ECE-656: Fall 2011

Lecture 14: The Boltzmann Transport Equation

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coupled current equations

$$J_x = \sigma \mathcal{E}_x - \sigma S \, dT_L / dx$$

$$J_x^q = T_L \sigma S \mathcal{E}_x - \kappa_0 \, dT_L / dx$$

$$\mathcal{E}_x = \rho J_x + S \frac{dT_L}{dx}$$

$$J_x^q = \pi J_x - \kappa_e \frac{dT}{dx}$$

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

$$\sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right)$$

$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T_L} \right) \sigma'(E) dE \Big/ \int \sigma'(E) dE$$

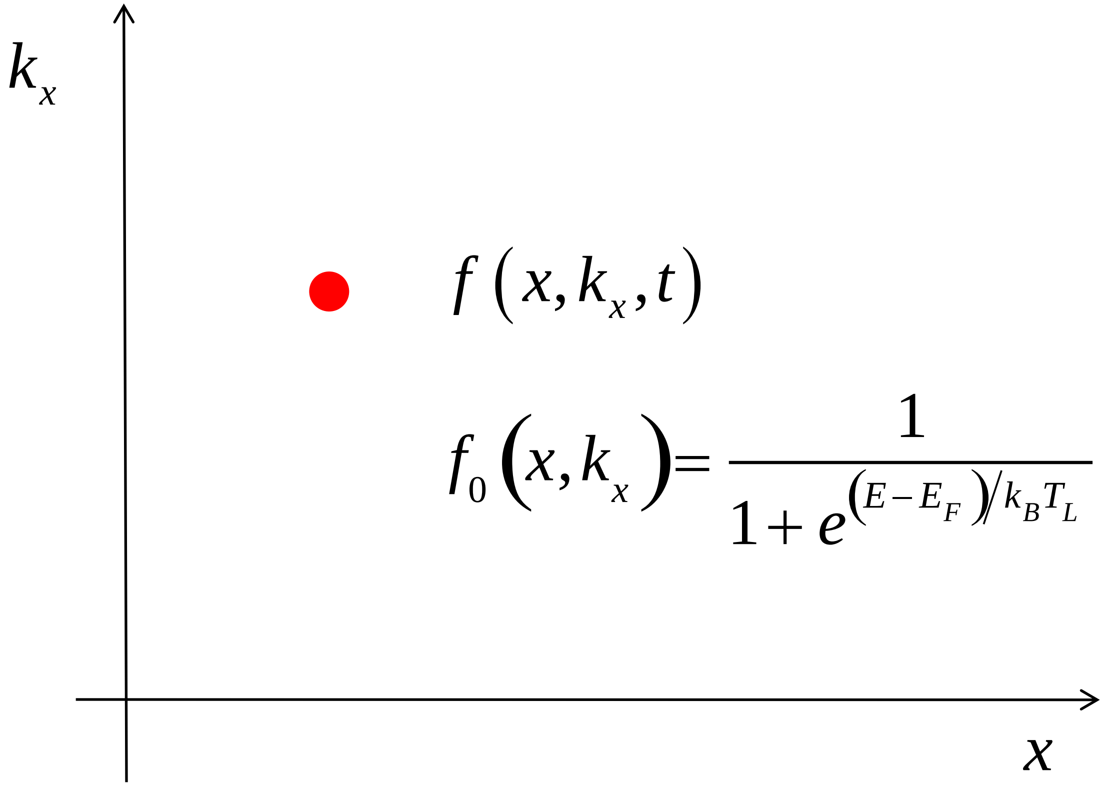
$$\pi = T_L S$$

$$\kappa_0 = T_L \left(\frac{k_B}{q} \right)^2 \int \left(\frac{E - E_F}{k_B T_L} \right)^2 \sigma'(E) dE$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

$f(r, k, t)$

$$\vec{J}_n(\vec{r}) = \frac{1}{A}\sum_{k}(-q)\vec{\upsilon}(\vec{k})\, f(\vec{r},\vec{k})$$



