Monte Carlo Method: Path Integral Formulation

Dragica Vasileska

Professor

Arizona State University

(8) MONTE CARLO AND PATH INTEGRAL METHODS

The path integral method for solving the BTE is a rather useful and intuitive procedure for describing the Monte Carlo method. In its general form, the BTE is:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_r f + (-e)\vec{\mathcal{E}} \cdot \nabla_p f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

$$= \sum_{i=1}^{N} \sum_{\vec{p}'} \left[\underbrace{S_i(\vec{p}', \vec{p})\, f(\vec{r}, \vec{p}', t)}_{\text{scattering into state } \vec{p}} - \underbrace{S_i(\vec{p}, \vec{p}')\, f(\vec{r}, \vec{p}, t)}_{\text{scattering out of state } \vec{p}} \right]$$

This form of the BTE is valid for non-degenerate semiconductors. The collision integral on the RHS can also be expressed as:

$$RHS = \sum_{\vec{p}'} \sum_{i=1}^{N} S_i(\vec{p}', \vec{p})\, f(\vec{r}, \vec{p}', t) - f(\vec{r}, \vec{p}, t) \sum_{\vec{p}'} \underbrace{\sum_{i=1}^{N} S_i(\vec{p}, \vec{p}')}_{\frac{1}{\tau(\vec{p})} \equiv \text{total scattering rate out of state } \vec{p}}$$

Hence:

$$RHS = \sum_{\vec{p}'} \sum_{i=1}^{N} S_i(\vec{p}', \vec{p}) f(\vec{r}, \vec{p}', t) - f(\vec{r}, \vec{p}, t)\left[\frac{1}{\tau(\vec{p})} + \Omega(\vec{p})\right] + f(\vec{r}, \vec{p}, t)\,\Omega(\vec{p})$$

self-scattering term

$$= \sum_{\vec{p}'} \sum_{i=1}^{N} S_i(\vec{p}', \vec{p}) f(\vec{r}, \vec{p}', t) - \Gamma(\vec{p}) f(\vec{r}, \vec{p}, t) + \sum_{\vec{p}'} f(\vec{r}, \vec{p}', t)\,\Omega(\vec{p})\,\delta_{\vec{p},\vec{p}'}$$

In this last expression, we have added a term $\Omega(\vec{p})$ such that the total scattering rate out of a state $\vec{p}$ is constant. To understand the meaning of this term, we need to go backwards, i.e. write $\Gamma(\vec{p})$ as:

$$\Gamma(\vec{p}) = \frac{1}{\tau(\vec{p})} + \Omega(\vec{p}) = \sum_{\vec{p}'} \sum_{i=1}^{N} S_i(\vec{p}, \vec{p}') + \sum_{\vec{p}'} \Omega(\vec{p})\,\delta_{\vec{p},\vec{p}'} =$$

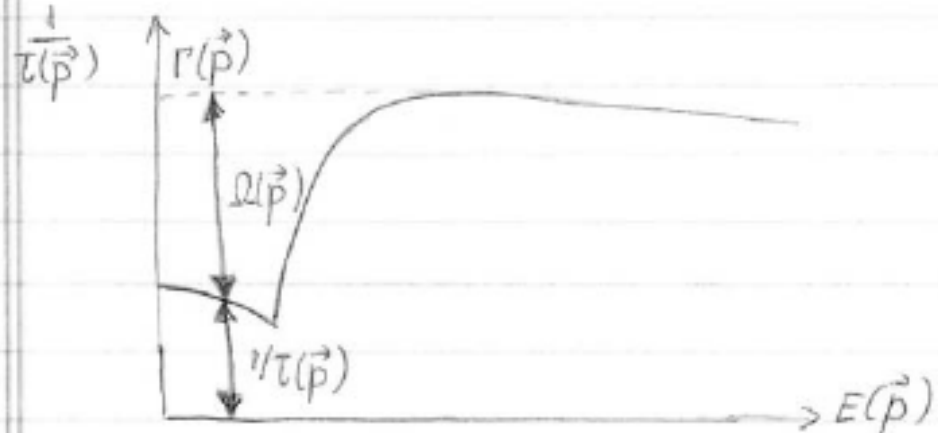
$$= \sum_{\vec{p}'} \left[\sum_{i=1}^{N} S_i(\vec{p}, \vec{p}') + \Omega(\vec{p})\,\delta_{\vec{p},\vec{p}'}\right]$$

We now define an effective transition rate:

$$S^{eff}(\vec{p},\vec{p}') = \sum_{n=1}^{N} S(\vec{p},\vec{p}') + \Omega(\vec{p})\,\delta_{\vec{p},\vec{p}'}$$

which consists of the sum of the N physical transition rates plus a term that has a momentum conserving δ-function. This second term has no effect on the carrier momentum and energy and is a fictitios scattering process called SELF-SCATTERING. The self-scattering can be calculated from:

$$\Gamma(\vec{p}) = \frac{1}{\tau(\vec{p})} + \Omega(\vec{p}) \Rightarrow \Omega(\vec{p}) = \Gamma(\vec{p}) - \frac{1}{\tau(\vec{p})}$$



With the above definitions for the self-scattering term, the BTE becomes:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_r f + (-e)\vec{\mathcal{E}} \cdot \nabla_p f + \Gamma(\vec{p}) f(\vec{r},\vec{p},t) =$$

$$= \sum_{p'} \left[\sum_{i=1}^{N} S_i(\vec{p}',\vec{p}) + \left(\Gamma(\vec{p}) - \frac{1}{\tau(\vec{p})}\right) \delta_{\vec{p},\vec{p}'} \right] f(\vec{r},\vec{p}',t)$$

For homogeneous samples, the BTE becomes:

$$\frac{\partial f}{\partial t} + (-e)\vec{\mathcal{E}} \nabla_p f + \Gamma(\vec{p}) f(\vec{p},t) = \tilde{I}(\vec{p},t) =$$

$$= \sum_{\vec{p}'} \left[\sum_{i=1}^{N} S_i(\vec{p}',\vec{p}) + \left(\Gamma(\vec{p}) - \frac{1}{\tau(\vec{p})}\right) \delta_{\vec{p},\vec{p}'} \right] f(\vec{p}',t)$$

In this last formulation of the BTE, the coordinate space (phase space) is fixed and the electrons move along given trajectory in response to the applied forces. With the introduction of the variables

$$\begin{cases} \tilde{t} = t \\ \tilde{p} = \vec{p} + e\vec{\mathcal{E}}t \end{cases}$$

we go to a description in which electrons are frozen in their positions and the coordinate system is moving. Then,

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial \tilde{t}}\frac{\partial \tilde{t}}{\partial t} + \frac{\partial f}{\partial \tilde{p}}\frac{\partial \tilde{p}}{\partial t} = \frac{\partial f}{\partial \tilde{t}} + e\vec{\mathcal{E}}\cdot\frac{\partial f}{\partial \tilde{p}}$$

$$\frac{\partial f}{\partial \vec{p}} = \frac{\partial f}{\partial \tilde{t}}\underbrace{\frac{\partial \tilde{t}}{\partial \vec{p}}}_{0} + \frac{\partial f}{\partial \tilde{p}}\frac{\partial \tilde{p}}{\partial \vec{p}} = \frac{\partial f}{\partial \tilde{p}}$$

In this notation, the BTE becomes:

$$\frac{\partial f}{\partial \tilde{t}} + \cancel{e\vec{\mathcal{E}}\cdot\frac{\partial f}{\partial \tilde{p}}} + \cancel{(-e\vec{\mathcal{E}})\cdot\left(\frac{\partial f}{\partial \tilde{p}}\right)} + \Gamma f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})$$

- The solution of the homogeneous equation, of the form:

$$\frac{\partial f}{\partial \tilde{t}} + \Gamma f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = 0$$

- The solution of the homogeneous equation, of the form:

$$\frac{\partial f}{\partial \tilde{t}} + \Gamma f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = 0$$

can be found using the separation of variables method, to be of the form:

$$\ln f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\Big|_0^{\tilde{t}} = -\Gamma \int_0^{\tilde{t}} d\tilde{t}$$

or: $\ln[f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) / f(\tilde{p}, 0)] = -\Gamma\tilde{t}$

to get:

$$f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = f(\tilde{p}, 0)\, e^{-\Gamma\tilde{t}}$$

Going back to the original coordinate system gives:

$$f(\vec{p} + e\vec{\mathcal{E}}t - e\vec{\mathcal{E}}t, t) = f(\vec{p} + e\vec{\mathcal{E}}t, 0)\, e^{-\Gamma t}$$

or:

$$f(\vec{p},t) = f(\vec{p} + e\vec{\mathcal{E}}t, 0)\, e^{-\Gamma t}$$

$f(\vec{p} + e\vec{\mathcal{E}}t, 0)$: initial state of an electron

$e^{-\Gamma t}$: probability of no scattering

This term is the transient term. It states that an electron initially in a state $(\vec{p} + e\vec{\mathcal{E}}t)$ at time $t=0$, has arrived in a state $\vec{p}$ at time t without scattering. This event occurs with a transition probability:

$$P(\vec{p},t,0) = e^{-\Gamma t}, \quad \text{for } \Gamma(\vec{p}) = \Gamma = \text{const.}$$

Note: for general case when $\Gamma(\vec{p})$ is not constant, we would have had:

$$P(\vec{p},t,0) = \exp\left[-\int_0^t \Gamma(\vec{p})\,dt'\right]$$

Also note that, if the initial momentum of the electron is $(\vec{p} + e\vec{\mathcal{E}}t)$, because of the drift motion and the acceleration by the electric field, the final electron momentum after time t equals to.

$$\vec{p}' = \vec{p} + e\vec{\mathcal{E}}t - e\vec{\mathcal{E}}t = \vec{p}.$$

- The next task is to find a general solution of the BTE for homogeneous systems. The homogeneous solution suggests that the general solution will also involve exponentials. For this purpose, we define a function:

$$f_1(\vec{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = f(\vec{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\, e^{r\tilde{t}}$$

which leads to:

$$f(\vec{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = f_1(\vec{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\, e^{-r\tilde{t}}$$

Then:

$$\frac{\partial f}{\partial \tilde{t}} = \frac{\partial f_1}{\partial \tilde{t}} e^{-r\tilde{t}} + f_1(-r) e^{-r\tilde{t}} = \frac{\partial f_1}{\partial \tilde{t}} e^{-r\tilde{t}} - r f_1(\vec{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) e^{-r\tilde{t}}$$

Substituting this result back into the BTE gives:

$$\frac{\partial f_1}{\partial \tilde{t}} e^{-r\tilde{t}} - r f_1(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\, e^{-r\tilde{t}} + r f_1(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\, e^{-r\tilde{t}} = \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})$$

or:

$$\frac{\partial f_1}{\partial \tilde{t}} = e^{r\tilde{t}}\, \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})$$

Solving this last equation for f_1 finally leads to:

$$f_1(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t})\Big|_0^{\tilde{t}} = \int_0^{\tilde{t}} d\tilde{t}_1\, e^{r\tilde{t}_1}\, \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}_1, \tilde{t}_1)$$

or:

$$f_1(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = f_1(\tilde{p}, 0) + \int_0^{\tilde{t}} d\tilde{t}_1\, e^{r\tilde{t}_1}\, \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}_1, \tilde{t}_1) \quad / \text{multiply by } e^{-r\tilde{t}}$$

Hence:

$$f(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}, \tilde{t}) = f(\tilde{p}, 0)\, e^{r\tilde{t}} + \int_0^{\tilde{t}} d\tilde{t}_1\, e^{-r(\tilde{t} - \tilde{t}_1)}\, \tilde{I}(\tilde{p} - e\vec{\mathcal{E}}\tilde{t}_1, \tilde{t}_1)$$

Returning back to the original coordinate system gives:

$$f(\vec{p}+e\vec{\mathcal{E}}t-e\vec{\mathcal{E}}t,t) = f(\vec{p}+e\vec{\mathcal{E}}t,0)\,e^{-\Gamma t} + \int_0^t dt_1\, e^{-\Gamma(t-t_1)}\,\tilde{I}(\vec{p}+e\vec{\mathcal{E}}t-e\vec{\mathcal{E}}t_1,t_1)$$

where $\tilde{I}(\vec{p},t) = \sum_{\vec{p}'} S_{eff}(\vec{p}',\vec{p})\,f(\vec{p}',t)$. Substituting this back gives:

$$f(\vec{p},t) = \underbrace{f(\vec{p}+e\vec{\mathcal{E}}t,0)\,e^{-\Gamma t}}_{\text{transient term}} + \int_0^t dt_1 \sum_{\vec{p}'} \underbrace{f(\vec{p}',t_1)}_{\substack{\text{probability that at time } t_1 \text{ a state } \vec{p}' \\ \text{is occupied by an electron.}}} \underbrace{S_{eff}(\vec{p}',\vec{p}+e\vec{\mathcal{E}}(t-t_1))}_{\substack{\text{Transition rate (probability) from state} \\ \vec{p}' \text{ to state } \vec{p}+e\vec{\mathcal{E}}(t-t_1)}} \underbrace{e^{-\Gamma(t-t_1)}}_{\substack{\text{probability that an electron will not undergo collision event in interval } (t-t_1).}}$$

This last expression is known as CHAMBERS-REES path integral. Rees innovation is the introduction of the fictitious scattering term.

• Ignoring the transient term, one can find the solution of the distribution function using the following iterative procedure that is obtained by time discretization, i.e. using $t = N\Delta t$, and $t_n = n\Delta t$. Then

$$f_N(\vec{p}) = \Delta t \sum_{m=0}^{N-1} \underbrace{\sum_{\vec{p}'} f_m(\vec{p}')\, S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}(N-m)\Delta t)}_{g_m(\vec{p} + e\vec{\mathcal{E}}(N-m)\Delta t)}\, e^{-\Gamma'(N-m)\Delta t}$$

The two step procedure is then found by using $N = 1$, which means that $t = \Delta t$, i.e.

$$f_1(\vec{p}) = \Delta t \underbrace{\sum_{\vec{p}'} f_0(\vec{p}')\, S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}\Delta t)}_{g_0(\vec{p} + e\vec{\mathcal{E}}\Delta t)}\, \underbrace{e^{-\Gamma\Delta t}}_{\text{integration over a trajectory, i.e. probability that no scattering occured within time integral } \Delta t. \text{ (free-fly)}}$$

$g_0(\vec{p} + e\vec{\mathcal{E}}\Delta t)$: intermediate function that describes the occupancy of a state $(\vec{p} + e\vec{\mathcal{E}}\Delta t)$ at time $t = 0$, which can be changed due to in-scattering events. (scatter)

Now, assume that $t = 2\Delta t$. This then gives:

$$f_2(\vec{p}) = \Delta t \sum_{m=0}^{} \sum_{\vec{p}'} f_m(\vec{p}') S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}(2-m)\Delta t)\, e^{-\Gamma(2-m)\Delta t}$$

$$= \Delta t \sum_{\vec{p}'} f_0(\vec{p}') S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}\, 2\Delta t)\, e^{-\Gamma(2\Delta t)} +$$

$$+ \Delta t \sum_{\vec{p}'} f_1(\vec{p}') S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}\,\Delta t)\, e^{-\Gamma\Delta t}$$

$$= \Delta t \left\{ \sum_{p'} f_0(\vec{p}') S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}(2\Delta t))\, e^{-\Gamma(2\Delta t)} + \right.$$

$$\left. + \sum_{p'} f_1(\vec{p}') S_{eff}(\vec{p}', \vec{p} + e\vec{\mathcal{E}}\,\Delta t)\, e^{-\Gamma\Delta t} \right\}$$

These examples suggest that the evaluation of $f_{n+1}(\vec{p})$ involves integration over trajectories, and the exponential factors just give the probability that no scattering has occured.

