ECE-656: Fall 2009

Lecture 17: BTE and Landauer

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acknowledgement

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outline

1) **BTE review**

2) Transport Distribution

3) Connection to Landauer

4) Modes

5) Mean-free-path

6) Summary

BTE

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C} f$$

The steady-state, near equilibrium BTE in the Relaxation Time Approximation is:

$$\vec{\upsilon} \bullet \nabla_r f_0 + \vec{F}_e \bullet \nabla_p f_0 = -\frac{\left(f - f_0\right)}{\tau_f} = -\frac{f_A}{\tau_f}$$

solution to the s.s., near eq. BTE

$$\vec{\upsilon} \bullet \nabla_r f_S + \vec{F}_e \bullet \nabla_p f_S = -\frac{f_A}{\tau_f}$$

$$f_A = \tau_f \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

anti-symmetric component

$$f_S = \frac{1}{1 + e^{(E - F_n)/k_B T}}$$

symmetric component

$$\vec{\mathcal{F}} = -\nabla_r F_n + T \left[E - F_n \right] \nabla_r \left(\frac{1}{T} \right)$$

generalized force

$$-\nabla_r F_n = -q \vec{\mathcal{E}}$$

when carrier density is constant

solution to the s.s., near eq. BTE

$$f_A = \tau_f \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \left[-\nabla_r F_n - \frac{(E - F_n)}{T} \nabla_r T \right]$$

$$\vec{J}_n(\vec{r}) = \frac{1}{\Omega} \sum_k (-q) \vec{\upsilon} f_A(\vec{r}, \vec{k})$$

$$\vec{J}_Q(\vec{r}) = \frac{1}{\Omega} \sum_k (E - F_n) \vec{\upsilon} f_A(\vec{r}, \vec{k})$$

$$J_i = \sigma_{ij} \mathcal{E}_j + [sg]_{ij} \partial_j T$$

$$J_i^Q = T [sg]_{ij} \mathcal{E}_j - \kappa_{ij}^0 \partial_j T$$

$$\mathcal{E}_j = \partial_j (F_n / q)$$

solution to the s.s., near eq. BTE

$$I_n(\vec{r}) = J_n(\vec{r})A$$

$$I_Q(\vec{r}) = J_Q(\vec{r})A$$

$$\Delta V_i = L\mathcal{E}_i \qquad \Delta T = L\,\partial_i T$$

$$G = \sigma\frac{A}{L} \qquad [SG] = [sg]\frac{A}{L}$$

$$T[SG] \qquad K = \kappa\frac{A}{L}$$

$$I = G\,\Delta V + [SG]\Delta T$$

$$I^Q = T[SG]\Delta V - K_0\Delta T$$

transport parameters (isotropic)

$$G_0 = \frac{q^2}{L^2}\sum_k \upsilon_x \upsilon_x \tau_f \left(-\frac{\partial f_S}{\partial E}\right)$$

$$[SG]_0 = \frac{q}{L^2}\sum_k \left\{\frac{(E-F_n)}{T}\upsilon_x \upsilon_x \tau_f \left(-\frac{\partial f_S}{\partial E}\right)\right\}$$

$$K_0 = \frac{1}{L^2}\sum_k \left\{\frac{(E-F_n)^2}{T}\upsilon_x \upsilon_x \tau_f \left(-\frac{\partial f_S}{\partial E}\right)\right\}$$

These three expressions involve a similar sum (or integral over *k*-space)

$$I_j = \frac{h}{2L^2}\sum_k \left(\frac{E-F_n}{k_B T}\right)^j \upsilon_x^2 \tau_f \left(-\frac{\partial f_S}{\partial E}\right)$$

transport parameters in k-space

$$G = \frac{2q^2}{h} I_0$$

$$[SG] = \frac{2qk_B}{h} I_1$$

$$K_0 = \frac{2k_B^2 T}{h} I_2$$

$$I_j = \frac{h}{2L^2} \sum_k \left(\frac{E - F_n}{k_B T} \right)^j \upsilon_x^2 \tau_f \left(-\frac{\partial f_S}{\partial E} \right)$$

$$I = G\,\Delta V + [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0 \Delta T$$