$$f(x, k_x, t)$$

$$f_0(x, k_x) = \frac{1}{1 + e^{(E - E_F)/k_B T_L}}$$

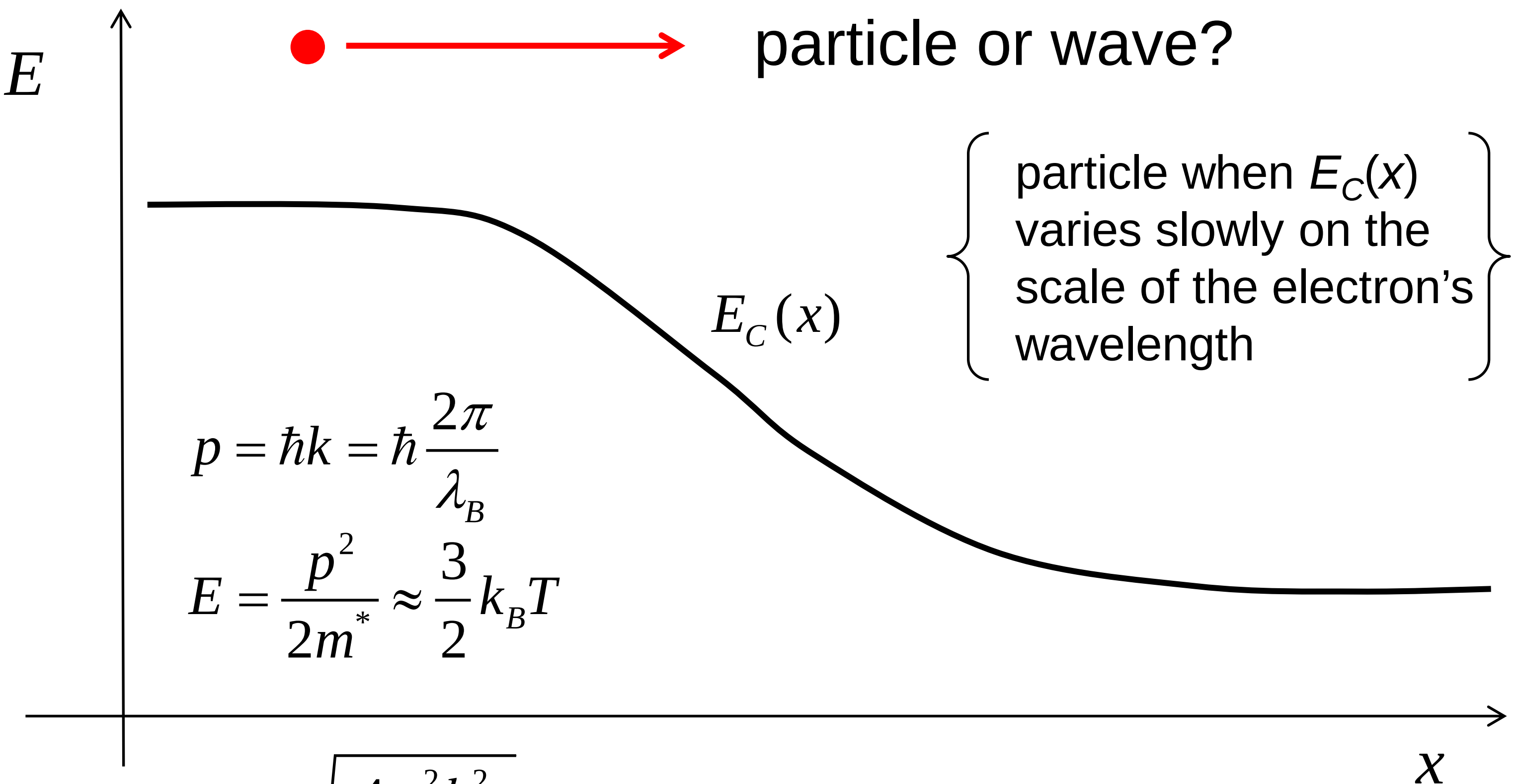
goals

1) Find an equation for $f(r, p, t)$ out of equilibrium
2) Learn how to solve it near equilibrium
3) Relate the results to our Landauer approach results – *in the diffusive limit*
4) Add a B-field and show how transport changes

outline

1) Introduction
2) **Equation of motion**
3) The BTE
4) Solving the s.s. BTE
5) Discussion
6) Summary

quantum vs. semi-classical transport



particle or wave?

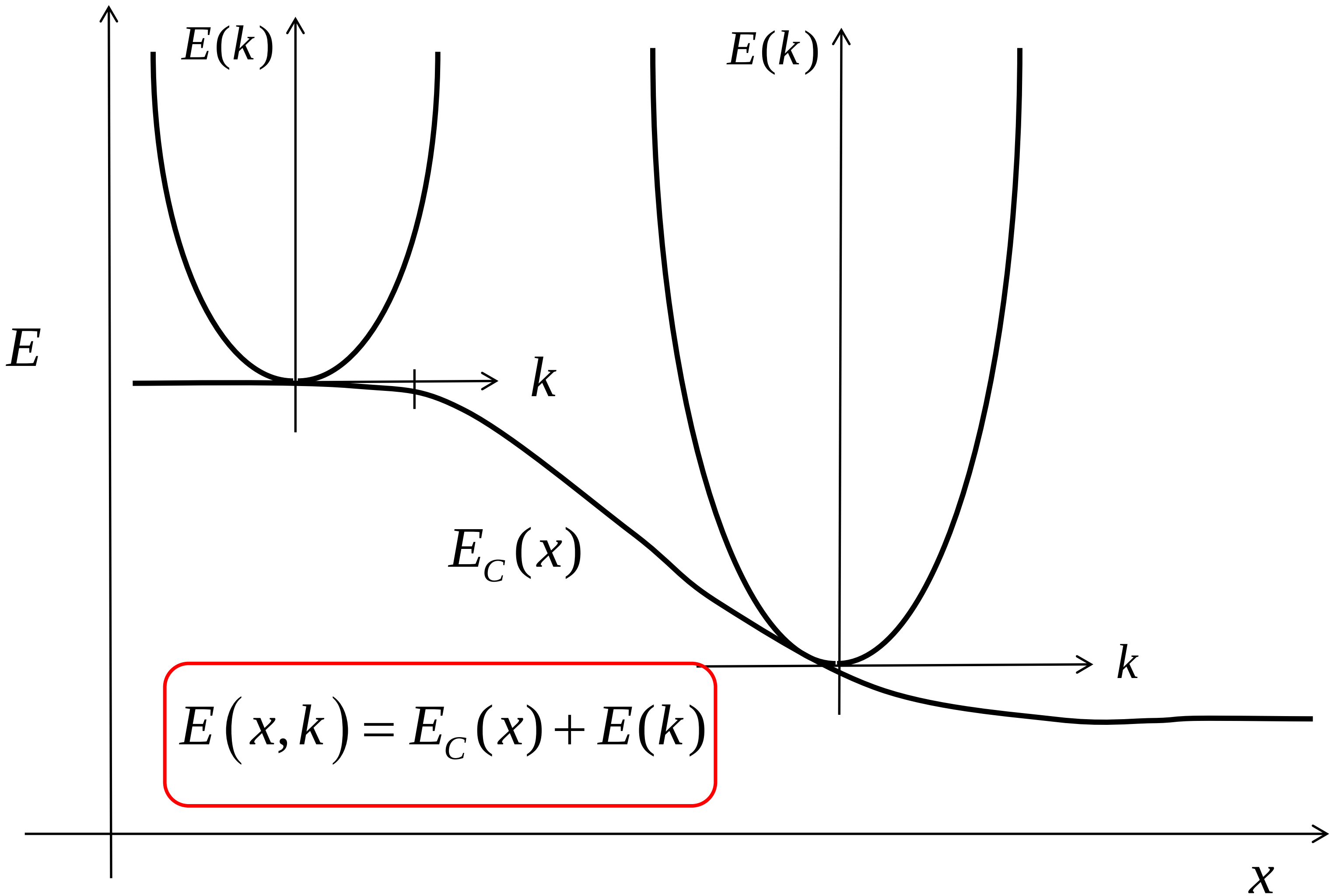
particle when $E_C(x)$ varies slowly on the scale of the electron's wavelength

