

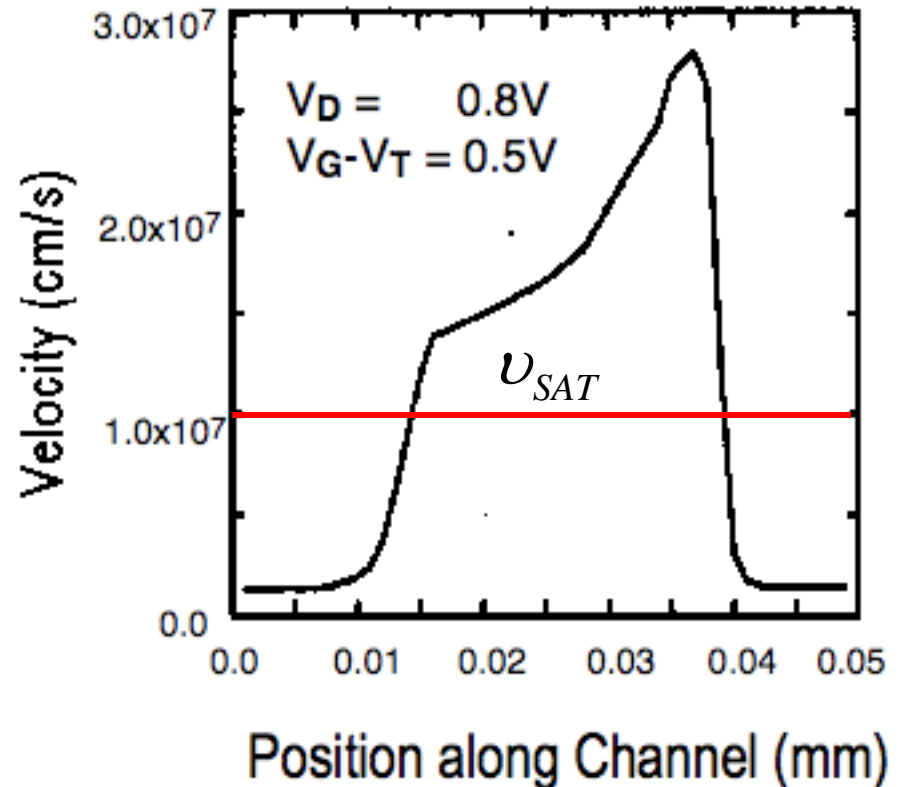
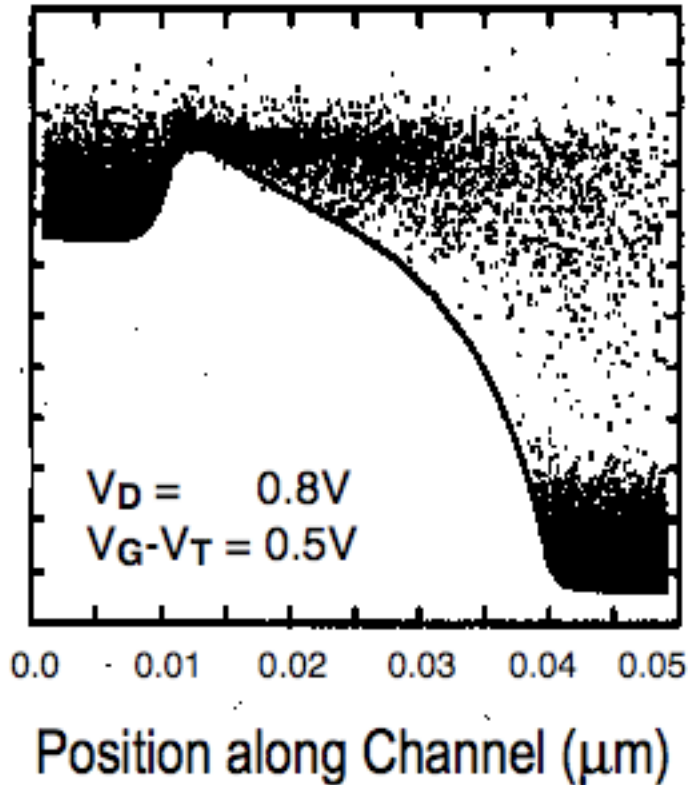
ECE-656: Fall 2011

