ECE-656: Fall 2009

Lecture 31: Monte Carlo Simulation

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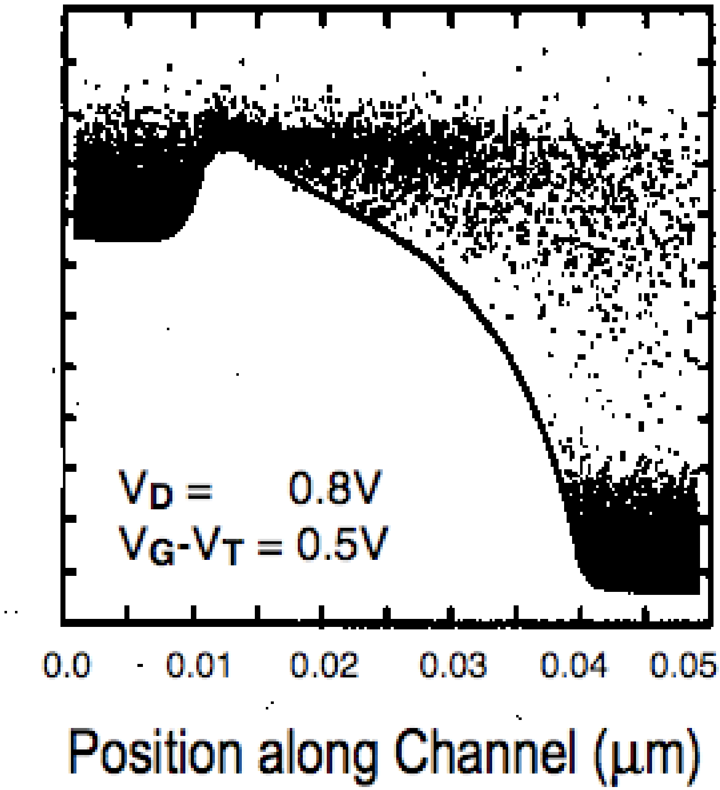
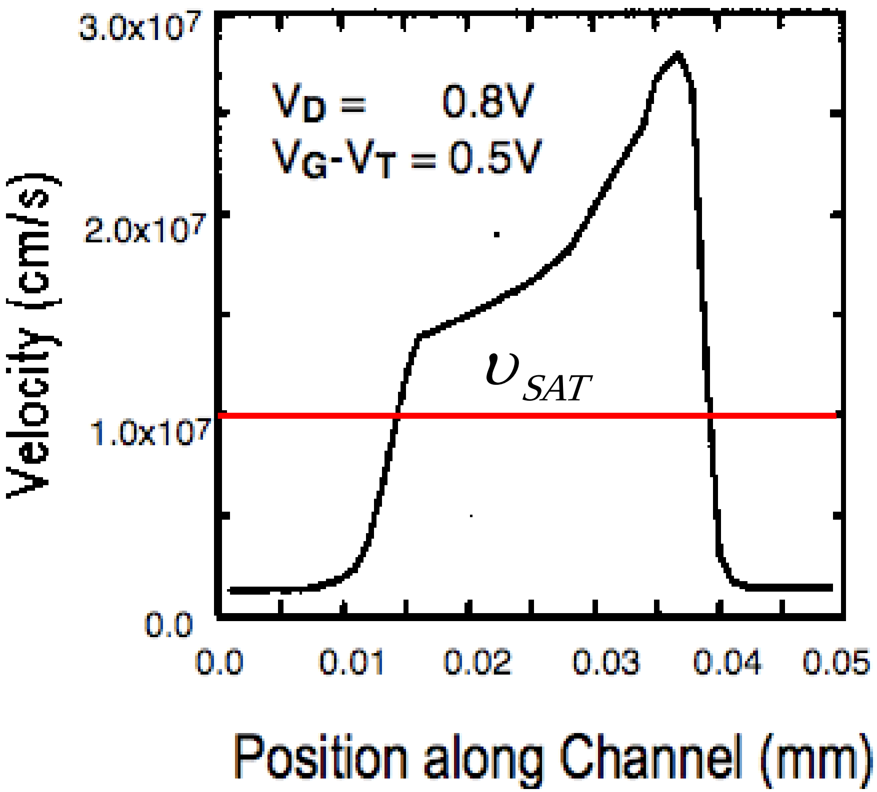
Damocles





Frank, Laux, and Fischetti, IEDM Tech. Dig., p. 553, 1992

outline

1) Introduction

2) **Review of carrier scattering**

3) Simulating carrier trajectories

4) Free flight

5) Collision

6) Update after collision

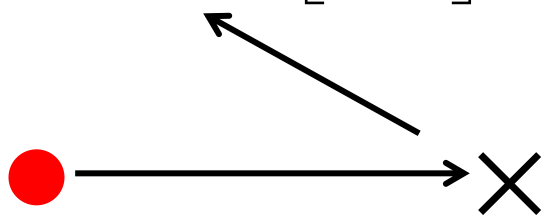
7) Putting it all together

8) Summary

carrier scattering

$$\vec{r}(t_C^+) = \vec{r}(t_C^-)$$
$$\vec{p}(t_C^+)$$
$$E\left[\vec{p}(t_C^+)\right]$$

$$\vec{r}(0)$$
$$\vec{p}(0)$$
$$E\left[\vec{p}(0)\right]$$

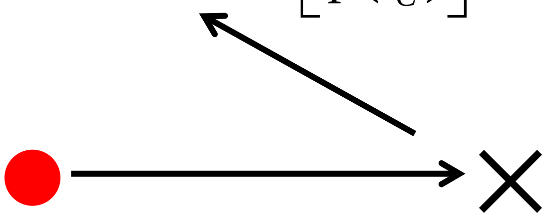


$$\vec{r}(t_C^-)$$
$$\vec{p}(t_C^-)$$
$$E\left[\vec{p}(t_C^-)\right]$$

1) Scattering events are assumed to be instantaneous - scattering changes the carrier's momentum (and energy) but not position.

2) Scattering events are treated quantum mechanically. Carrier motion between scattering events is treated semi-classically

carrier scattering



Elastic scattering:

$$E\left[\vec{p}(t_C^+)\right] = E\left[\vec{p}(t_C^-)\right]$$

Inelastic scattering:

$$E\left[\vec{p}(t_C^+)\right] \neq E\left[\vec{p}(t_C^-)\right]$$

Isotropic scattering:

-no preferred direction

Scattering rate:

$$\frac{1}{\tau(E_i)} : \; D\left(E_f\right)$$

total scattering rate

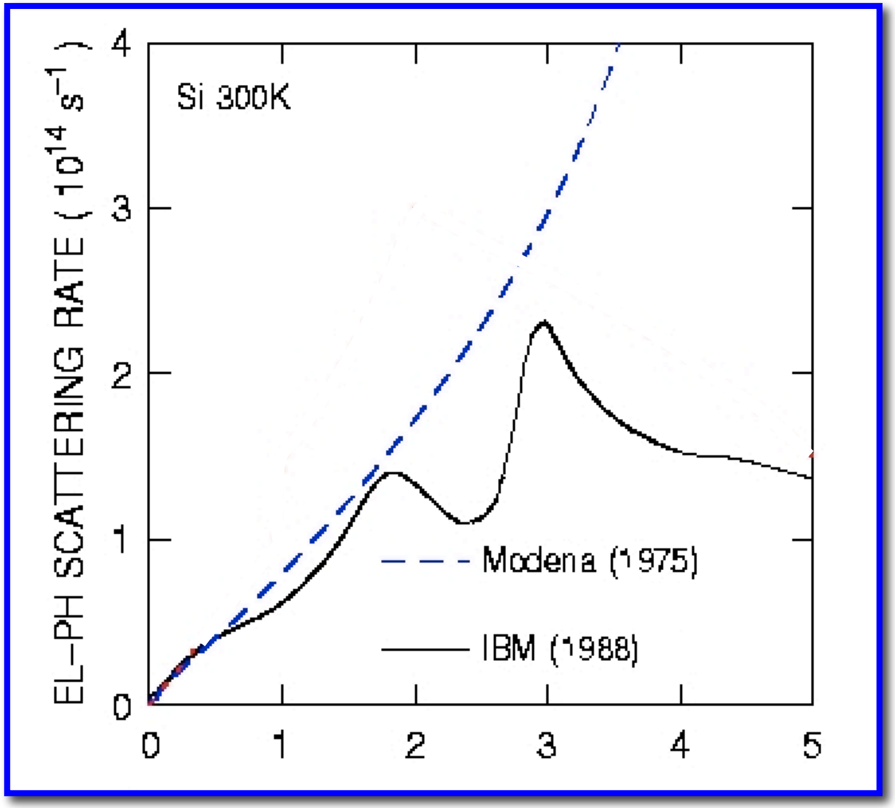
$$\frac{1}{\tau(E_i)} = \sum_{k=1}^{N} \frac{1}{\tau_k(E_i)} = \Gamma(E_i)$$

scattering mechanisms:

- ionized impurity
- acoustic phonon emission
- acoustic phonon absorption
- optical phonon ems
- optical phonon abs
- intervalley
- electron-electron
- electron-hole
- “polar optical phonon”
- surface roughness
- etc.