$$p = \hbar k = \hbar \frac{2\pi}{\lambda_B}$$

$$E = \frac{p^2}{2m^*} \approx \frac{3}{2} k_B T$$

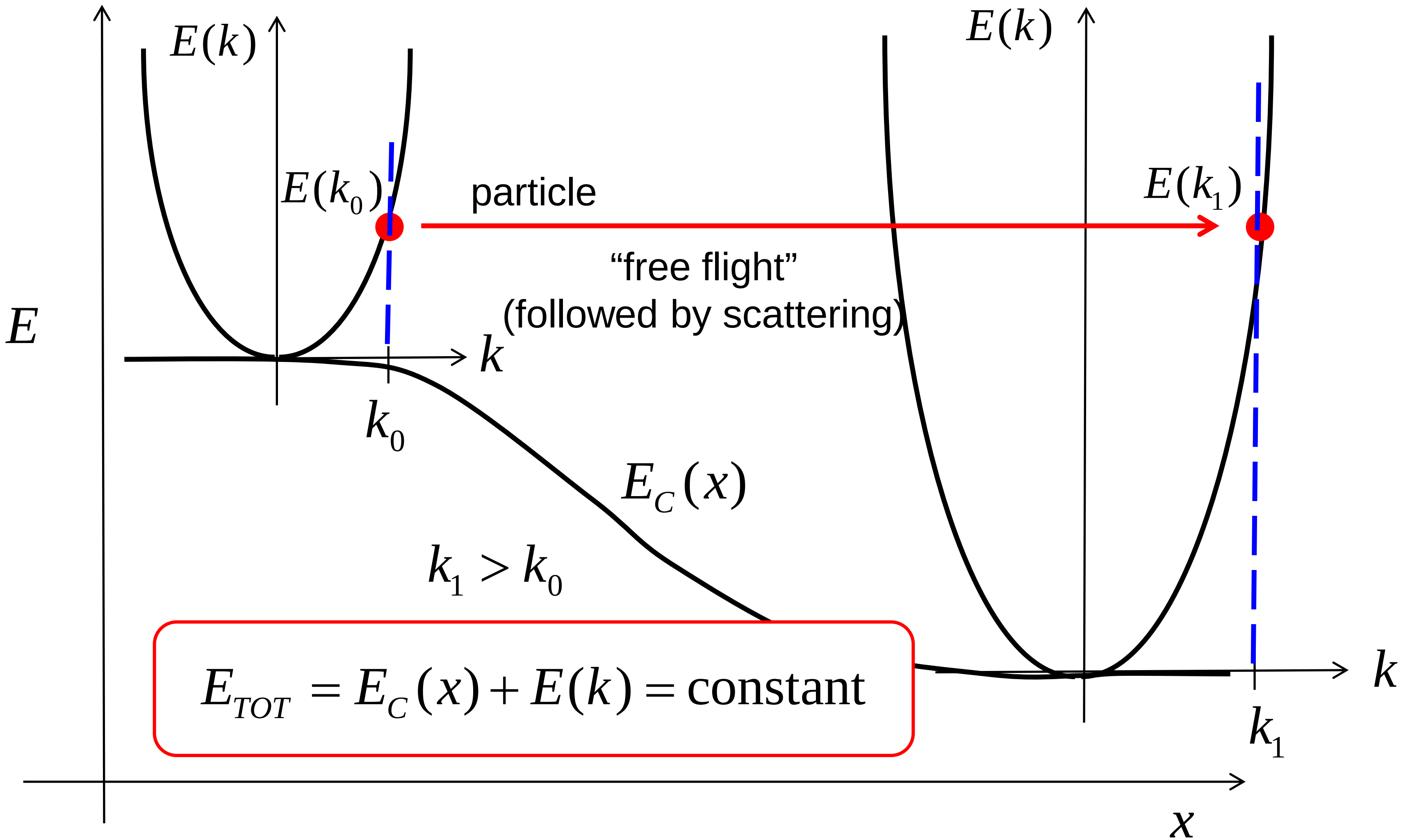
$$\lambda_B = \sqrt{\frac{4\pi^2 \hbar^2}{3m^* k_B T}} \simeq 10\text{nm (electrons in Si at 300K)}$$

semi-classical transport



$$E(x,k) = E_C(x) + E(k)$$

semi-classical transport



semi-classical transport

$$E_{TOT} = E_C(x) + E(k)$$

$$\frac{dE_{TOT}\left(x,k\right)}{dt} = 0 = \frac{dE_C(x)}{dx}\frac{dx}{dt} + \frac{dE(k)}{dk_x}\frac{dk_x}{dt}$$

$$0 = \frac{dE_C(x)}{dx}\upsilon_x + \frac{1}{\hbar}\frac{dE}{dk_x}\frac{d\left(\hbar k_x\right)}{dt}$$

