ECE-656: Fall 2011

Lecture 34a:

Monte Carlo Simulation

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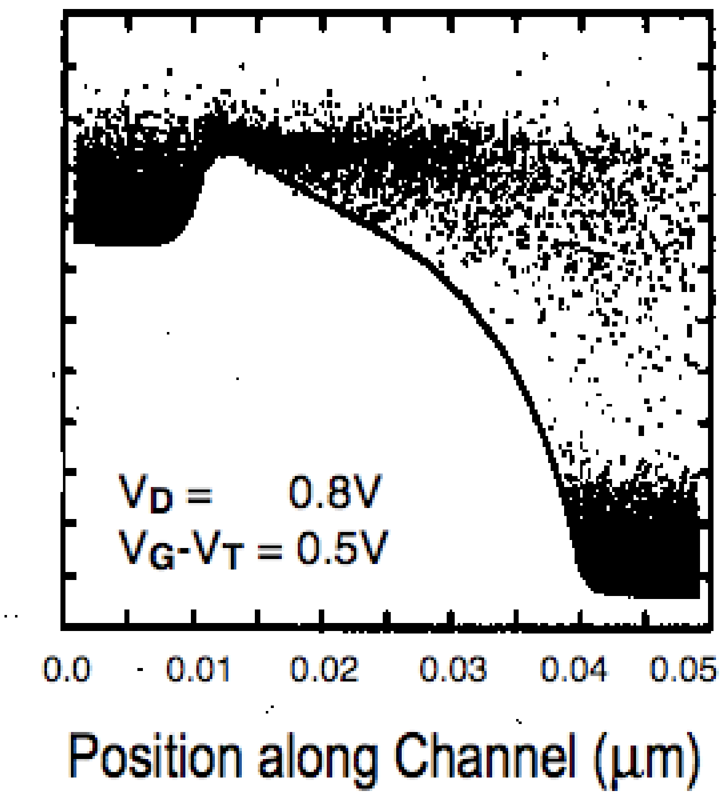
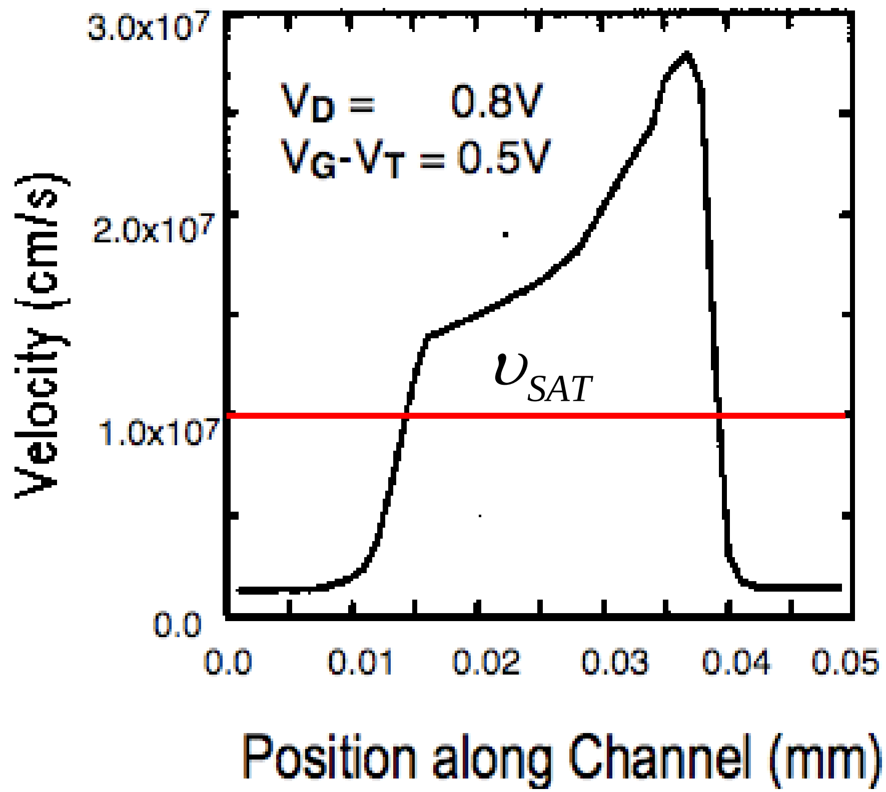
11/16/11

