ECE-656: Fall 2009

Lecture 12: Boltzmann Transport Equation

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

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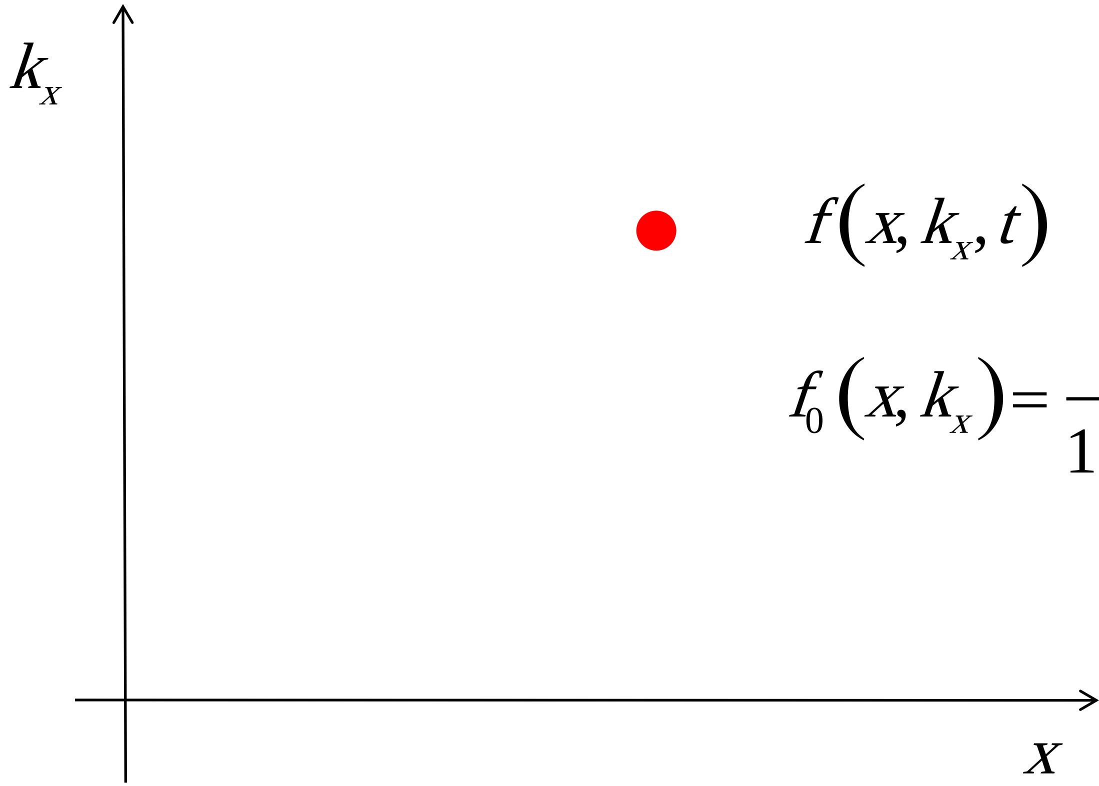
$f(r, k, t)$



$$f\left(x, k_x, t\right)$$

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

finding *f*(*r*, *k*, *t*): by analogy

$$\frac{\partial n}{\partial t} = -\nabla \bullet \frac{\vec{J}_n}{(-q)} + G_n - R_n$$

$$\vec{J}_n = qn\langle \vec{\upsilon} \rangle = qn\left\langle \frac{d\vec{r}}{dt} \right\rangle$$

$$\frac{\partial f}{\partial t} = -\nabla \cdot (\vec{\upsilon} f) + (G - R)$$

$$\vec{J} = f\left(\frac{d\vec{r}}{dt} + \frac{d\vec{k}}{dt} \right)$$

$$\nabla \cdot \vec{\upsilon} f = \nabla_r \cdot (\vec{\upsilon} f) + \nabla_k \cdot \left(\frac{d\vec{k}}{dt} f \right)$$

$$= \vec{\upsilon} \cdot \nabla_r f + \nabla_k \cdot \left(\frac{d\vec{k}}{dt} f \right)$$

$$\hbar \frac{d\vec{k}}{dt} = \vec{F}_e = -q\vec{\mathcal{E}}$$

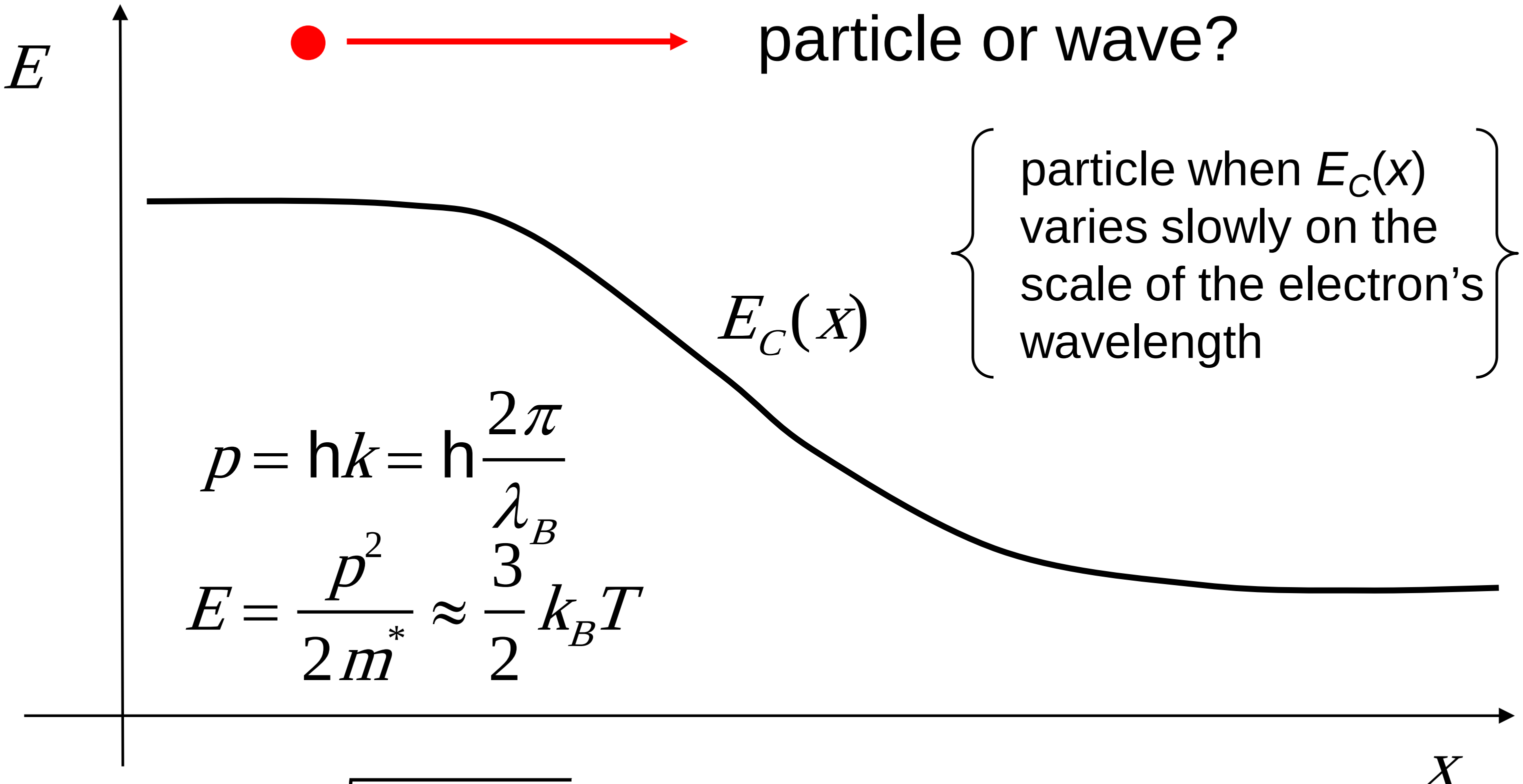
$$(G - R) = \left.\frac{df}{dt}\right|_{coll} + \left.\frac{df}{dt}\right|_{other}$$