Lecture 34a:

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

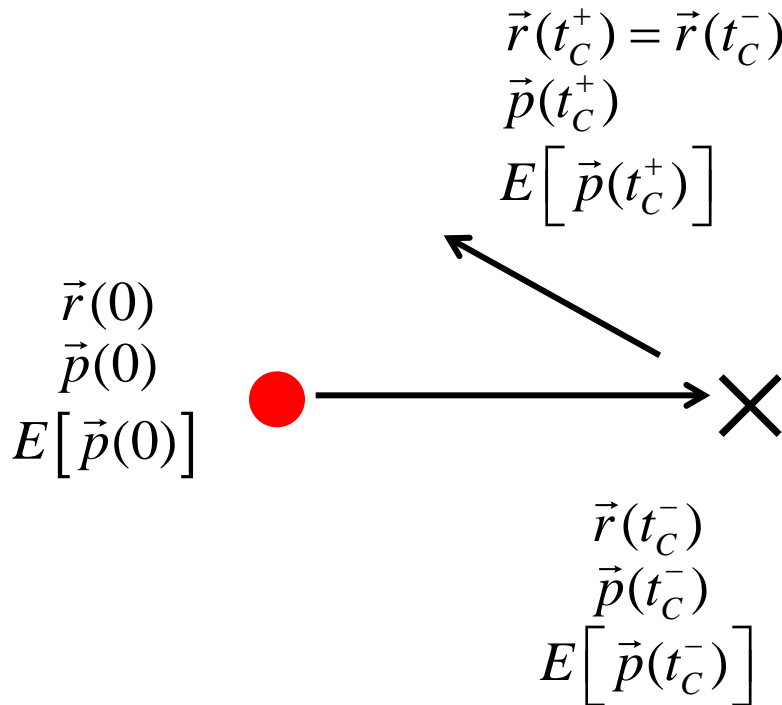
(Reference: Chapter 6, Lundstrom, FCT)



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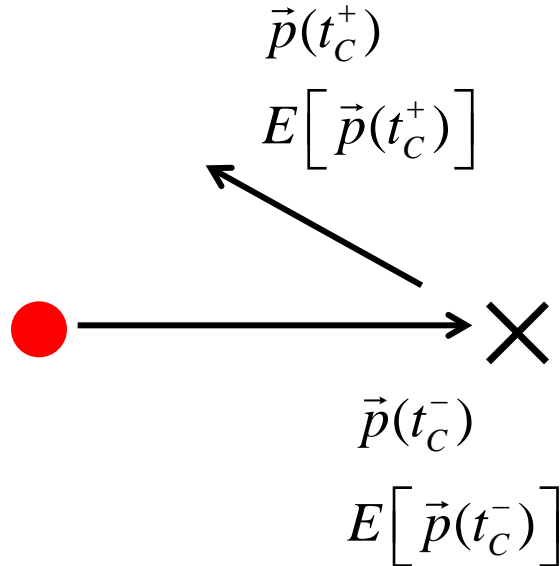
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carrier scattering



- 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



Scattering rate:

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

Elastic scattering:

$$E[\vec{p}(t_c^+)] = E[\vec{p}(t_c^-)]$$

Inelastic scattering:

$$E[\vec{p}(t_c^+)] \neq E[\vec{p}(t_c^-)]$$

Isotropic scattering:

-no preferred direction

Anisotropic scattering:

-preferred direction

total scattering rate

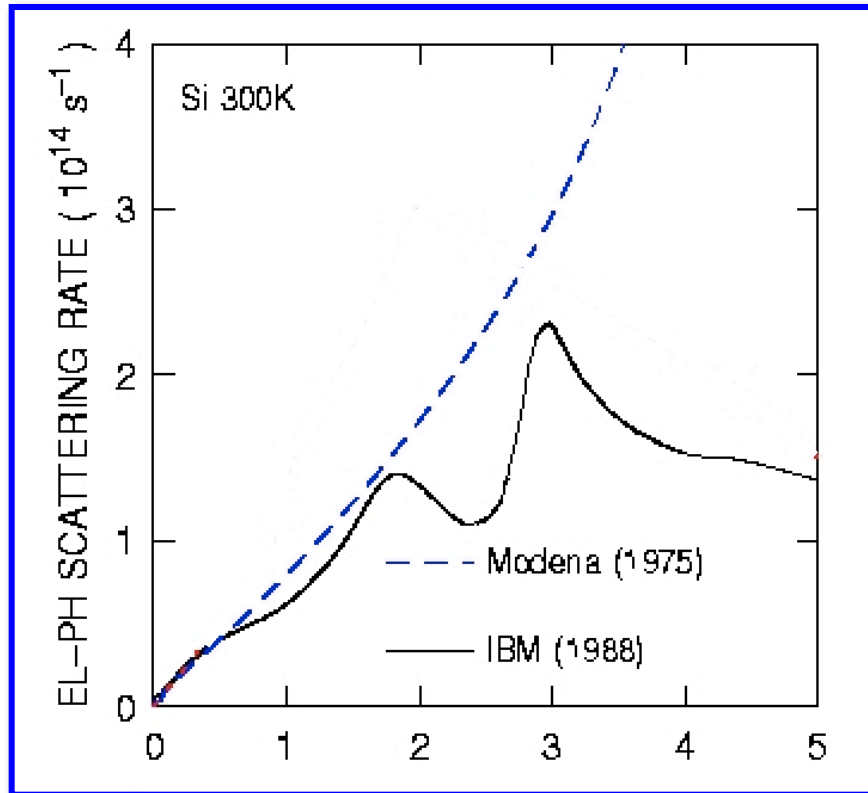
$$\frac{1}{\tau(E_i)} = \sum_{k=1}^N \frac{1}{\tau_k(E_i)} = \Gamma(E_i)$$

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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outline