Damocles





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

outline

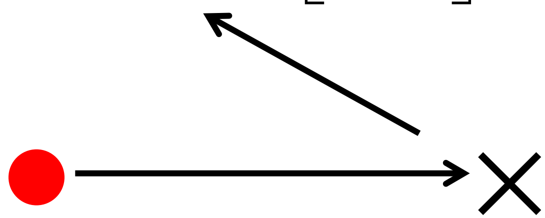
1. Introduction
2. **Review of carrier scattering**
3. Simulating carrier trajectories
4. Free flight
5. Collision
6. Update after collision
7. Putting it all together
8. Summary

(Reference: Chapter 6, Lundstrom, FCT)

carrier scattering

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

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



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

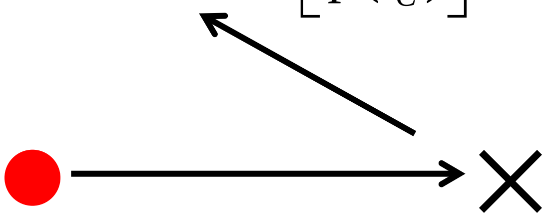
1) Scattering events are assumed to be instantaneous - scattering changes the carrier's momentum (and energy) but not position.

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

carrier scattering

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

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



$$\vec{p}(t_C^-)$$

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

Scattering rate:

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

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

Anisotropic scattering:

-preferred direction

total scattering rate

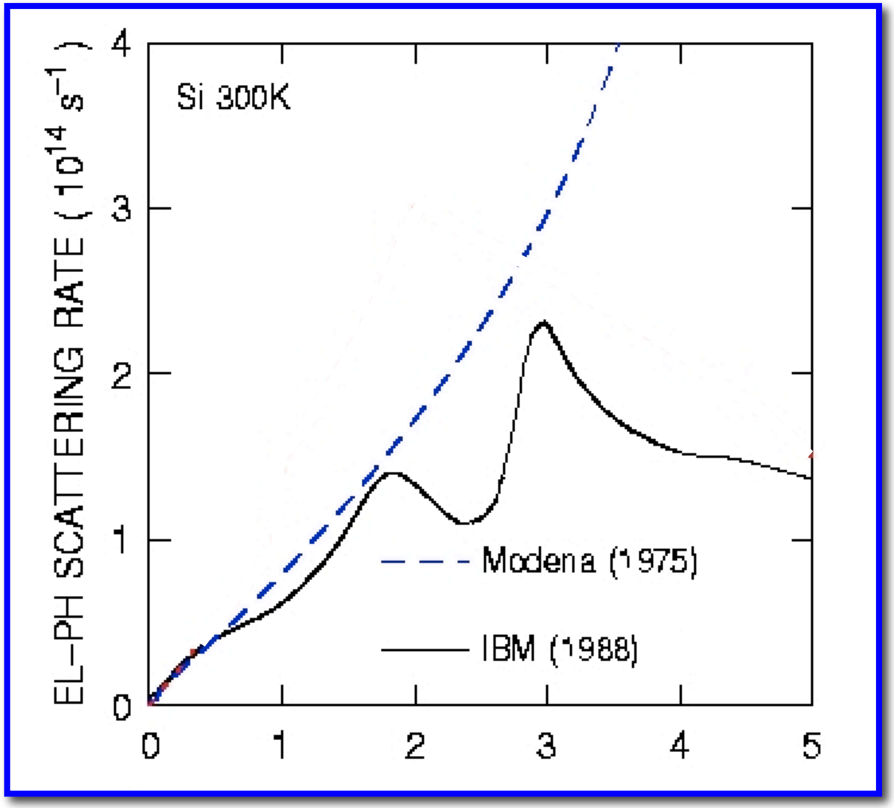
$$\frac{1}{\tau(E_i)} = \sum_{k=1}^{N} \frac{1}{\tau_k(E_i)} = \Gamma(E_i)$$