inverted equations

$$G = 1/R$$

$$S = -[SG]/G$$

$$K_e = K_0 - T[SG]^2/G$$

$$I_j = \frac{h}{2L^2}\sum_k \left(\frac{E-F_n}{k_B T}\right)^j \upsilon_x^2 \tau_f \left(-\frac{\partial f_S}{\partial E}\right)$$

$$\Delta V = RI - S\,\Delta T$$

$$I_Q = TS\,I - K_e \Delta T$$

$$R = \left(\frac{2q^2}{h} I_0\right)^{-1}$$

$$S = \left(\frac{k_B}{-q}\right)\frac{I_1}{I_0}$$

$$K_e = \frac{2k_B^2 T}{h}\left\{I_2 - \frac{I_1^2}{I_0}\right\}$$

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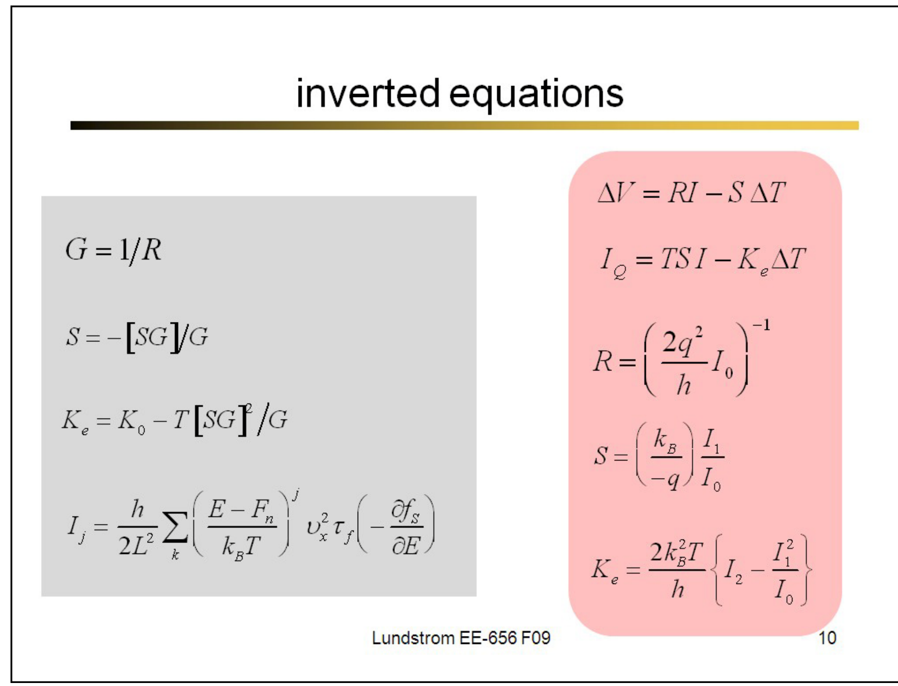
integration over energy

In the Landauer approach, we integrate over **energy** channels rather than summing over *k*-space. (The advantage is that even for materials with no *E*(*k*), we can compute the IV)

$$G=\int_{-\infty}^{+\infty} G(E)dE=\frac{2q^2}{h}\int_{-\infty}^{+\infty} T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$



How do we express the BTE results as an integral over energy?

converting k-space sums to energy integrals

$$H = 2\sum_{\vec{k}} h\left(\vec{k}\right)$$

$$H = \int H(E)\,dE$$

$$H(E) = 2\sum_{\vec{k}} h\left(\vec{k}\right)\delta\left(E - E_k\right)$$

(factor of 2 for spin)

(factor of 2 for spin)

Proof:

$$H = \int dE \sum_{\vec{k}} 2h\left(\vec{k}\right)\delta\left(E - E_k\right) = 2\sum_{\vec{k}} h\left(\vec{k}\right)\int \delta\left(E - E_k\right)dE = 2\sum_{\vec{k}} h\left(\vec{k}\right)$$

converting k-space sums to energy integrals

$$G_0 = \frac{q^2}{L^2} \sum_{k} \upsilon_x \upsilon_x \tau_f \left(-\frac{\partial f_S}{\partial E} \right)$$

$$G = \frac{2q^2}{h} \frac{h}{2L^2} (2) \sum_{k} \upsilon_x^2 \tau_f \left(-\frac{\partial f_S}{\partial E} \right)$$