DESCRIPTION OF THE SINGLE-PARTICLE MONTE CARLO

(a) Length of the particle free-flights:

The electron wavevector changes continuously during free-flight because of the applied electric field. Hence, if $P[\vec{k}(t)]dt$ is the probability that an electron in a state $\vec{k}$ suffers a collision during the time interval dt, the probability that an electron which had a collision at time $t=0$ has not yet undergone another collision after time t is:

$$e^{-\int_0^t P[\vec{k}(t')]\,dt'}$$

Therefore, the probability $P(t)$ that the electron will suffer its next collision during dt around t is given by:

$$P(t)dt = P[\vec{k}(t)] \exp\left[-\int_0^t P[\vec{k}(t')]\,dt'\right] dt$$

Therefore, the probability $P(t)$ that the electron will suffer its next collision during dt around t is given by:

$$P(t)dt = P[\vec{k}(t)] \exp\left[-\int_0^t P[\vec{k}(t')]dt'\right] dt$$

Now, if Γ is the maximum value of $P[\vec{k}]$ in the region of k-space of interest, then $P[\vec{k}(t)] = \Gamma$ and:

$$P(t)dt = \Gamma e^{-\Gamma t} dt$$

The integrated probability density is:

$$\int_0^\infty \Gamma e^{-\Gamma t} dt = -e^{-\Gamma t}\Big|_0^\infty = 1 \quad ; \text{ which should have been expected.}$$

Single Particle and Ensemble Monte Carlo

Dragica Vasileska

Professor

Arizona State University

Kinetic Transport

- We use *N* particles, which are a representation of the total particles in our region of interest
- This provides a *phase space* of 6*N* dimensions
- A phase space distribution function has these 6*N* variables
- Our “normal” Boltzmann distribution has only 6 variables (plus time)
- The configuration of *N* particles in 6 variable space gives us a 1-particle distribution (probability) in *configuration space*
- The projection from a 6N distribution in phase space to a single particle distribution in configuration space is a difficult problem in statistical physics (e.g., BBGKY heirarchy), and uncoupling the projections requires assumptions.

Equilibrium and Nonequilibrium Kinetic Transport

- **(Near) Equilibrium transport: almost no change in the one particle distribution, or in the *correlation functions***

- **Non-equilibrium transport: significant changes in the one particle distribution function—the system is no longer stationary, and the Einstein relation is violated…. In particular, the "ergodic theorem" is no longer correct (time averages are no longer equivalent to ensemble averages; only the latter are correct).**

Monte Carlo Method Described

1. Some General Considerations

There are basically two types of Monte Carlo simulations:

- Statistical systems in which an energy functional is minimized (simulated annealing, etc.)

- Kinetic transport in which particle flow is studied (von Neumann neutron transport in ‘45, Kurosawa electron transport ‘65,…)

This is the approach we use in device modeling and carrier transport in semiconductors.

It is related to the mathematical use of Monte Carlo to integrate a function.

BTE Solution

- The Monte Carlo method is a stochastic method for solving the Boltzmann Transport equation.
- Semiclassical particle motion is assumed to be decomposed into:

  – free flights (subject to external forces)

$$\mathrm{k}(t) = \mathrm{k}(0) - e(\mathrm{v} \times \mathrm{B} + \mathrm{E})t / \hbar$$

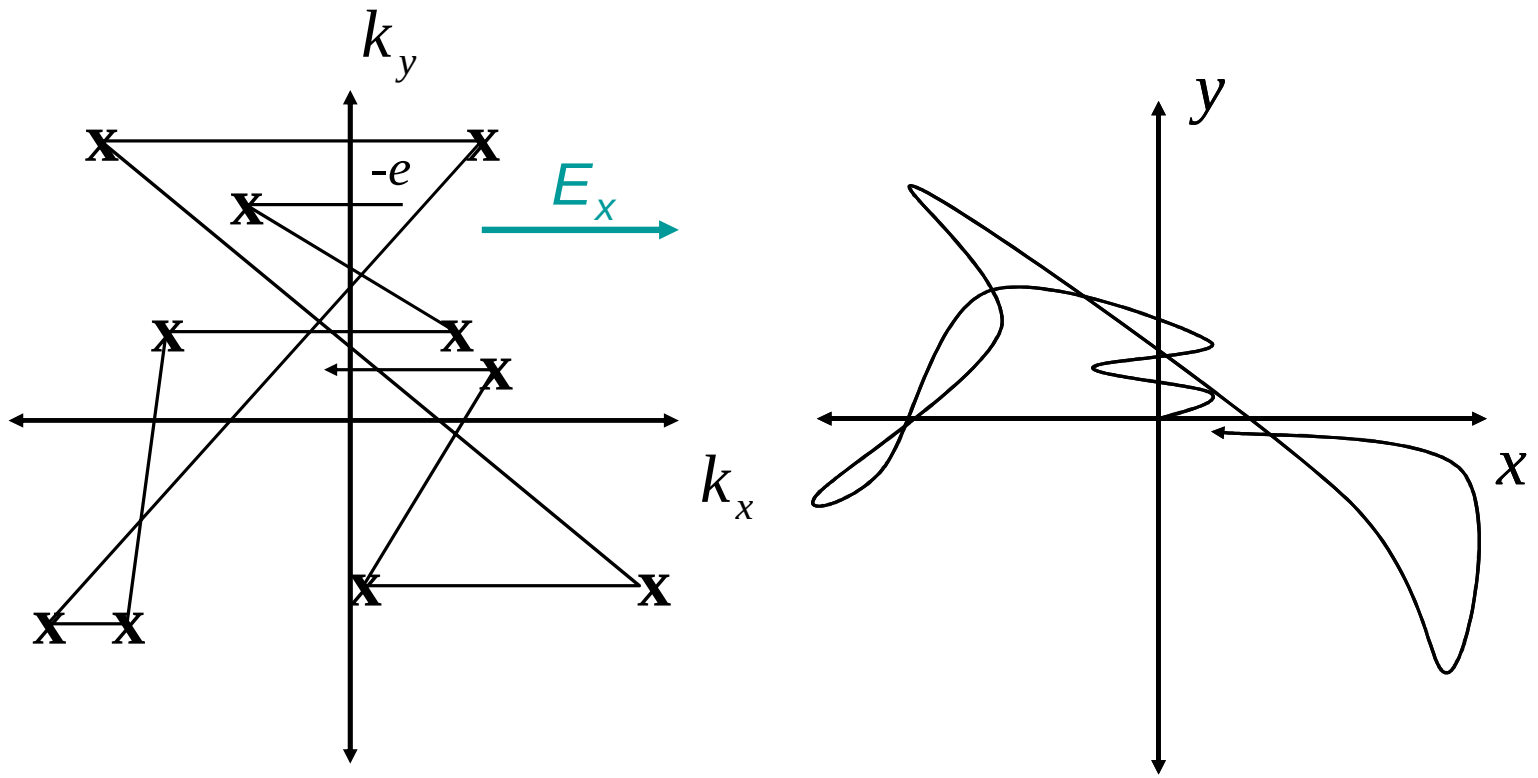
  – Instantaneous, memory-less, scattering events (Elastic, inelastic, intercarrier, electron-photon, etc.)

References:

1) C. Jacoboni and L. Reggiani, *Rev. Mod. Phys.* 55, no. 3, pp. 645-705, 1983

2) C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, 1990

Particle Trajectories in Phase Space



Particle trajectories in **k**-space and real space

Monte Carlo Integration

(M. H. Kalas and P. A. Whitlock, "Monte Carlo Methods," John Wiley, 1986)

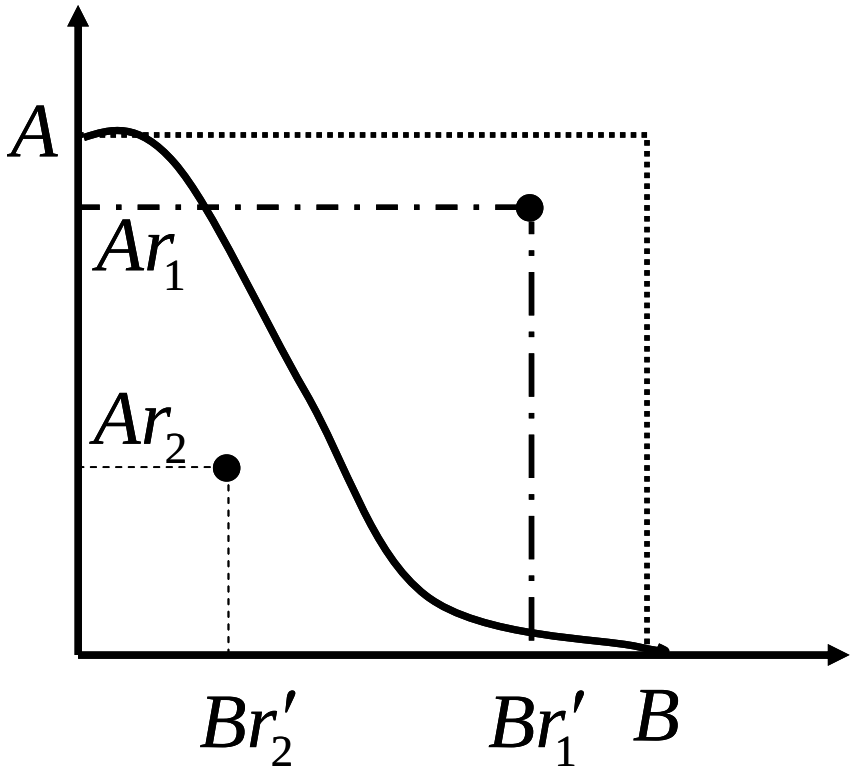
Suppose we want to integrate: $g(x) = Ae^{-(x/L)^2} \quad 0 < x < B$

Monte Carlo Algorithm:

- Define ceiling function
  $$g(x) = A$$
- Generate pairs of random numbers: r_1, r_1'

  If $Ar_1 > g(Br_1')$ *reject*
  If $Ar_2 < g(Br_2')$ *accept*

- Ratio of accepted to total times area *AB* is integral



Monte Carlo Algorithm

Typical algorithm for accomplishing this goal is:

```
acceptnum=0
do 10 i=1,nsampltot
        xval=rand( )*Bmax
        yval=rand( )*Amax
        gy=Amas*exp(-(xval/Lg)**2)
        if (gy.gt.yval) acceptnum=acceptnum+1
10     continue
area=Amax*Bmax*acceptnum/nsampltot
```

Here rand( ) is a generic call to a random number generator (either intrinsic or subroutine). Ideally it produces a uniformly distributed random number between 0 and 1

Monte Carlo Integration of a Function

Consider the integral

$$g = \int_a^b F(x)dx$$

A Monte Carlo approach uses random numbers, say 10 chosen in the interval

$$x_i \subset [a,b] \rightarrow x_i = a + r_i(b-a)$$
$$r_i \subset [0,1]$$

Then

$$g \cong (b-a)\frac{1}{10}\sum_{i=1}^{10} F(x_i)$$

Various weightings can be used (preferentially choose x_i in regions where *F* is large) to improve the estimate of *g*.

Direct Technique

- If *P*(r) is a uniform distribution between 0 and 1 then:

$$r = \int_0^r dr' P(r') = F = \int_a^{x_r} f(x)dx \,/\, \int_a^b f(x)dx$$

  where x_r is a random number sampled from $f(x)$. x_r is found by inverting this integration.

- Example, for constant $f(x)$ is given below:

$$r = (x_r - a)/(b-a) \quad or \quad x_r = a + r(b-a)$$

Rejection Technique

- For most cases of interest, the integral cannot be easily inverted. As in the case of Monte Carlo integration, a *rejection* technique may be employed.
- Choose a maximum value *C,* such that $C > f(x)$ for all x in the interval (a,b).
- As in the case of Monte Carlo integration, pairs of random numbers are chosen, one between *a* and *b*

$$x_1 = a + r_1(b - a)$$

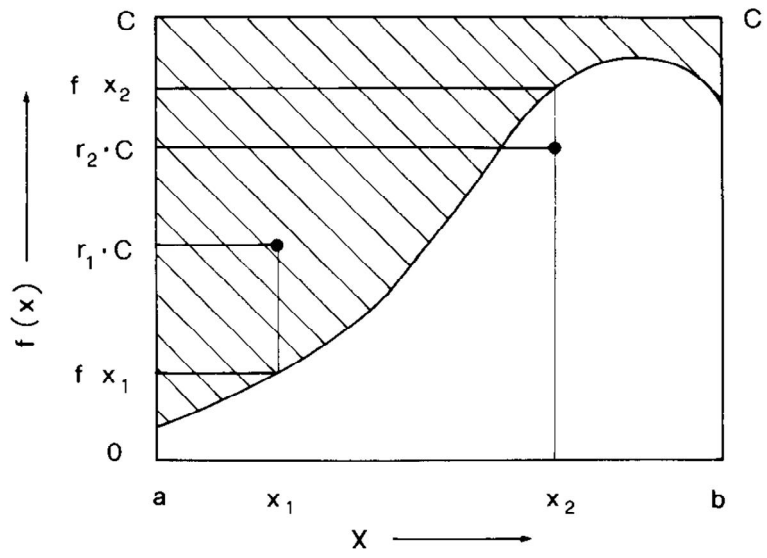
and another between 0 and *C* :

$$f_1 = r_1' C$$

- If

$$f_1 \le f(x_1)$$

the number x_1 is accepted as a suitable sample, otherwise it is rejected.



Combined Technique

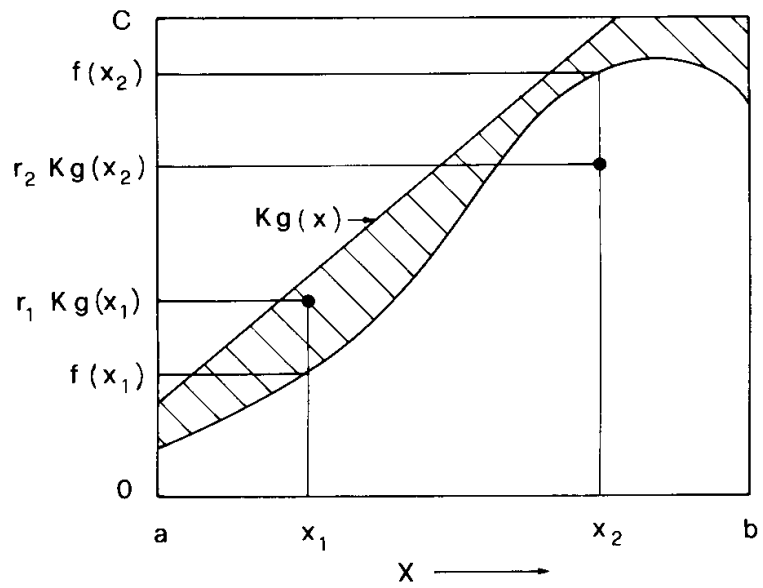
- If the probability function is singular in nature, the simple rejection technique with a constant ceiling function may be inefficient. If a ceiling function may be defined such that

$$Kg(x) \geq f(x)$$

over the range of interest, and random numbers may be sample from *g* using the direct technique, then a combined technique may be used, where if:

$$r_1 Kg(x_1) \leq f(x_1)$$

the random number x_1 is accepted.