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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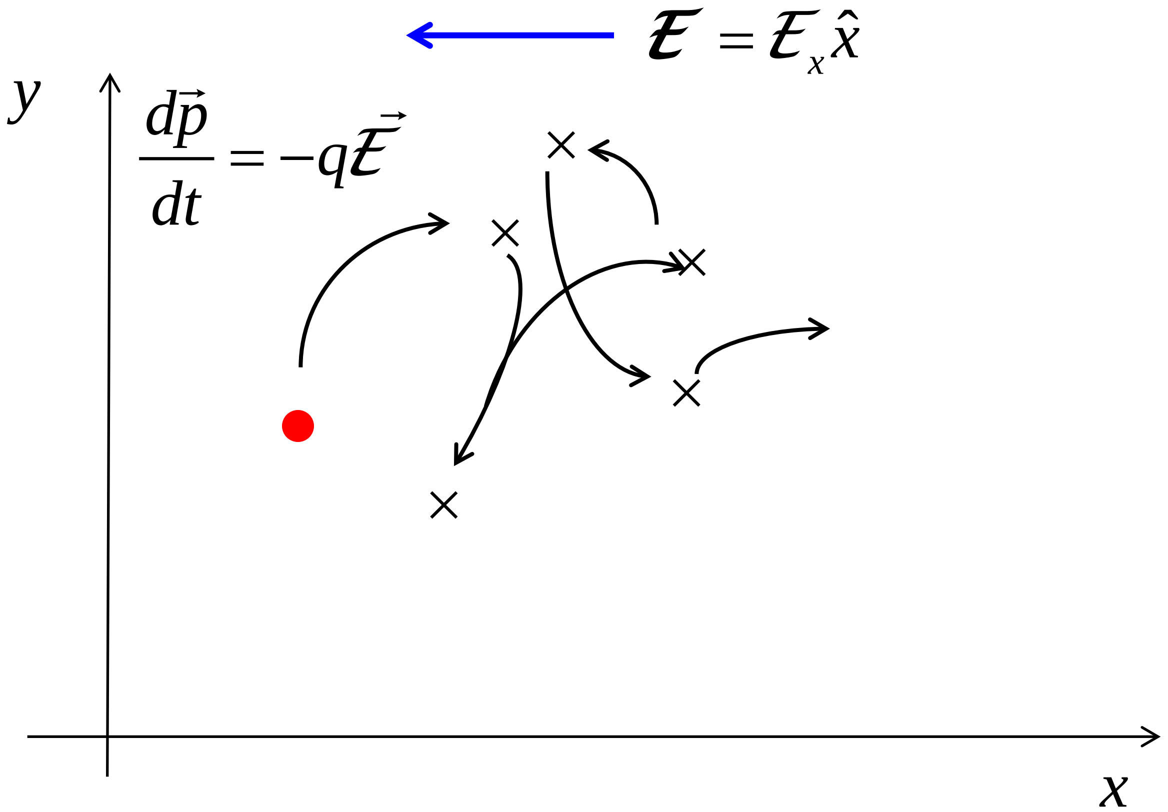
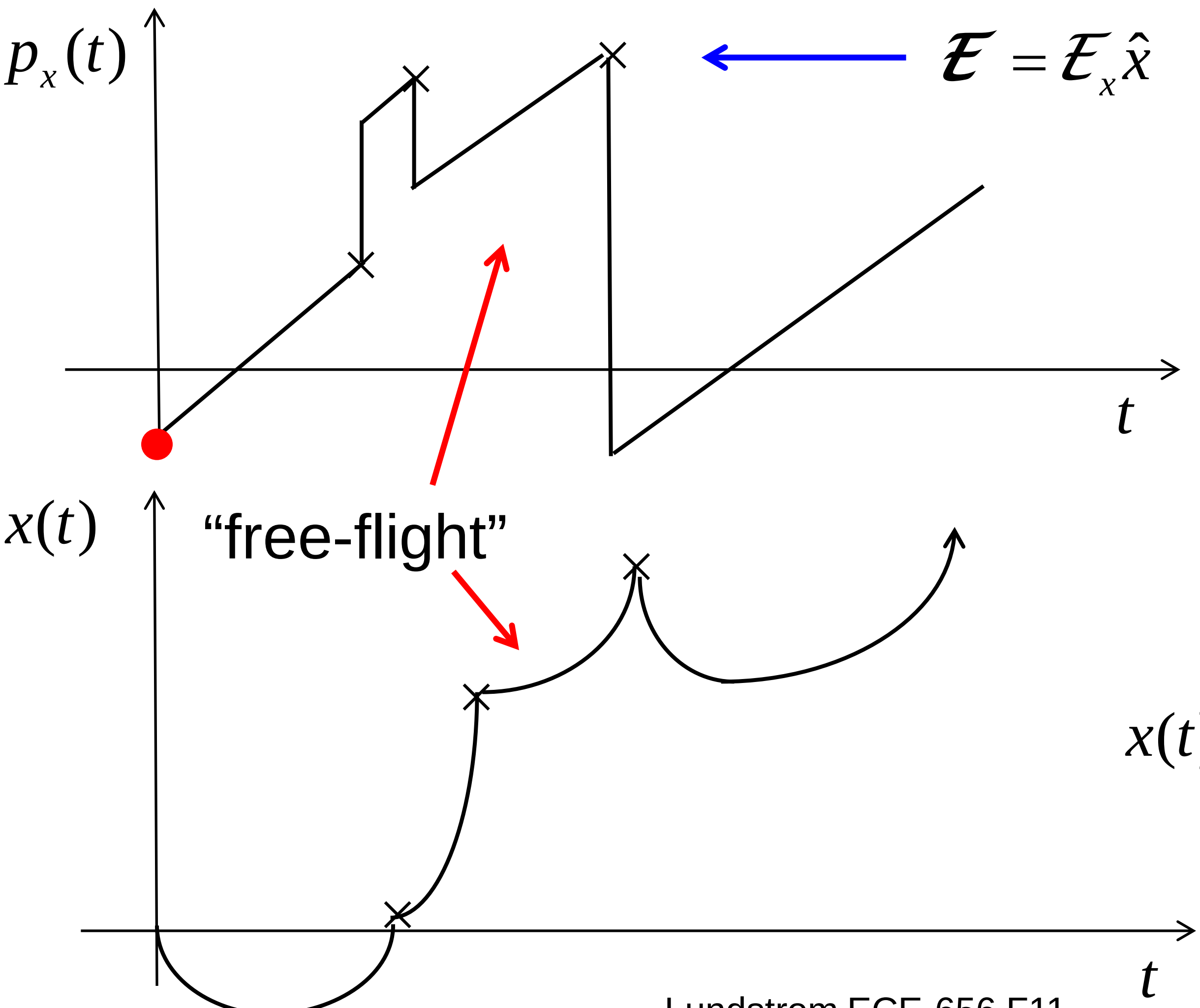
carrier trajectories in 2D



