$$

so that

$$m^*(k) = \frac{\hbar^2}{2a^2 t} \sec ka$$

- (b) What are the effective masses near the bottom and top of the bands? Explain the dependence of these masses on a and t .

The effective mass at the bottom of the band is $\frac{\hbar^2}{2a^2 t}$, and that at the top of the band is $\frac{-\hbar^2}{2a^2 t}$. When coupling t increases, the electrons are more easily able to move from one atom to another, and so the effective mass reduces; t can be interpreted as a probability of electrons hopping from one atom to a neighbouring one. When a increases at constant t , each hop takes the electron further, so it effectively moves through space quicker, again resulting in a lower effective mass.

- (c) What is the average value of $(m^*(k))^{-1}$ over the band?

$(m^*(k))^{-1} \propto \cos ka$, so its average value over the band is zero. Note that the mobility $\propto (m^*(k))^{-1}$, so this implies the band-averaged mobility is zero. This corresponds to the fully general result that a completely filled band does not conduct because contributions from the bottom of the band cancel those from the top.

2. Sketching density of states of real metals

For a simple cubic lattice with only nearest neighbour coupling, the density of states of a tight-binding model is $E(\vec{k}) = E_0 - 2t \cos k_x a - 2t \cos k_y a - 2t \cos k_z a$, where \vec{k} is in the Brillouin zone $[-\pi/a, \pi/a]^3$.

- (a) What is band width and total number of states per unit cell for this band?

The minimum energy is $E_0 - 6t$ for $\vec{k} = 0$, while the maximum energy is $E_0 + 6t$ for $k_x = k_y = k_z = \pm\pi/a$, so that the bandwidth is $12t$. The total number of states is 2/cell including spin; regardless of shape of band.

- (b) It is not easy to calculate the DOS of this dispersion relation, so let us try to approximate it. By Taylor expanding, show that $E \approx E_a + \hbar^2(\vec{k} - \vec{k}_a)^2/(2m_a)$ for some E_a , \vec{k}_a and m_a near the bottom and top of the band. What is the effective mass m_a at each of these band edges?

Expanding near $\vec{k} = 0$, we can Taylor expand to:

$$E(\vec{k}) = E_0 - 2t \left(1 - \frac{(k_x a)^2}{2}\right) - 2t \left(1 - \frac{(k_y a)^2}{2}\right) - 2t \left(1 - \frac{(k_z a)^2}{2}\right)$$

$$= E_0 - 6t + a^2 t k^2$$

Similarly expanding near $\vec{k}_0 = (\pi/a, \pi/a, \pi/a)$

$$\begin{aligned} E(\vec{k}) &= E_0 - 2t \left(-1 + \frac{(k_x a - \pi)^2}{2} \right) - 2t \left(-1 + \frac{(k_y a - \pi)^2}{2} \right) - 2t \left(-1 + \frac{(k_z a - \pi)^2}{2} \right) \\ &= E_0 + 6t - a^2 t (\vec{k} - \vec{k}_0)^2 \end{aligned}$$

So that corresponds to an effective mass of $\pm \hbar^2/(2a^2 t)$ near the band edges (+ for bottom, - for top edge), exactly as in the 1D tight-binding model.

- (c) Using the above, construct an approximation for the density of states of the form $g(E) = \frac{A}{1+B((E-E_0)/(6t))^2} \sqrt{(E-E_{\min})(E_{\max}-E)}$ for $E_{\min} \leq E \leq E_{\max}$ and 0 otherwise. Select A and B to produce the correct density of states near the band edges, as well as the correct number of states/cell, and plot the resulting DOS. (You will need to solve for A and B numerically.)