$$0 = \frac{dE_C(x)}{dx}\upsilon_x + \upsilon_x\frac{d\left(\hbar k_x\right)}{dt}$$

$$\frac{d\left(\hbar k_x\right)}{dt} = F_e = -\frac{dE_C(x)}{dx}$$

semi-classical transport

$$\frac{d\left(\hbar\vec{k}\right)}{dt} = -\nabla_r E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r})$$

$$\left\{ \frac{d\vec{p}}{dt} = \vec{F}_e \right\}$$

$$\hbar\vec{k}(t) = \hbar\vec{k}(0) + \int_0^t -q\vec{\mathcal{E}}(t')dt'$$

$$\vec{\upsilon}_g(t) = \frac{1}{\hbar}\nabla_k E\left[\vec{k}(t)\right]$$

$$\vec{r}(t) = \vec{r}(0) + \int_0^t \vec{\upsilon}_g(t')dt'$$

equations of motion for "semi-classical transport"

E_C varies slowly on the scale of the electron's wavelength.

no effective mass!

exercise: equations of motion for m*(x)

i) assume:

$$E(k,\vec{r}) \approx \frac{\hbar^2 k^2}{2m^*(\vec{r})}$$

ii) assume that m* varies slowly with position

iii) derive the equation of motion in *k*-space

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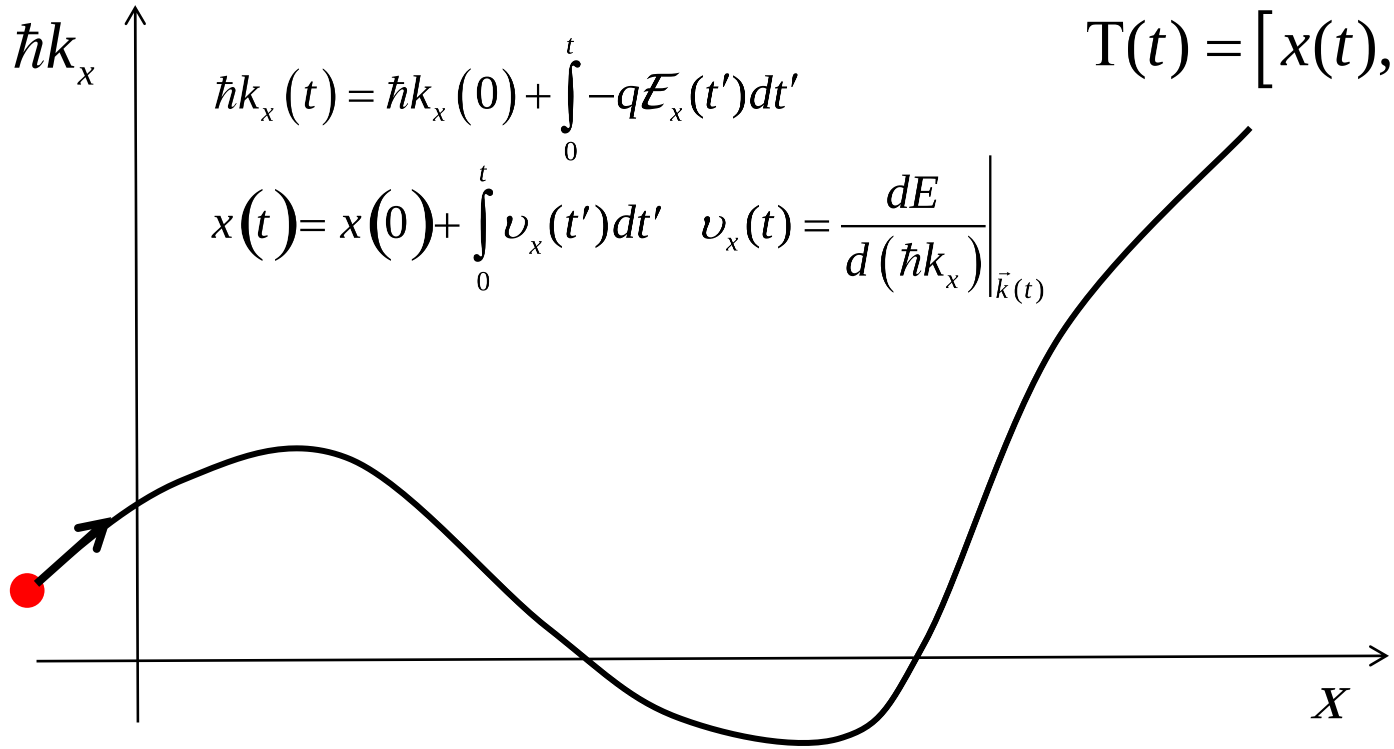
trajectories in phase space