the (2) is for spin

$$\Sigma(E) = \frac{h}{L^2} \sum_{\vec{k}} \upsilon_x^2 \tau_f \delta(E - E_k)$$

$$G = \frac{2q^2}{h} I_0$$

$$I_0 = \int \Sigma(E) \left(-\frac{\partial f_S}{\partial E} \right) dE$$

$$\Sigma(E) = \frac{h}{L^2} \sum_{\vec{k}} \upsilon_x^2 \tau_f \delta(E - E_k)$$

transport parameters in energy-space

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \Sigma(E) \left(-\frac{\partial f_S}{\partial E} \right) dE$$

$$\Sigma(E) = \frac{h}{L^2} \sum_k \upsilon_x^2 \tau_f \delta(E - E_k)$$

$\sqcap$

$$\Delta V = RI - S\,\Delta T$$

$$I_Q = TS\,I - K_e \Delta T$$

$$R = \left(\frac{2q^2}{h} I_0 \right)^{-1}$$

$$S = \left(\frac{k_B}{-q} \right) \frac{I_1}{I_0}$$

$$K_e = \frac{2k_B^2 T}{h} \left\{ I_2 - \frac{I_1^2}{I_0} \right\}$$

transport parameters: Landauer

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \bar{T}(E) \left(-\frac{\partial f_S}{\partial E} \right) dE$$

$$\bar{T}(E) = T(E) M(E)$$

$$\Delta V = RI - S\,\Delta T$$

$$I_Q = TS\,I - K_e \Delta T$$

$$R = \left(\frac{2q^2}{h} I_0 \right)^{-1}$$

$$S = \left(\frac{k_B}{-q} \right) \frac{I_1}{I_0}$$

$$K_e = \frac{2k_B^2 T}{h} \left\{ I_2 - \frac{I_1^2}{I_0} \right\}$$

BTE and Landauer

From the BTE, we find the TE coefficients from an integral:

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \Sigma(E) \left(-\frac{\partial f_S}{\partial E} \right) dE \qquad \Sigma(E) = \frac{h}{L^2} \sum_k \upsilon_x^2 \tau_f \delta(E - E_k)$$

From the Landauer approach, we find the TE coefficients from a similar integral:

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \bar{T}(E) \left(-\frac{\partial f_S}{\partial E} \right) dE \qquad \bar{T}(E) = T(E) M(E)$$

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derivation

$$\Sigma(E) = \frac{h}{L^2}\sum_{\vec{k}} \upsilon_x^2 \tau_f \delta\left(E - E_k\right) = T(E)M(E)$$

How are *T*(*E*) and *M*(*E*) defined?

Define the average *x*-directed velocity:

$$\left\langle \left|\upsilon_x\right| \right\rangle = \frac{\sum_{\vec{k}} \left|\upsilon_x\right| \delta\left(E - E_k\right)}{\sum_{\vec{k}} \delta\left(E - E_k\right)}$$

average velocity, 1D

$$\langle |\upsilon_x| \rangle = \frac{\sum_k |\upsilon_x| \delta(E - E_k)}{\sum_k \delta(E - E_k)}$$

$$\langle |\upsilon_x| \rangle = \upsilon_x(E)$$

$$\langle |\upsilon_x| \rangle = \frac{\frac{L}{\pi}\int_{-k}^{+k} dk |\upsilon_x| \delta(E - E_k)}{\frac{L}{\pi}\int_{-k}^{+k} dk\, \delta(E - E_k)} = \frac{\frac{2L}{\pi\hbar}\int_{0}^{+k} \frac{d(\hbar k)}{dE} \upsilon_x \delta(E - E_k) dE}{\frac{2L}{\pi\hbar}\int_{0}^{+k} \frac{d(\hbar k)}{dE} \delta(E - E_k) dE}$$

$$= \frac{\int_{0}^{+k} \delta(E - E_k) dE}{\int_{0}^{+k} \frac{1}{\upsilon_x(E)} \delta(E - E_k) dE} = \upsilon_x(E)$$

parabolic bands, 2D

$$\langle|\upsilon_x|\rangle = \frac{\sum_k |\upsilon_x| \delta(E - E_k)}{\sum_k \delta(E - E_k)}$$