total scattering rate

typical scattering rates vs. energy



http://www.research.ibm.com/DAMOCLES/html_files/sirates.html#history

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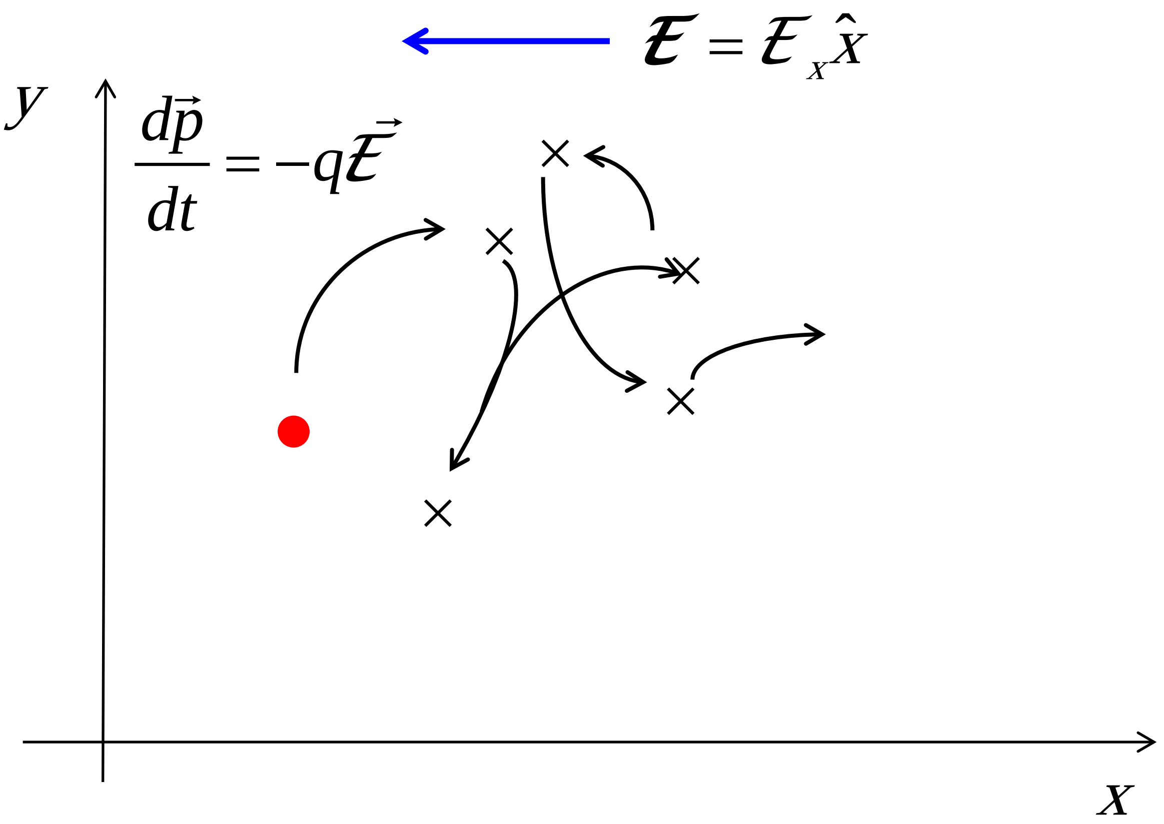
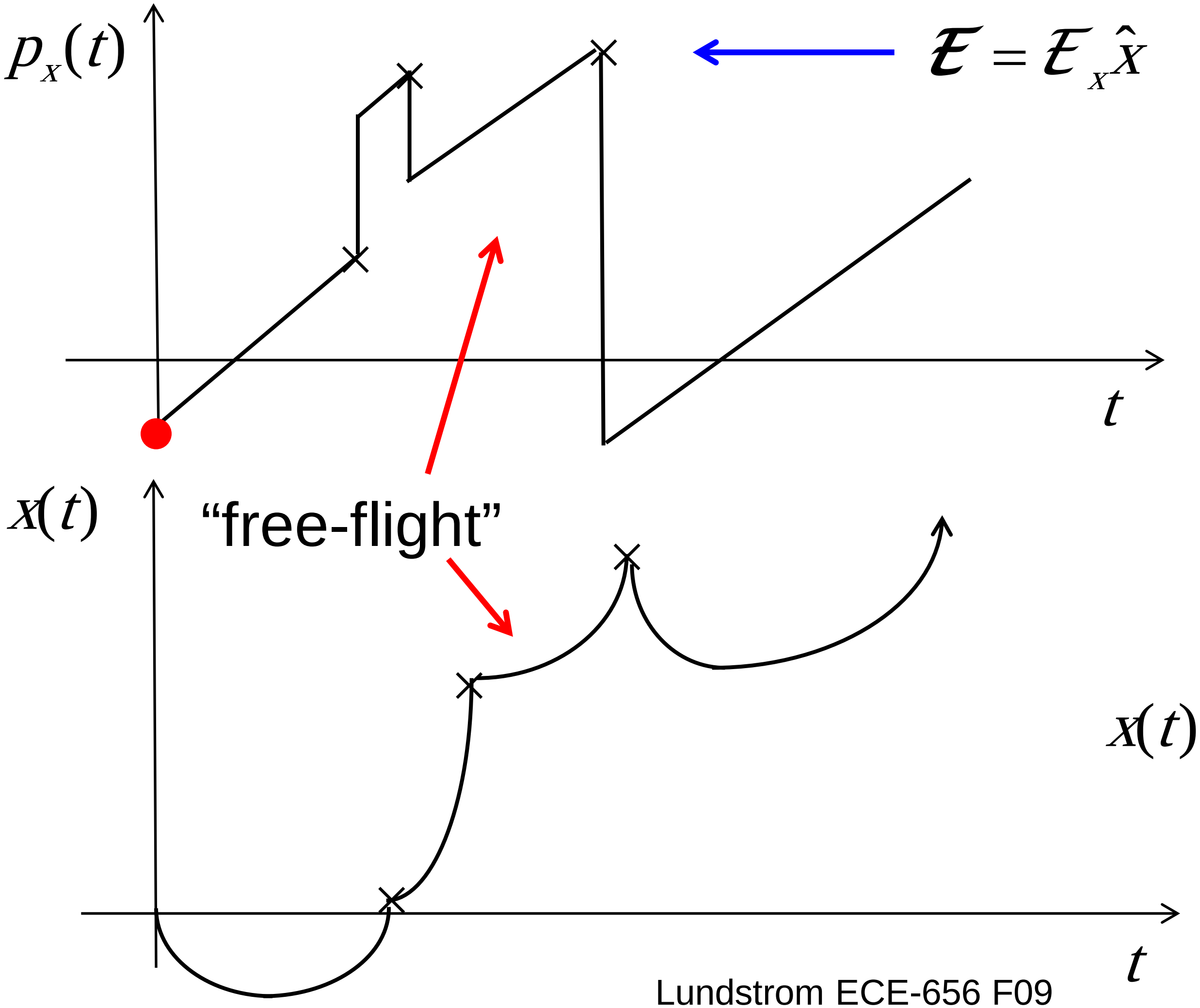
carrier trajectories in 2D



carrier trajectories in phase space



$$\frac{dp_x}{dt} = -q\mathcal{E}_x$$

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

$$x(t) = x(0) + \int_0^{t_C} \upsilon_x(t)\,dt$$

MC algorithm

1) "free flight" for t_C seconds.
2) update $E(t_C^-)$ and $r\ (t_C^-)$
3) identify collision
4) update $E(t_C^+)$ and $p\ (t_C^+)$
5) Set t = 0 and repeat