Averages of important parameters are evaluated periodically by *ensemble averages*:

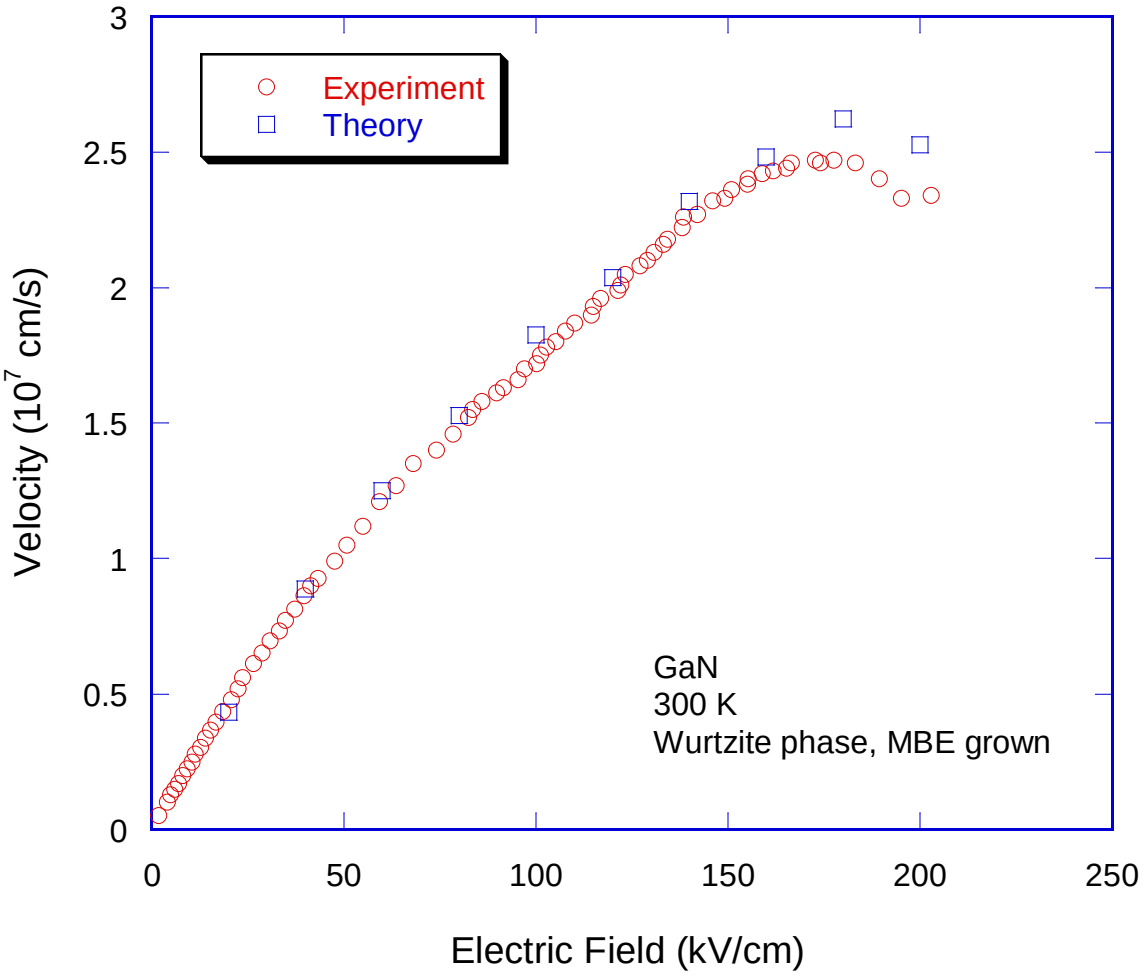
$$\langle A \rangle = \frac{1}{N} \sum_{i \subset N} A_i$$

This average *may* be position dependent:

$$\langle A(x) \rangle = \frac{1}{N(x)} \sum_{i \subset R(x)} A_i$$

The ensemble average evolves with time, and is the parametrically described *distribution function*.

Example: Velocity of Hot Carriers in GaN



The Monte Carlo simulation:

The weightings of initial distributions, and scattering processes assures that the ensemble evolves according to a master equation with collisions—the scattering probabilities provide the correct weightings for the collision integrals.

On the short-time basis, the proper equation is the Prigogine-Resibois equation (not the Boltzmann equation), but on the long-time limit, this evolves into the Boltzmann equation.

Monte Carlo Method Described

2. Generation of the random flight time

Generation of Random Flight Times

- The probability of an electron scattering in a small time interval *dt* is $\Gamma(\mathbf{k})dt$, where $\Gamma(\mathbf{k})$ is the *total* transition rate per unit time. Time dependence originates from the change in $\mathbf{k}(t)$ during acceleration by external forces

$$\mathbf{k}(t) = \mathbf{k}(0) - e(\mathbf{E} + \mathbf{v} \times \mathbf{B})t / \hbar$$

  where ***v*** is the velocity of the particle.

- The probability that an electron has not scattered after scattering at $t = 0$ is:

$$P_n(t) = e^{-\int_0^t dt' \Gamma(\mathbf{k}(t'))}$$

- It is this (unnormalized) probability that we utilize as a non-uniform distribution of *free flight times* over a semi-infinite interval 0 to ∞. We want to sample random flight times from this non-uniform distribution using uniformly distributed random numbers over the interval 0 to 1, corresponding to typical numerical random number generators.

Generation of Random Flight Times

Hence, we choose a random number

$$r_{i,1} = e^{-\int_0^t dt' \Gamma(\mathbf{k}(t'))}$$

***i*th particle** — **first random number**

We have a problem with this integral!

We solve this by introducing a new, fictitious scattering process which does not change energy or momentum:

$$\Gamma_{ss}(k) = \Gamma_S(E)\delta(\mathbf{x}' - \mathbf{x})\delta(\mathbf{k}' - \mathbf{k})$$

Generation of Random Flight Times

$$r_{i,1} = e^{-\int_0^t dt\,\Gamma(\mathbf{k}(t'))}$$

$$\Gamma(k) = \sum_i \Gamma_i(k)$$

The sum runs over all the real scattering processes. To this we add the fictitious self-scattering which is chosen to have a nice property:

$$\Gamma_{new} = \Gamma_0$$

$$\Gamma_{ss}(k) \equiv \Gamma_0 - \sum_{\substack{real \\ scatterers}} \Gamma_i(k)$$

Self-Scattering

- The use of the full integral form of the free-flight probability density function is tedious (unless **k** is invariant during the free flight).
- The introduction of *self-scattering* (Rees, *J. Phys. Chem. Solids* **30**, 643, 1969) simplifies the procedure considerably.
- The properties of the self-scattering mechanism are that it does not change either the energy or the momentum of the particle.
- The self-scattering rate adjusts itself in time so that the total scattering rate is constant. Under these circumstances, one has that:

$$\Gamma = \Gamma(\mathrm{k}(t)) + \Gamma_{self}(\mathrm{k}(t)) \qquad P(t)dt = \Gamma e^{-\int_0^t dt'\Gamma} dt = \Gamma e^{-\Gamma t} dt$$

Self-Scattering (cont'd)

- Random flight times t_r may be generated from $P(t)$ above using the direct method to get:

$$r = e^{-\Gamma t_r} \qquad t_r = -\frac{1}{\Gamma}\ln(1-r) = -\frac{1}{\Gamma}\ln(r)$$

  where r is a uniform random between 0 and 1 (and therefore r and 1-r are the same).

- Γ must be chosen (a priori) such that $\Gamma > \Gamma(\mathbf{k}(t))$ during the entire flight.

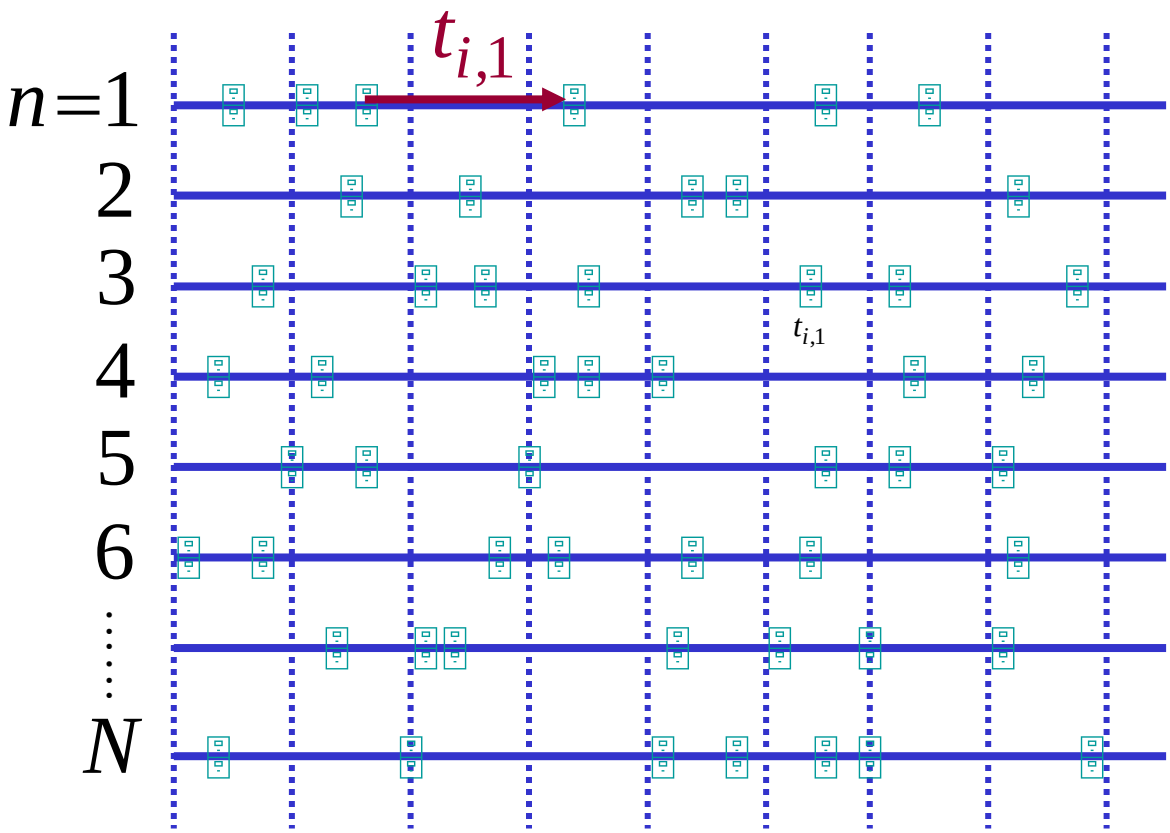
- Choosing a new t_r after every collision generates a random walk in k-space over which statistics concerning the occupancy of the various states **k** are collected.

Monte Carlo Method Described

3. Free-Flight Scatter Sequence

An ensemble Monte Carlo approach is used by considering *N* particles simultaneously