$$\frac{\partial f}{\partial t} = -\vec{\upsilon} \cdot \nabla_r f - \frac{1}{\hbar}\vec{F}_e \bullet \nabla_k f + \left.\frac{df}{dt}\right|_{coll}$$

outline

1) Introduction
2) **Semi-classical electron dynamics**
3) Boltzmann Transport Equation (BTE)
4) Scattering
5) Discussion
6) Summary

quantum vs. semi-classical



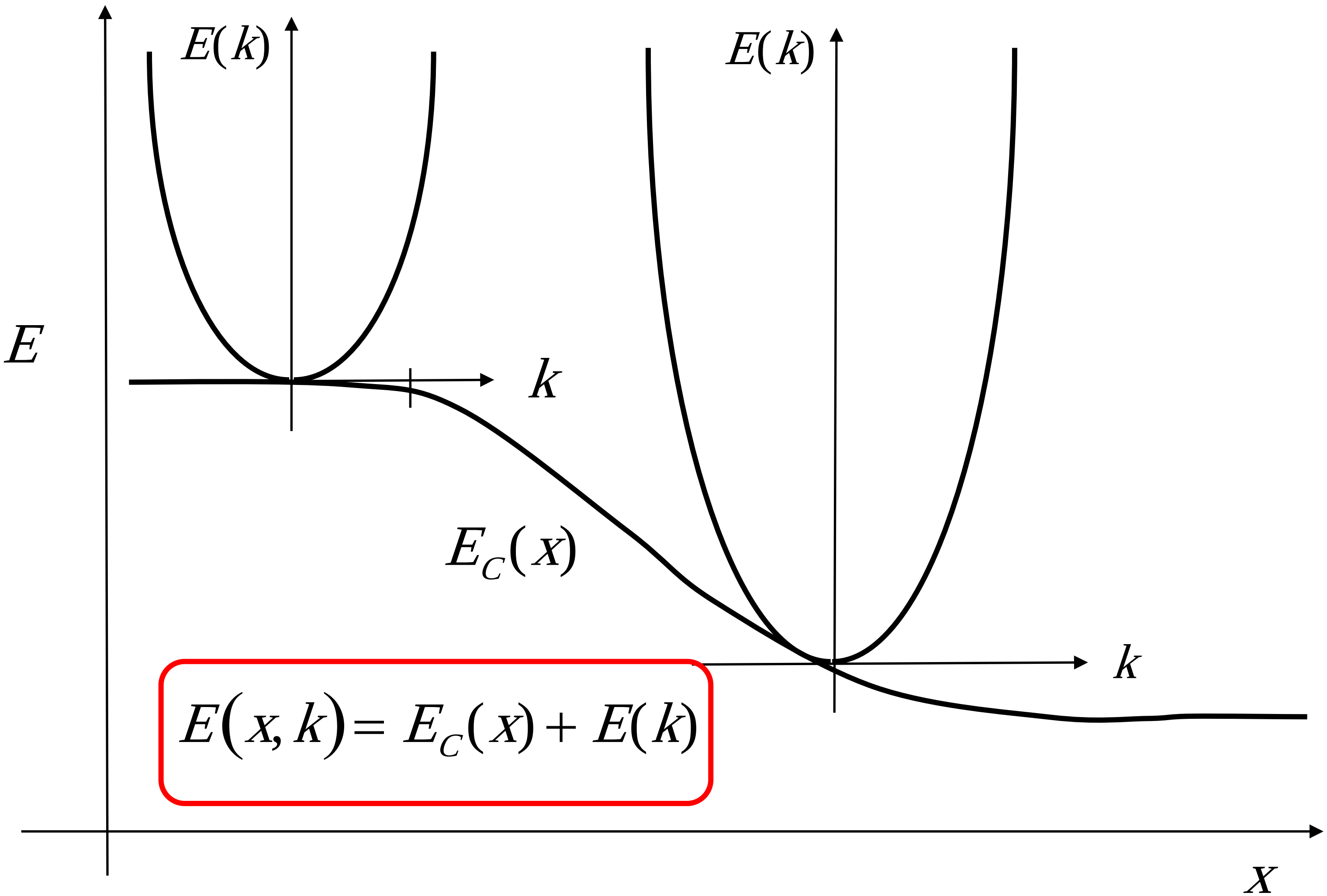
particle when $E_C(x)$ varies slowly on the scale of the electron's wavelength