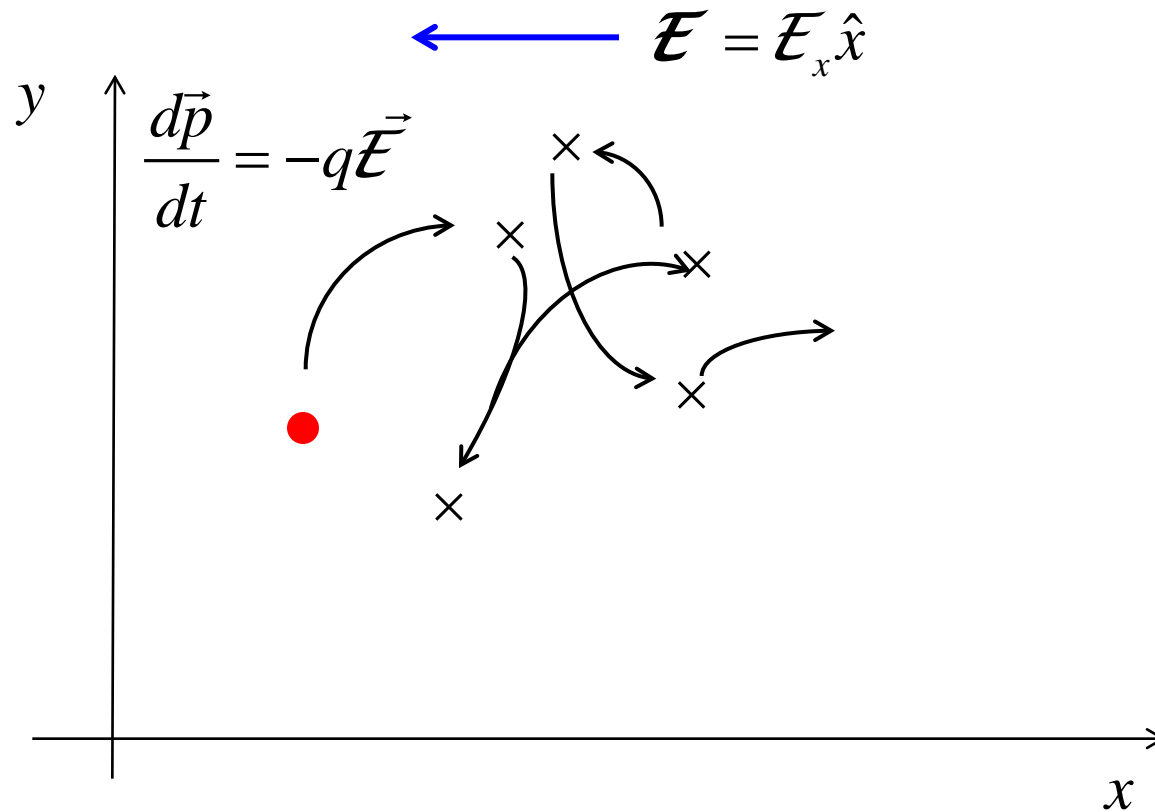
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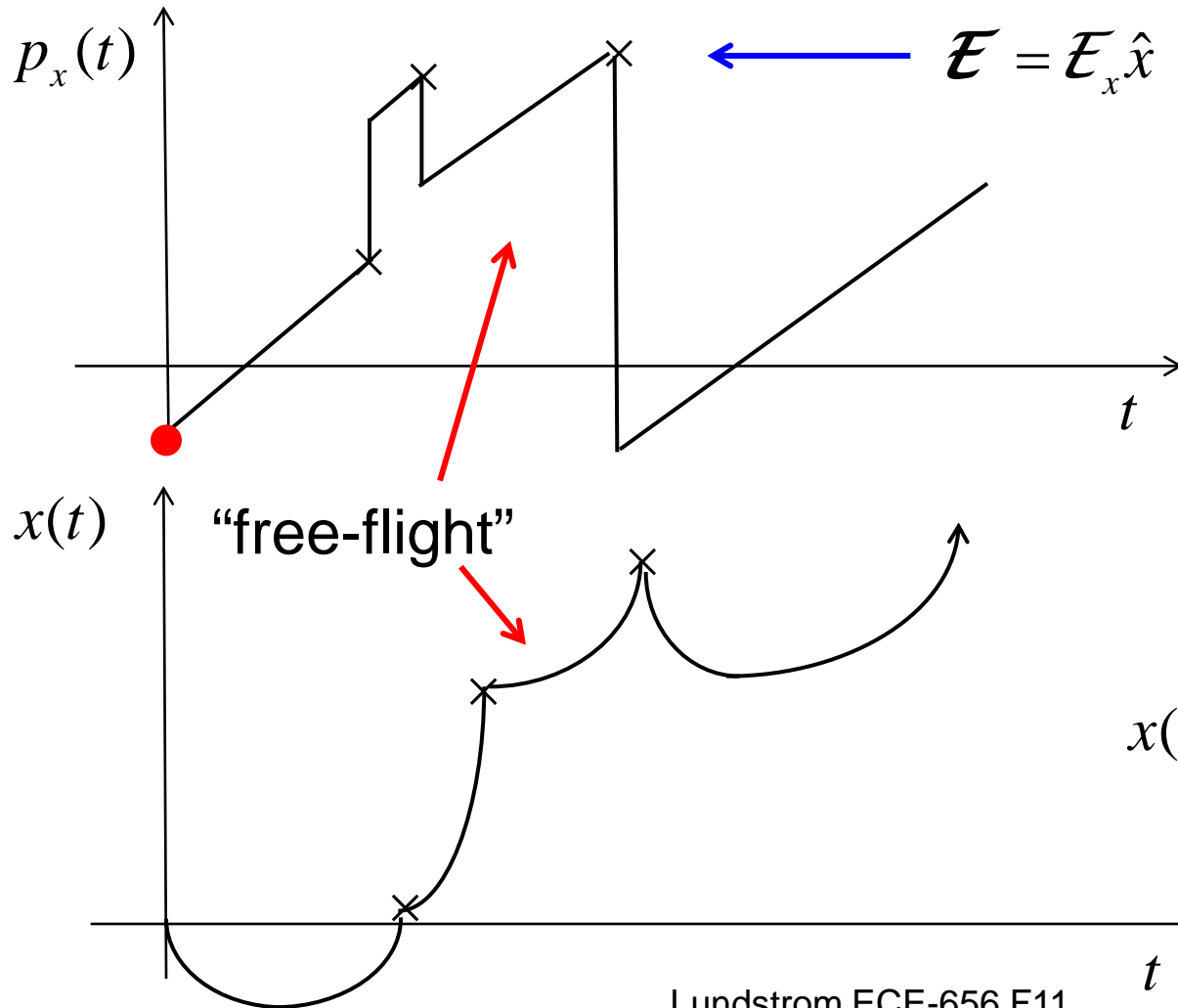