$$\langle|\upsilon_x|\rangle = \frac{\int_0^\infty k\,dk \int_0^{2\pi} d\theta |\upsilon_x| \delta(E - E_k)}{\int_0^\infty k\,dk \int_0^{2\pi} d\theta\, \delta(E - E_k)} = \frac{\int_0^\infty k\,dk \int_0^{2\pi} d\theta\, \upsilon(E) |\cos\theta| \delta(E - E_k)}{\int_0^\infty k\,dk \int_0^{2\pi} d\theta\, \delta(E - E_k)}$$

$$E_k = \frac{\hbar^2 k^2}{2m^*} \rightarrow kdk = \frac{m^*}{\hbar^2} dE_k$$

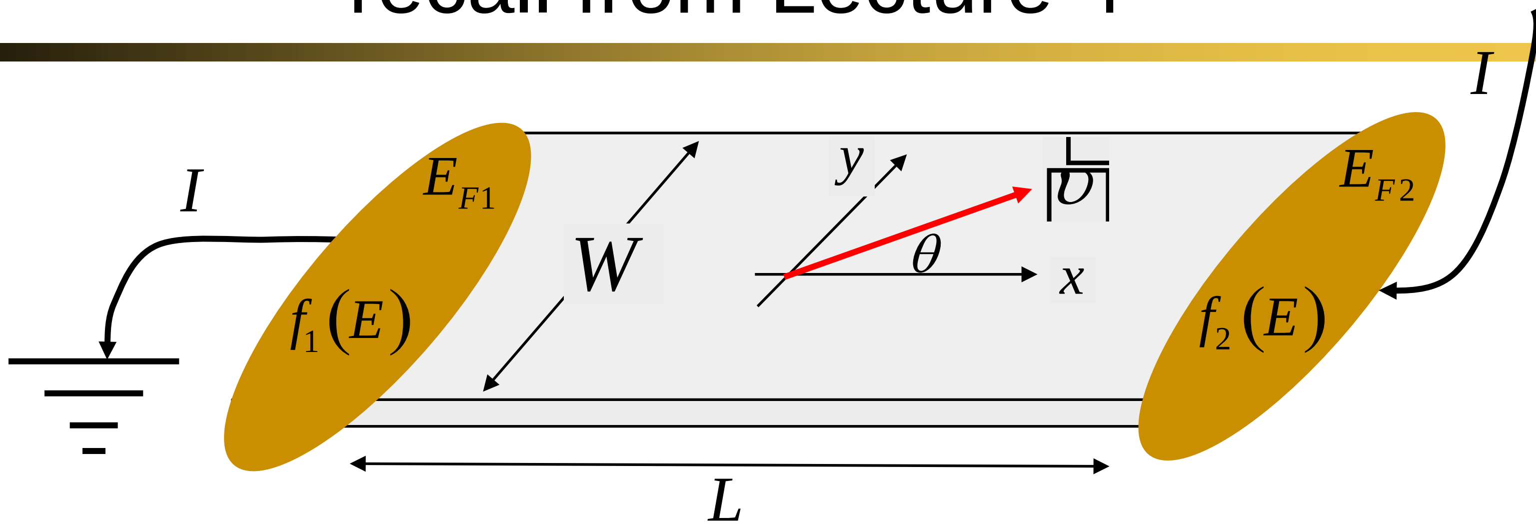
parabolic bands, 2D

$$\langle|\upsilon_x|\rangle = \frac{\int_0^\infty k\,dk \int_0^{2\pi} d\theta\, \upsilon(E)|\cos\theta|\,\delta(E-E_k)}{\int_0^\infty k\,dk \int_0^{2\pi} d\theta\, \delta(E-E_k)} = \frac{\int_0^\infty \upsilon(E)\delta(E-E_k)dE_k \int_{-\pi/2}^{+\pi/2} \cos\theta\, d\theta}{\int_0^\infty \delta(E-E_k)dE_k \int_{-\pi/2}^{+\pi/2} d\theta}$$

$$\langle|\upsilon_x|\rangle = \frac{2}{\pi}\frac{\int_0^\infty \upsilon(E_k)\delta(E-E_k)dE_k}{\int_0^\infty \delta(E-E_k)dE_k}$$