r_1

r_2

r_3, r_4

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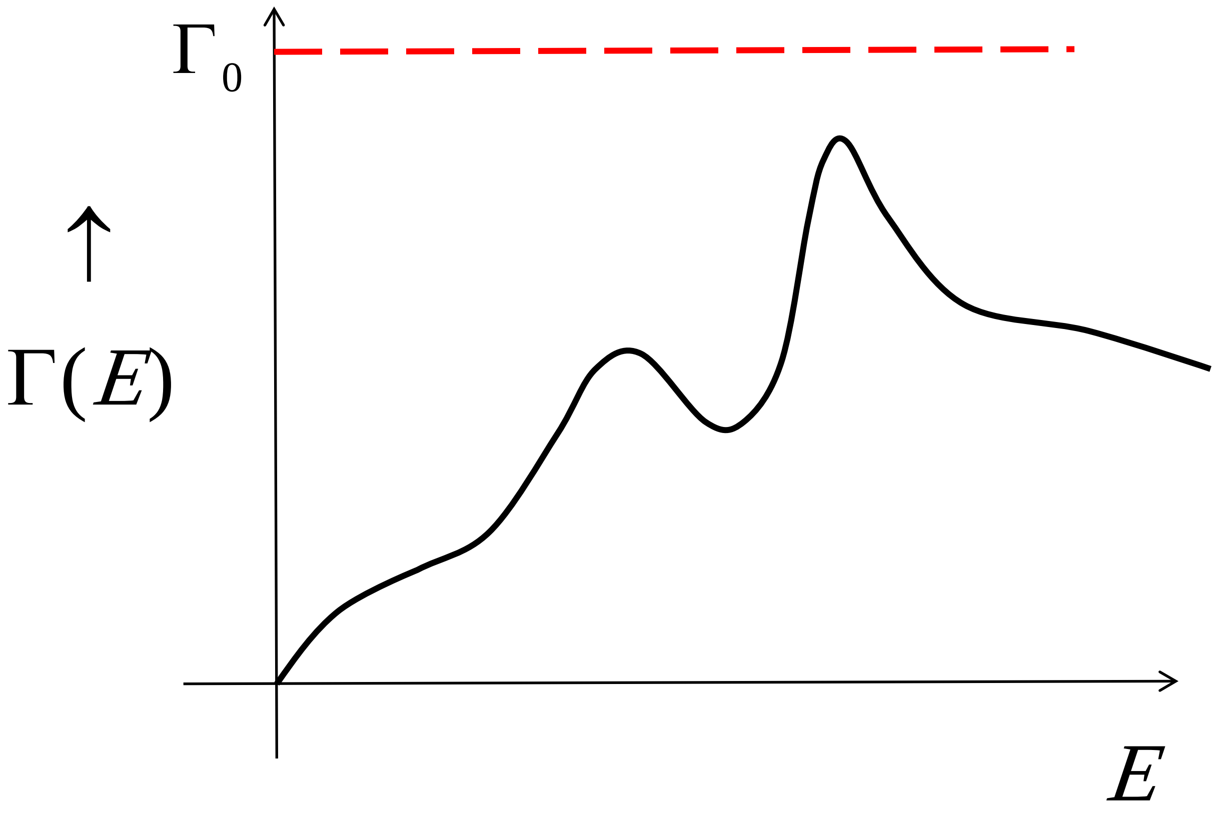
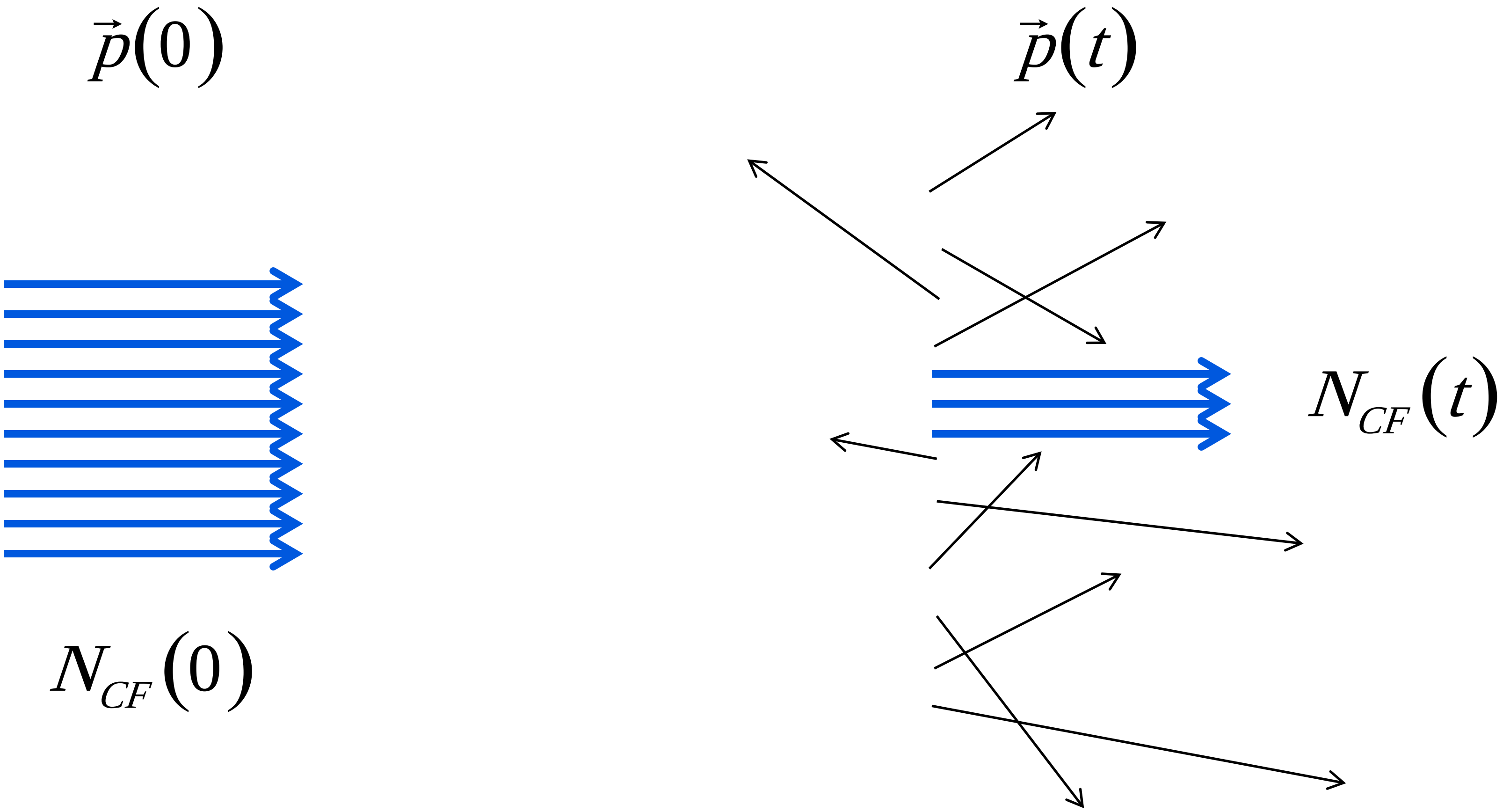
free flight



free flight



free flight time

How many carriers survive until time *t* + *dt* without scattering?

$$N_{CF}\left(t+dt\right) = N_{CF}(t) - N_{CF}(t)\Gamma_0 dt$$

$$\frac{dN_{CF}\left(t\right)}{dt} = -N_{CF}(t)\Gamma_0$$

$$N_{CF}(t) = N_{CF}(0)e^{-\Gamma_0 t}$$

$$\frac{N_{CF}(t)}{N_{CF}(0)} = e^{-\Gamma_0 t} \qquad \langle \tau \rangle = 1/\Gamma_0$$

free flight time

What is the probability that a carrier survives until time, *t*, <u>and then scatters</u> between *t* and *t* + *dt* ?

$$\mathcal{P}(t)dt = \left(\frac{N_{CF}(t)}{N_{CF}(0)}\right)\Gamma_0 dt = e^{-\Gamma_0 t}\Gamma_0 dt$$

free-flight time probability density function

If we have a random number generator that produces random numbers with a probability distribution, $\mathcal{P}(r)$, how do we use it to choose free flight times?

$$\mathcal{P}(t)dt = e^{-\Gamma_0 t}\Gamma_0 dt = \mathcal{P}(r)dr$$

free flight times

Assume a random number generator that produces random numbers uniformly distributed between 0 and 1.

$$\mathcal{P}(r)dr = e^{-\Gamma_0 t}\Gamma_0 dt$$

$$dr = e^{-\Gamma_0 t}\Gamma_0 dt$$

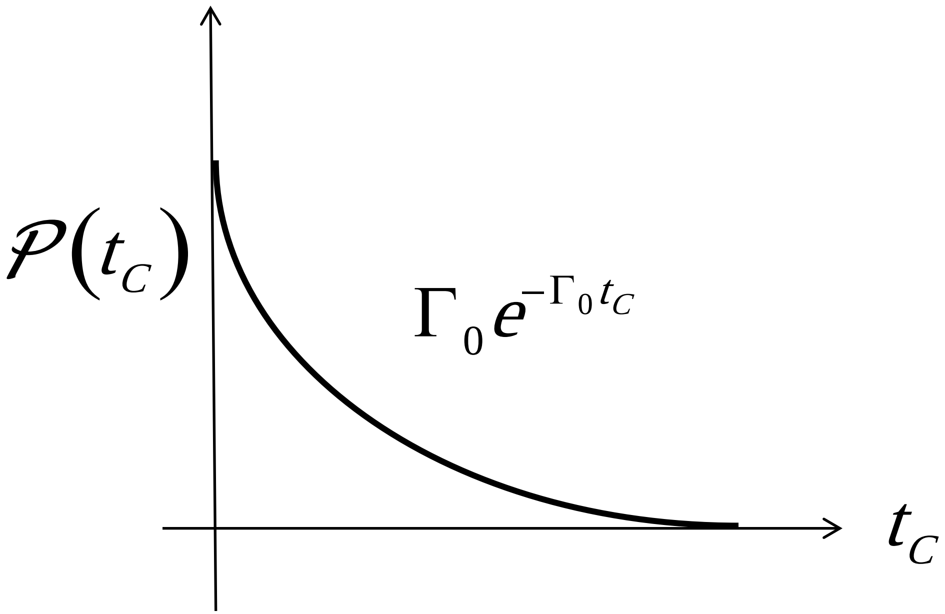
$$\int_0^{r_C} dr = r_c = \int_0^{t_C} e^{-\Gamma_0 t}\Gamma_0 dt = -e^{-\Gamma_0 t}\Big|_0^{t_C} = \left(1 - e^{-\Gamma_0 t_C}\right)$$