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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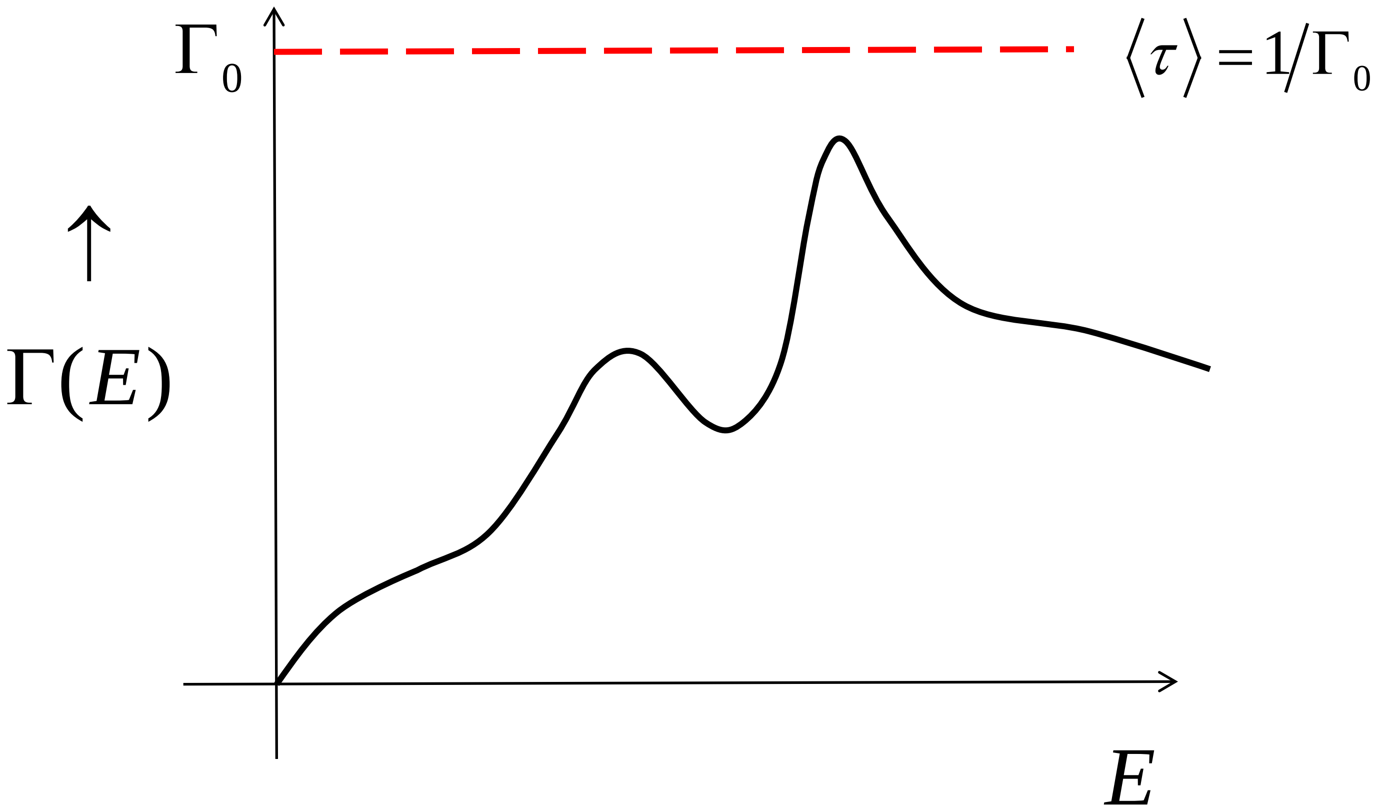
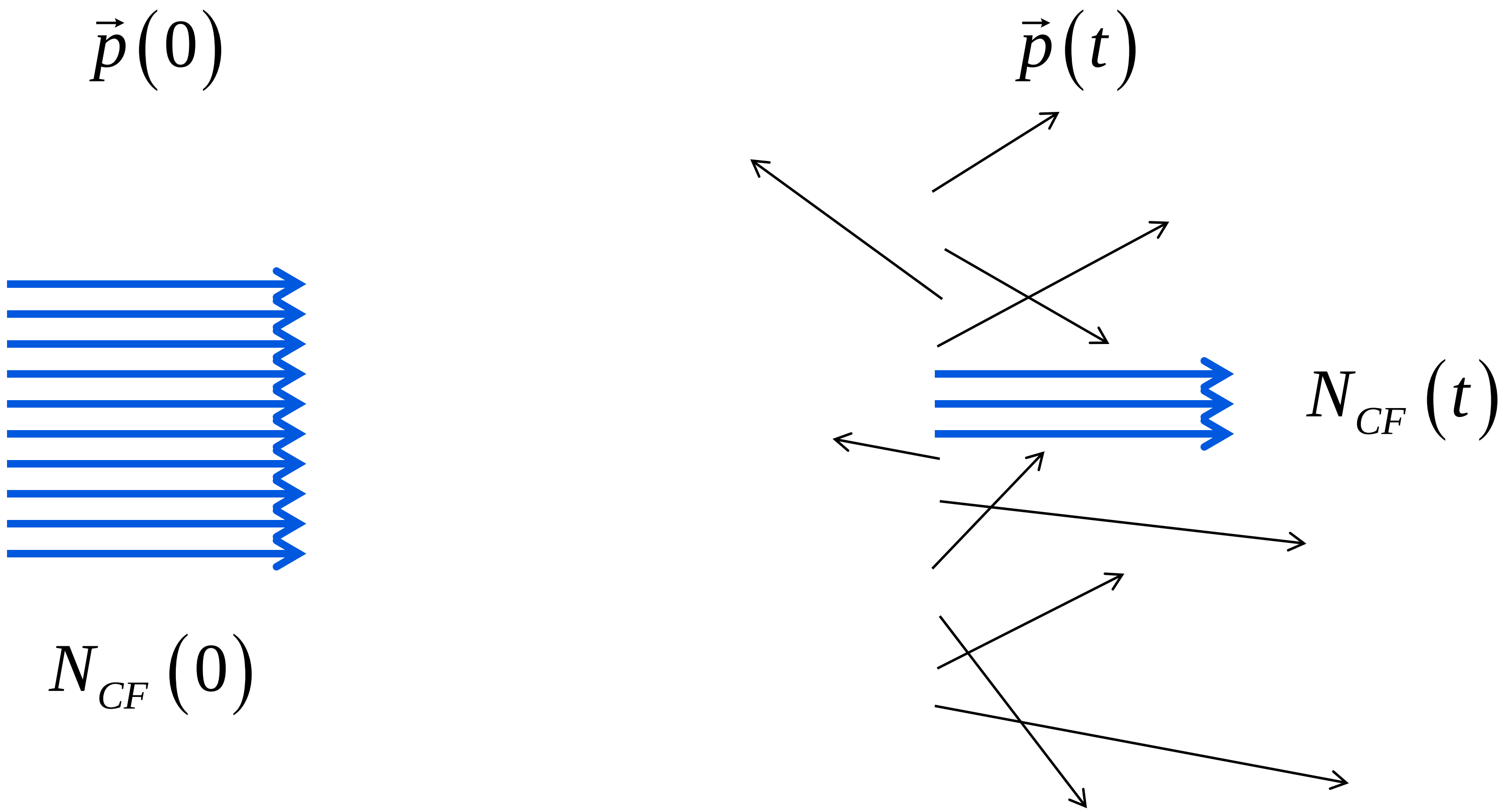
free flight