$$\langle|\upsilon_x|\rangle = \frac{2}{\pi}\upsilon(E)$$

recall from Lecture 4



$$M_{2D}(E) = \gamma\,\pi\,D_{2D}(E)/2 \qquad D_{2D}(E) = A\left(m^*/\pi h^2\right) \qquad \left(E(k) = h^2k^2/2m^*\right)$$

$$\gamma = h/\langle\tau\rangle$$

$$\gamma = \frac{h}{L/\langle\upsilon_x\rangle} = \frac{h\upsilon\langle\cos\theta\rangle}{L}$$

$$\langle\cos\theta\rangle = \frac{\int_{-\pi/2}^{+\pi/2}\cos\theta\, d\theta}{\pi}$$

$$\langle\cos\theta\rangle = \frac{2}{\pi}$$

$$\langle\upsilon_x\rangle = \upsilon(E)\langle\cos\theta\rangle = \frac{2}{\pi}\upsilon(E)$$

parabolic bands, 3D

We leave this as an exercise.

The point is that:

$$\langle |\upsilon_x| \rangle = \frac{\sum_{\vec{k}} |\upsilon_x| \delta(E - E_k)}{\sum_{\vec{k}} \delta(E - E_k)}$$

is simply the average *x*-directed velocity at energy, *E*, in 1D, 2D, or 3D.

so where are we?

$$\Sigma(E) = \frac{h}{L^2} \sum_{k} \upsilon_x^2 \tau_f \delta(E - E_k) = T(E)M(E)$$

Define the average *x*-directed velocity:

$$\langle |\upsilon_x| \rangle = \frac{\sum_{k} |\upsilon_x| \delta(E - E_k)}{\sum_{k} \delta(E - E_k)}$$

derivation

$$\Sigma(E) = \frac{h}{L^2} \sum_{k} \upsilon_x^2 \tau_f \delta(E - E_k)$$

$$\Sigma(E) = \frac{h}{L^2} \frac{\sum_{k} \upsilon_x^2 \tau_f \delta(E - E_k)}{\sum_{k} \delta(E - E_k)} \sum_{k} \delta(E - E_k)$$

$$\Sigma(E) = \frac{h}{L^2} \left\langle \upsilon_x^2 \tau_f \right\rangle D(E)$$

$$\Sigma(E) = \frac{h}{L^2} \frac{\left\langle \upsilon_x^2 \tau_f \right\rangle}{\left\langle |\upsilon_x| \right\rangle} \left\langle |\upsilon_x| \right\rangle D(E) = \frac{h}{L^2} \frac{\left\langle \upsilon_x^2 \tau_f \right\rangle}{\left\langle |\upsilon_x| \right\rangle} \sum_{k} |\upsilon_x| \delta(E - E_k)$$

$$\left\langle |\upsilon_x| \right\rangle = \frac{\sum_{k} |\upsilon_x| \delta(E - E_k)}{\sum_{k} \delta(E - E_k)}$$

$$\left\langle \upsilon_x^2 \tau_f \right\rangle \equiv \frac{\sum_{k} \upsilon_x^2 \tau_f \delta(E - E_k)}{\sum_{k} \delta(E - E_k)}$$

derivation (ii)

$$\Sigma(E)=\frac{h}{L^2}\frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle}\sum_{\vec{k}}|\upsilon_x|\delta(E-E_k)=\frac{2}{L}\frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle}\frac{h}{2L}\sum_{\vec{k}}|\upsilon_x|\delta(E-E_k)$$

$$\langle\langle \lambda(E) \rangle\rangle \equiv 2\frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle}$$

$$M(E)=\frac{h}{2L}\sum_{\vec{k}}|\upsilon_x|\delta(E-E_k)$$

$$\Sigma(E)=\frac{\langle\langle \lambda(E) \rangle\rangle}{L}M(E)=T(E)M(E)$$ ✓

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modes: 1D

$$M(E) = \frac{h}{2L}\sum_{k}|\upsilon_x|\,\delta(E - E_k)$$

Let's work this out in 1D and you will find: $M(E) = 1$ ✓

modes: 2D

$$M(E) = \frac{h}{2L}\sum_{k}|\upsilon_x|\delta(E - E_k)$$

Let's work this out in 2D…..