$$p_x = \hbar k_x$$

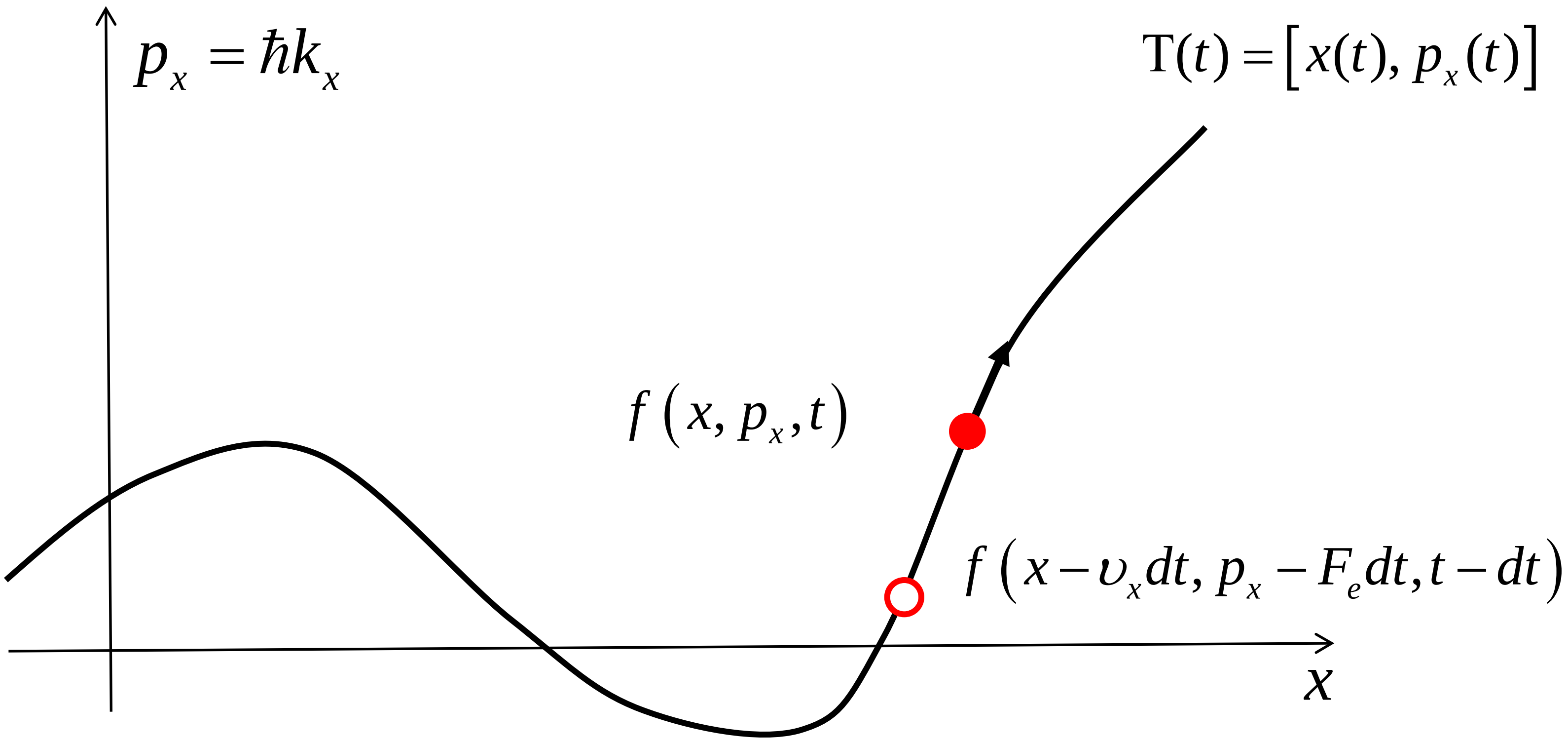
$$T(t) = \left[x(t), p_x(t) \right]$$

$$\hbar k_x(t) = \hbar k_x(0) + \int_0^t -q\mathcal{E}_x(t')dt'$$

$$x(t) = x(0) + \int_0^t \upsilon_x(t')dt' \qquad \upsilon_x(t) = \left.\frac{dE}{d(\hbar k_x)}\right|_{\vec{k}(t)}$$



Boltzmann Transport Equation (BTE)



$$f\left(x, p_x, t\right) = f\left(x - \upsilon_x dt, p_x - F_e dt, t - dt\right)$$

$$\frac{df}{dt} = 0$$

Boltzmann Transport Equation (BTE)

$$f\left(x, p_x, t\right) \qquad \frac{df}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial p_x}\frac{dp_x}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\upsilon_x + \frac{\partial f}{\partial p_x}F_x = 0$$

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = 0$$

$$\vec{F}_e = -q\vec{\mathcal{E}} - q\vec{\upsilon} \times \vec{B}$$

$$\nabla_r f = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$$

$$\nabla_p f = \frac{\partial f}{\partial p_x}\hat{p}_x + \frac{\partial f}{\partial p_y}\hat{p}_y + \frac{\partial f}{\partial p_z}\hat{p}_z$$

$$\vec{p} = \hbar\vec{k}$$

result

$$f\left(\vec{r},\vec{p},t\right)$$

$$\frac{\partial f\left(\vec{r},\vec{p},t\right)}{\partial t}+\left\{\vec{\upsilon}\bullet\nabla_{r}f+\vec{F}_{e}\bullet\nabla_{p}f\right\}=G\left(\vec{r},\vec{p},t\right)-R\left(\vec{r},\vec{p},t\right)$$

optical absorption, impact ionization, etc.
and carrier scattering

Boltzmann Transport Equation (BTE)

$f\left(\vec{r},\vec{p},t\right):$

$$\frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_r f+\vec{F}_e\bullet\nabla_p f=0$$

neglected scattering!

assumptions:

1) semi-classical treatment of electrons in a crystal with *E*(*k*)