$$t_C = \frac{1}{\Gamma_0}\ln\left(1 - r_C\right)$$

free flight distribution

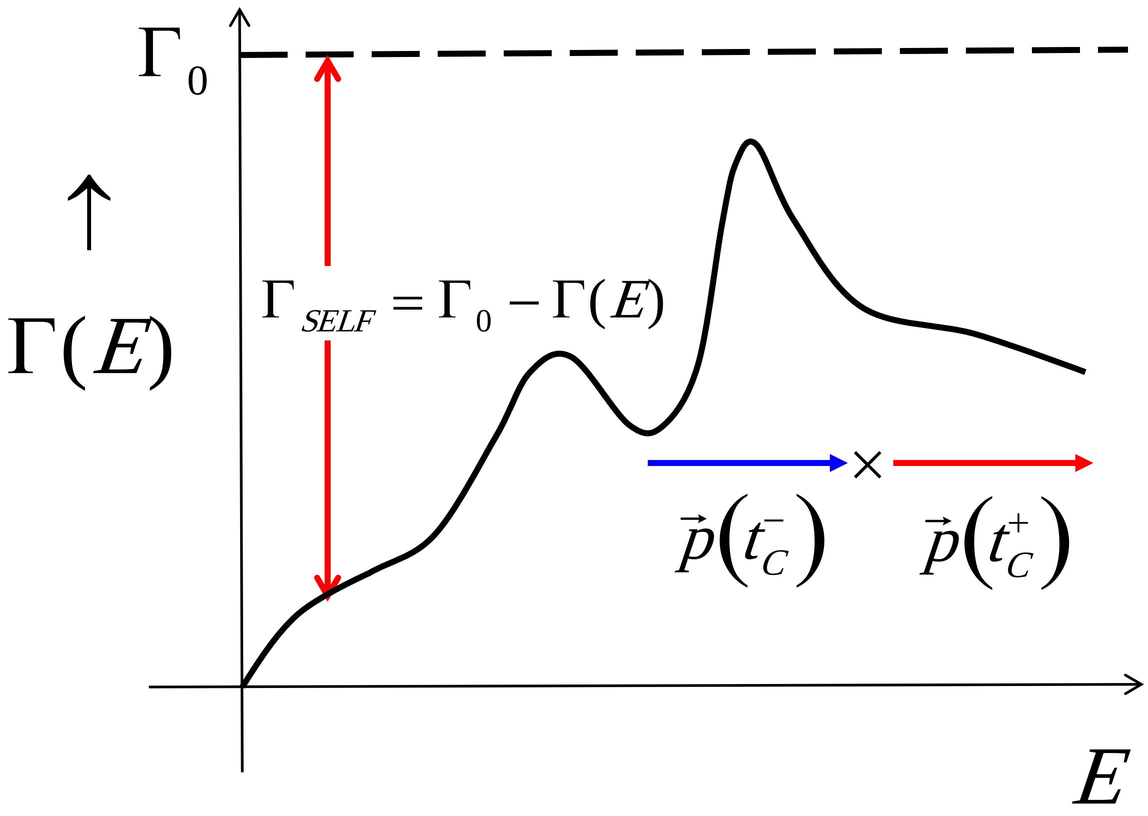
$$t_C = \frac{1}{\Gamma_0} \ln(r_1)$$

$$\langle t_C \rangle = \frac{1}{\Gamma_0}$$



but, the scattering rate is not constant with energy!

free flight



$$\Gamma(E) = \sum_{k=1}^{N} \frac{1}{\tau_k(E)}$$

$$\Gamma_0 = \sum_{k=1}^{N+1} \frac{1}{\tau_k(E)}$$

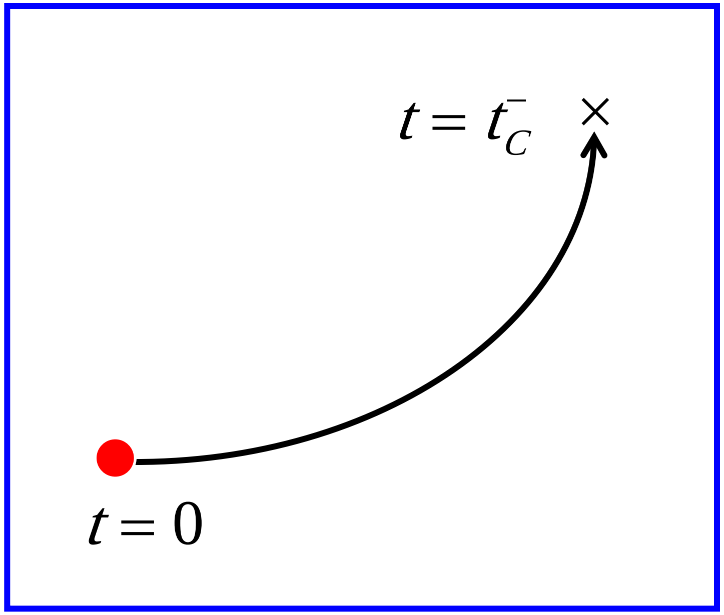
$$t_C = \frac{1}{\Gamma_0} \ln(r_1)$$

update at end of free-flight

$$\vec{p}\left(t_C^-\right) = \vec{p}(0) - q\vec{\mathcal{E}}\, t_C$$

$$E\left(t_C^-\right) = E\left[\,\vec{p}(t_C^-)\right]$$

$$\vec{r}\left(t_C^-\right) = r(0) + \vec{\upsilon}\left(0\right)t_C$$



1) what collision terminated the free flight?

2) how does the collision affect the carrier's momentum and energy?

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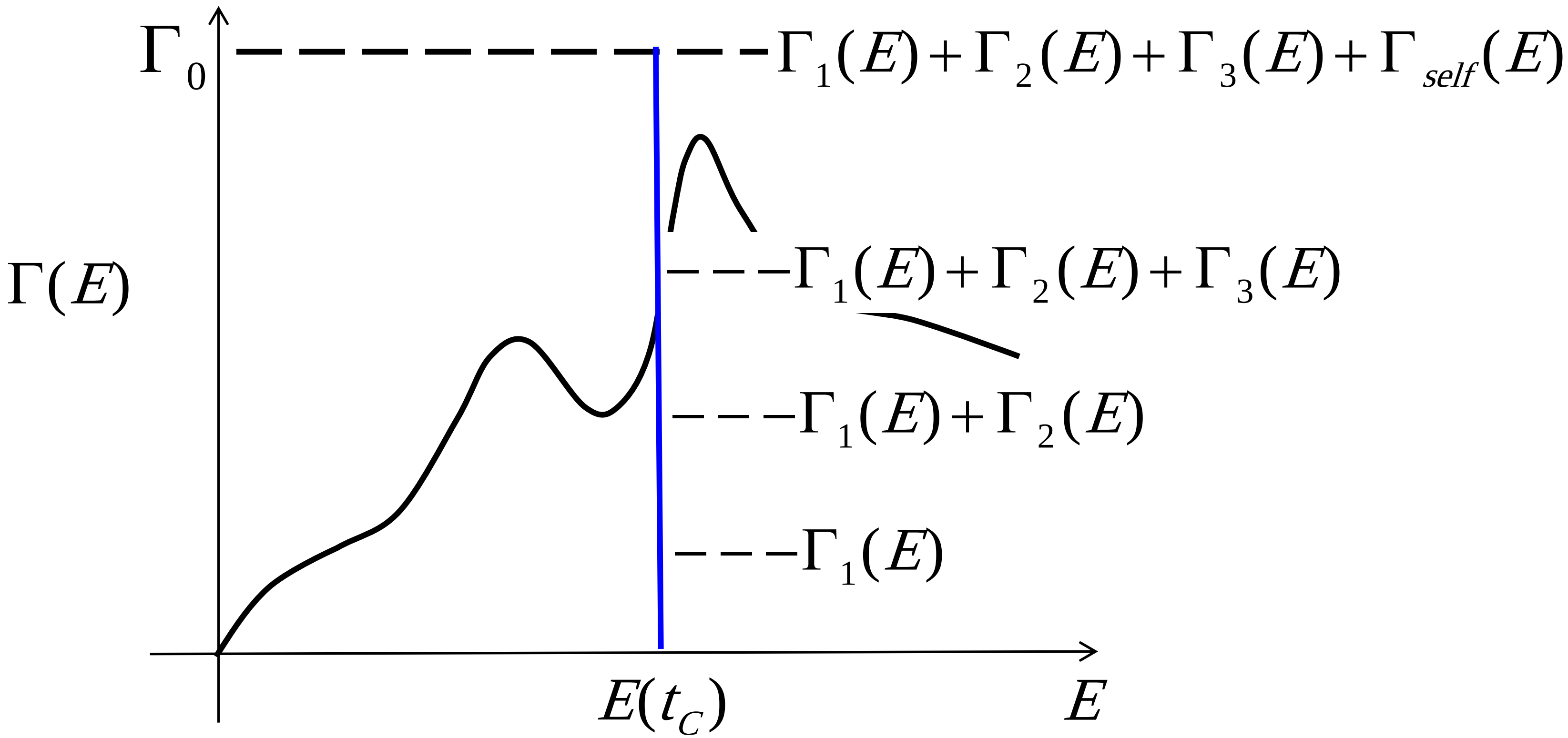
collision

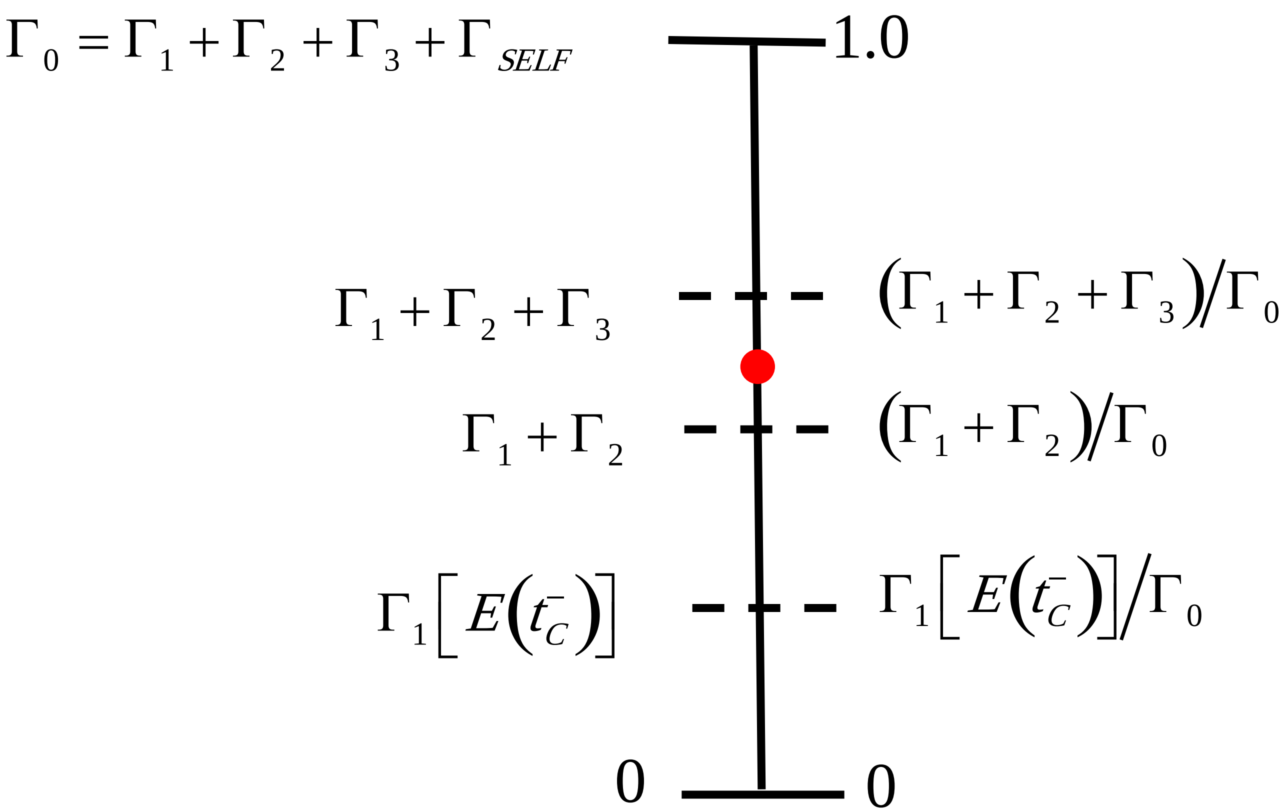
As an example, assume that there are 3 scattering mechanisms, plus self-scattering.