$$E_k = \frac{\hbar^2 k^2}{2m^*}$$

$$\upsilon_k = \sqrt{\frac{2E_k}{m^*}}$$

$$M(E) = \frac{h}{2L}\frac{A}{4\pi^2}\int_0^{\infty} k\,dk\int_0^{2\pi} d\theta|\upsilon_x|\delta(E - E_k)$$

$$= \frac{h}{2L}\frac{WL}{4\pi^2}2\int_0^{\infty} k\,dk\int_{-\pi/2}^{+\pi/2} d\theta\,\upsilon\cos\theta\,\delta(E - E_k)$$

$$= \frac{hW}{2\pi^2}\int_0^{\infty} k\,dk\,\upsilon(E)\delta(E - E_k) = \frac{hW}{2\pi^2}\int_0^{\infty}\frac{m^*}{\hbar^2}dE_k\sqrt{\frac{2E_k}{m^*}}\delta(E - E_k)$$

$$= W\frac{\sqrt{2m^*E}}{\pi\hbar}$$

modes: 3D

$$M(E) = \frac{h}{2L} \sum_{\vec{k}} |\upsilon_x| \delta(E - E_k)$$

As an exercise, work this out in 3D and show…..

$$M_{3D}(E) = A \frac{m^*}{2\pi h^2} E$$

an alternate view

$$M(E) = \frac{h}{2L}\sum_{\vec{k}} |\upsilon_x| \delta(E - E_k)$$

$\square$

$$M(E) = \frac{h}{2L} 2 \sum_{k_z}\sum_{k_y}\sum_{k_x>0} \upsilon_x \delta(E - E_k)$$

$$= \frac{h}{L}\sum_{k_z}\sum_{k_y} \frac{L}{2\pi}\int_0^\infty dk_x \upsilon_x \delta(E - E_k)$$

$$= \sum_{k_z}\sum_{k_y} \int_0^\infty \frac{d(hk_x)}{dE_k} \upsilon_x \delta(E - E_k) dE_k$$

$$= \sum_{k_z}\sum_{k_y} \Theta(E - E_k)$$

$\square$

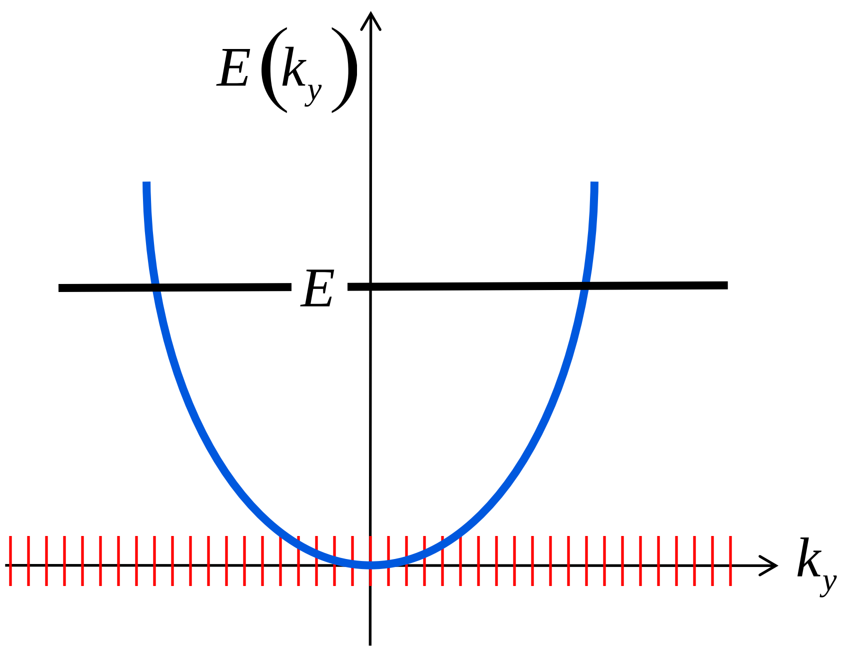
$$M(E) = \frac{h}{2L}\sum_{\vec{k}} |\upsilon_x| \delta(E - E_k)$$

$$= \sum_{k_\perp} \Theta(E - E_k)$$

$\square$

interpretation

$$M(E) = \sum_{k_\perp} \Theta(E - E_k)$$



Consider a 2D conductor with transport in the *x*-direction. Then the sum is simply the number of *k*-states in the transverse direction with energy less than *E*.