Our density of states ansatz is $g(E) = A \sqrt{(E-E_0+6t)(E_0+6t-E)}/(1+B((E-E_0)/(6t))^2)$ for $|E-E_0| < 6t$ and 0 otherwise. Since we have a parabolic dispersion near each band edge with m^* calculated above, we expect a DOS profile $g(E) \approx (\sqrt{2m^*}/2\pi\hbar)^3 4\pi \sqrt{|E-E_a|}$ near each band edge energy E_a . Expanding the ansatz near the bottom edge, we find

$$\frac{A}{1+B} \sqrt{(E-E_0+6t)(12t)} \approx \left(\frac{1}{2\pi a \sqrt{t}} \right)^3 4\pi \sqrt{E-E_0+6t}$$

which yields $\frac{A}{1+B} \approx \frac{1}{4\pi^2 \sqrt{3} a^3 t^2}$. (The top edge would yield the same condition by symmetry.)

Integrating from the minimum to the maximum energy of the band, we find

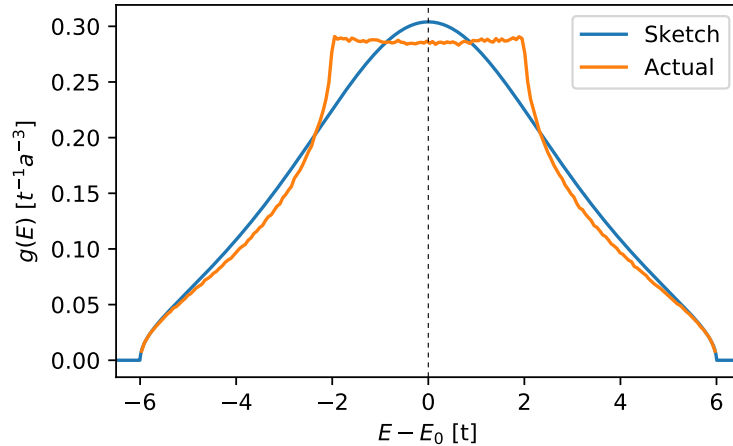
$$\begin{aligned} \frac{2}{a^3} &= \int_{E_0-6t}^{E_0+6t} dE g(E) \\ &= \int_{E_0-6t}^{E_0+6t} dE \frac{A \sqrt{(E-E_0+6t)(E_0+6t-E)}}{1+B((E-E_0)/(6t))^2} \\ &= 2A(6t)^2 \int_0^1 dx \frac{\sqrt{1-x^2}}{1+Bx^2} \quad \left(x \equiv \frac{E-E_0}{6t} \right) \\ &= 2A(6t)^2 \frac{\pi \sqrt{1+B}-1}{B} \\ &= 36\pi A t^2 \frac{\sqrt{1+B}-1}{B} \end{aligned}$$

which yields $A \frac{\sqrt{1+B}-1}{B} = \frac{2}{36\pi a^3 t^2}$.

Dividing the two conditions yields $(1+B) \frac{\sqrt{1+B}-1}{B} = \frac{2\pi}{3\sqrt{3}}$, which can be solved numerically to $B = 2.46$. Substituting, $A = 0.051/(a^3 t^2)$. Putting these together

$$g(E) \approx \frac{0.304 \sqrt{1-x^2}}{a^3 t (1+2.46x^2)}$$

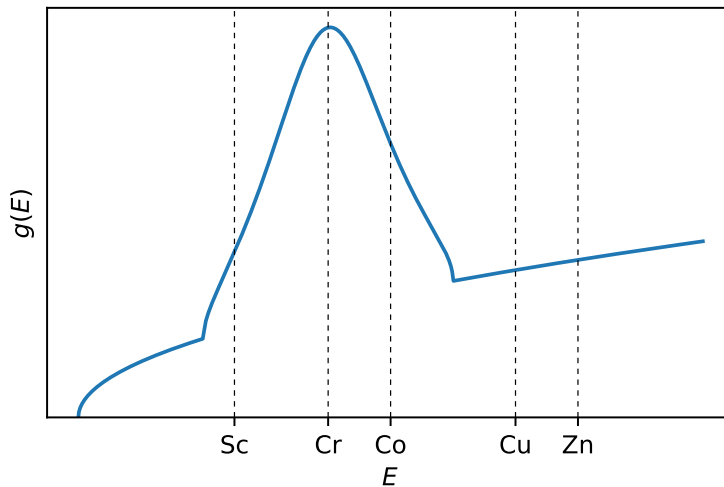
with $x = (E-E_0)/6t$, which agrees reasonably well with a Monte Carlo numerical estimate shown below.