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

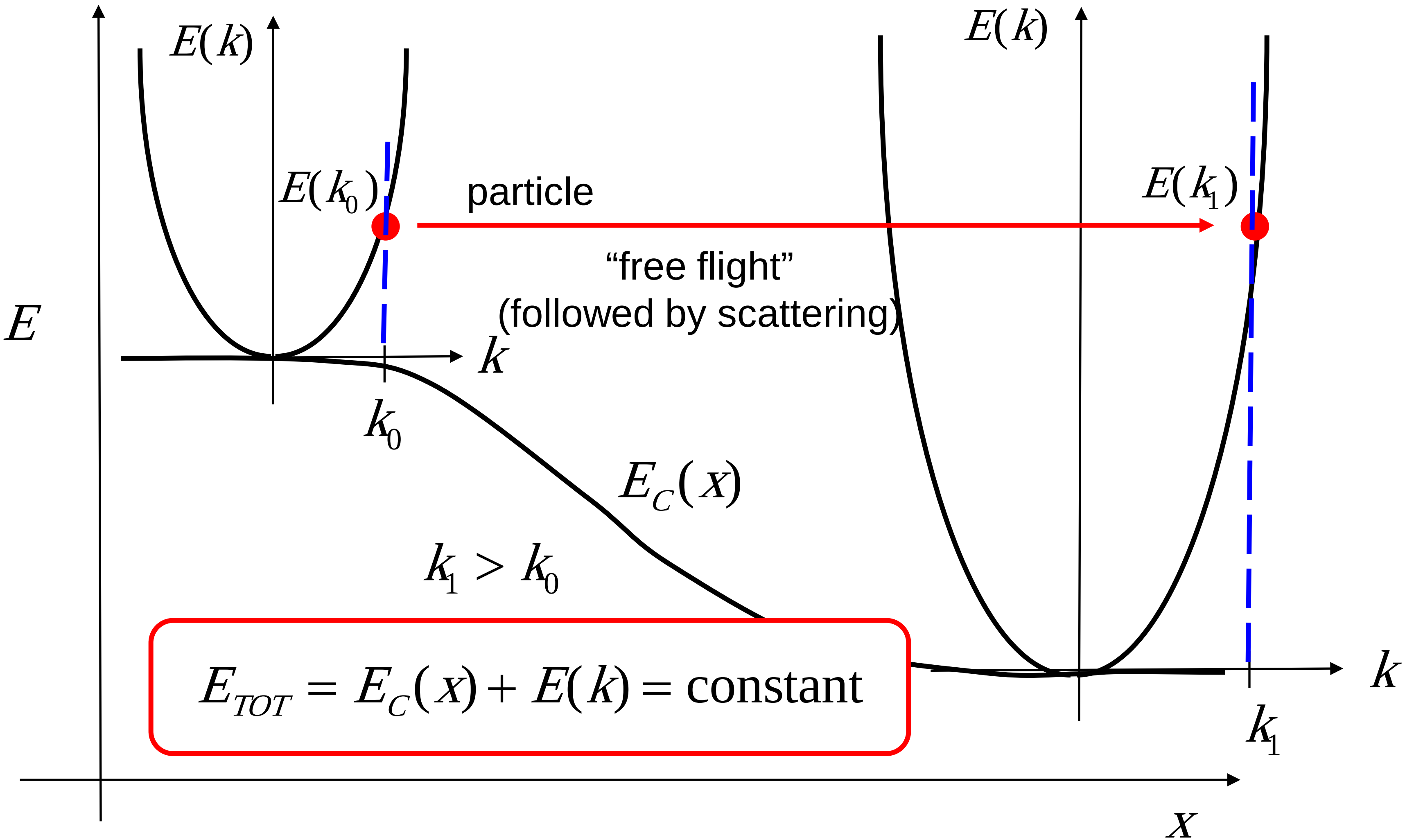
$$E = \frac{p^2}{2m^*} \approx \frac{3}{2} k_B T$$

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

semi-classical transport



semi-classical transport



semi-classical transport

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

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

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

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

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

semi-classical transport

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

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

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

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

equations of motion for semi-classical transport

exercise: equations of motion when *m**(*x*)

i) assume:

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

ii) assume that m* varies <u>slowly</u> with position

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

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2) Semiclassical electron dynamics