Exercise: Work the sum out in 2D and show that the result is the same as that obtained from:

$$M(E) = \frac{h}{2L} \sum_{k} |\upsilon_x| \delta(E - E_k)$$

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mean-free-path

$$\langle\langle \lambda(E) \rangle\rangle \equiv 2\frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle}$$

Note that this is an "average" over angle at a specific energy, *E.*

The double braces are to help remember that this is a specially-defined "average."

If we work this out in 1D, 2D, and 3D for parabolic energy bands.

$$\langle\langle \lambda(E) \rangle\rangle = 2\upsilon(E)\tau_f(E) \qquad \text{(1D)}$$

$$\langle\langle \lambda(E) \rangle\rangle = (\pi/2)\upsilon(E)\tau_f(E) \qquad \text{(2D)}$$

$$\langle\langle \lambda(E) \rangle\rangle = (4/3)\upsilon(E)\tau_f(E) \qquad \text{(3D)}$$

example: mean-free-path in 2D

$$\langle\langle\lambda(E)\rangle\rangle \equiv \frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle} = 2\,\frac{\frac{1}{2}\upsilon^2(E)\tau_f(E)}{\frac{2}{\pi}\upsilon(E)} = \frac{\pi}{2}\upsilon(E)\tau_f(E)$$

Assume an isotropic band.

$$\langle |\upsilon_x| \rangle = \frac{2}{\pi}\upsilon(E)$$

$$\langle \upsilon_x^2 \tau_f \rangle = \frac{\sum_k \upsilon_x^2 \tau_f \delta(E - E_k)}{\sum_k \delta(E - E_k)} = \frac{\frac{A}{2\pi}\int_0^{2\pi} \cos^2\theta \, d\theta \int_0^{\infty} \upsilon^2(E_k)\tau_f(E_k)\delta(E - E_k)\, dE}{\frac{A}{2\pi}\int_0^{2\pi} d\theta \int_0^{\infty} \delta(E - E_k)\, dE}$$

$$= \frac{1}{2}\upsilon^2(E)\tau_f(E)$$

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key results

$$\Delta V = RI - S\,\Delta T$$

$$I_Q = TS\,I - K_e \Delta T$$

$$R = \left(\frac{2q^2}{h} I_0 \right)^{-1}$$

$$S = \left(\frac{k_B}{-q} \right) \frac{I_1}{I_0}$$

$$K_e = \frac{2k_B^2 T}{h} \left\{ I_2 - \frac{I_1^2}{I_0} \right\}$$

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \Sigma(E) \left(-\frac{\partial f_S}{\partial E} \right) dE$$

$$I_j = \int \left(\frac{E - F_n}{k_B T} \right)^j \bar{T}(E) \left(-\frac{\partial f_S}{\partial E} \right) dE$$

$$\Sigma(E) = \frac{h}{2L^2} \sum_{\vec{k}} \upsilon_x^2 \tau_f \delta\left(E - E_k\right)$$

$$\bar{T}(E) = T(E) M(E)$$

key results

$$M(E) = \sum_{k_\perp} \Theta(E - E_k)$$

$$T(E) = \frac{\langle\langle \lambda(E) \rangle\rangle}{L}$$

$$\Sigma(E) = \frac{h}{2L^2} \sum_{k} \upsilon_x^2 \tau_f \delta(E - E_k)$$

$$\bar{T}(E) = T(E) M(E)$$

$$\langle\langle \lambda(E) \rangle\rangle \equiv 2 \frac{\langle \upsilon_x^2 \tau_f \rangle}{\langle |\upsilon_x| \rangle}$$

$$\langle\langle \lambda(E) \rangle\rangle = 2\upsilon(E)\tau_f(E) \qquad \text{(1D)}$$

$$\langle\langle \lambda(E) \rangle\rangle = (\pi/2)\upsilon(E)\tau_f(E) \qquad \text{(2D)}$$

$$\langle\langle \lambda(E) \rangle\rangle = (4/3)\upsilon(E)\tau_f(E) \qquad \text{(3D)}$$

questions

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