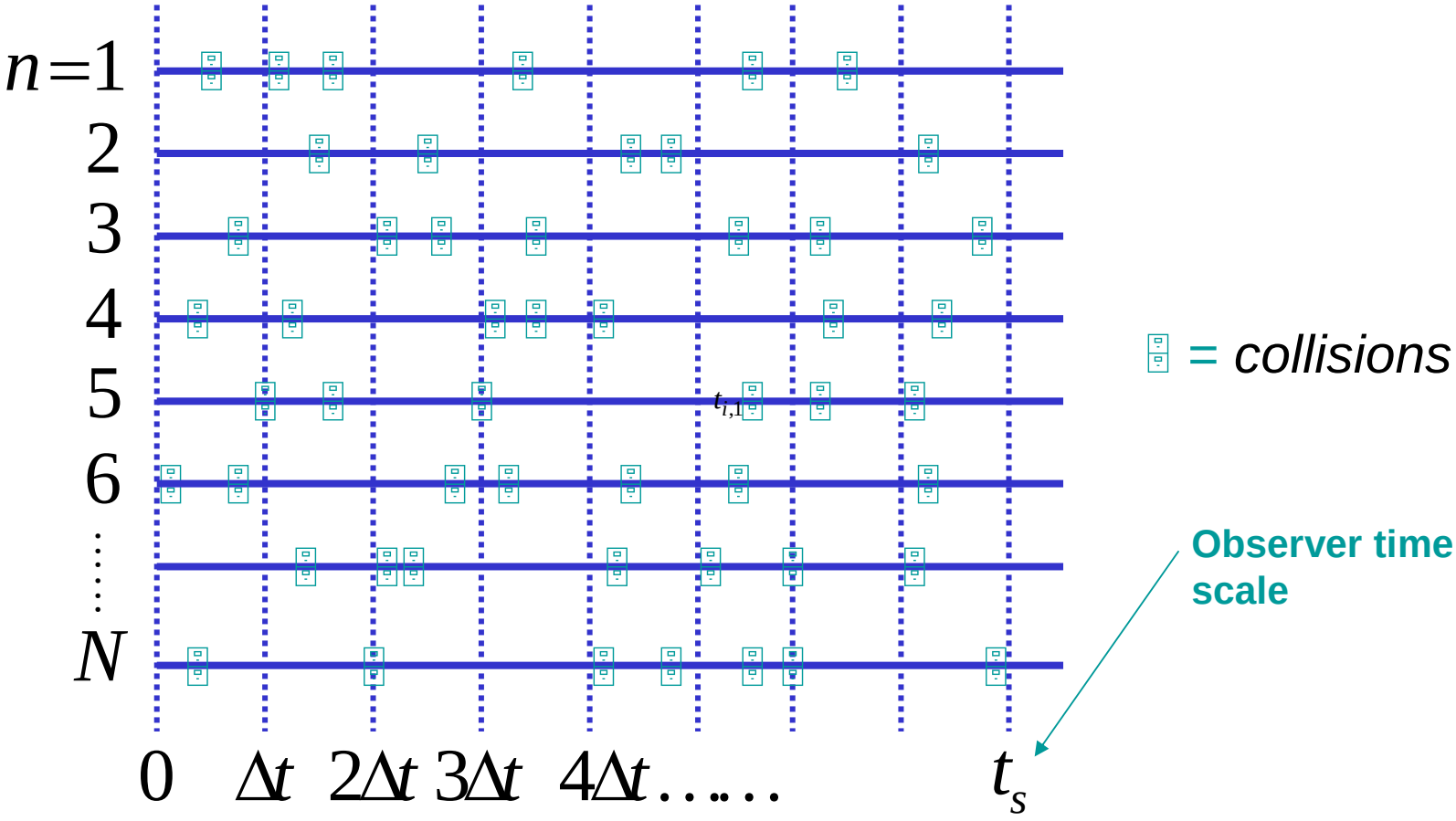
Particle time scale



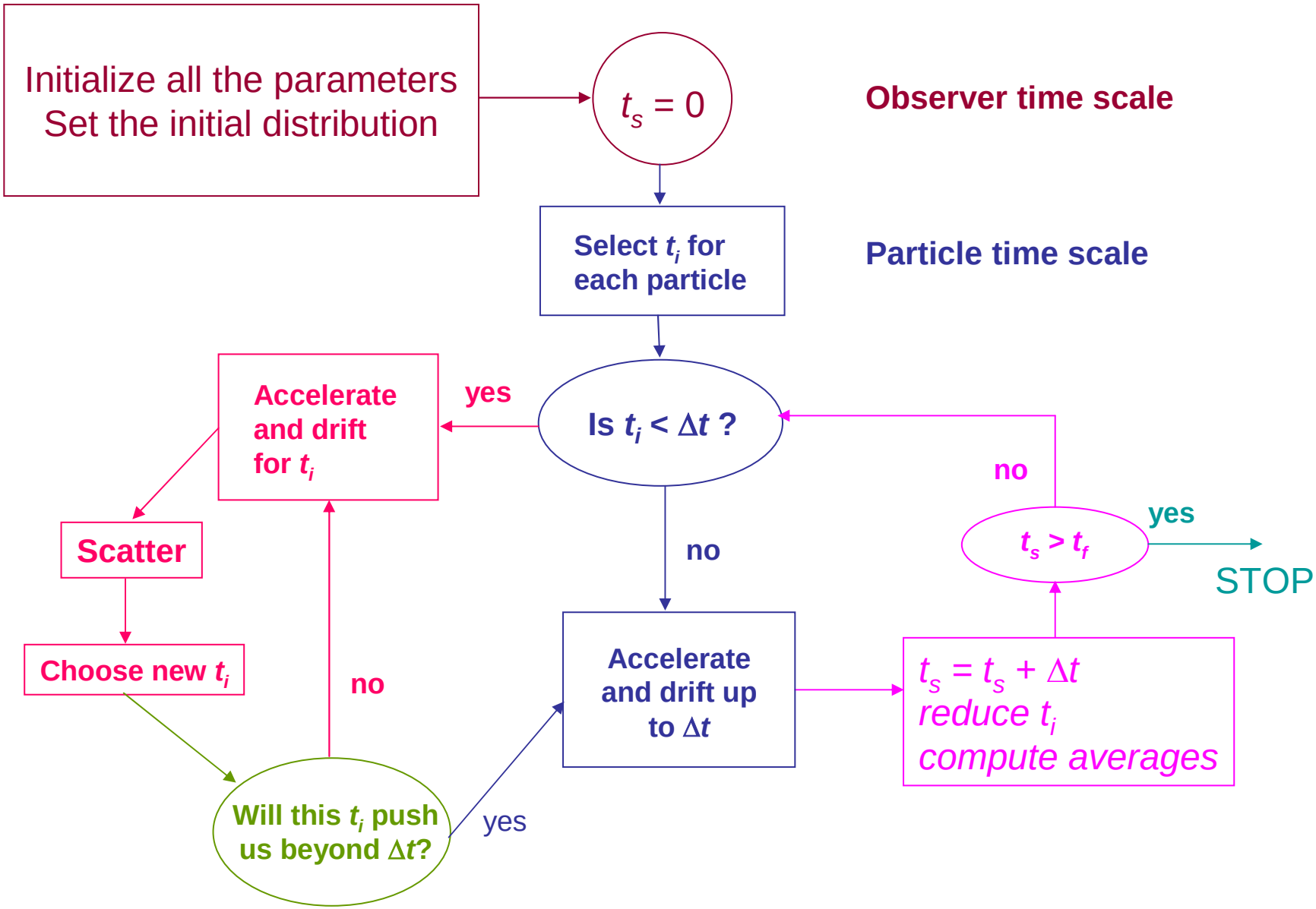
However, we need a second time scale, which provides the times at which the ensemble is "stopped" and averages are computed.

= *collisions*

An ensemble Monte Carlo approach is used by considering *N* particles simultaneously, and introducing a time step, Δt, at which the motion of all the particles is synchronized



In this approach, we will always reference t_i to the current time t_s.


Initialize all the parameters
Set the initial distribution
$t_s = 0$
Observer time scale
Select t_i for each particle
Particle time scale
Is $t_i < \Delta t$?
yes
Accelerate and drift for t_i
Scatter
Choose new t_i
Will this t_i push us beyond Δt?
no
yes
Accelerate and drift up to Δt
$t_s = t_s + \Delta t$
reduce t_i
compute averages
$t_s > t_f$
yes
STOP
no
no

$$\mathbf{k}(t_s + t_i) = \mathbf{k}(t_s) - (e\mathbf{E}/\hbar)t_i$$

Update position, energy

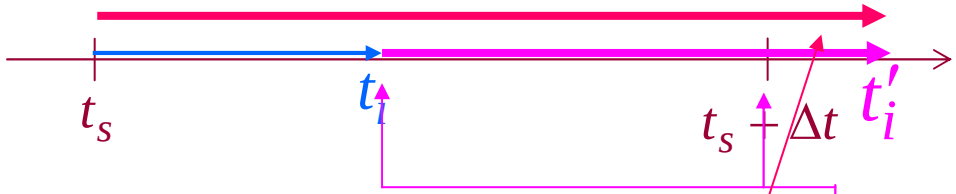
Scatter $\longrightarrow$ $\mathbf{k}'(t_s + t_i)$

$E(k')$

Choose a new t_i'

There are now 2 possibilities!

1



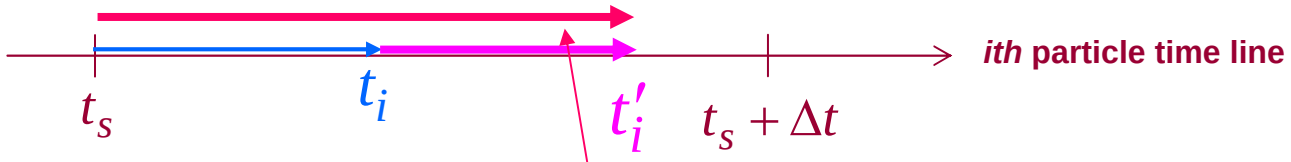
$$\mathbf{k}(t_s + \Delta t) = \mathbf{k}(t_s + t_i) - (e\mathbf{E}/\hbar)(\Delta t - t_i)$$

Update position, energy

$$new \quad t_i = t_{i,old} + t_i'$$

This keeps t_i referenced to the current time t_s.

2



$$\mathbf{k}(t_s + \Delta t) = \mathbf{k}(t_s + t_i) - (e\mathbf{E}/\hbar)t_i'$$

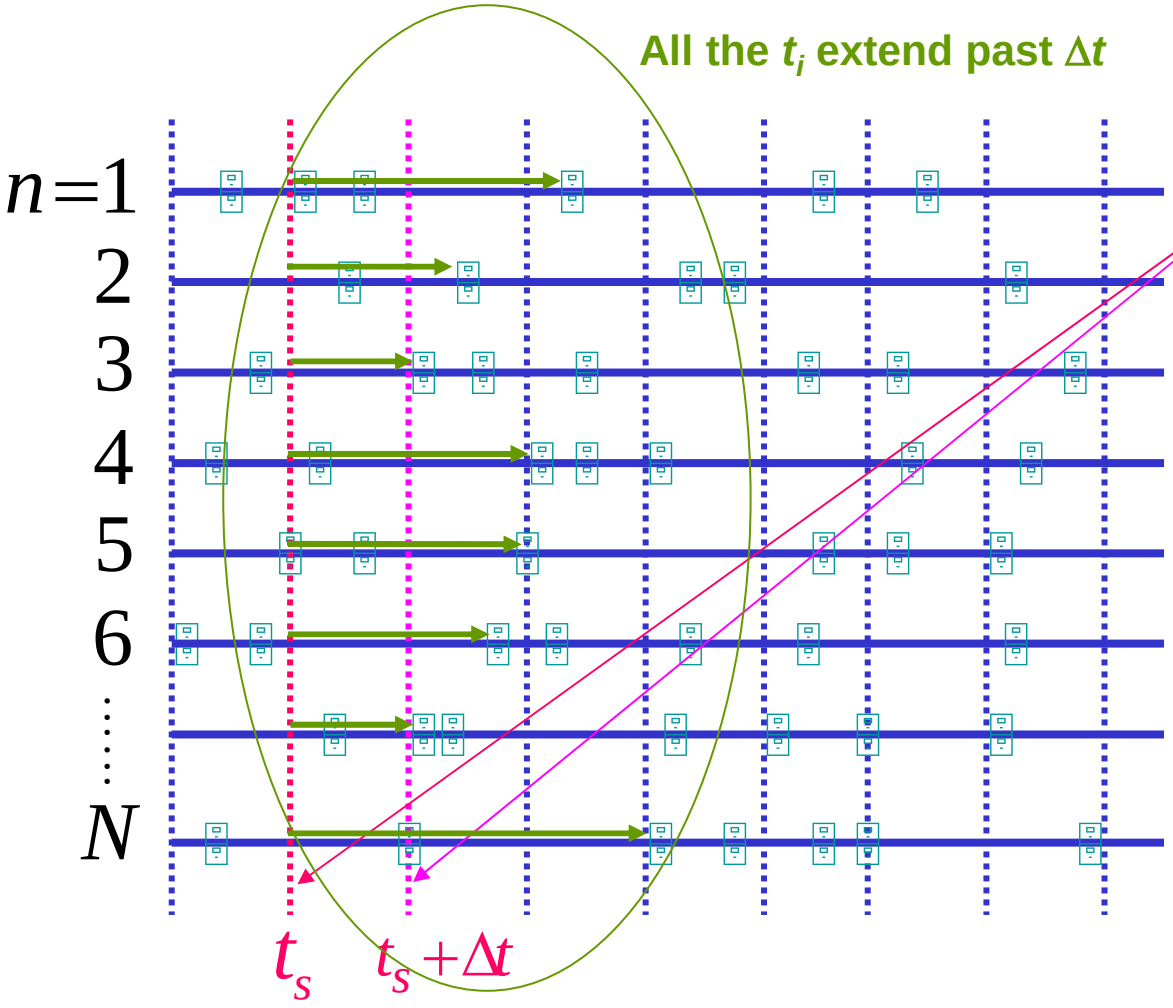
Update position, energy

$$new \quad t_i = t_{i,old} + t_i'$$

Return to Scatter process, which picks new

Scatter $\longrightarrow$ $\mathbf{k}'(t_s + t_i)$

$E(k')$

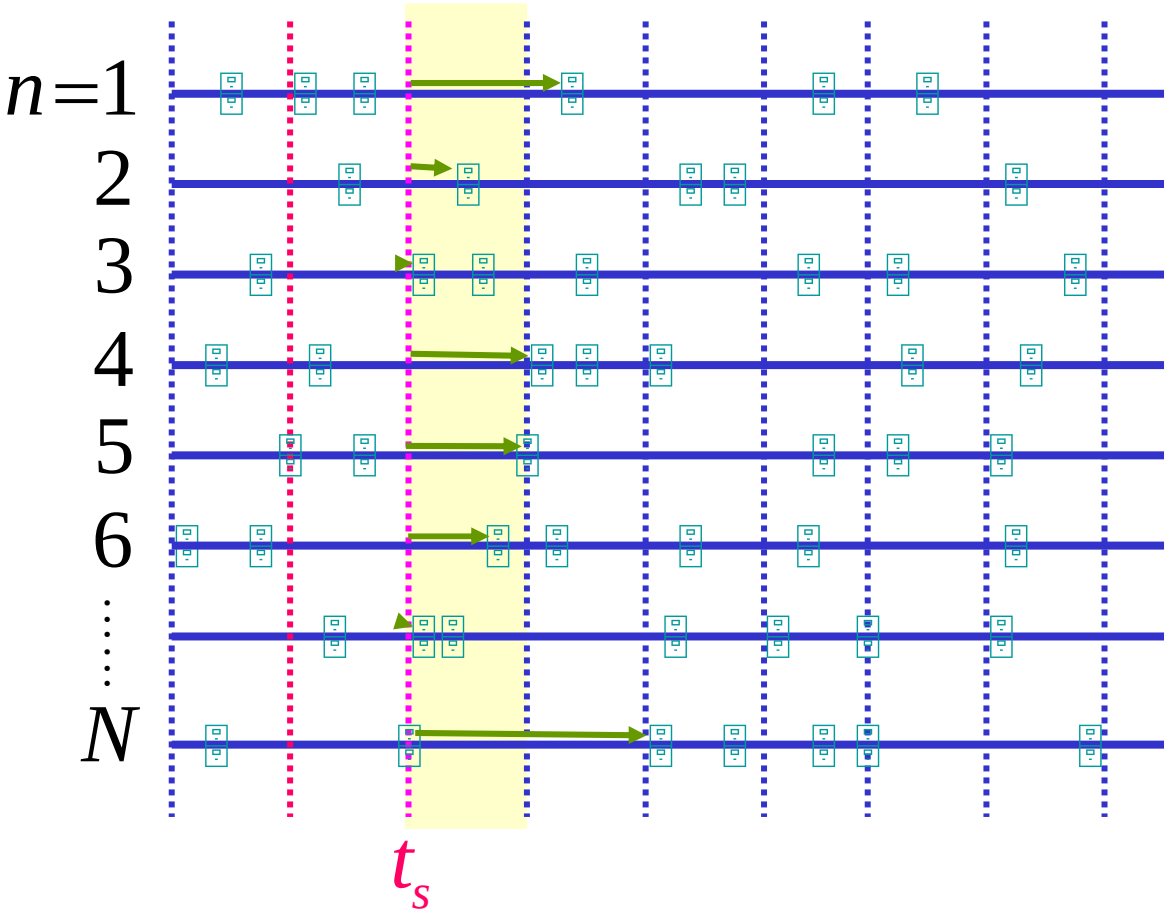


We update the reference time

$$t_s = t_s + \Delta t$$

We now have to change the reference point for the t_i

$$t_i = t_i - \Delta t$$



If our time has not yet finished, we can now return to the start of the scattering selection loop, examining the next increment of the reference time.

Before Returning to the Scattering Selection Loop
Compute the Averages

$$v_d(t_s) = \frac{\hbar}{N}\sum_{i=1}^{N}\frac{k_i(t_s)}{m_c\left(1+2E_i(t_s)/E_{gap}\right)}$$

$$x_{avg} = \frac{1}{N}\sum_{i=1}^{N} x_i(t_s)$$

$$E_{avg} = \frac{1}{N}\sum_{i=1}^{N} E_i(t_s)$$

Monte Carlo Method Described

4. Choice of the scattering terminating free-flight

Choice of Scattering Event Terminating Free Flight

- At the end of the free flight t_i, the type of scattering which ends the flight (either real or self-scattering) must be chosen according to the relative probabilities for each mechanism.