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5) Discussion

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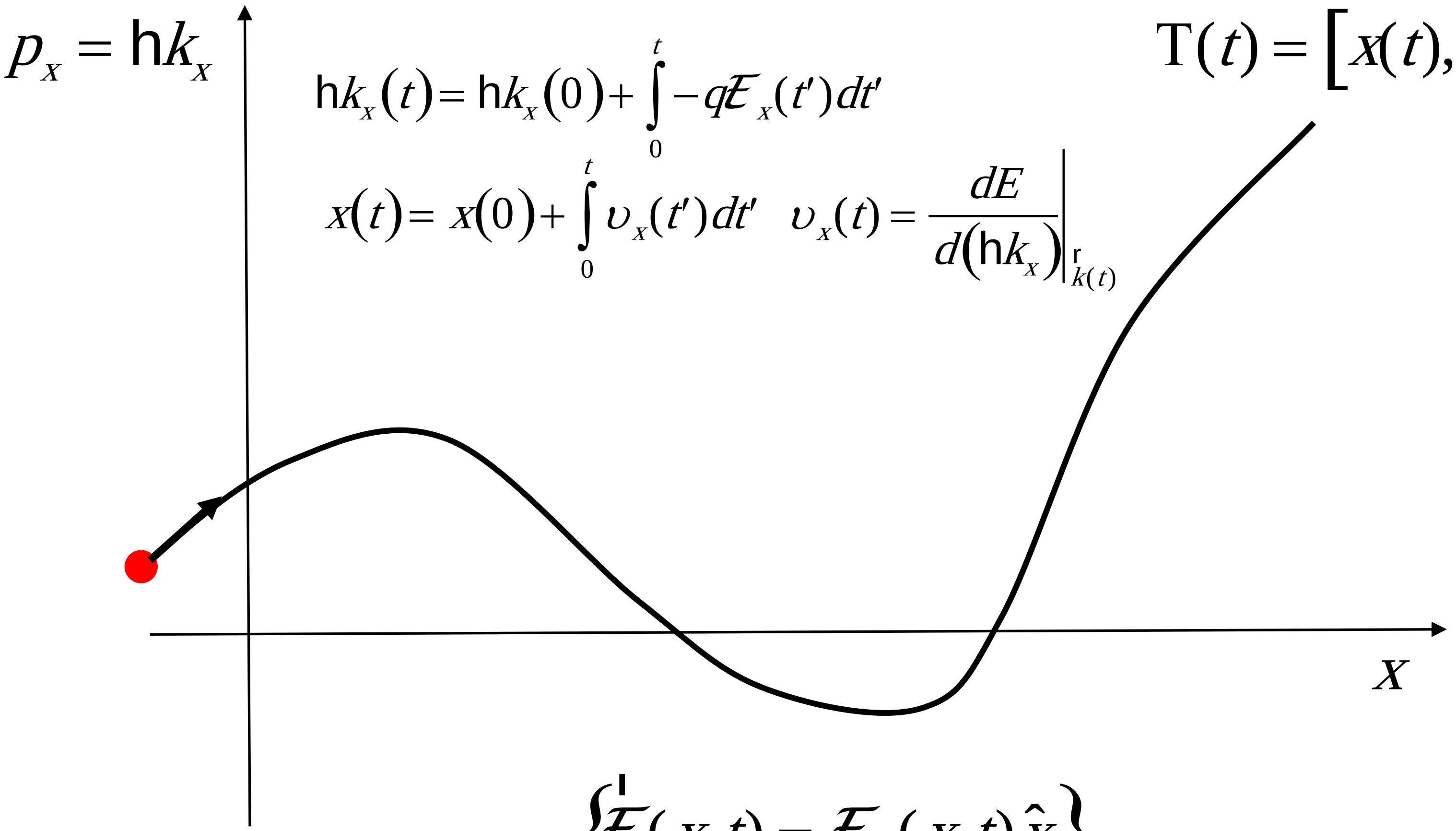
trajectories in phase space



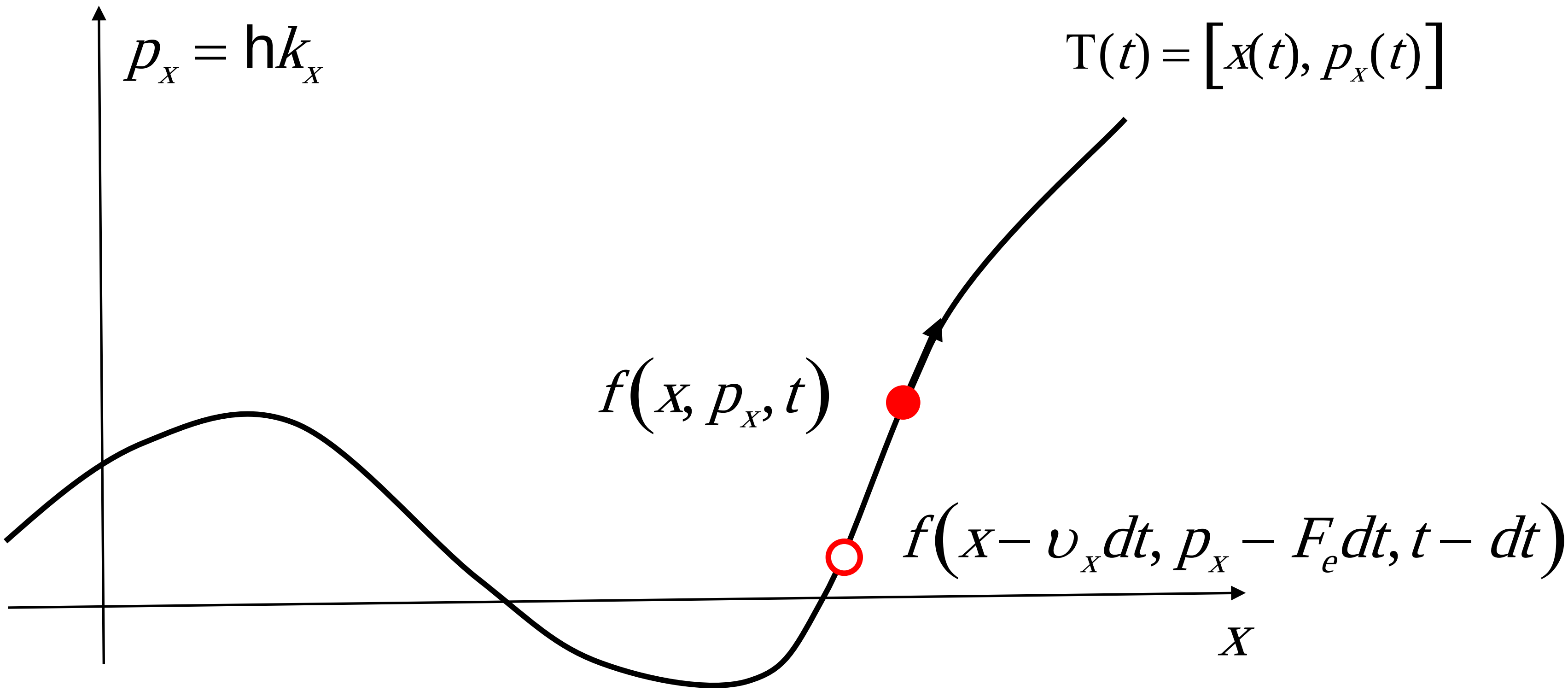
$$\mathrm{T}(t) = \left[x(t),\, p_x(t)\right]$$

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

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

$$\left\{\vec{\mathcal{E}}(x,t) = \mathcal{E}_x(x,t)\,\hat{x}\right\}$$

Boltzmann Transport Equation (BTE)



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

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

Boltzmann Transport Equation (BTE)