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carrier trajectories in 2D



carrier trajectories in phase space



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

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

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

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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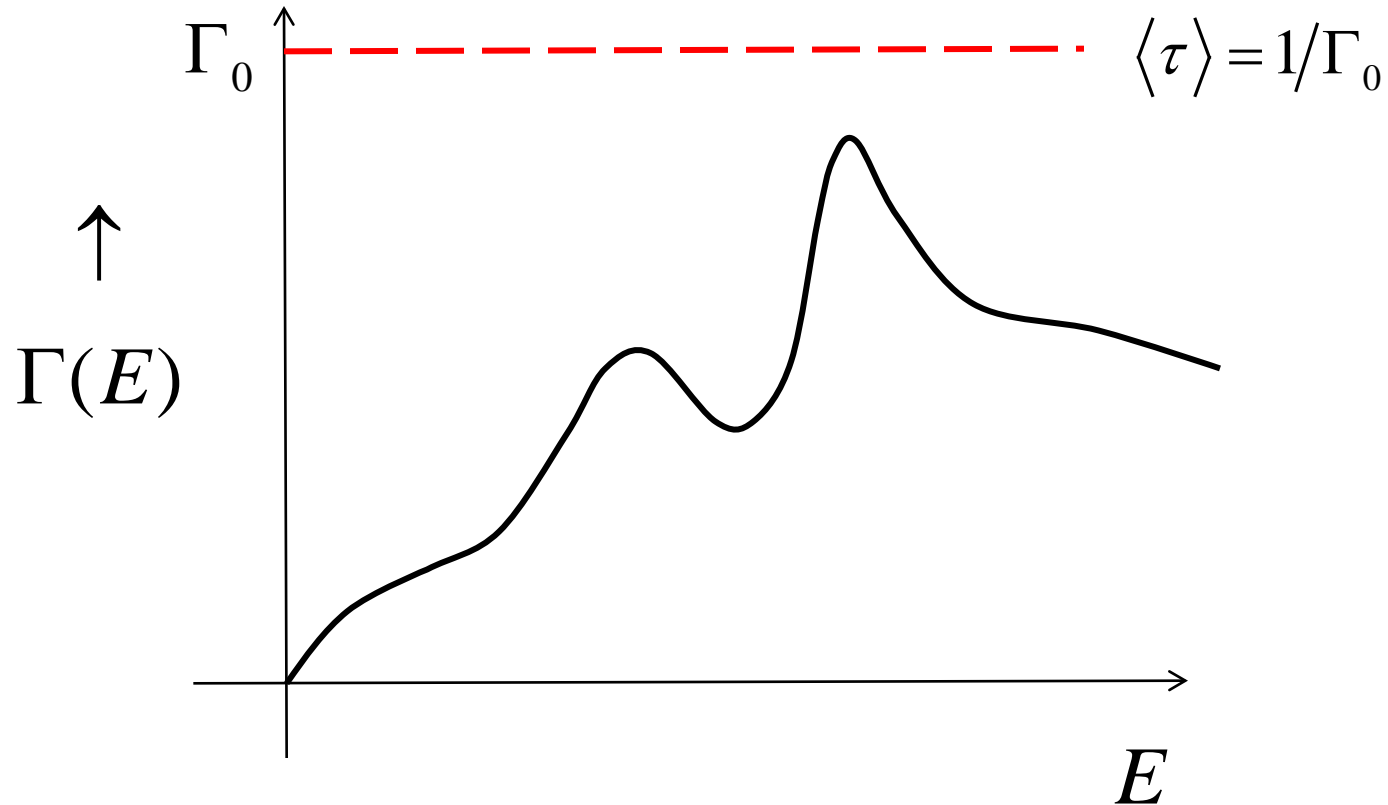
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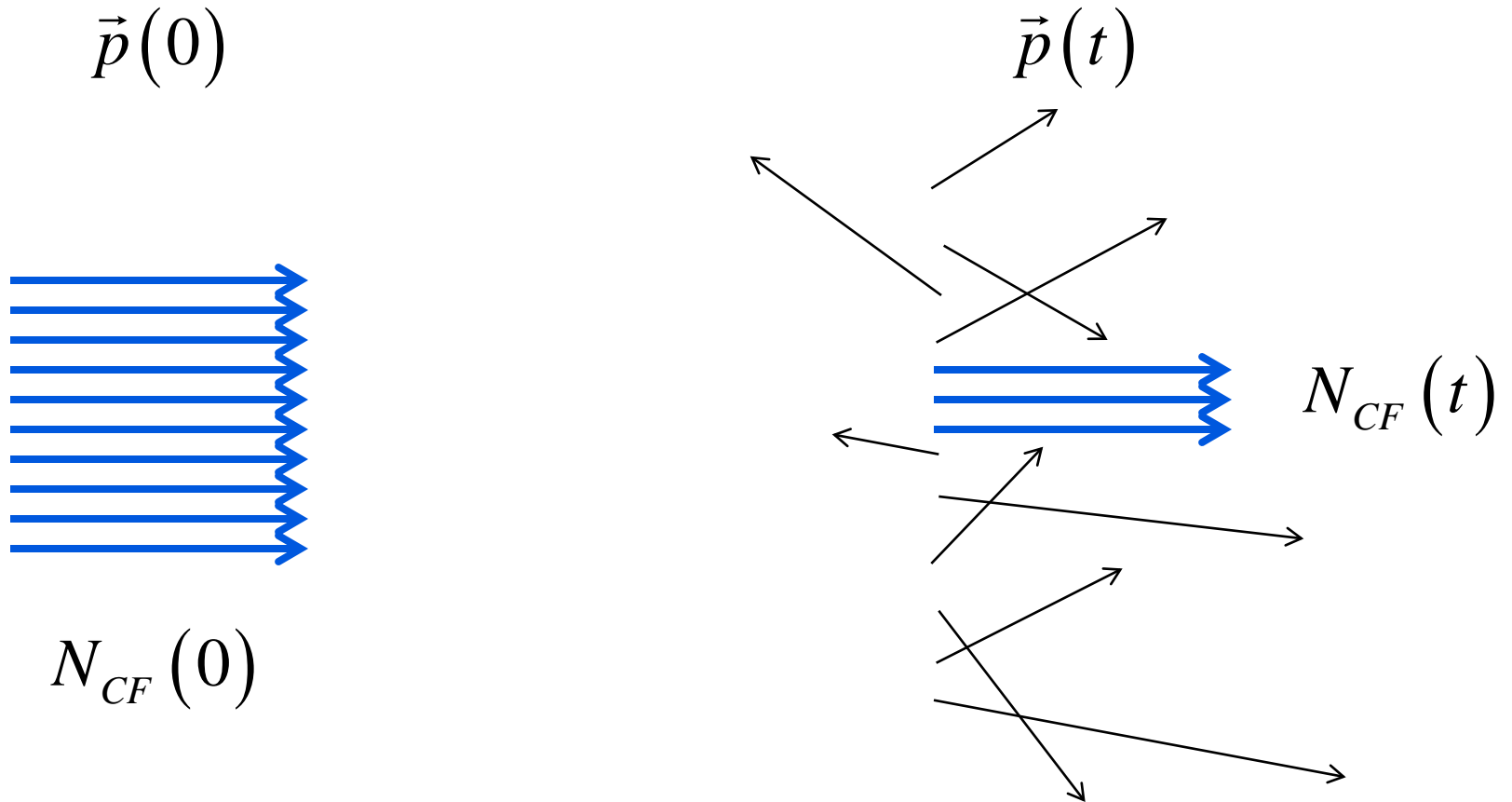
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free flight