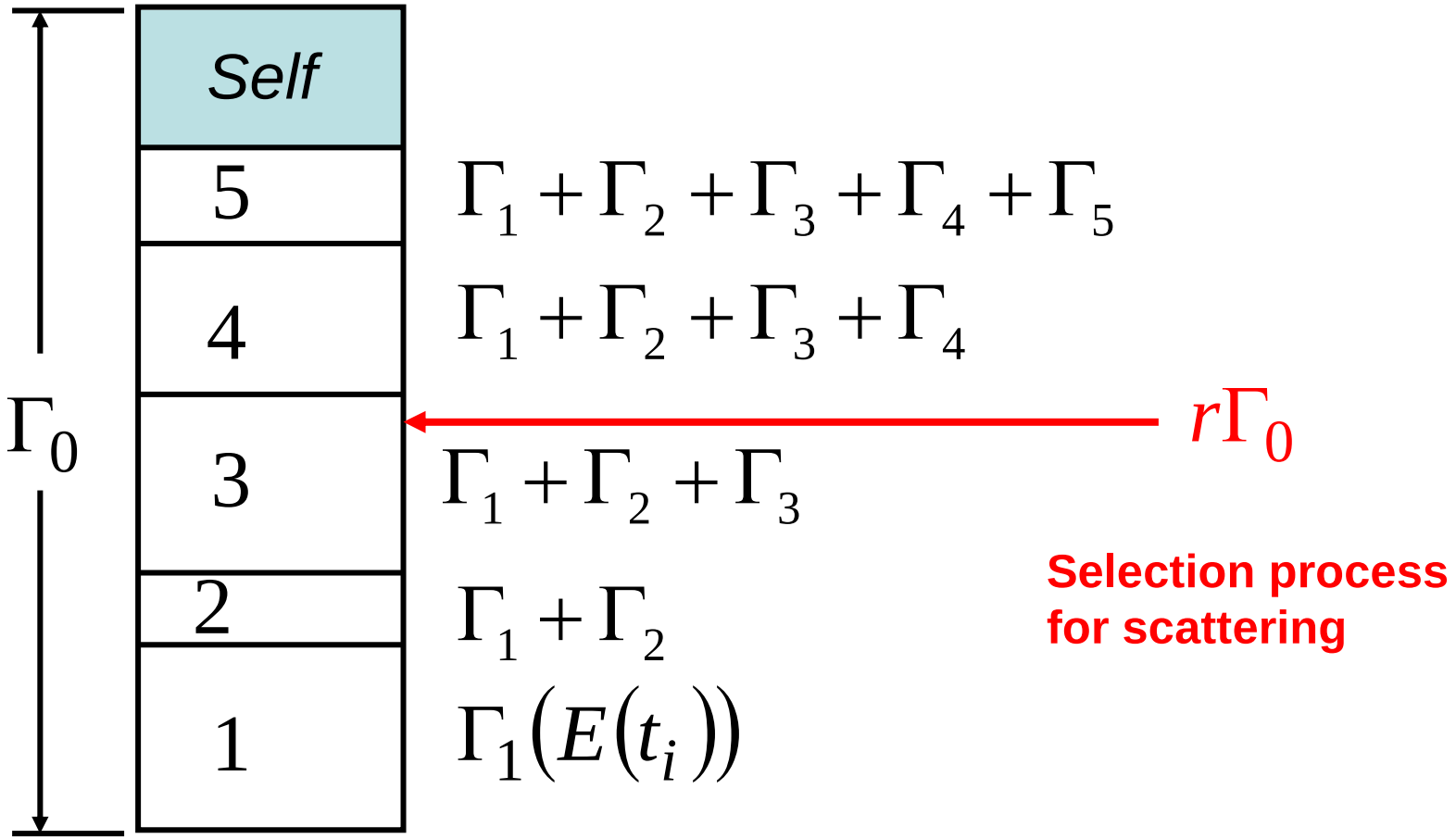
- Assume that the total scattering rate for each scattering mechanism is a function only of the energy, E, of the particle at the end of the free flight

$$\Gamma = \Gamma_{self}(E) + \Gamma_i(E) + \Gamma_{ac}(E) + \Gamma_{pop}(E) + \ldots$$

- where the rates due to the real scattering mechanisms are typically stored in a lookup table.

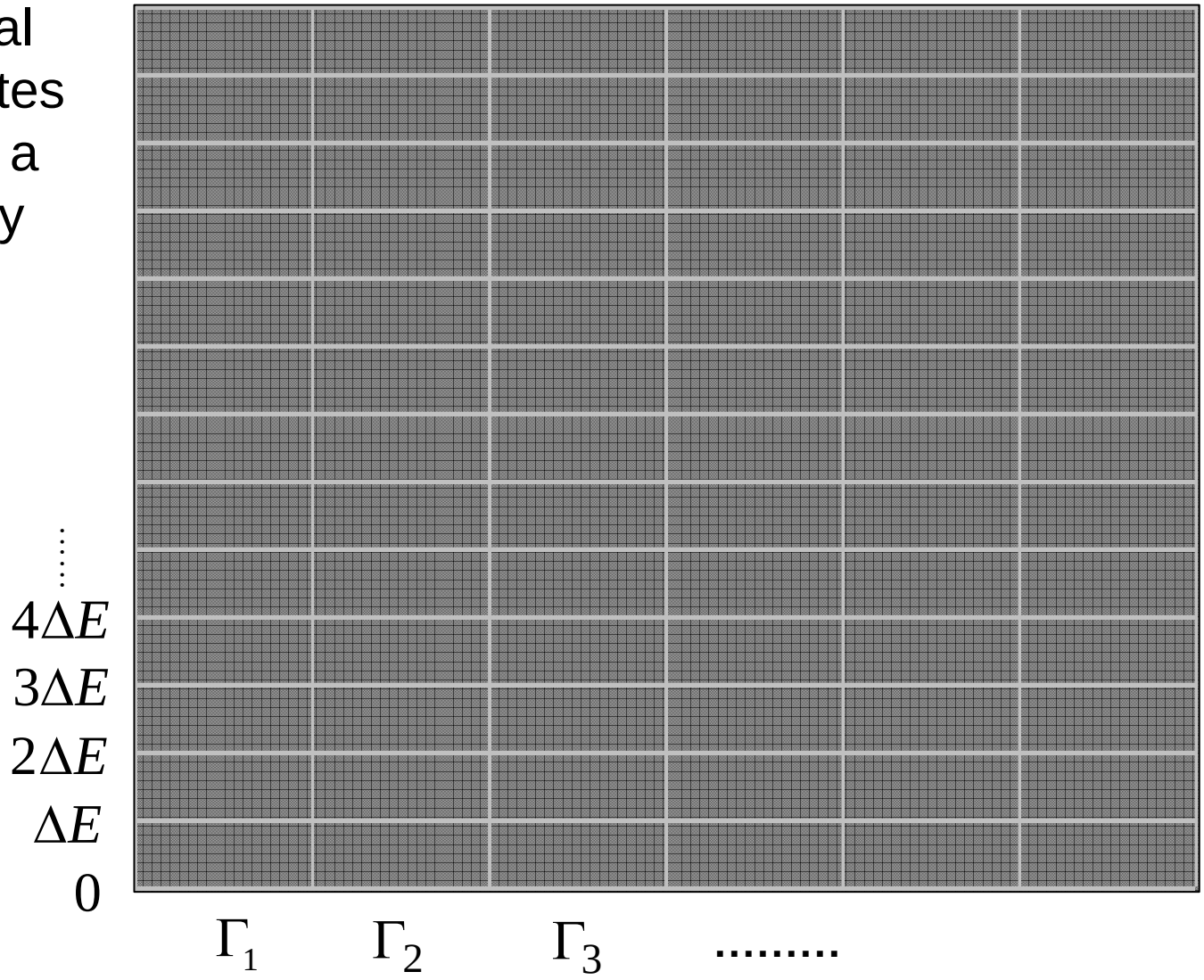
- A histogram is formed of the scattering rates, and a random number $r\Gamma$ is used as a pointer to select the right mechanism. This is schematically shown on the next slide.

We can make a table of the scattering processes at the energy of the particle at the scattering time:



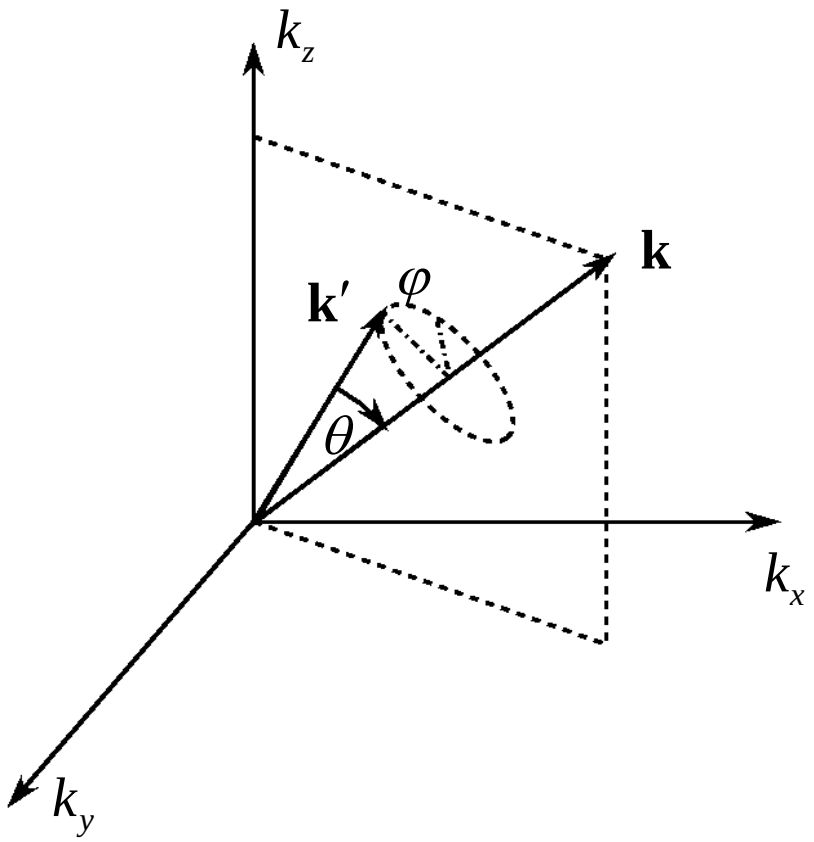
Look-up table of scattering rates:

Store the total scattering rates in a table for a grid in energy

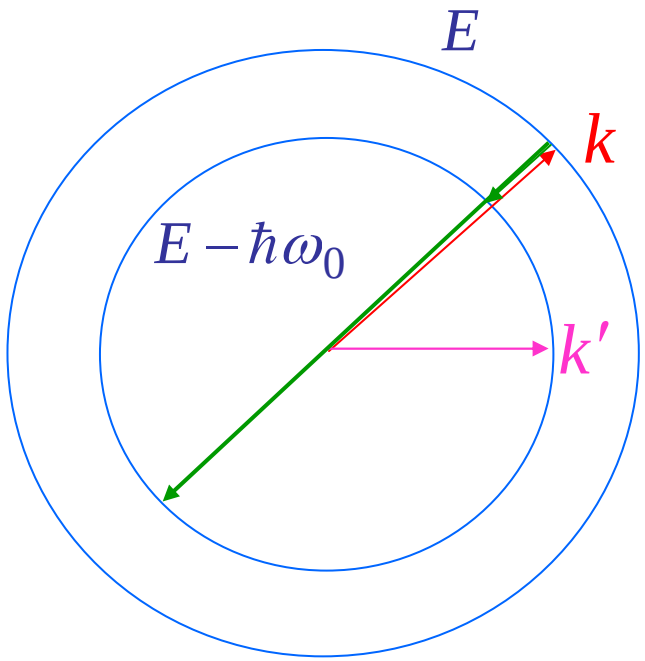


Once we have selected a scattering process, we must now find the final state of the carrier, after the scattering event:

- Final state energy E' is determined through conservation of energy.
- Azimuthal angle ϕ of **k** relative to **k** $'$ selected randomly between 0 and 2π.
- Polar angle θ is selected
  - according to the angular dependence of the scattering cross-section



Consider phonon emission



minimum *q*

$$q_{\min} = k - k'$$

maximum *q*

$$q_{\max} = k + k'$$

If the scattering is isotropic, any state on the final energy shell is equally likely, and θ is chosen randomly between 0 and π.

Coulomb Scattering is Anisotropic
(Polar LO phonons, impurities, carrier-carrier…)

$$P(\vartheta) \sim \frac{1}{q^2} = \frac{1}{\left|\mathbf{k}-\mathbf{k}'\right|^2}$$

$$= \frac{2m^*/\hbar^2}{E(k)+E(k')-\sqrt{E(k)E(k')}\cos\vartheta}$$

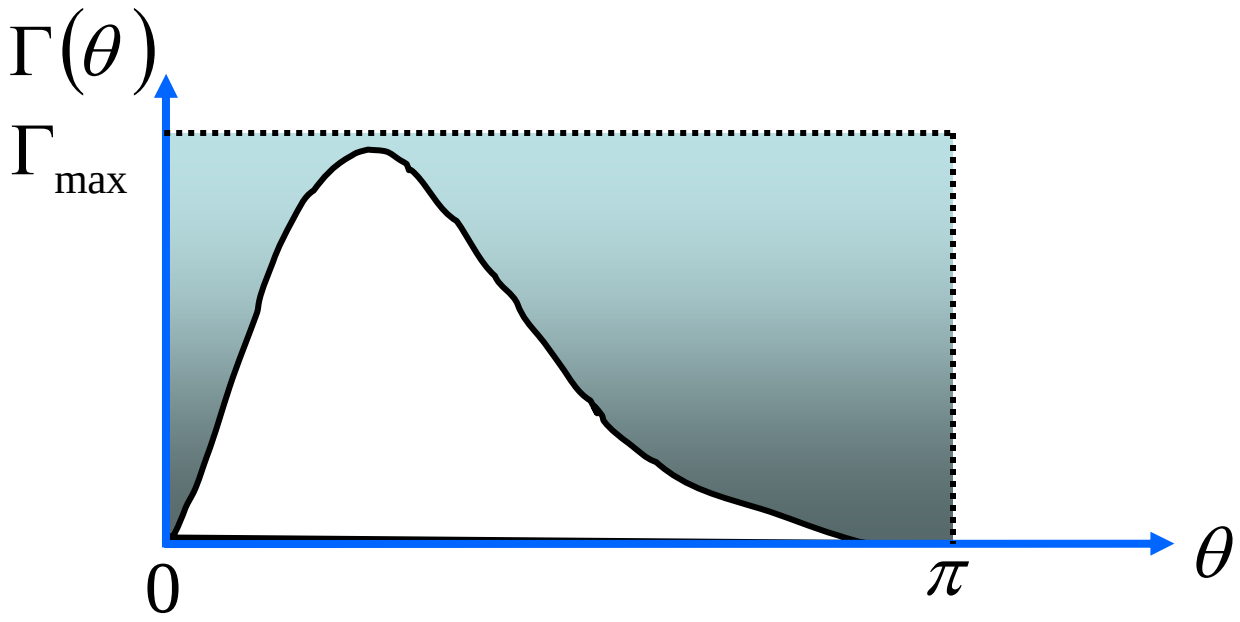
$$E(k') = E(k) \pm \hbar\omega_0$$

This assumes parabolic bands. For non-parabolic bands (hyperbolic bands), we make the replacement:

$$E(x) \rightarrow E(x)\left[1+2E(x)/E_{gap}\right]$$

Below is an example given for the choice of the polar angle for POP scattering:

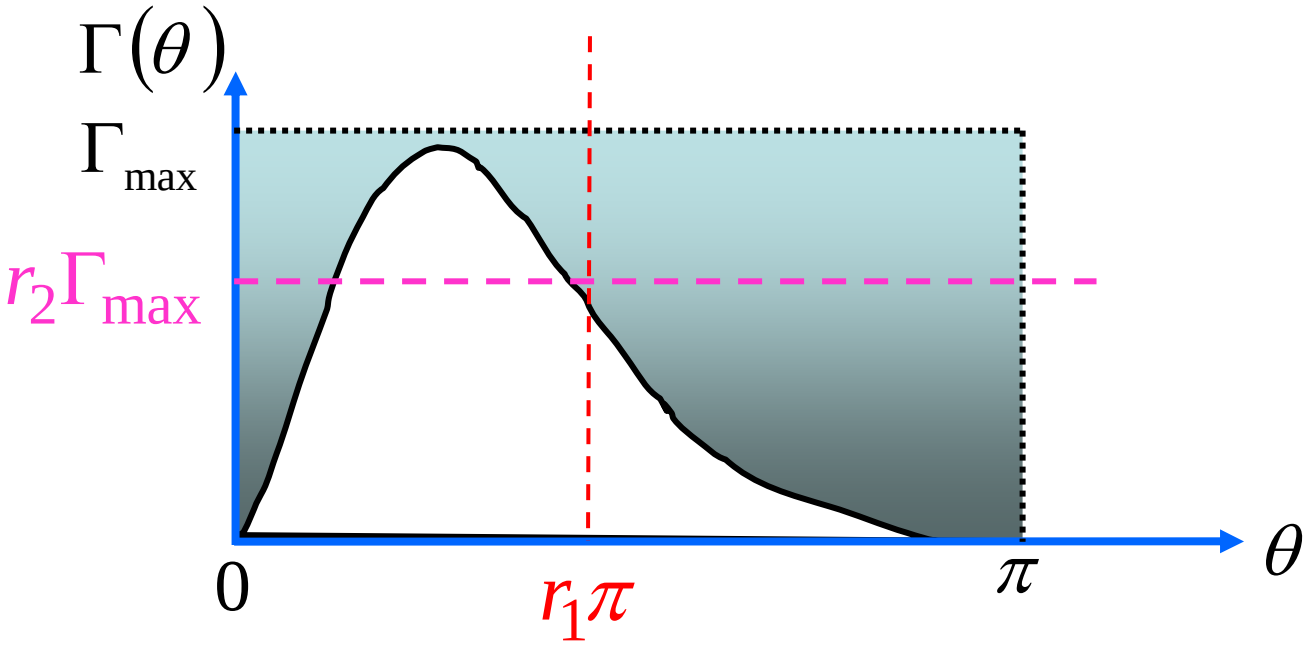
$$\Gamma_{POP}(\theta)d\theta \sim \frac{\sin(\theta)d\theta}{\left(E + E' - 2\sqrt{EE'}\cos\theta\right)}$$



We may find θ by two methods: (1) a rejection technique, or (2) direct integration.