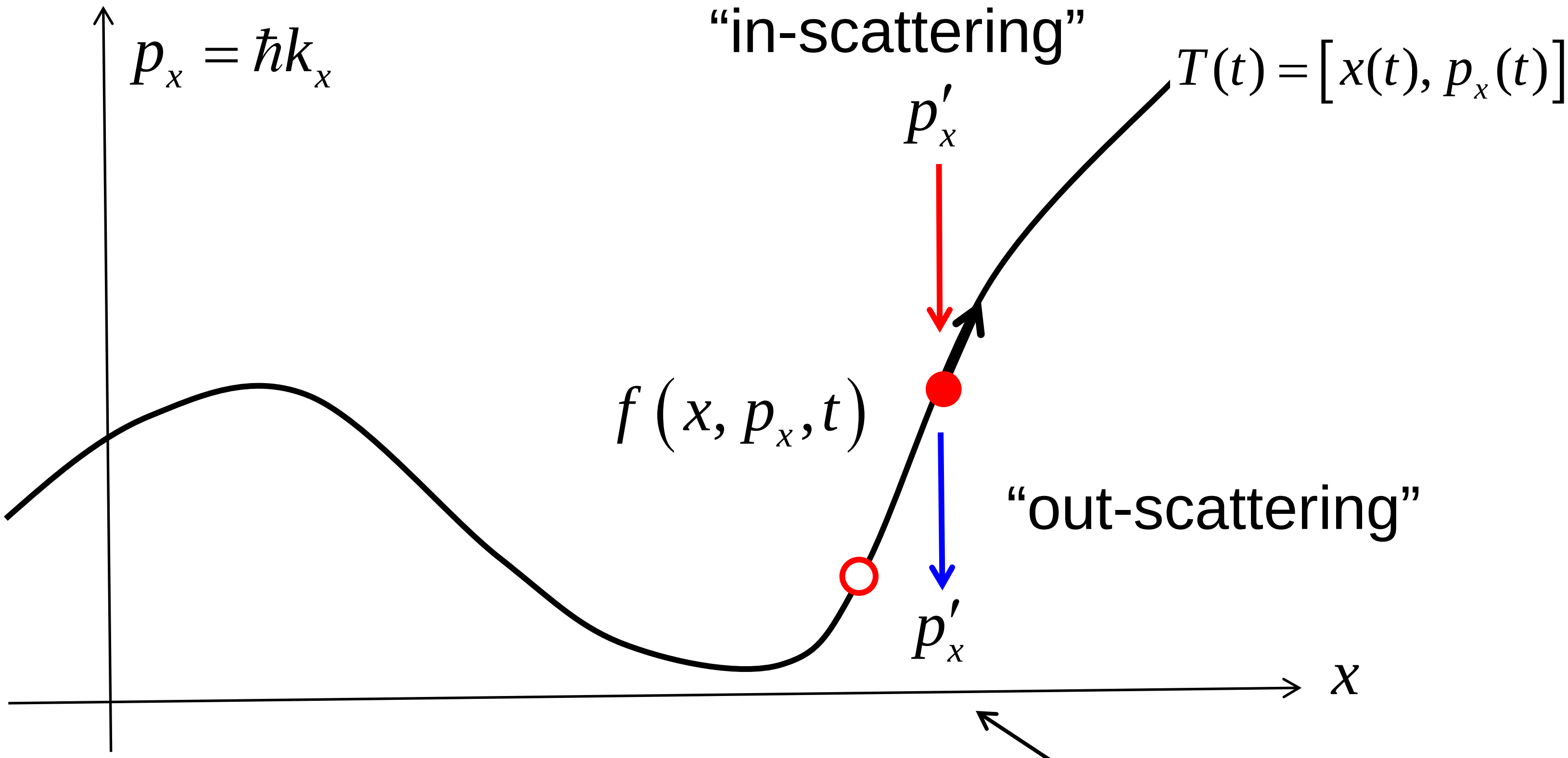
$$\frac{d\left(\hbar\vec{k}\right)}{dt}=-\nabla E_C(\vec{r})=-q\vec{\mathcal{E}}(\vec{r}) \qquad E=E_C(\vec{r})+E\left(\vec{k}\right)$$

$$\upsilon_g\left(t\right)=\frac{1}{\hbar}\nabla_k E\left[k\left(t\right)\right] \qquad \Delta p_x\Delta x\geq\hbar$$

2) neglected generation-recombination

3) neglected e-e correlations (mean-field-approximation)

in and out-scattering



$$\left.\frac{df}{dt}\right|_{coll} = \hat{C}f = \text{in-scattering - out-scattering}$$

position, x, does not change

scattering operator

$$\left.\frac{df}{dt}\right|_{coll} = \hat{C}f\left(\vec{r},\vec{p},t\right) = \text{in-scattering rate - out-scattering rate}$$

$$\text{in-scattering rate} = \sum_{p'} S\left(\vec{p}' \to \vec{p}\right) f\left(\vec{p}'\right)\left[1 - f\left(\vec{p}\right)\right]$$

$$\text{out-scattering rate} = \sum_{p'} S\left(\vec{p} \to \vec{p}'\right) f\left(\vec{p}\right)\left[1 - f\left(\vec{p}'\right)\right]$$

$$\hat{C}f\left(\vec{r},\vec{p},t\right) = \sum_{p'} S\left(\vec{p}' \to \vec{p}\right) f\left(\vec{p}'\right)\left[1 - f\left(\vec{p}\right)\right] - \sum_{p'} S\left(\vec{p} \to \vec{p}'\right) f\left(\vec{p}\right)\left[1 - f\left(\vec{p}'\right)\right]$$

nondegenerate scattering operator

$$\hat{C}f(\vec{r},\vec{p},t) = \sum_{p'} S(\vec{p}\,' \to \vec{p}) f(\vec{p}\,')\left[1 - f(\vec{p})\right] - \sum_{p'} S(\vec{p} \to \vec{p}\,') f(\vec{p})\left[1 - f(\vec{p}\,')\right]$$

probability that the state at p' is occupied

probability that the state at p is empty

$$\hat{C}f(\vec{r},\vec{p},t) = \sum_{p'} S(\vec{p}\,' \to \vec{p}) f(\vec{p}\,') - \sum_{p'} S(\vec{p} \to \vec{p}\,') f(\vec{p})$$

non-degenerate scattering operator
(assumes final state empty)

conservation of carriers

We are discussing scattering mechanisms that move carriers around in *k*-space. They do not create or destroy carriers.

