SOLUTIONS: ECE 656 Homework (Week 9)

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1) It is sometimes said that Fick's Law of diffusion, $J = -D\, dn/dx$, only applies when the region of interest is many mean-free-paths long. Is this true?

   1a) Follow the derivation in Lecture 12, Fall 2011 and show that this is not the case; i.e. show that it works in the ballistic limit, diffusive limit, and in between.

Solution:

Let' re-visit the derivation:

At the left of the slab we have

$$n^+(0) = F^+(0)/\langle \upsilon_x^+ \rangle \qquad \text{(i)}$$

At the right of the slab

$$n^-(0) = F^-(0)/\langle \upsilon_x^+ \rangle \qquad \text{(ii)}$$

or

$$n(0) = (1+R)F^+(0)/\langle \upsilon_x^+ \rangle = n(0) = (2-\mathcal{T})F^+(0)/\langle \upsilon_x^+ \rangle \qquad \text{(iii)}$$

Note that our derivation of the transmission made no assumptions about the length of the slab as compared to the mean-free-path – it couldbe much longer than a mfp, much shorter, or comparable to the mfp.

At the right side of the slab, we have:

$$n^+(L) = I^+(L)/\langle \upsilon_x^+ \rangle = \mathcal{T} F^+(0)/\langle \upsilon_x^+ \rangle \qquad \text{(iv)}$$

and

$$n^-(0) = 0 \qquad \text{(v)}$$

so

$$n(L) = n^+(L) + n^-(L) = \mathcal{T} F^+(0)/\langle \upsilon_x^+ \rangle \qquad \text{(vi)}$$

Now subtract (vi) from (iii) to find

$$n(0) - n(L) = \frac{F^+(0)}{\langle \upsilon_x^+ \rangle} 2(1-\mathcal{T}), \qquad \text{(vii)}$$

solve for $F^+(0)$ and then for the current, $F^+(0)$ to find

$$F = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{\mathcal{T} L}{1-\mathcal{T}} \times \left[\frac{n(0)-n(L)}{L} \right] = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{\mathcal{T} L}{1-\mathcal{T}} \times \left(-\frac{dn}{dx} \right) \quad \text{(viii)}$$

This looks like Fick's law

$$F = -D\left(-\frac{dn}{dx} \right) \quad \text{(ix)}$$

with

$$D = \frac{\langle \upsilon_x^+ \rangle}{2} \frac{\mathcal{T} L}{1-\mathcal{T}} \quad \text{(x)}$$

Using

$$\mathcal{T} = \frac{\lambda}{\lambda + L}, \quad \text{(xi)}$$

we find

$$\boxed{\begin{aligned} F &= -D\left(-\frac{dn}{dx} \right) \\ D &= \frac{\langle \upsilon_x^+ \rangle \lambda}{2} \end{aligned}}, \quad \text{(xii)}$$

which is Fick's Law with the bulk diffusion coefficient. We still have made no assumption that the region is long compared to the ballistic limit. Apparently, Fick's Law holds all the way to the ballistic limit.

1b) Make a sketch of $n(x)$ vs. x in the a) diffusive limit, b) in the ballistic limit, and c) in between.

Solution:

Use (iii) and (iv):

$$n(0) = (2-\mathcal{T}) F^+(0) \big/ \langle \upsilon_x^+ \rangle$$

$$n(L) = \mathcal{T} F^+(0) \big/ \langle \upsilon_x^+ \rangle$$

a) diffusive limit: $\mathcal{T} \to 0$

$$n(0) \to 2F^+(0)\big/\langle \upsilon_x^+ \rangle$$
$$n(L) \to 0$$

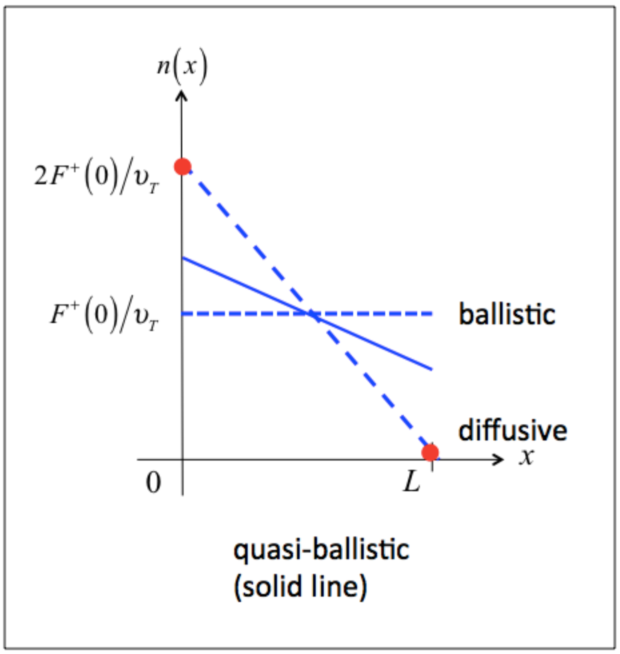
b) ballistic limit: $\mathcal{T} \to 1$

$$n(0) \to F^+(0)\big/\langle \upsilon_x^+ \rangle$$
$$n(L) \to F^+(0)\big/\langle \upsilon_x^+ \rangle = n(0)$$