Rejection Technique

We choose two new random numbers r_1 and r_2.



If $\Gamma(r_1\pi) > r_2\Gamma_{max}$, we accept the process with $\theta = r_1\pi$, otherwise we reject this angle and choose 2 new random numbers and try again.

Direct Integration for Inelastic Processes

$$r = \frac{\int_0^{\vartheta} \Gamma(\vartheta')\,d\vartheta'}{\int_0^{\pi} \Gamma(\vartheta')\,d\vartheta'} = \frac{\ln\left\{\dfrac{E(k)+E(k')-2\sqrt{E(k)E(k')}\cos\vartheta}{E(k)+E(k')-2\sqrt{E(k)E(k')}}\right\}}{\ln\left\{\dfrac{E(k)+E(k')+2\sqrt{E(k)E(k')}}{E(k)+E(k')-2\sqrt{E(k)E(k')}}\right\}}$$

$$\left\{\frac{E(k)+E(k')-2\sqrt{E(k)E(k')}\cos\vartheta}{E(k)+E(k')-2\sqrt{E(k)E(k')}}\right\} = \left\{\frac{E(k)+E(k')+2\sqrt{E(k)E(k')}}{E(k)+E(k')-2\sqrt{E(k)E(k')}}\right\}^{r}$$

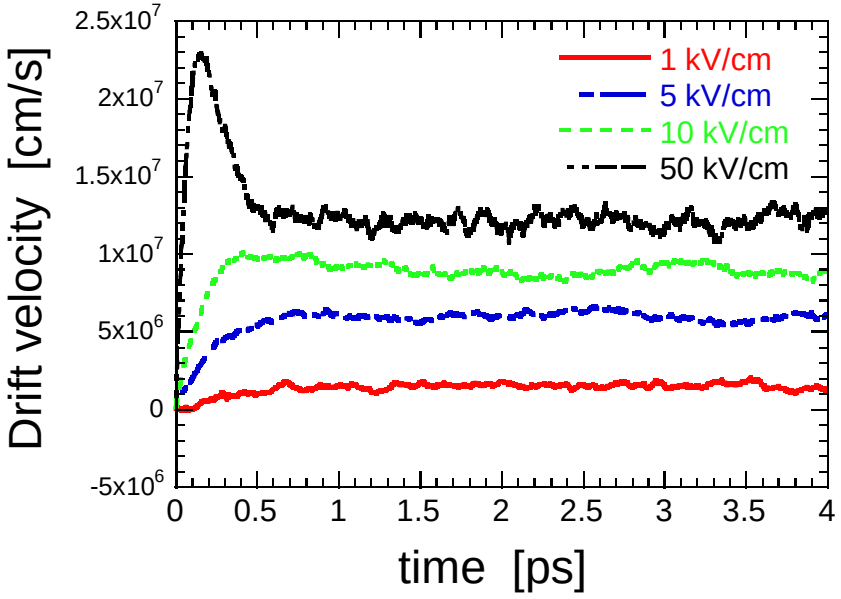
$$\cos\vartheta = \frac{(1+\xi)-(1+2\xi)^{r}}{\xi}$$

$$\xi = \frac{2kk'}{(k-k')^{2}} = \frac{2\sqrt{E(k)E(k')}}{E(k)+E(k')-2\sqrt{E(k)E(k')}}$$

Monte Carlo Method Described

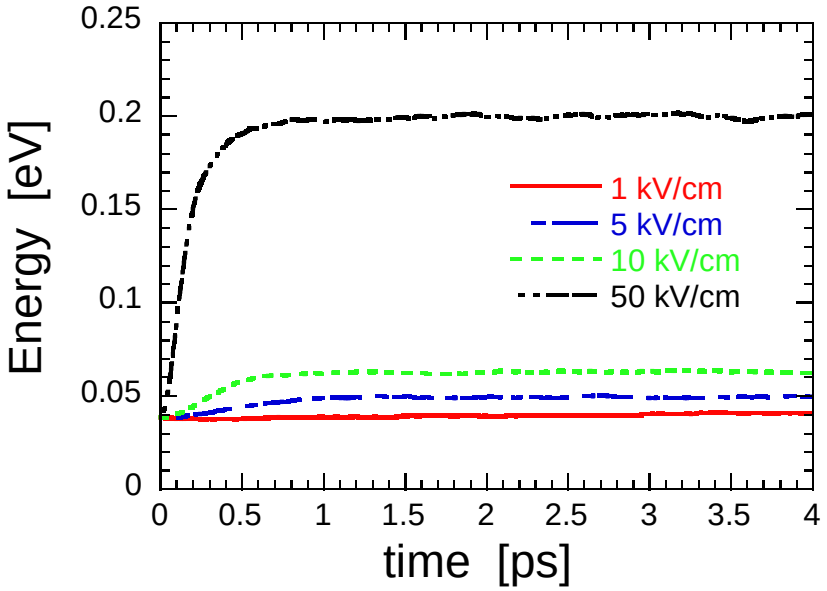
5. Representative Monte Carlo Results

Transient simulation results for Si

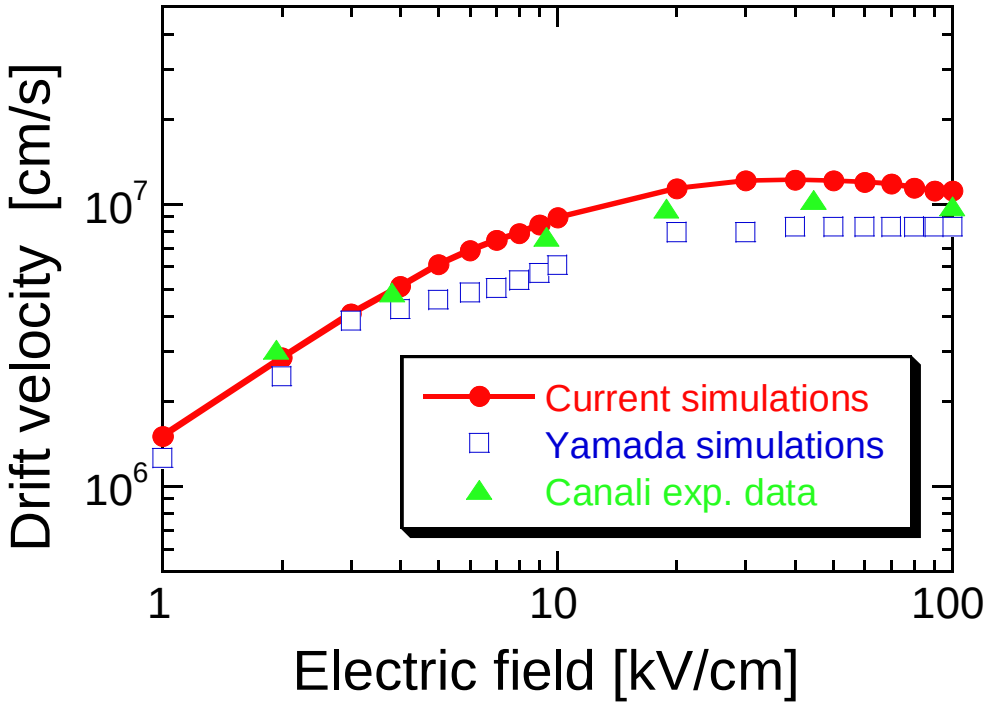


Time evolution of mean drift velocity. Electric field is: (a) 1.0 kV/cm, (b) 5.0 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.

Time evolution of the average electron kinetic energy. The electric field equals: (a) 1 kV/cm, (b) 5 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.



Steady-state simulation results for Si bulk



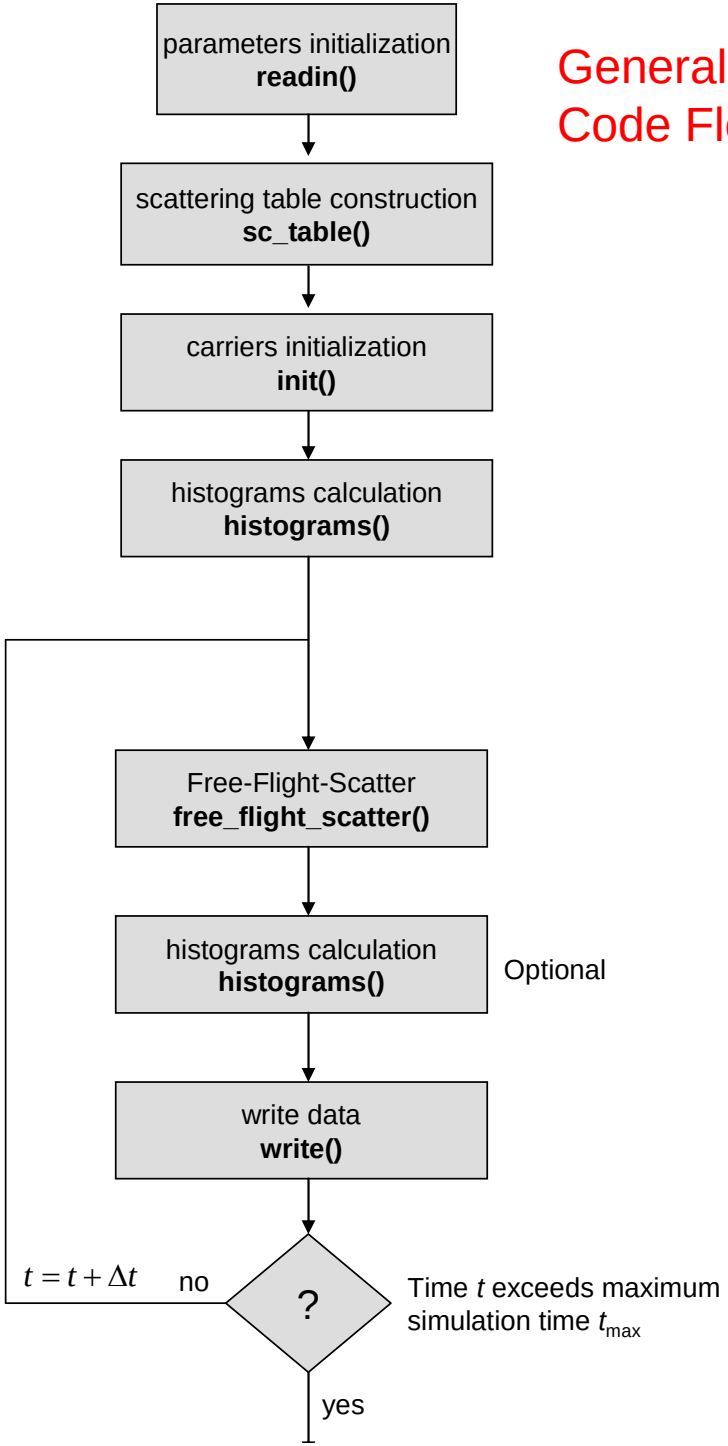
Mean drift velocity characteristics with respect to applied electric field. Also shown in this figure are the simulation results by Yamada *et al*. [1] and Canali [2] experimental data.

[1] T. Yamada, J.-R. Zhou, H. Miyata and D. K. Ferry, *Phys. Rev. B*, Vol. **49**, 1875 (1994).
[2] C. Canali, G. Ottaviani, and A. Alberigi-Quaranta, *J. Phys. Chem. Solids*, Vol. **32**, 1707 (1971).