free flight



free flight time

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

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

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

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

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

free flight time

What is the probability that a carrier survives until time, t , and then scatters 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.

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

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

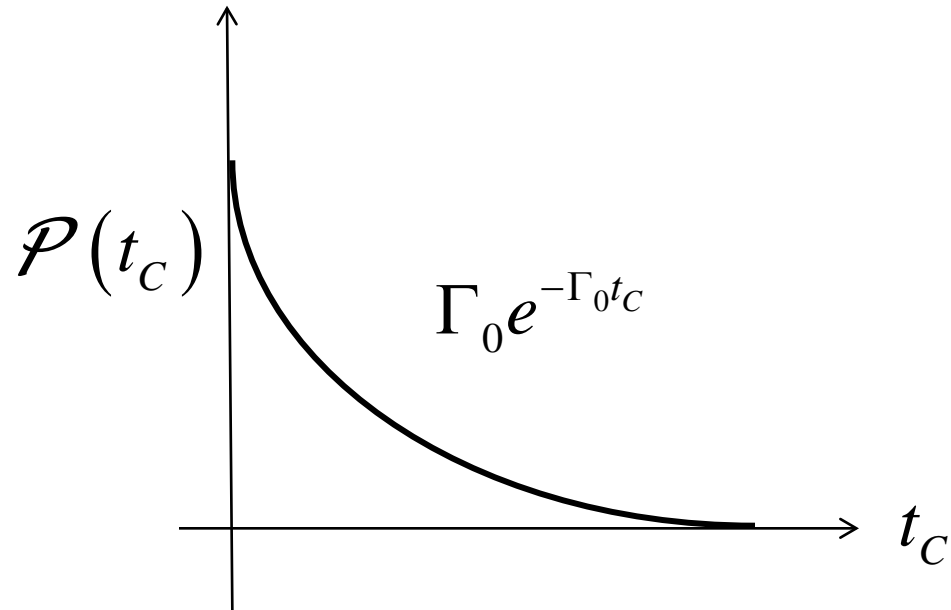
$$\int_0^{r_c} dr = r_c = \int_0^{t_c} e^{-\Gamma_0 t} \Gamma_0 dt = -e^{-\Gamma_0 t} \Big|_0^{t_c} = (1 - e^{-\Gamma_0 t_c})$$