$$\sum_p \hat{C} f(\vec{r}, \vec{p}, t) = 0$$

$$\sum_p \left\{ \sum_{p'} S(\vec{p}', \vec{p}) f(\vec{p}') - \sum_{p'} S(\vec{p}, \vec{p}') f(\vec{p}) \right\} = \sum_{p,p'} S(\vec{p}', \vec{p}) f(\vec{p}') - \sum_{p,p'} S(\vec{p}, \vec{p}') f(\vec{p})$$

$$\sum_{p,p'} S(\vec{p}', \vec{p}) f(\vec{p}') = \sum_{p',p} S(\vec{p}', \vec{p}) f(\vec{p}')$$ (interchange order of summation)

$$\sum_{p,p'} S(\vec{p}', \vec{p}) f(\vec{p}') = \sum_{p,p'} S(\vec{p}, \vec{p}') f(\vec{p})$$ (interchange labels of dummy indices)

Relaxation Time Approximation (RTA)

$$\hat{C}f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_m}\right)$$

$$\delta f = f(\vec{p}) - f_0(\vec{p})$$

$$\hat{C}f = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\hat{C}f = \frac{f_0(\vec{p})}{\tau_m} - \frac{f(\vec{p})}{\tau_m}$$

in-scattering – out-scattering

See Lundstrom: pp. 139-141. The RTA can be justified when the scattering is **isotropic and/or elastic** in which case the proper time to use is the “momentum relaxation time.”

meaning of the RTA

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\frac{\delta f}{\tau_m}$$

Assume spatial uniformity, no *E*-field.

$$\frac{\partial f}{\partial t} = -\frac{\delta f}{\tau_m}$$

$$\delta f = f - f_0$$

$$\frac{\partial(\delta f)}{\partial t} = -\frac{\delta f}{\tau_m}$$

$$\delta f(t) = \delta f(0) e^{-t/\tau_m}$$

Perturbations decay away exponentially with a characteristic time, τ_m

steady-state BTE in 1D

$$\upsilon_x \frac{\partial f}{\partial x} + F_x \frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m}$$

RTA

no B-fields for now

$$F_x = -q\mathcal{E}_x$$

$$f(\vec{p}) = f_0(\vec{p}) + \delta f(\vec{p})$$

$$\left| f_0(\vec{p}) \right| >> \left| \delta f(\vec{p}) \right|$$

$$\delta f(\vec{p}) = f(\vec{p}) - f_0(\vec{p})$$

near-equilibrium

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near eq., s.s BTE

$$\vec{\upsilon} \bullet \nabla_r f - q\vec{\mathcal{E}} \bullet \nabla_p f = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\nabla_r f \approx \nabla_r f_0 \qquad \nabla_p f \approx \nabla_p f_0$$

$$\vec{\upsilon} \bullet \nabla_r f_0 - q\vec{\mathcal{E}} \bullet \nabla_p f_0 = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\delta f(\vec{p}) = -\tau_m \vec{\upsilon} \bullet \nabla_r f_0 + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_0$$

BTE solution

$$\delta f = -\tau_m \vec{\upsilon} \bullet \nabla_r f_0 + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_0$$

$$f_0(\vec{p}) = \frac{1}{1+e^{\Theta}} \qquad \Theta(\vec{r},\vec{p}) = \left[E(\vec{r},\vec{p}) - F_n(\vec{r})\right] / k_B T_L$$

$$= \left[E_C(\vec{r}) + E(\vec{p}) - F_n(\vec{r})\right] / k_B T_L$$

$$\nabla_r f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_r \Theta$$

$$\nabla_p f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_p \Theta$$

$$\frac{\partial f_0}{\partial \Theta} = k_B T_L \frac{\partial f_0}{\partial E}$$

$$\delta f = \tau_m k_B T_L \left(-\frac{\partial f_0}{\partial E}\right)\left[\vec{\upsilon} \bullet \nabla_r \Theta - q\vec{\mathcal{E}} \bullet \nabla_p \Theta\right]$$

BTE solution

$$\delta f = \tau_m k_B T_L \left(-\frac{\partial f_0}{\partial E}\right)\left[\vec{\upsilon} \bullet \nabla_r \Theta - q\vec{\mathcal{E}} \bullet \nabla_p \Theta\right]$$

$$\Theta(\vec{r},\vec{p}) = \left[E_C(\vec{r}) + E(\vec{p}) - F_n(\vec{r})\right] / k_B T_L$$

$$\nabla_r \Theta = \frac{1}{k_B T_L}\left[\nabla_r E_C - \nabla_r F_n\right] + \left[E_C + E(\vec{p}) - F_n\right]\nabla_r\left(\frac{1}{k_B T_L}\right) \qquad \nabla_p \Theta = \frac{\vec{\upsilon}(\vec{p})}{k_B T_L}$$

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E}\right)\vec{\upsilon} \bullet \left\{-\nabla_r F_n + T_L\left[E_C + E(\vec{p}) - F_n\right]\nabla_r\left(\frac{1}{T_L}\right)\right\}$$

generalized force

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

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

"generalized force"

The two forces driving current flow are gradients in QFL and gradients in (inverse) temperature. In Lecture 4, we saw that ($f_1 - f_2$) produces current flow and that differences in Fermi level and temperature cause differences in *f*.