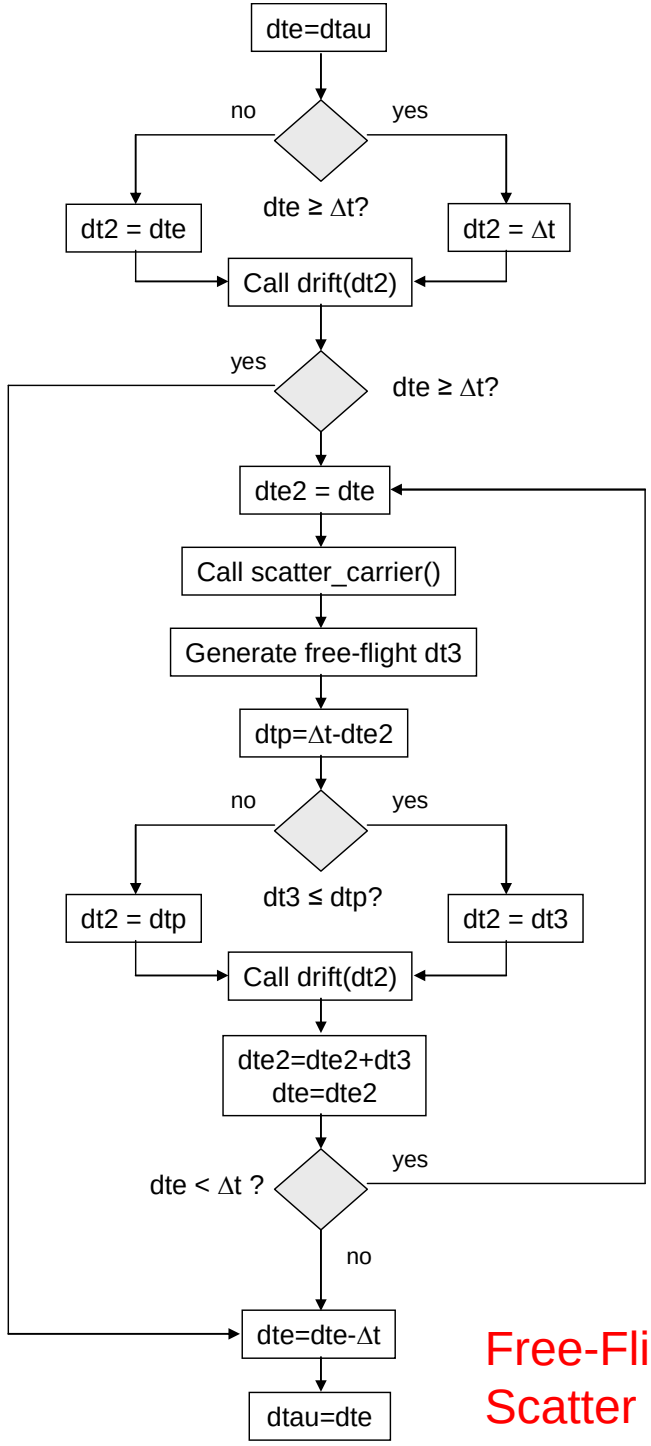
Monte Carlo Method Described

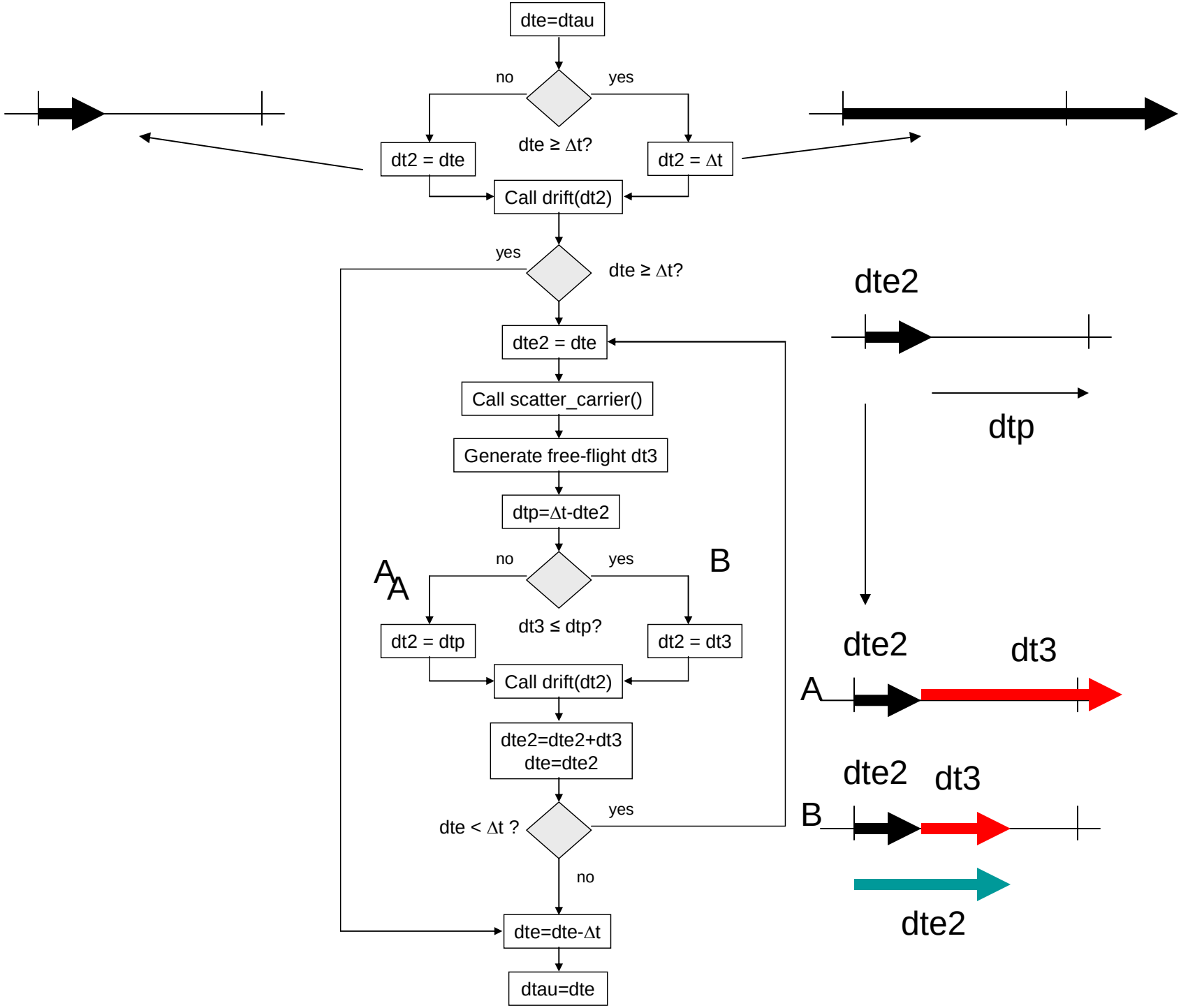
6. Code Details Description and Sample Simulation Results for GaAs

General Code Flowchart

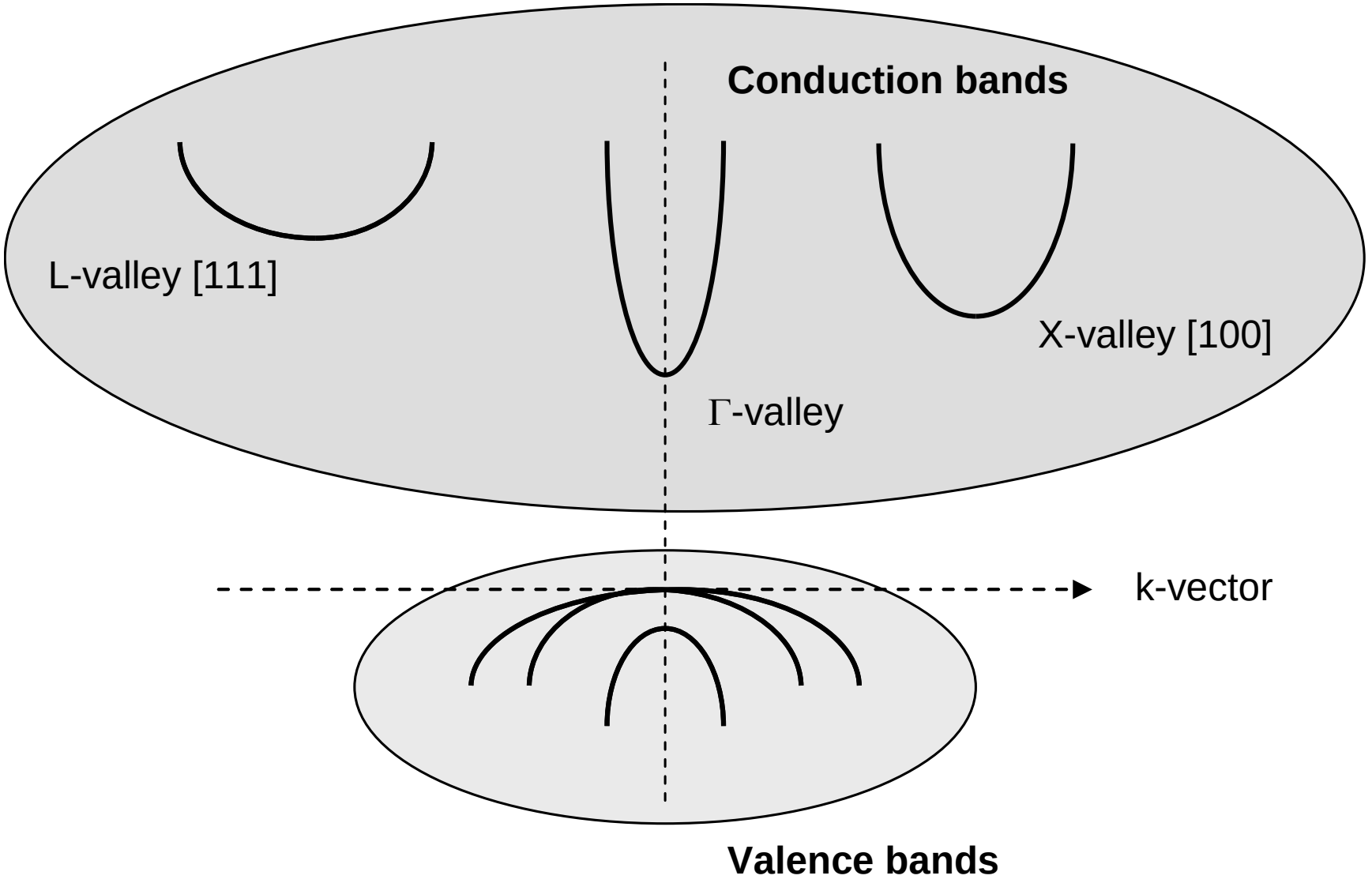


Free-Flight Scatter Routine

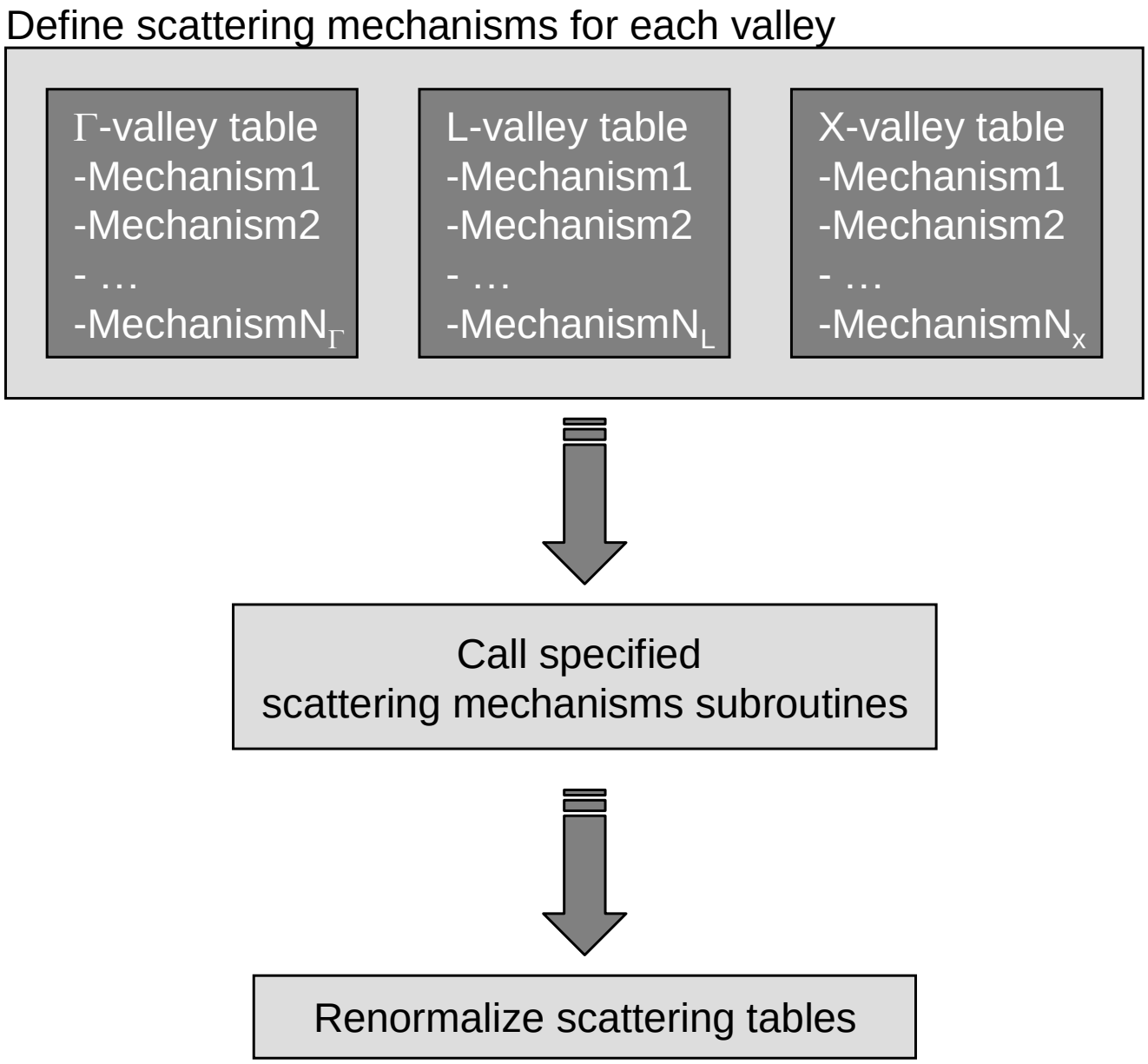


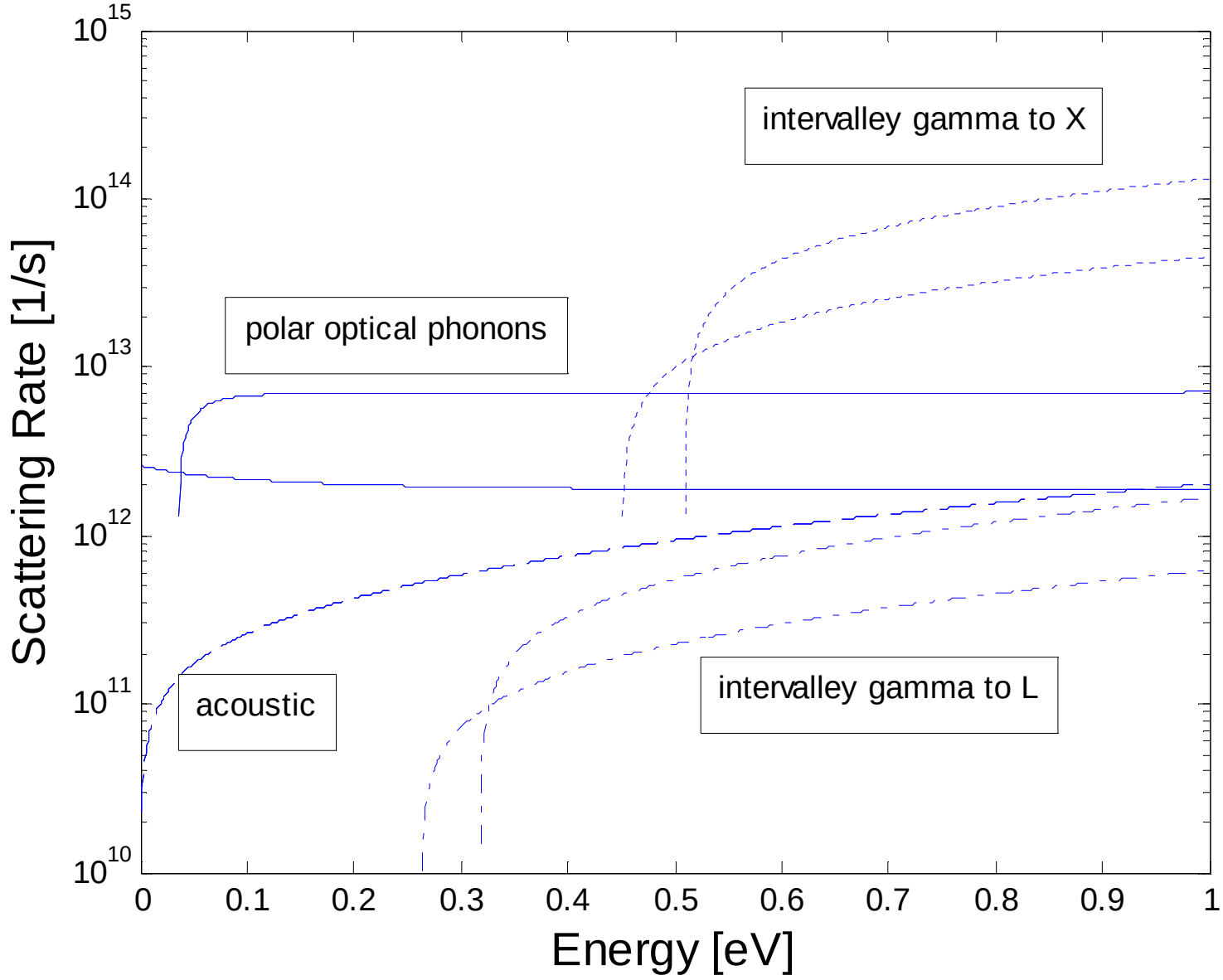

dte=dtau
no
yes
dte ≥ Δt?
dt2 = dte
dt2 = Δt
Call drift(dt2)
yes
dte ≥ Δt?
dte2 = dte
Call scatter_carrier()
Generate free-flight dt3
dtp=Δt-dte2
no
yes
A
A
B
dt3 ≤ dtp?
dt2 = dtp
dt2 = dt3
Call drift(dt2)
dte2=dte2+dt3
dte=dte2
dte < Δt ?
yes
no
dte=dte-Δt
dtau=dte
dte2
dtp
dte2
dt3
A
dte2
dt3
B
dte2