$$\Gamma(E) = \Gamma_1(E) + \Gamma_2(E) + \Gamma_3(E) + \Gamma_{SELF}(E) = \Gamma_0$$



collision

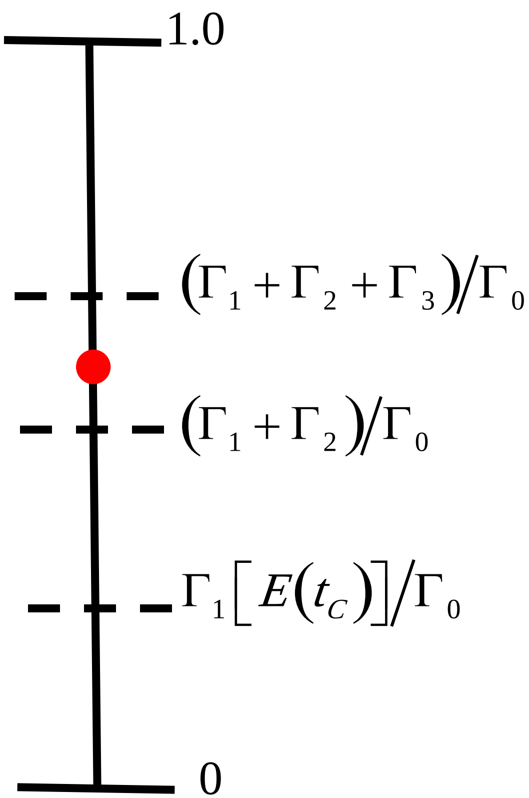
$$\Gamma(E)=\Gamma_1(E)+\Gamma_2(E)+\Gamma_3(E)+\Gamma_{SELF}(E)=\Gamma_0$$



choose random number between 0 and 1

collision

$$\Gamma(E) = \Gamma_1(E) + \Gamma_2(E) + \Gamma_3(E) + \Gamma_{SELF}(E) = \Gamma_0$$



$0 < r_2 < \Gamma_1/\Gamma_0$ process 1

$\Gamma_1/\Gamma_0 < r_2 < (\Gamma_1 + \Gamma_2)/\Gamma_0$ process 2

$(\Gamma_1 + \Gamma_2)/\Gamma_0 < r_2 < (\Gamma_1 + \Gamma_2 + \Gamma_3)/\Gamma_0$ process 3

$(\Gamma_1 + \Gamma_2 + \Gamma_3)/\Gamma_0 < r_2 < 1.0$ self-scattering

choose random number uniformly distributed between 0 and 1

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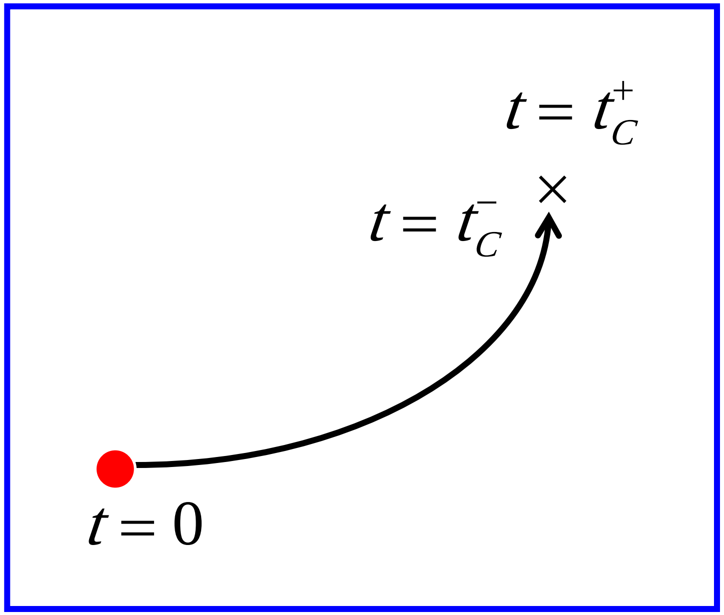
update after scattering

$$\vec{r}\left(t_C^+\right) = \vec{r}\left(t_C^-\right)$$

$$E\left(t_C^+\right) = E\left(t_C^-\right) + \Delta E_i$$

$$\Delta E_i = 0, \pm\hbar\omega_0, \text{etc}$$

$$\vec{p}\left(t_C^+\right) = ?$$



We know the magnitude of *p* from the known energy after the collision, but how do we determine the direction?

update after scattering: 1D

$$\vec{p}\left(t_C\right)$$

i) forward scattering by phonon absorption

$$\vec{p}\left(t_C^+\right)$$

ii) backward scattering by phonon absorption

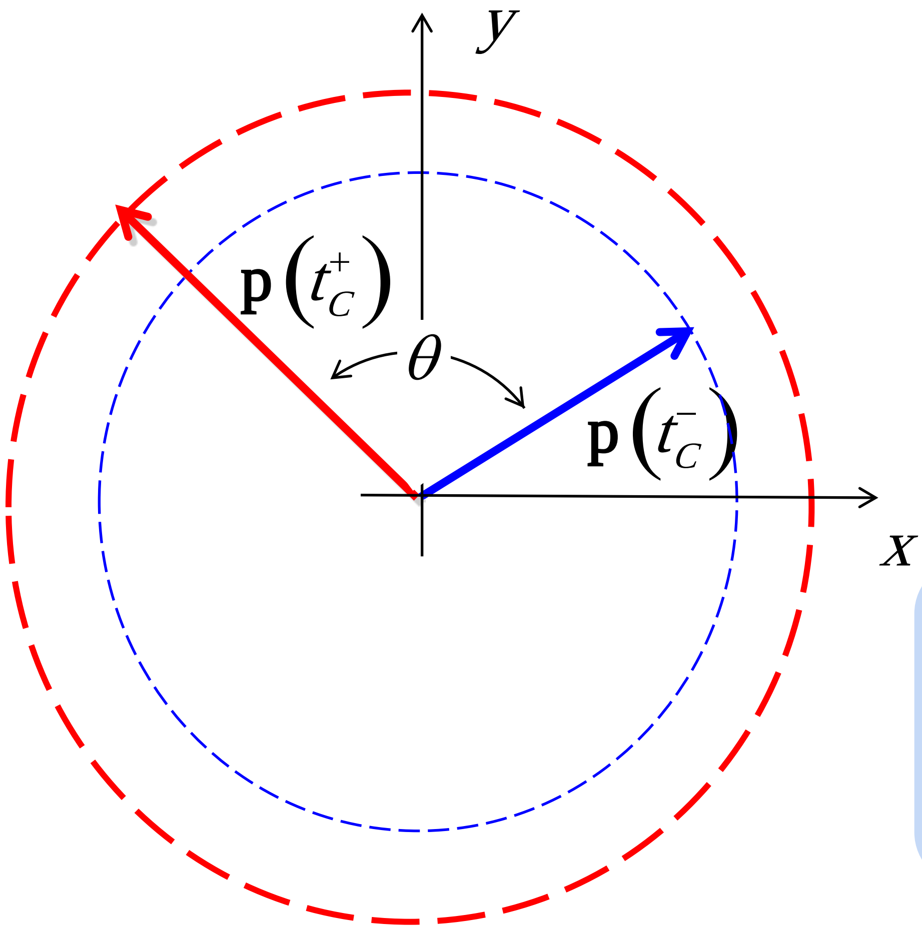
$$\vec{p}\left(t_C^+\right)$$

If scattering is isotropic, then forward and backward scattering are equally probable.