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another look at the solution…

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}} \rightarrow \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \upsilon_x \mathcal{F}_x$$

$$\vec{\mathcal{F}} = -\nabla_r F_n + T_L \left[E_C + E(k) - F_n \right] \nabla_r \left(\frac{1}{T_L} \right) \rightarrow -\frac{dF_n}{dx} = -q\mathcal{E}_x$$

$$\delta f = q \tau_m \mathcal{E}_x \left(\frac{\partial f_0}{\partial E} \right) \upsilon_x$$

$$\delta f = q \tau_m \mathcal{E}_x \left(\frac{\partial f_0}{\partial p_x} \right) \left(\frac{\partial p_x}{\partial E} \right) \upsilon_x = q \tau_m \mathcal{E}_x \left(\frac{\partial f_0}{\partial p_x} \right)$$

another look at the solution…

$$\delta f = \left(\frac{\partial f_0}{\partial p_x}\right) q\tau_m \mathcal{E}_x \qquad f = f_0 + \delta f = f_0 + \left(\frac{\partial f_0}{\partial p_x}\right) q\tau_m \mathcal{E}_x$$

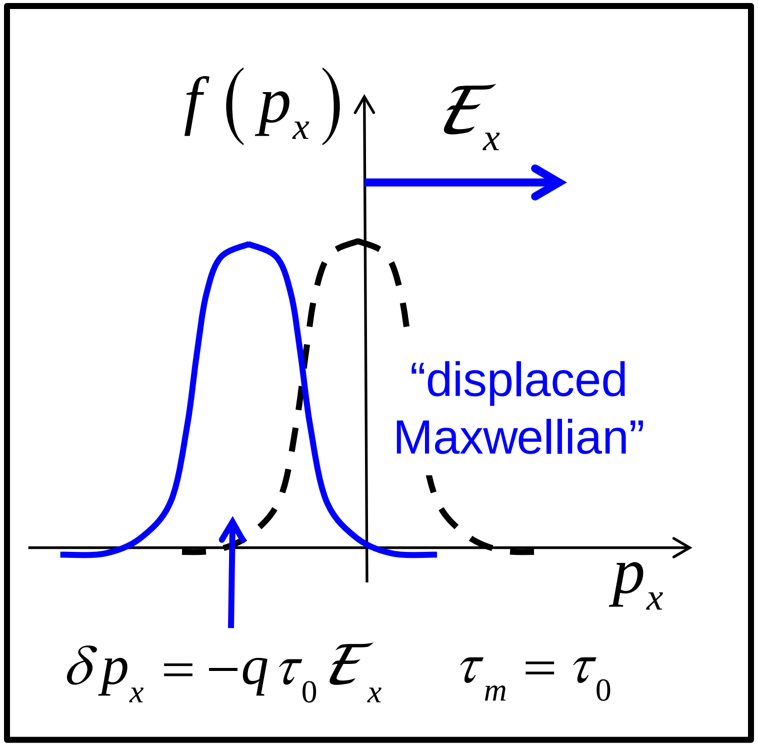
Recall:

$$g(x+dx) \approx g(x) + \frac{\partial g}{\partial x}dx + \ldots$$

$$f(\vec{p}) = f_0(\vec{p} + dp_x\hat{x})$$

$$dp_x = q\tau_m \mathcal{E}_x$$

So the distribution has been displaced by p_d is a direction ***opposite*** to the electric field



now what?

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

We have solved the BTE,
now what do we do with the solution?

moments

$$n(\vec{r}) = \frac{1}{\Omega}\sum_{k} f_0(\vec{r},\vec{k}) + \delta f(\vec{r},\vec{k}) \approx \frac{1}{\Omega}\sum_{k} f_0(\vec{r},\vec{k})$$

$$\vec{J}_n(\vec{r}) = \frac{1}{A}\sum_{k}(-q)\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

$$\vec{J}_W(\vec{r}) = \frac{1}{A}\sum_{k} E(\vec{k})\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

$$\vec{J}_Q(\vec{r}) = \frac{1}{A}\sum_{k}\left(E(k) - F_n\right)\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

To evaluate these quantities, we need to work out sums in *k*-space.

moments

$$n(\vec{r}) = \frac{1}{\Omega}\sum_k f_0(\vec{r},\vec{k}) + \delta f(\vec{r},\vec{k}) \approx \frac{1}{\Omega}\sum_k f_0(\vec{r},\vec{k})$$

$$\vec{J}_n(\vec{r}) = \frac{1}{A}\sum_k (-q)\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

$$\vec{J}_W(\vec{r}) = \frac{1}{A}\sum_k E(\vec{k})\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

$$\vec{J}_Q(\vec{r}) = \frac{1}{A}\sum_k \left(E(k) - F_n\right)\vec{\upsilon}(\vec{k})\delta f(\vec{r},\vec{k})$$

To evaluate these quantities, we need to work out sums in *k*-space.

recall lecture 4

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summary

1) Semi-classical transport assumes a bulk bandstructure with a slowly varying applied potential.

2) Semiclassical transport ignores quantum reflections and assumes that position and momentum can both be precisely specified.

3) The Boltzmann Transport Equation can be solved to find the probability that states in the device are occupied.

4) In equilibrium, the solution to the BTE is the Fermi function.

summary

BTE:

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

$$\hat{C}f(\vec{r}, \vec{p}, t) = \sum_{p'} S(\vec{p}', \vec{p}) f(\vec{p}')\left[1 - f(\vec{p})\right] - \sum_{p'} S(\vec{p}, \vec{p}') f(\vec{p})\left[1 - f(\vec{p}')\right]$$

RTA:

$$\hat{C}f = -\left(f(\vec{p}) - f_0(\vec{p})\right)\big/\tau_m$$

Solution:

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E}\right) \vec{\upsilon} \bullet \vec{\mathcal{F}} \qquad \vec{\mathcal{F}} = -\nabla_r F_n + T_L \left[E_C + E(k) - F_n\right] \nabla_r \left(\frac{1}{T_L}\right)$$

questions

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