$$t_c = -\frac{1}{\Gamma_0} \ln(1 - r_c)$$

free flight distribution

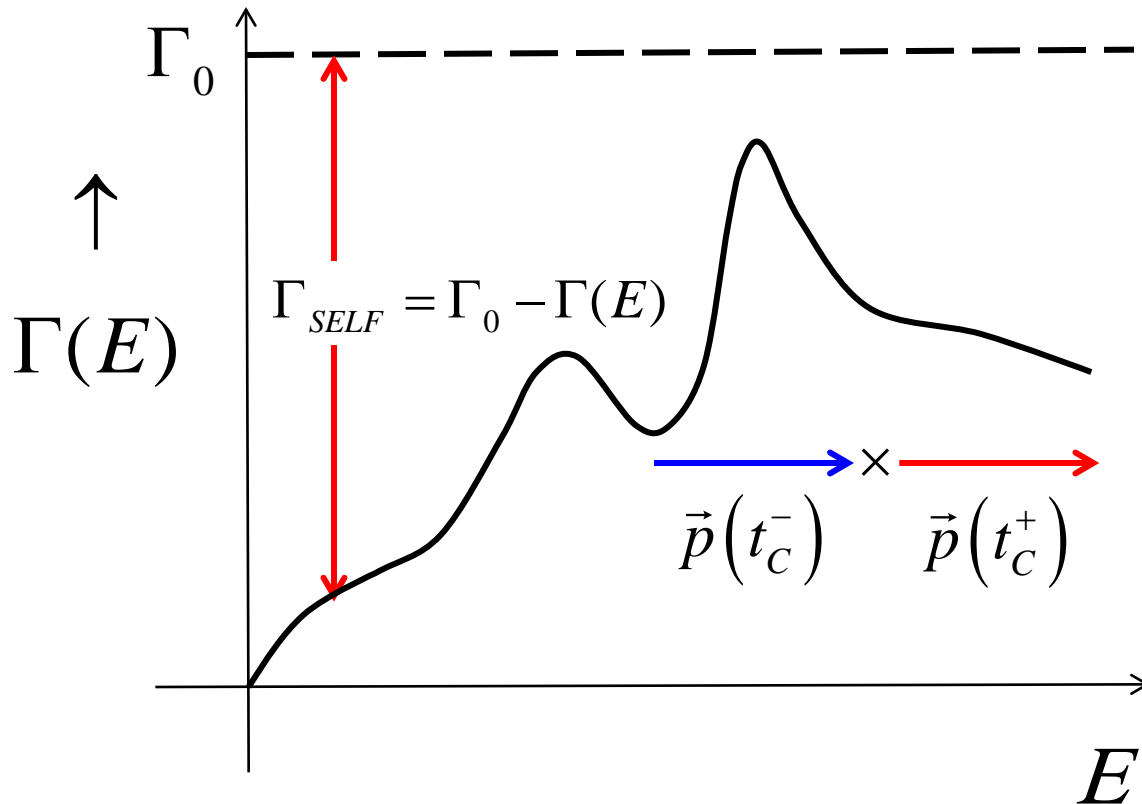
$$t_C = -\frac{1}{\Gamma_0} \ln(r_1)$$

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



but, the scattering rate is not constant with energy!

free flight



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

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

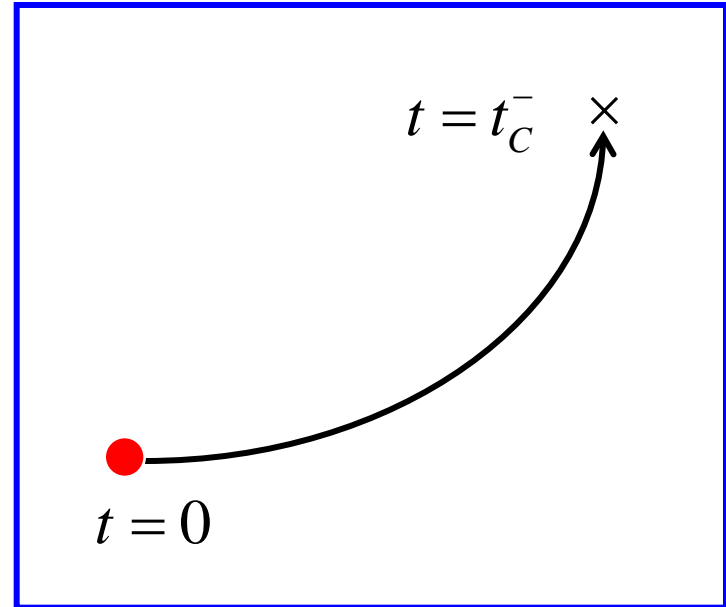
$$t_c = -\frac{1}{\Gamma_0} \ln(r_1)$$

update at end of free-flight

$$\vec{p}(t_c^-) = \vec{p}(0) - q\vec{E}t_c$$

$$E(t_c^-) = E[\vec{p}(t_c^-)]$$

$$\vec{r}(t_c^-) = r(0) + \vec{v}(0)t_c$$



- 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...