$$0 < r_3 \le 0.5: \quad \vec{p}\left(t_C^+\right) = \vec{p}\left(t_C^-\right)$$

$$0.5 < r_2 \le 1.0: \quad \vec{p}\left(t_C^+\right) = -\vec{p}\left(t_C^-\right)$$

update after scattering: 2D



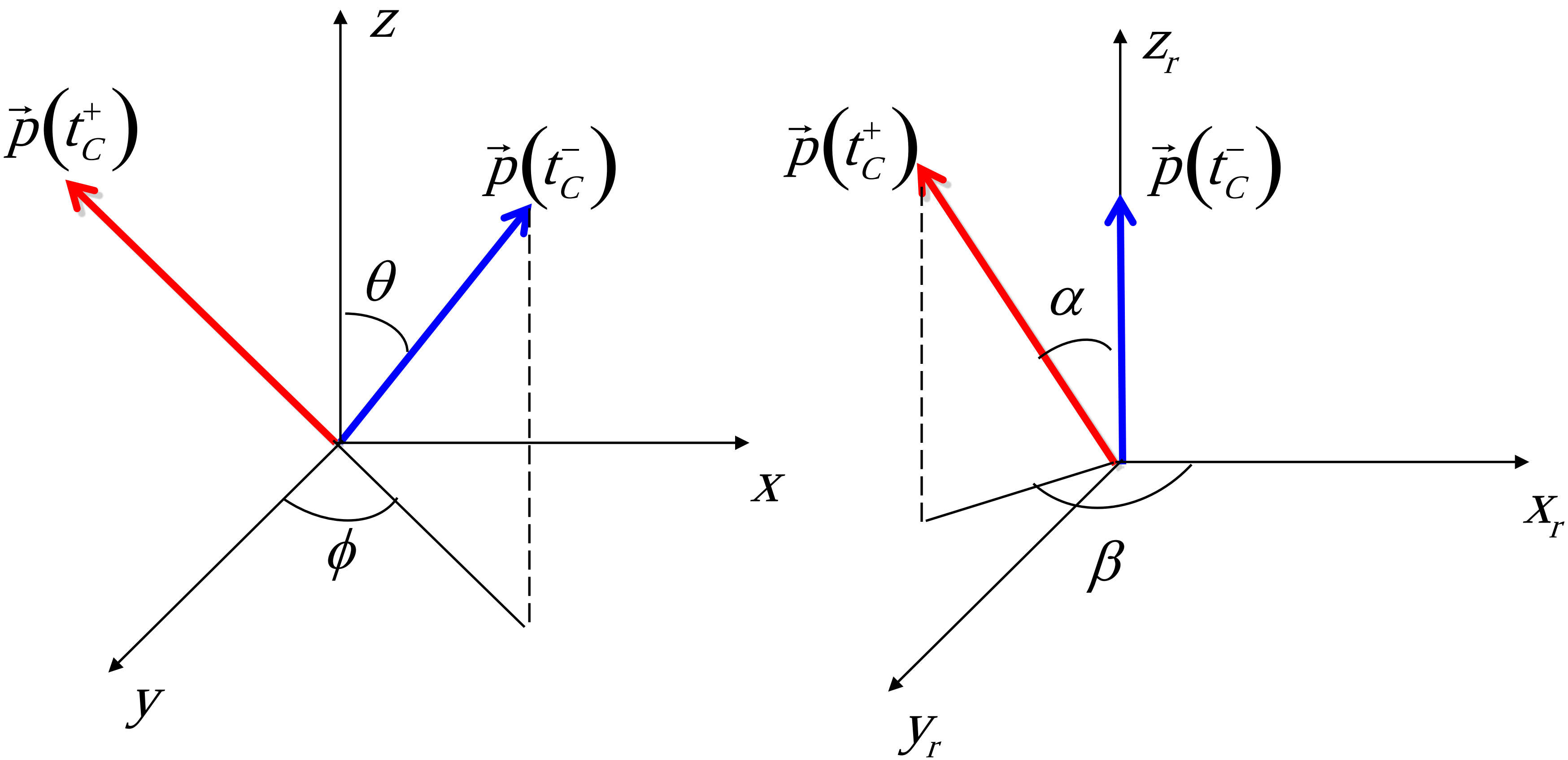
assume isotropic scattering

(e.g. optical phonon abs)

$$\theta = 2\pi r_3$$

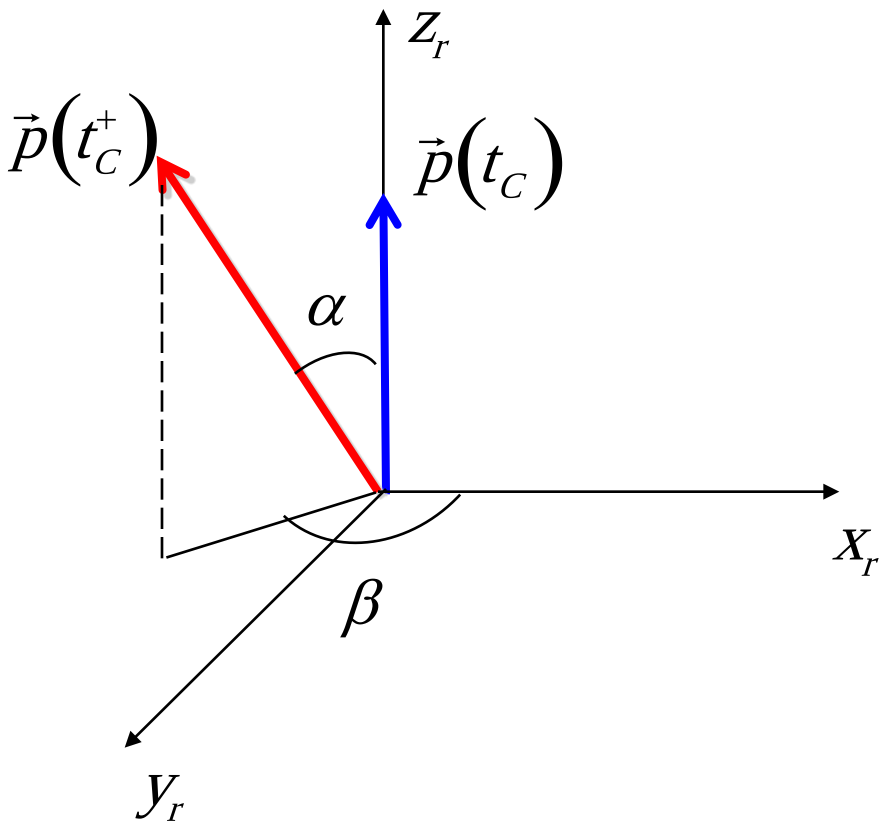
r_3 is a random number uniformly distributed between 0 and 1

update after scattering: 3D



need two random numbers to select $(\alpha,\beta)\rightarrow(\theta,\phi)$

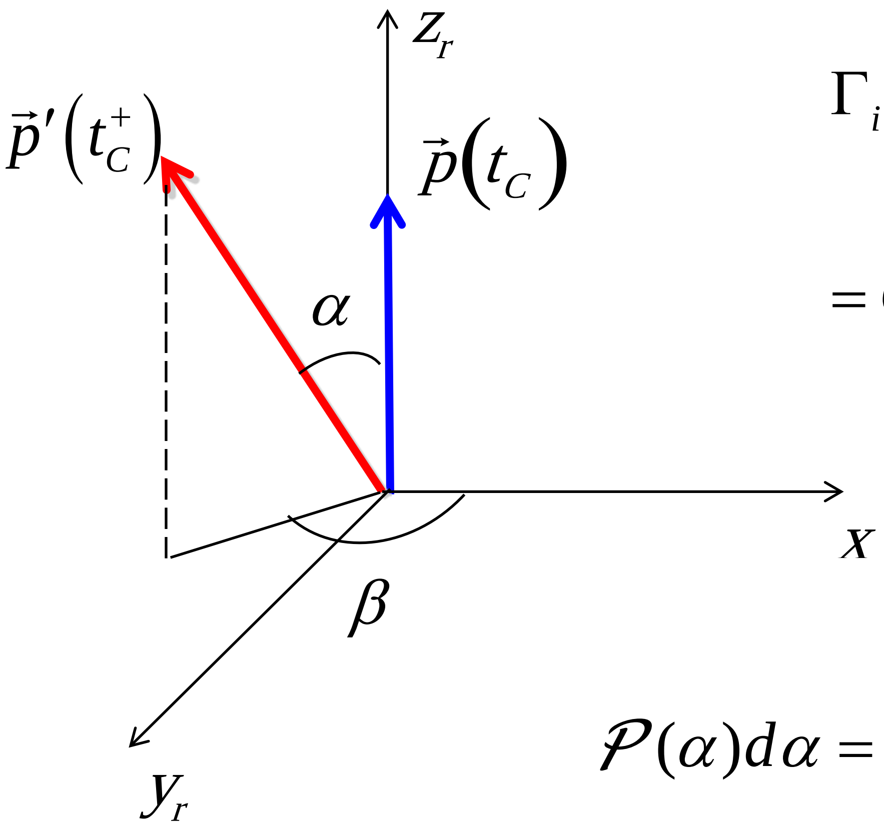
update after scattering: 3D



$$\beta = 2\pi r_3$$

r_3 is a random number uniformly distributed between 0 and 1

update after scattering: 3D

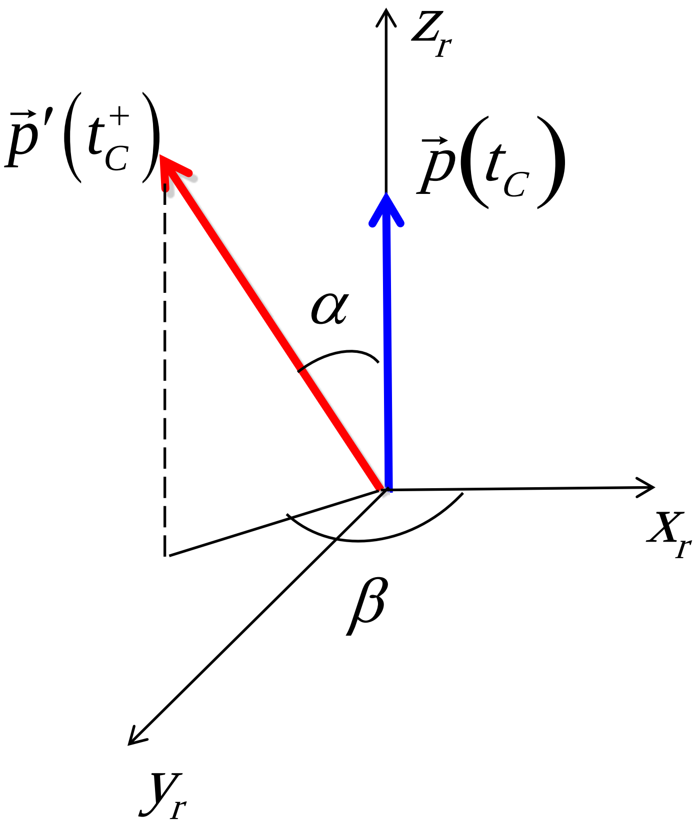


$$\Gamma_i = \frac{1}{\tau_i} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}')$$