c) in between: $0 < \mathcal{T} < 1$

$$F^+(0)\big/\langle \upsilon_x^+ \rangle < n(0) < 2F^+(0)\big/\langle \upsilon_x^+ \rangle$$

$$0 < n(L) < F^+(0)\big/\langle \upsilon_x^+ \rangle$$



1c) Explain why the simple application of Fick's Law often leads to incorrect results.

Solution:

It is very common to apply the boundary condition, $n(L) = 0$, but this assumes diffusive transport. It is not Fick's Law that is wrong, it is the boundary condition. It is more physical to impose boundary conditions from the fluxes incident from the two sides, not the carrier densities on the two sides.

2) For electrons, the bandstructure is a plot of energy, $E(\vec{k})$, vs. wavevector, $\vec{k}$. For phonons, the dispersion is a plot of phonon energy, $\hbar\omega(\vec{q})$, vs. phonon wavector, $\vec{q}$. For electrons, we often approximate the bandstructure with simple, parabolic bands,

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$$

For phonons, we can sometimes approximate the phonon dispersion with the Debye approximation,

$$\hbar\omega = \hbar\upsilon_D q\,,$$

where υ_D is the Debye velocity (an average of the longitudinal and transverse acoustive celocities.)

2a) Compute the density-of-states, $D_{ph}(\hbar\omega)$, for phonons in the Debye model.

Solution:

Equate the DOS in q-space to energy space:

$$\frac{1}{\Omega} N_q dq = D_{ph}(\hbar\omega)\, d(\hbar\omega) \qquad \text{(i)}$$

$$\frac{1}{\Omega} N_q dq = \frac{1}{8\pi^3} \times 3\left(4\pi q^2\right) dq = D_{ph}(\hbar\omega)\, d(\hbar\omega) \qquad \text{(ii)}$$

Note that there is no factor of 2 for spin in this case, but we have a factor of three because of the three polarizations, longitudinal and two transverse acoustic phonons.

From the dispersion,

$$\hbar\omega = \hbar\upsilon_D q \qquad \text{(iii)}$$

we have

$$q^2 = \left(\frac{\hbar\omega}{\hbar\upsilon_D}\right)^2 \qquad \text{(iv)}$$

and

$$dq = \frac{d(\hbar\omega)}{\hbar\upsilon_D} \qquad \text{(v)}$$

Using (iv) and (v) in (ii), we find

$$D_{ph}(\hbar\omega)d(\hbar\omega) = \frac{3}{2\pi^2}q^2 dq = \frac{3}{2\pi^2}\left(\frac{\hbar\omega}{\hbar\upsilon_D}\right)^2 \frac{d(\hbar\omega)}{\hbar\upsilon_D} \qquad \text{(vi)}$$

so the final answer is

$$\boxed{D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2(\hbar\upsilon_D)^3} \quad \left(\text{J-m}^3\right)^{-1}} \qquad \text{(vii)}$$

2b) Compute the distribution of channels, $M_{ph}(\hbar\omega)$, for phonons in the Debye model.

Solution:

Begin with the definition:

$$M_{ph}(\hbar\omega) = \frac{h}{2}\langle \upsilon_x^+ \rangle D_{ph}(\hbar\omega) \qquad \text{(viii)}$$

From the dispersion, (iii), we find

$$\upsilon(\hbar\omega) = \upsilon_D \qquad \text{(ix)}$$

and the average over angles in 3D gives

$$\langle \upsilon_x^+ \rangle = \frac{\upsilon_D}{2} \qquad \text{(x)}$$

Now using (x) in (viii), we find

$$M_{ph}(\hbar\omega) = \frac{h}{2}\langle \upsilon_x^+ \rangle D_{ph}(\hbar\omega) = \frac{h}{2}\frac{\upsilon_D}{2}\frac{3(\hbar\omega)^2}{2\pi^2(\hbar\upsilon_D)^3} \qquad \text{(xi)}$$

$$\boxed{M_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{4\pi(\hbar\upsilon_D)^2}} \qquad \text{(xii)}$$