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

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

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

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

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

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

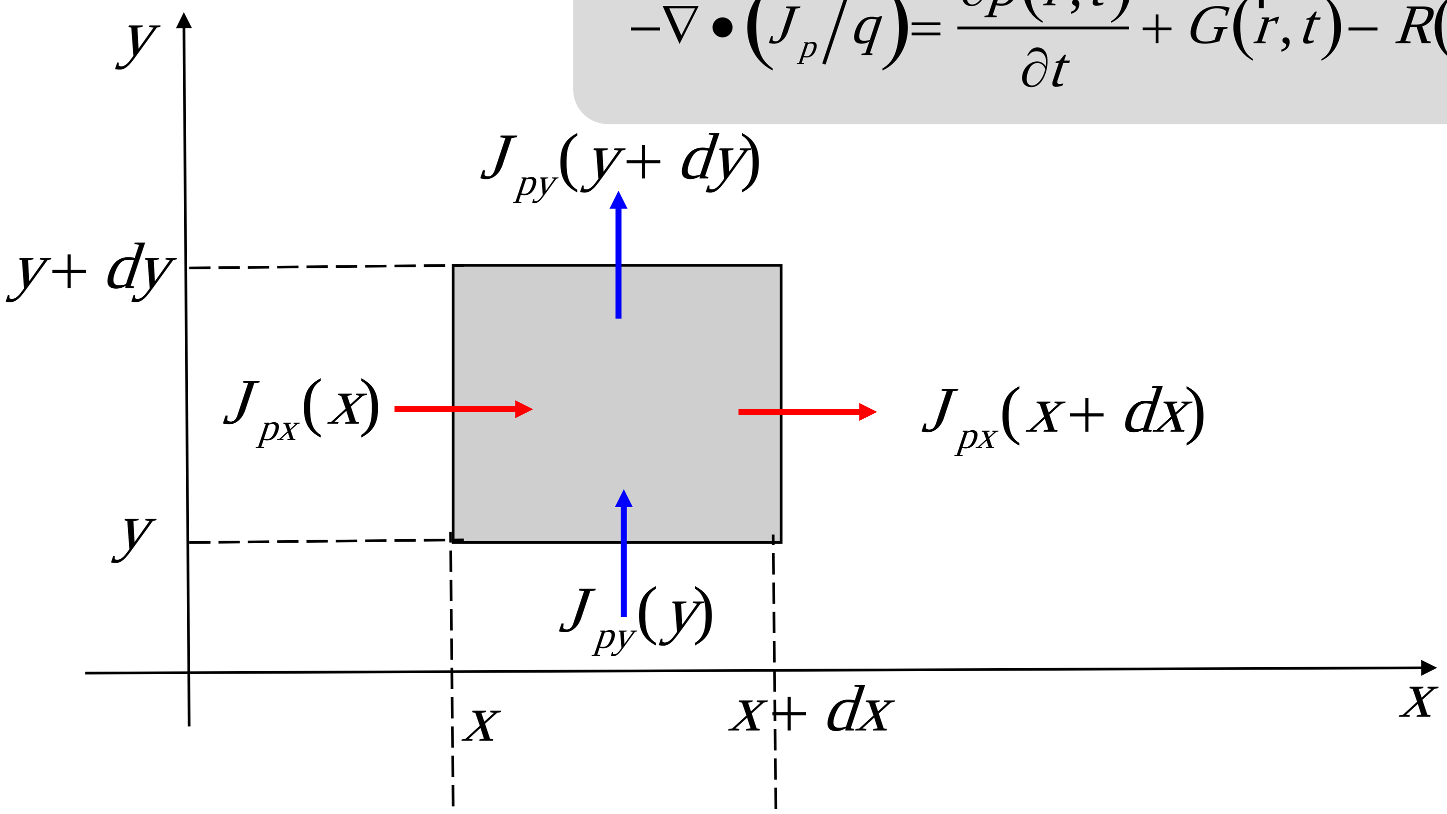
$$\nabla_p f = \frac{\partial f}{\partial p_x}\hat{p}_x + \frac{\partial f}{\partial p_y}\hat{p}_y + \frac{\partial f}{\partial p_z}\hat{p}_z$$

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

another view: continuity equation

$$p(\vec{r},t)$$

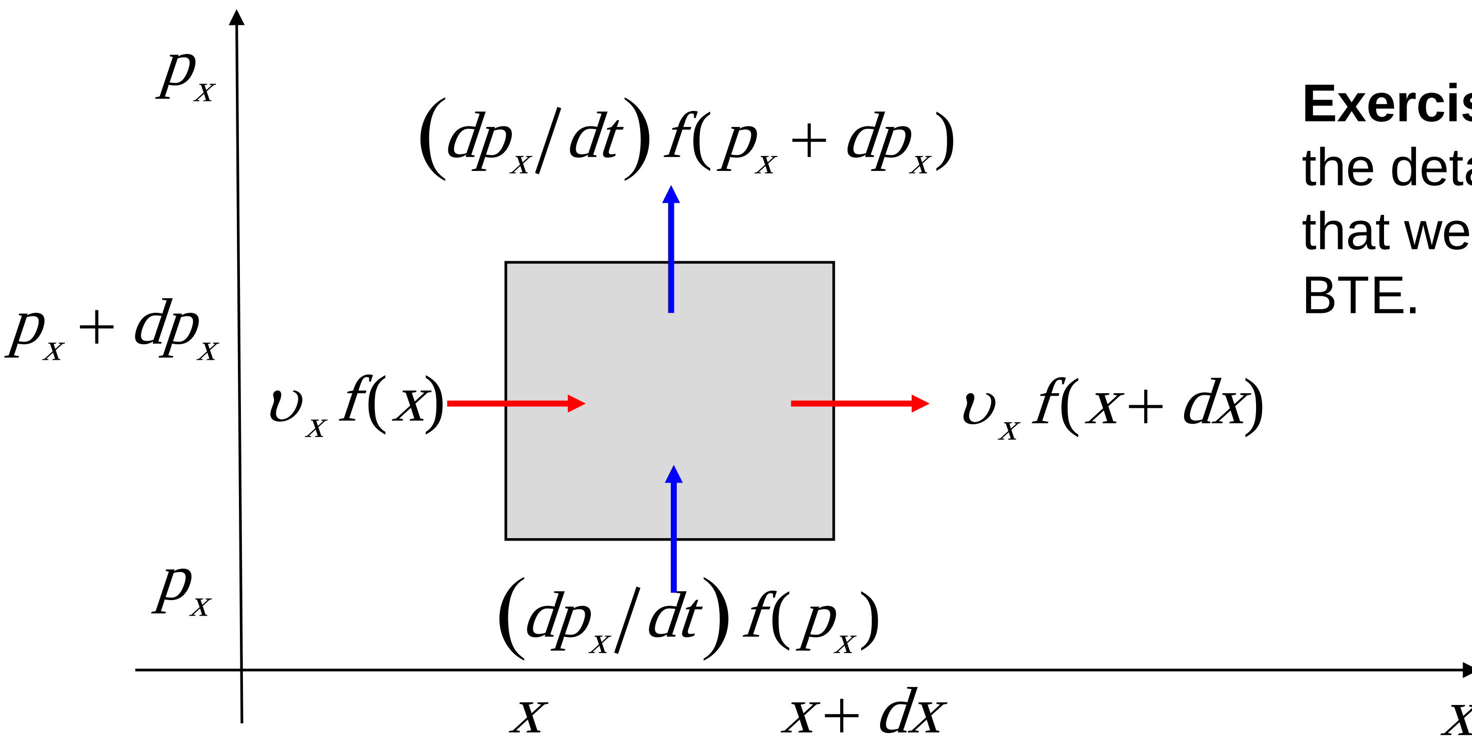
$$-\nabla \bullet \left(\vec{J}_p/q\right) = \frac{\partial p(\vec{r},t)}{\partial t} + G(\vec{r},t) - R(\vec{r},t)$$