$$= C\int_0^{2\pi} d\beta \int_0^{\pi}\int_0^{\infty} S(\vec{p}, \vec{p}')\sin\alpha\, d\alpha\; p'^2 dp'$$

$$\mathcal{P}(\alpha)d\alpha = \frac{C\int_0^{2\pi} d\beta \int_0^{\infty} S(\vec{p}, \vec{p}')\sin\alpha\, d\alpha\, p'^2 dp'}{C\int_0^{2\pi} d\beta \int_0^{\pi}\int_0^{\infty} S(\vec{p}, \vec{p}')\sin\alpha\, d\alpha\, p'^2 dp'}$$

update after scattering: 3D

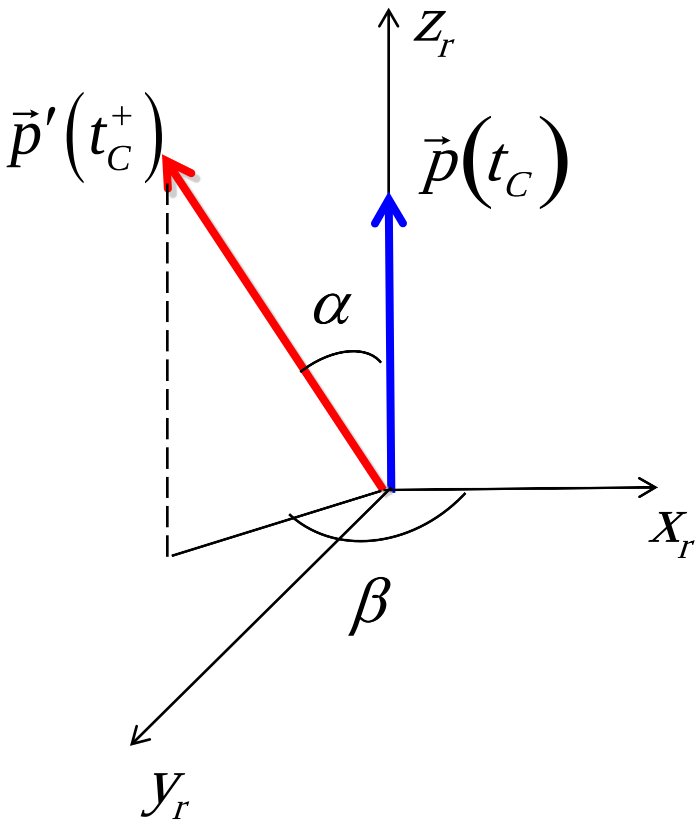


$$\mathcal{P}(\alpha)d\alpha = \frac{\int_0^\infty S\left(\vec{p},\vec{p}'\right)\sin\alpha\, d\alpha\, p'^2 dp'}{\int_0^\pi \int_0^\infty S\left(\vec{p},\vec{p}'\right)\sin\alpha\, d\alpha\, p'^2 dp'}$$

example: isotropic scattering

$$\mathcal{P}(\alpha)d\alpha = \frac{\sin\alpha\, d\alpha}{\int_0^\pi \sin\alpha\, d\alpha} = \frac{\sin\alpha\, d\alpha}{-\cos\alpha\big|_0^\pi}$$

update after scattering: 3D



example: isotropic scattering

$$\mathcal{P}(\alpha)d\alpha = \frac{\sin\alpha\, d\alpha}{2} = \mathcal{P}(r)dr$$

$$\int_0^{r_4} dr = r_4 = \int_0^{\alpha} \frac{\sin\alpha\, d\alpha}{2} = \left.\frac{-\cos\alpha}{2}\right|_0^{\alpha}$$

$$2r_4 = 1 - \cos\alpha$$

$$\boxed{\cos\alpha = 1 - 2r_4}$$

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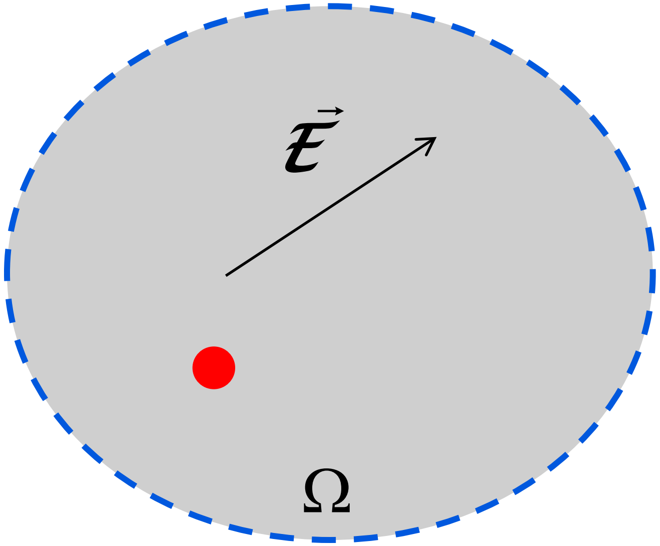
MC simulation of a bulk semiconductor



initialize $\vec{p}(t=0)$

1) select: $t_C = -\dfrac{1}{\Gamma_0}\ln r_1$

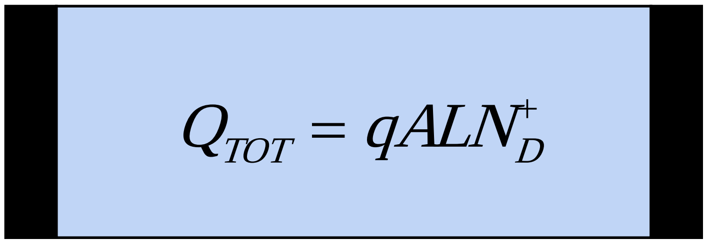
2) update: $\vec{r}\left(t_C^-\right), \vec{p}\left(t_C^-\right), E\left(t_C^-\right)$

3) identify scattering event: r_2

4) update: $E\left(t_C^+\right), \vec{p}\left(t_C^+\right), \theta, \phi \quad r_3, r_4$

5) repeat

MC simulation of a device



$$Q_{super} = \frac{N_{electrons}}{N_{sim}} \times (-q)$$

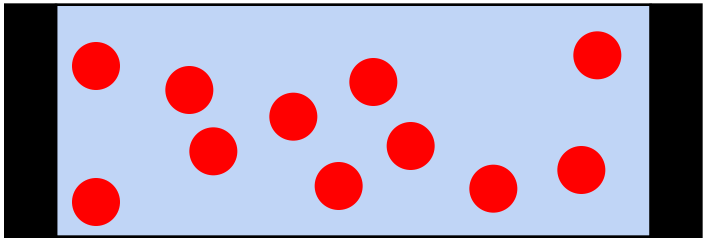
1) Load up device with *N* “super electrons”

example:

$$A = 1\mu\text{m} \times 1\mu\text{m} \quad L = 10\ \mu\text{m} \quad N_D = 10^{18}\ \text{cm}^{-3}$$