free flight



free flight time

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

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

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

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

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

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.

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

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

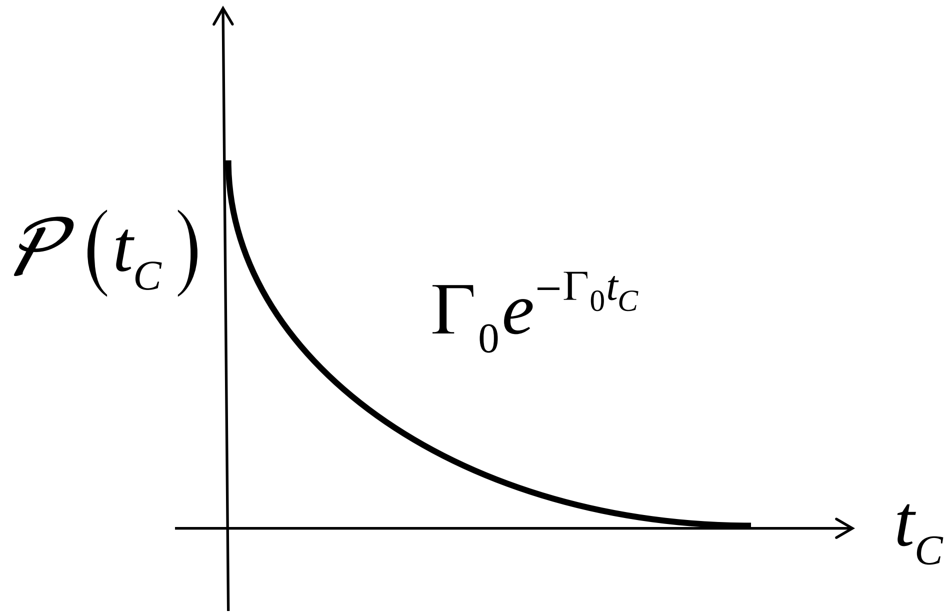
$$\int_0^{r_C} dr = r_c = \int_0^{t_C} e^{-\Gamma_0 t}\Gamma_0 dt = -e^{-\Gamma_0 t}\Big|_0^{t_C} = \left(1 - e^{-\Gamma_0 t_C}\right)$$