continuity equation view

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

$$-\nabla \bullet \left[\left(\upsilon_x \hat{x} f + \upsilon_{p_x} \hat{p}_x f \right) \right] = \frac{\partial f(x, p_x, t)}{\partial t} + G(x, p_x, t) - R(x, p_x, t)$$



Exercise: work out the details and show that we get the same BTE.

result

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

$$\frac{\partial f\left(x, p_x, t\right)}{\partial t} + \left\{\vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f\right\} = G\left(\vec{r}, \vec{p}, t\right) - R\left(\vec{r}, \vec{p}, t\right)$$

optical absorption, impact ionization, etc.
and carrier scattering

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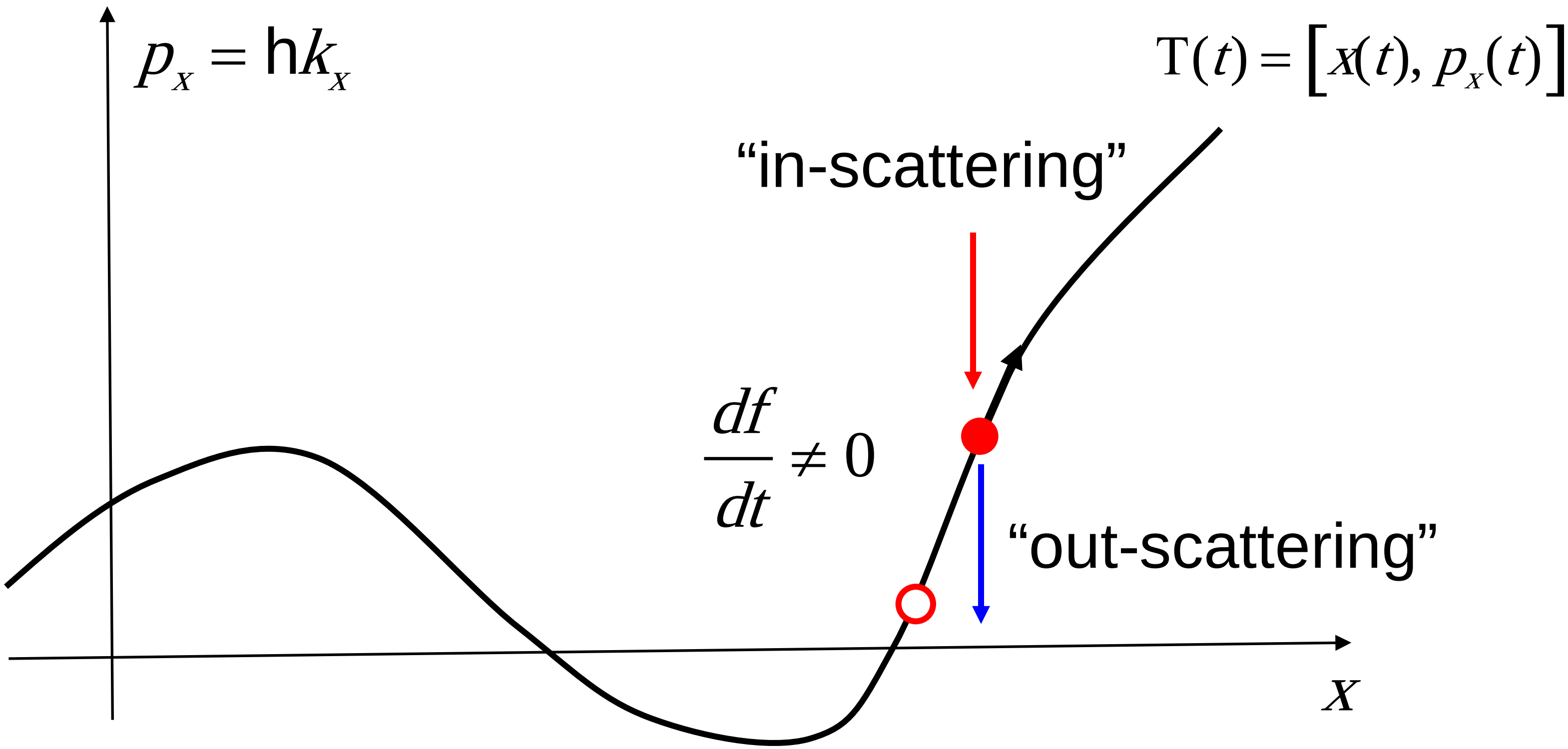
carrier scattering



$$\frac{df}{dt} = \left.\frac{df}{dt}\right|_{coll} = \hat{C}f$$

Boltzmann Transport Equation (BTE)

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

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

assumptions:

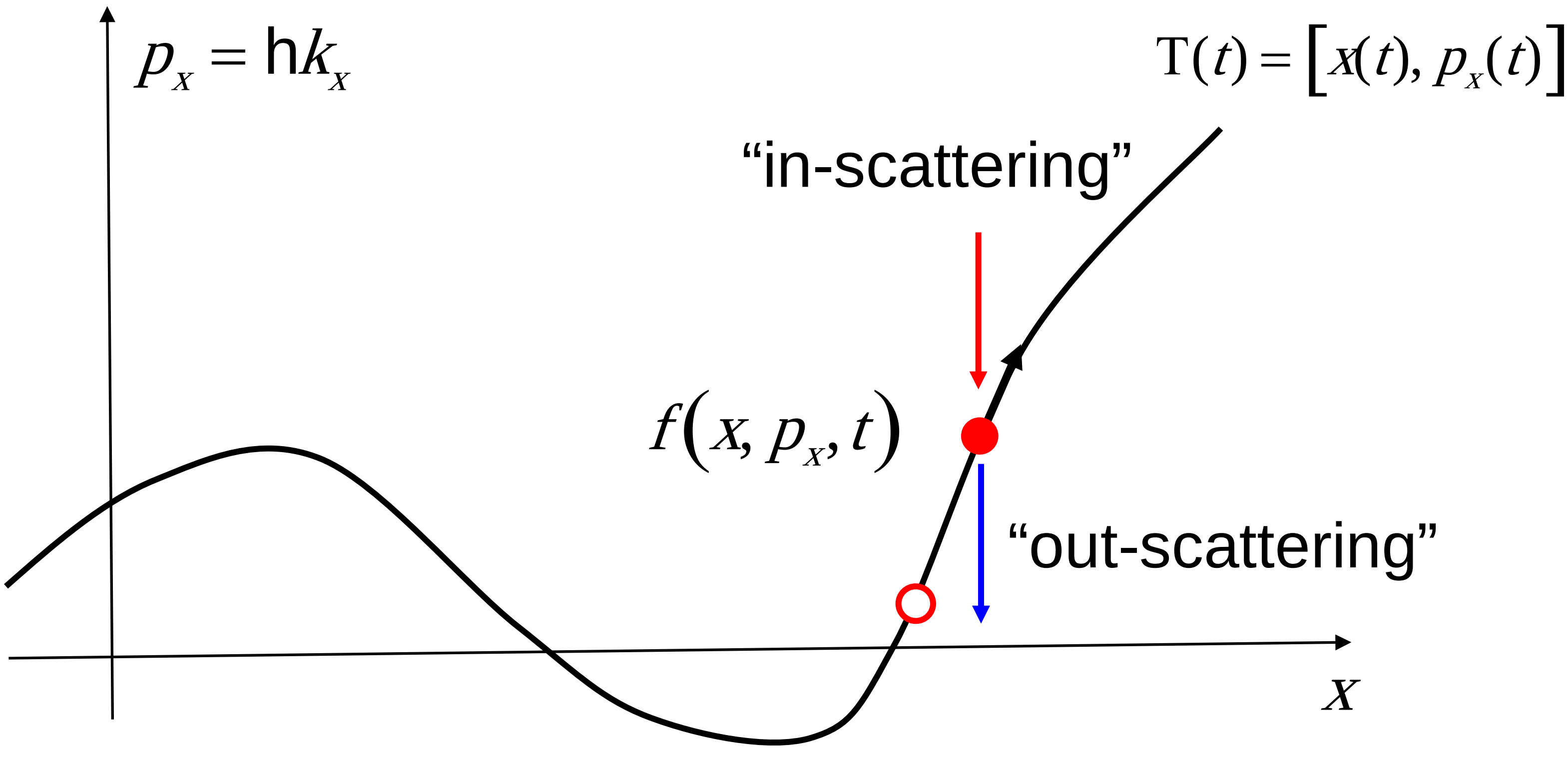
1) semi-classical treatment of electrons:

$$\frac{d(\hbar\vec{k})}{dt} = -\nabla E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r}) \quad E = E_C(\vec{r}) + E(\vec{k}) \quad \Delta p_x \Delta x \geq \hbar$$

2) neglected generation-recombination

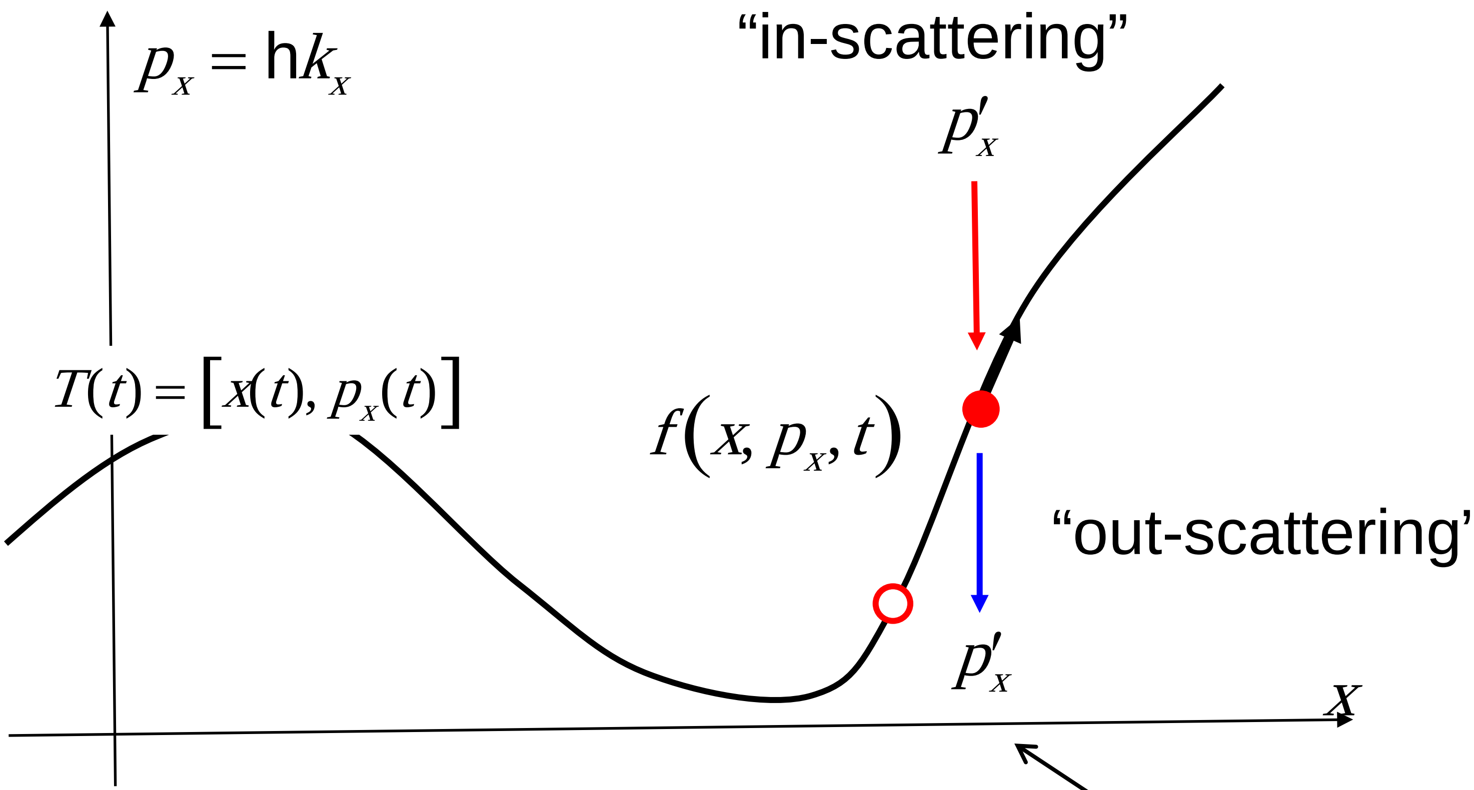
3) neglected e-e correlations (mean-field-approximation)