The idea here was to reproduce the edge features and the norm of the DOS, somewhat analogous to the Debye model we used for the phonons.

- (d) Assume that the transition metals have tight-binding d electrons with a free-electron like s band. Schematically sketch the density of states, and indicate the Fermi level position for each element in the 3d transition series, Sc ($3d^1 4s^2$) to Zn ($3d^{10} 4s^2$).

The net DOS should have a strong contribution due to d electrons in shape similar to what we derived above, superimposed on a free-electron parabolic contribution. The Fermi level should be close to the lower energy end of the d contribution for Sc and its should be close to the middle for the $d^5 s^1$ Cr. The Fermi level should be above the d region for $d^{10} s^1$ Cu as well as $d^{10} s^2$ Zn.



3. Resistivity of the best conductors

Silver, copper, gold and aluminum are the four best conductors at room temperature among the elemental metals, with resistivities of 16, 17, 23 and 27 nΩm respectively. They are all face-centered cubic metals with lattice constants of 4.09, 3.61, 4.08 and 4.05 Å respectively.

- (a) Assuming these are free electron metals, calculate the carrier density, Fermi energy, Fermi velocity and density of states at the Fermi level for all four of them. If the relaxation time τ had been equal for all four, which should have been the best conductor?

Based on the valence configurations $d^{10} s^1$ for the noble metals and $s^2 p^1$ for Al, these will be free electron metals with $Z_{\text{val}} = 1$ and 3 valence electrons per unit cell respectively. The carrier

density is then $n = 4Z_{\text{val}}/a^3$, because of 4 atoms per cubic unit in FCC. From this we calculate $k_F = (3\pi^2 n)^{1/3}$, $v_F = \hbar k_F/m$ and $E_F = mv_F^2/2$, with $m =$ the free electron mass for a free electron model. The density of states at the Fermi level is $mk_F/(\hbar^2 \pi^2)$. Evaluating the above expressions, we find

Metal	n [nm ⁻³]	v_F [10 ⁶ m/s]	E_F [eV]	$g(E_F)$ [eV ⁻¹ nm ⁻³]
Ag	58	1.4	5.5	15.9
Cu	85	1.6	7.1	18.0
Au	59	1.4	5.5	15.9
Al	181	2.0	11.7	23.2

The conductivity is proportional to $g(E_F)v_F^2$, and both $g(E_F)$ and $v_F \propto k_F$ for a free electron model, so that $\sigma \propto k_F^3 \propto n$. In fact, for a free electron model, Drude theory continues to hold, so that $\sigma = ne^2\tau/m$. Aluminum has the highest n , followed by copper, so if τ had remained the same, those two should have been the best conductors.

- (b) Calculate the τ based on the experimental resistivity numbers given above. What other material properties could one look at to explain this trend?

Using the Drude formula, which remains exactly valid for a quantum free electron model, we can calculate $\tau = m/(\rho ne^2)$ with the results:

Metal	ρ [nΩm]	n [nm ⁻³]	τ [fs]
Ag	16	58	37
Cu	17	85	24
Au	23	59	26
Al	27	181	7

This variation of τ depends on many factors. As discussed in class, Fermi golden rule for e-ph scattering rate $\propto g(E_F)$ so the high DOS in Al and then Cu decrease the relaxation time τ . The remaining variation in τ results from the phonon properties. Al has low elastic moduli, which results in larger amplitude phonons for the same energy and stronger e-ph coupling ($c_{\text{e-ph}}$ in our derivation). Au is heavy, which results in a low sound velocity and hence low energy phonons (low Debye temperature), which can be more easily excited at the same temperature, enhancing the Bose occupation factors in the scattering rate and reducing τ . Essentially, a light and high-modulus material will have the largest τ .