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

free flight distribution

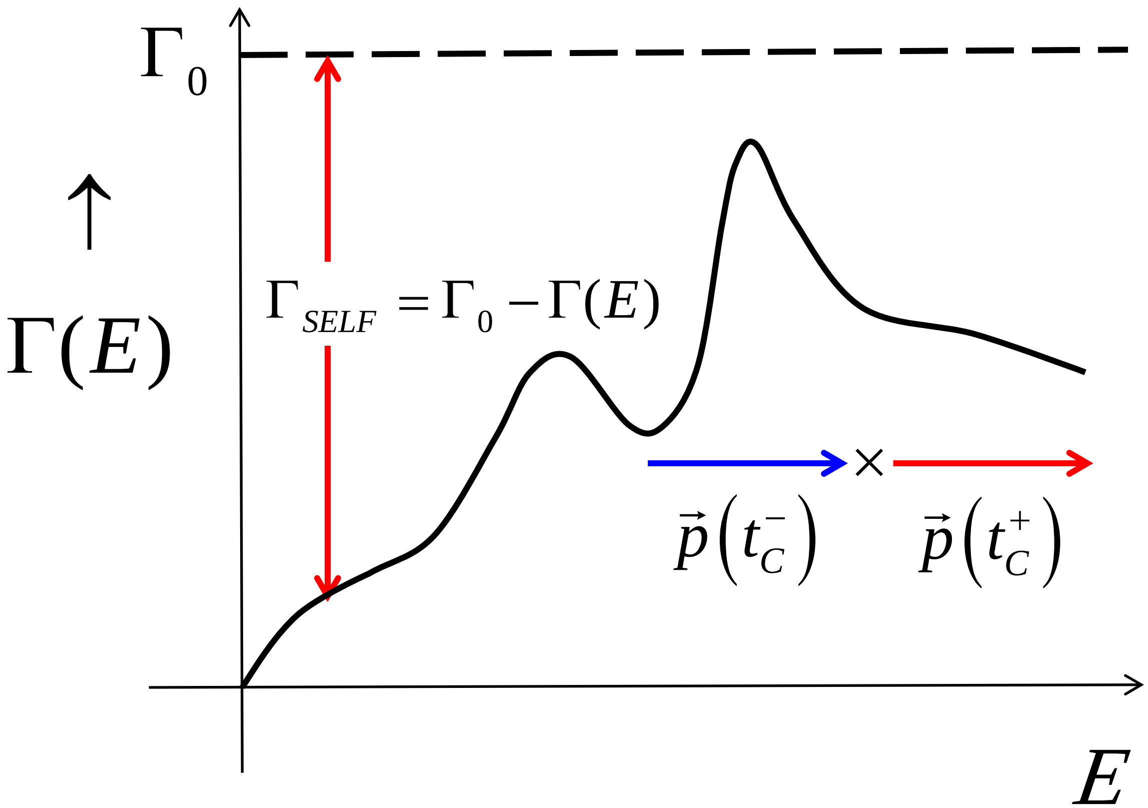
$$t_C = -\frac{1}{\Gamma_0}\ln\left(r_1\right)$$

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



but, the scattering rate is not constant with energy!

free flight



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

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

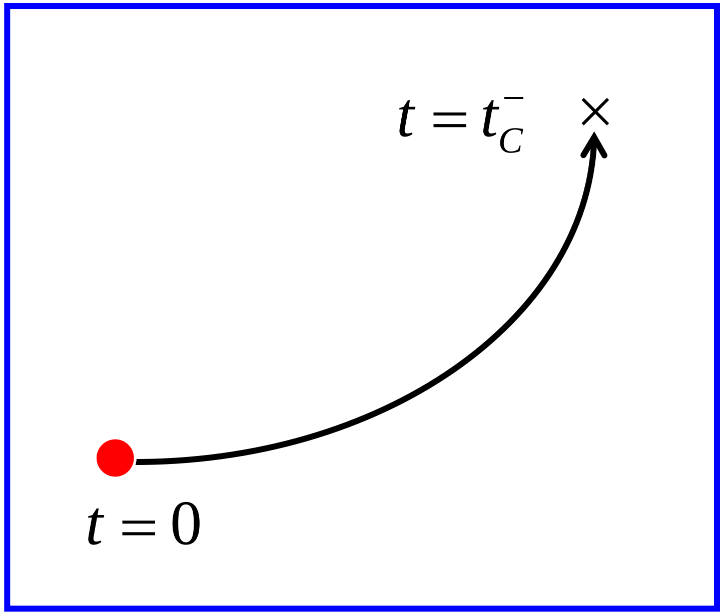
$$t_C = -\frac{1}{\Gamma_0} \ln\left(r_1\right)$$

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?

L32 outline

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collision

To be continued next lecture…