carrier scattering



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

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

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

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

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

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

non-degenerate scattering operator

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

probability that the state at p' is occupied

probability that the state at p is empty

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

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.

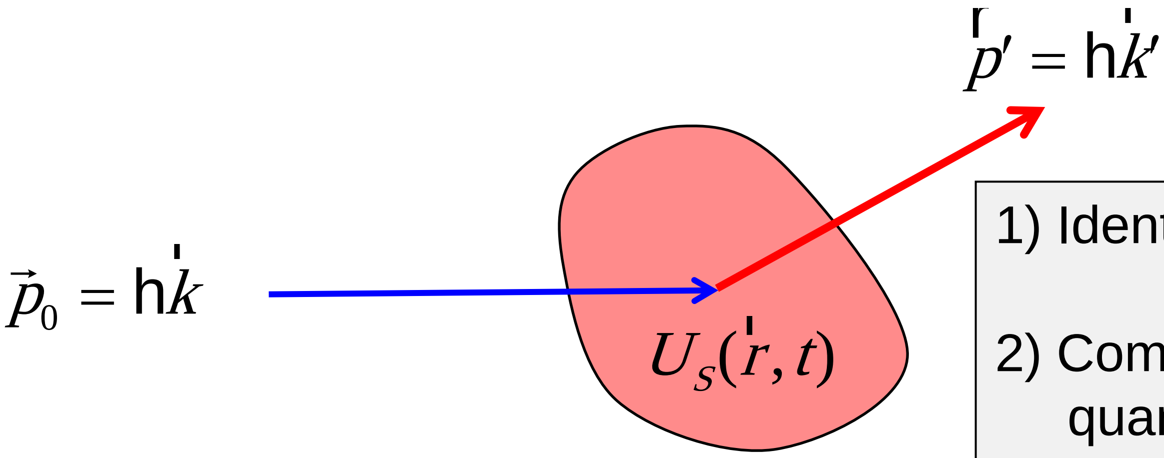
$$\sum_{p} \hat{C} f(\vec{r}, \vec{p}, t) = 0$$

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

$$\sum_{p,p'} S(\vec{p}', \vec{p})\, f(\vec{p}') = \sum_{p',p} S(\vec{p}', \vec{p})\, f(\vec{p}')$$ (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)

determining *S*(p, p')



1) Identify scattering potential

2) Compute transition rate quantum mechanically (typically using Fermi's Golden Rule)

$S(\vec{p}, \vec{p}')$ Transition rate: Probability per unit time that a carrier with momentum, *p*, makes a transition to *p'* (**assuming** that *p* is occupied and that *p'* is empty).

$S(\vec{p}_0, \vec{p}')\, f(\vec{p}_0)\left[1 - f(\vec{p}')\right]$ Actual rate of transitions

outline

the BTE

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

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

$$\sum_{p'} S(\vec{p}', \vec{p}) f(\vec{p}')[1 - f(\vec{p})] - \sum_{p'} S(\vec{p}, \vec{p}') f(\vec{p})[1 - f(\vec{p}')]$$

Six-dimensional integro-differential equation for *f*(*r*, *p*, *t*).

solving the BTE

(x, y, z) 3 independent variables

(k_x, k_y, k_z) 3 more independent variables

+ time….. 7 dimensional

$(100 \times 100 \times 100) \times (100 \times 100 \times 100) \times 10 = 10^{13}$ unknowns!

"curse of dimensionality"

A difficult problem ... We will need to make approximations in order to solve the BTE.

using $f(x, k_x, t)$

$$n(x,t) = \frac{1}{\Omega}\int_{-\infty}^{\infty} f(x,k,t) N_k d^3k$$

$$J(x,t) = \frac{1}{\Omega}\int_{-\infty}^{\infty} (-q)\upsilon_x(k) \times f(x,k,t) N_k d^3k$$

$$P_x(x,t) = \frac{1}{\Omega}\int_{-\infty}^{\infty} m^* \upsilon(k) \times f(x,k,t) N_k d^3k$$

$$W(x,t) = \frac{1}{\Omega}\int_{-\infty}^{\infty} \left(E - E_C\right) \times f(x,k,t) N_k d^3k$$

....

assumptions

1) Semi-classical treatment of electrons:

Electrons respond semi-classically to the local electric field. Quantum transport models (like the NEGF approach) remove this assumption.

2) Neglected generation-recombination:

But can add for specific problems (e.g. photoexcitation, impact ionization, etc.

3) Neglected e-e correlations

So-called ensemble Monte Carlo (or molecular dynamics) simulations can treat these many body effects.

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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.

questions

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