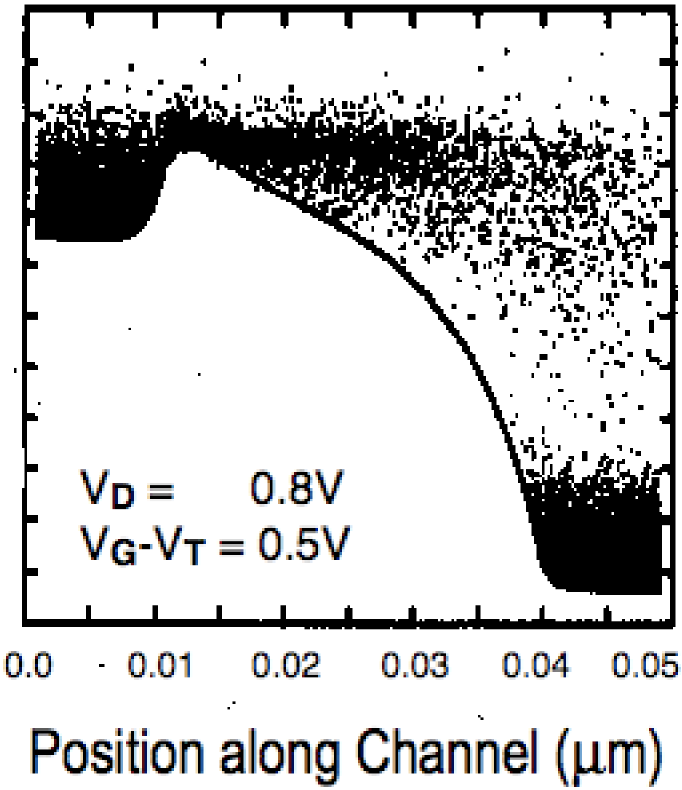
$$Q_{TOT} = 10^7 \times (-q)$$

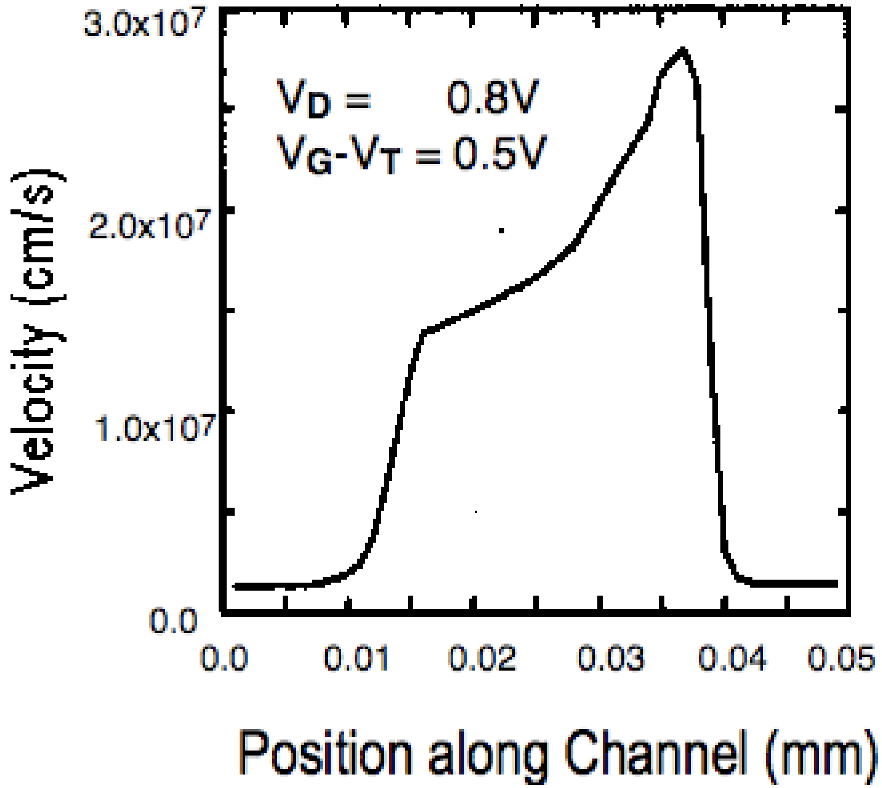
MC simulation of a device



1) load up device with *N* “super electrons”
2) track all electron trajectories for ⊗T (replace electrons that leave the device
3) collect statistics
4) solve Poisson equation for new self-consistent potential
5) repeat until steady-state

Damocles





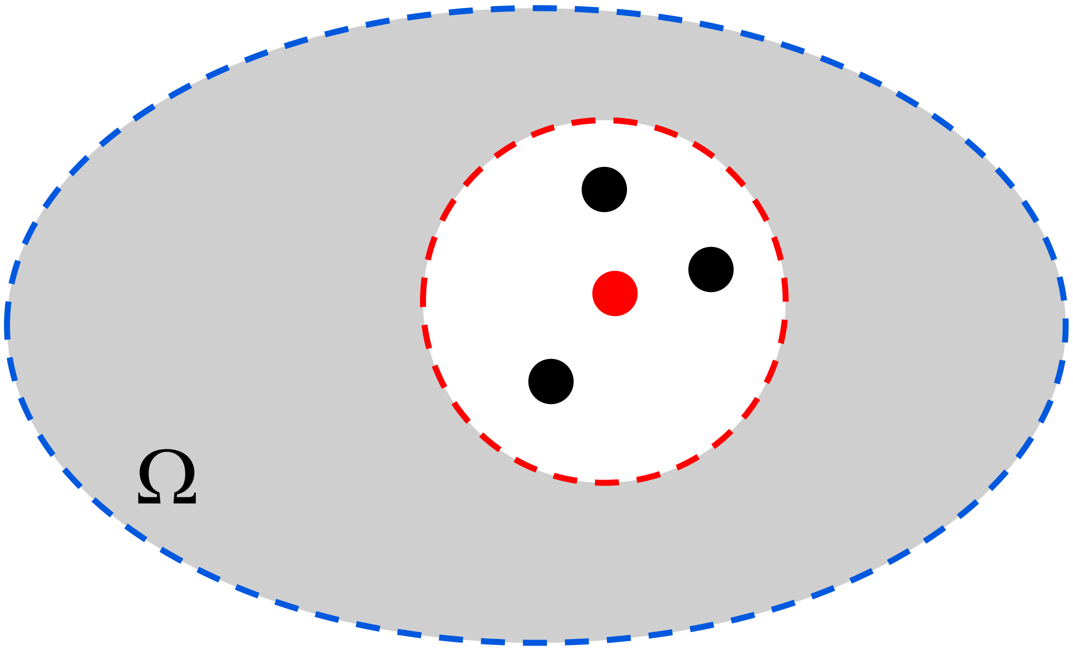
Frank, Laux, and Fischetti, IEDM Tech. Dig., p. 553, 1992

comments

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f - q\vec{\mathcal{E}} \bullet \nabla_p f = \hat{C}f$$

a six-dimensional, time-dependent problem in 3D

"curse of dimensionality"

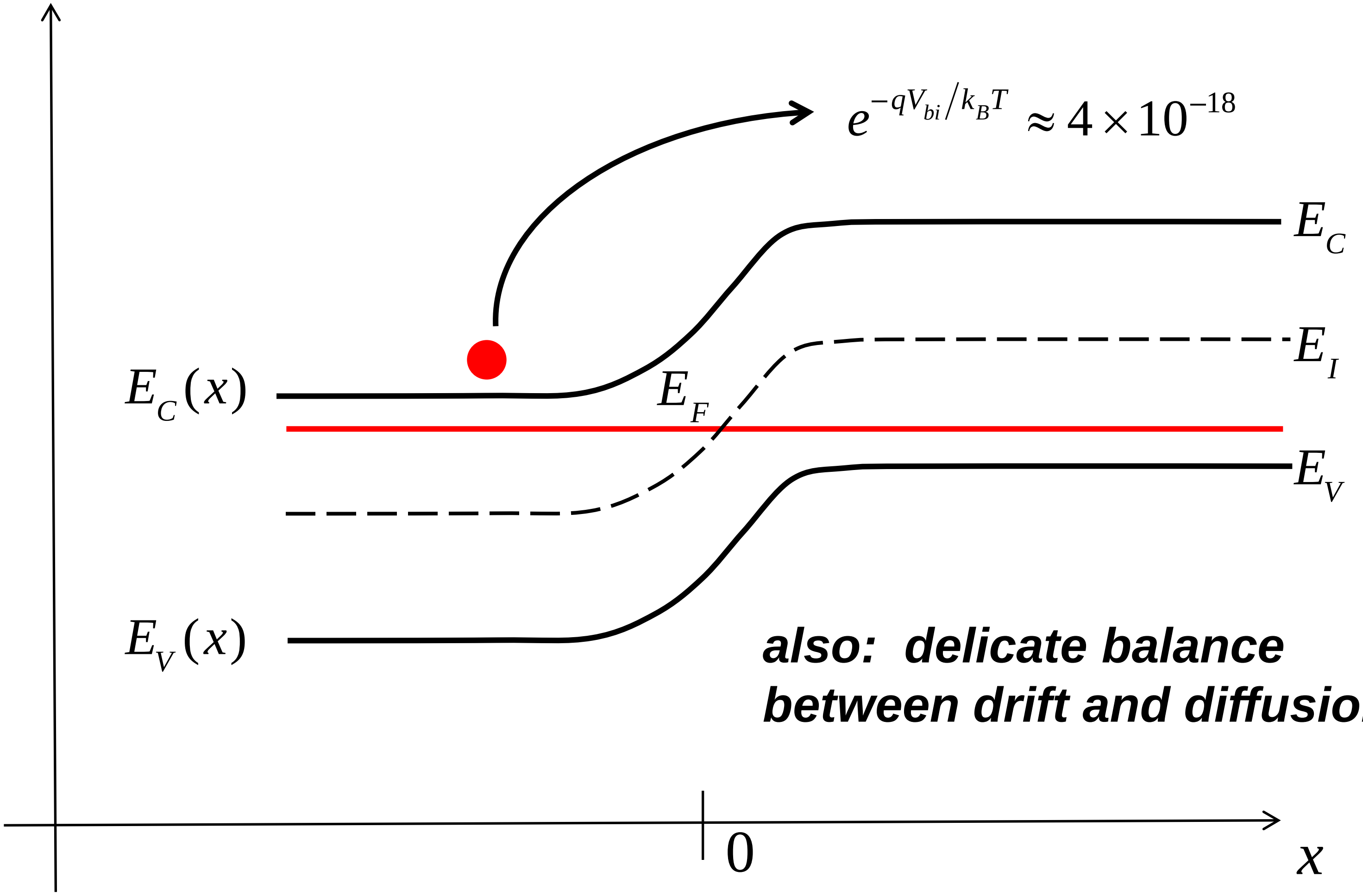


1) long range forces due to the average charge in the device (from Poisson's equation)

2) short-range (Coulomb) forces

$$F = \frac{q_1 q_2}{4\pi\varepsilon r_{12}^2}$$

near-equilibrium



also: delicate balance between drift and diffusion

Monte Carlo simulation and the BTE

One can show (see Lundstrom, Sec. 6.8) that Monte Carlo simulation provides a solution to the BTE -

except when short range e-e scattering is included in which case it goes beyond the BTE by treating particle-particle correlations.

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summary

1) Monte Carlo simulation is a technique to solve the BTE (can go beyond by treating correlations)

2) Details of bandstructure and scattering are readily included

3) But rare events can be hard to treat

4) When applicable, MC simulation typically provides the most accurate solutions of the BTE

5) For a description of a state-of-the-art MC simulator:

http://www.research.ibm.com/DAMOCLES/home.html

questions

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