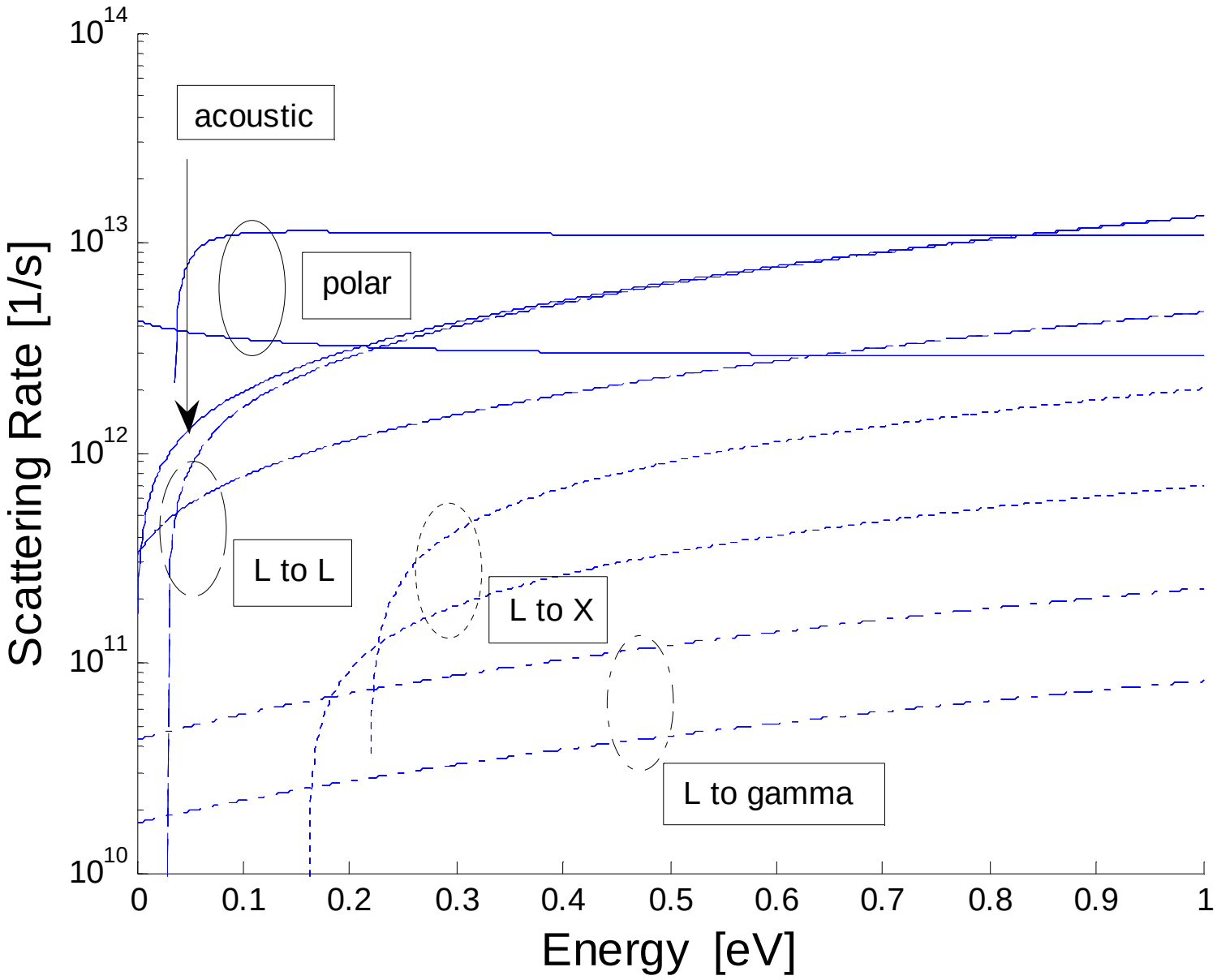
Model Bandstructure for GaAs

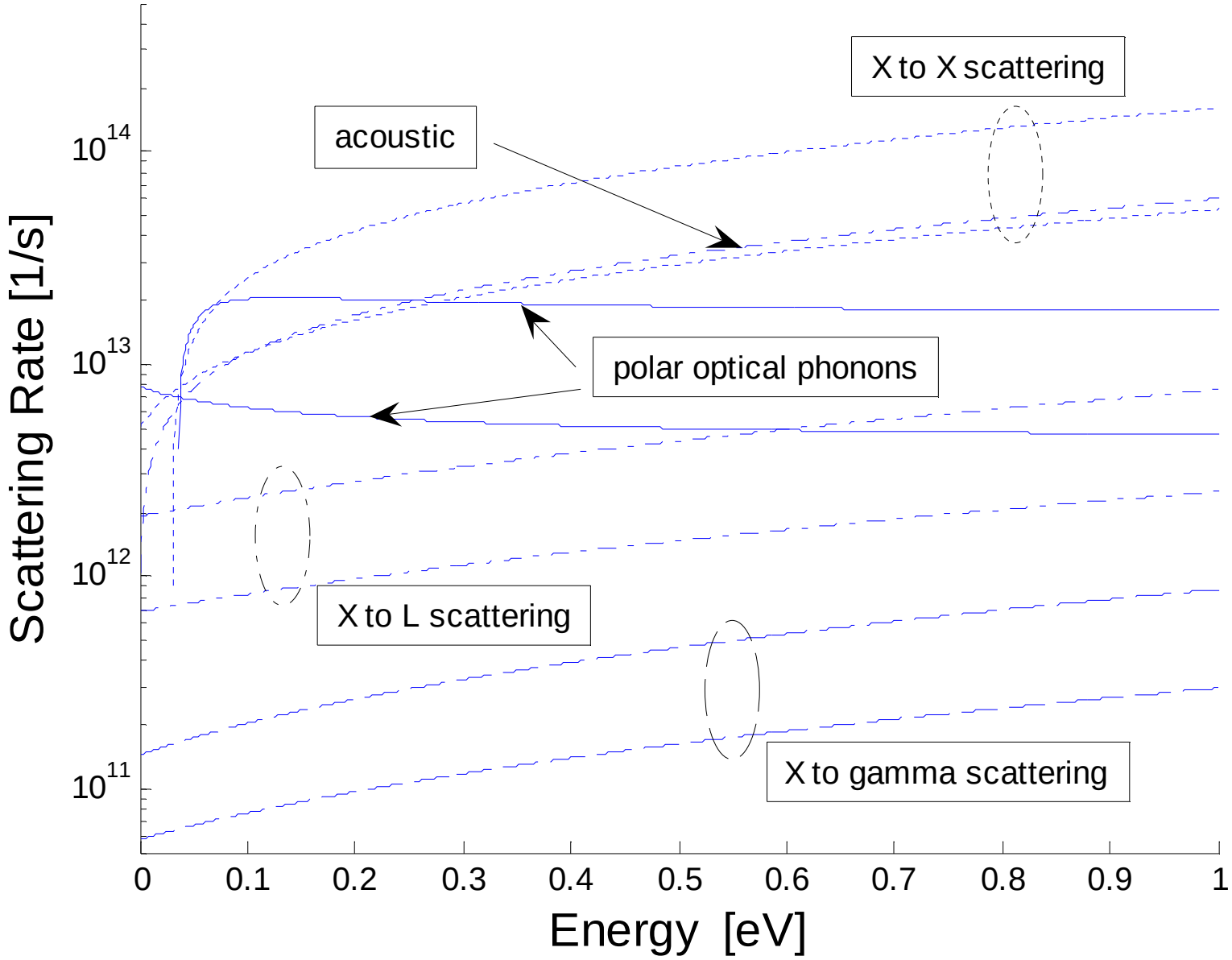


Scattering Tables Creation

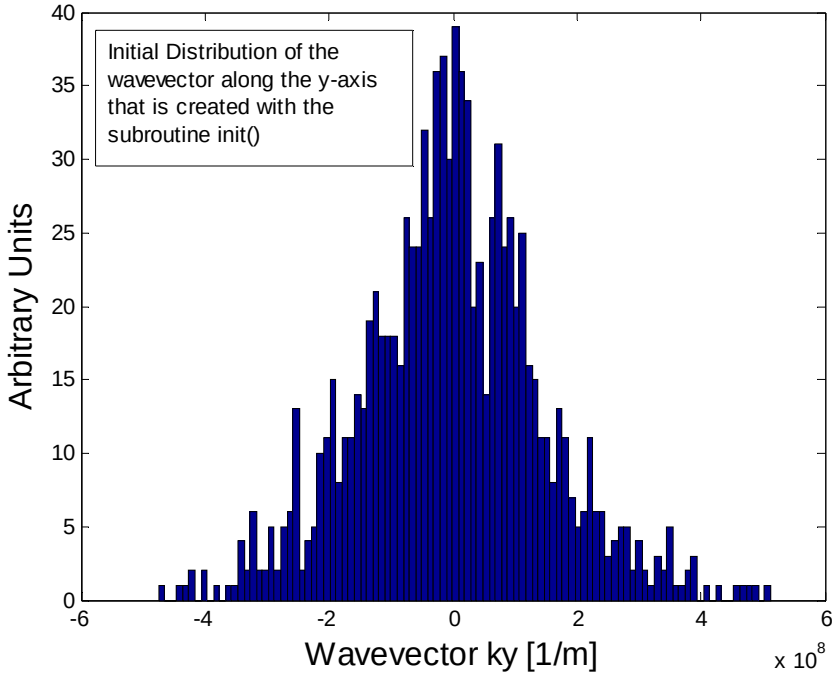


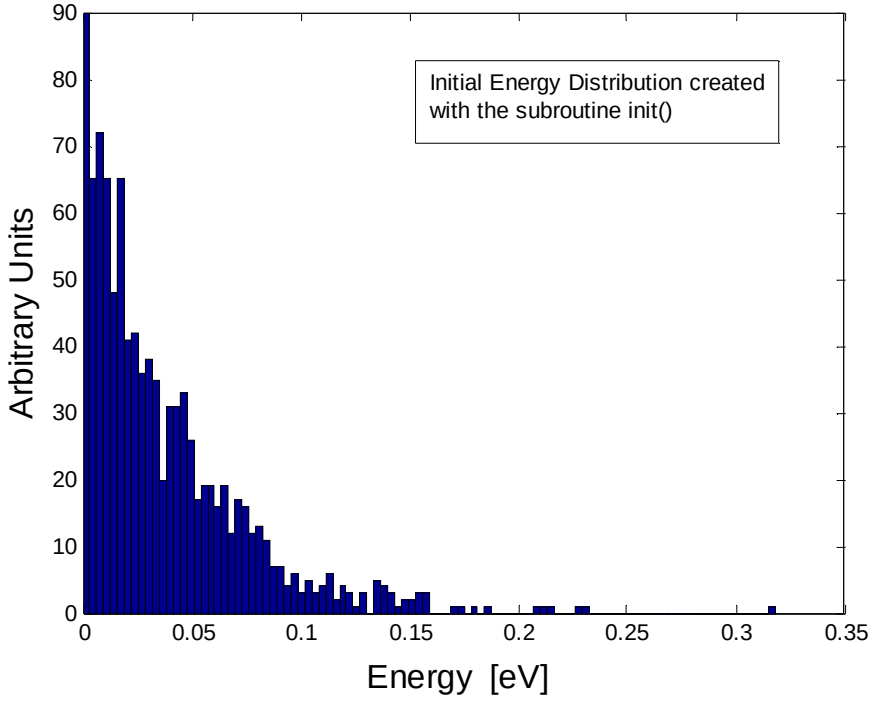

Scattering Rate [1/s]
10^{15}
10^{14}
10^{13}
10^{12}
10^{11}
10^{10}
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Energy [eV]
intervalley gamma to X
polar optical phonons
acoustic
intervalley gamma to L


Scattering Rate [1/s]
10^14
10^13
10^12
10^11
10^10
acoustic
polar
L to L
L to X
L to gamma
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Energy [eV]


X to X scattering
acoustic
polar optical phonons
X to L scattering
X to gamma scattering
Scattering Rate [1/s]
10^{14}
10^{13}
10^{12}
10^{11}
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Energy [eV]

Initial carrier wavevector and energy



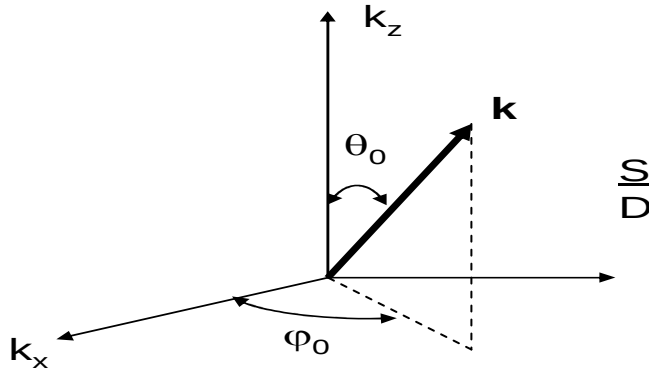



```
e = -(1.5*Vt)*log(ran(iso))
k=smh*sqrt(e*(1.+af*e))
fai=two_pi*ran(iso)
ct=1.-2.*ran(iso)
st=sqrt(1.-ct*ct)
kx=k*st*cos(fai)
ky=k*st*sin(fai)
kz=k*ct
```

1. Isotropic scattering processes

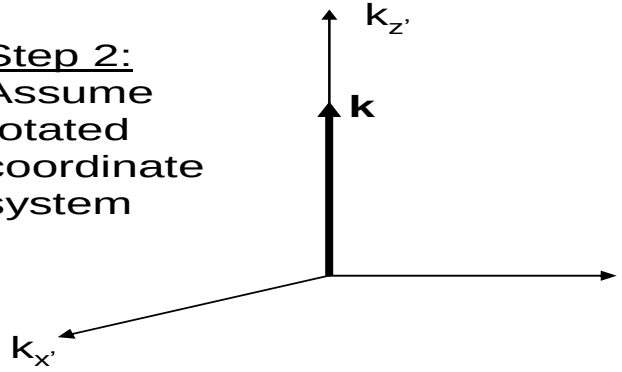
$$\cos\theta = 1 - 2r, \quad \varphi = 2\pi r$$

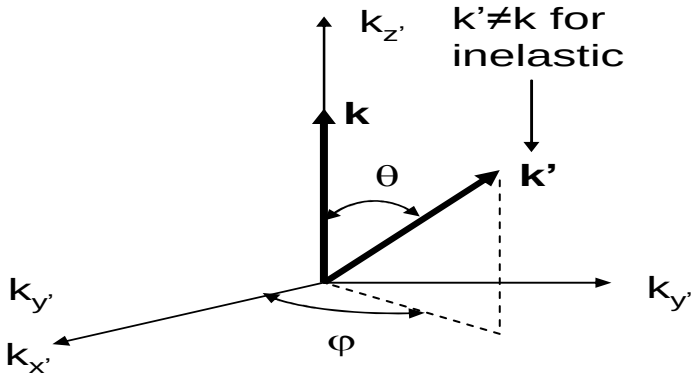
2. Anisotropic scattering processes (Coulomb, POP)



Step 1:
Determine θ_o and φ_o

Step 2:
Assume rotated coordinate system





Step 3:
perform scattering

$$\cos\theta = \frac{(1+\xi) - (1+2\xi)^r}{\xi}, \quad \xi = \frac{2\sqrt{E_k(E_k \pm \hbar\omega_0)}}{\left(\sqrt{E_k} - \sqrt{E_k \pm \hbar\omega_0}\right)^2} \quad \text{POP}$$

$$\cos\theta = 1 - \frac{2r}{1 + 4k^2 L_D^2 (1-r)} \quad \text{Coulomb}$$

$\varphi=2\pi r$ for both

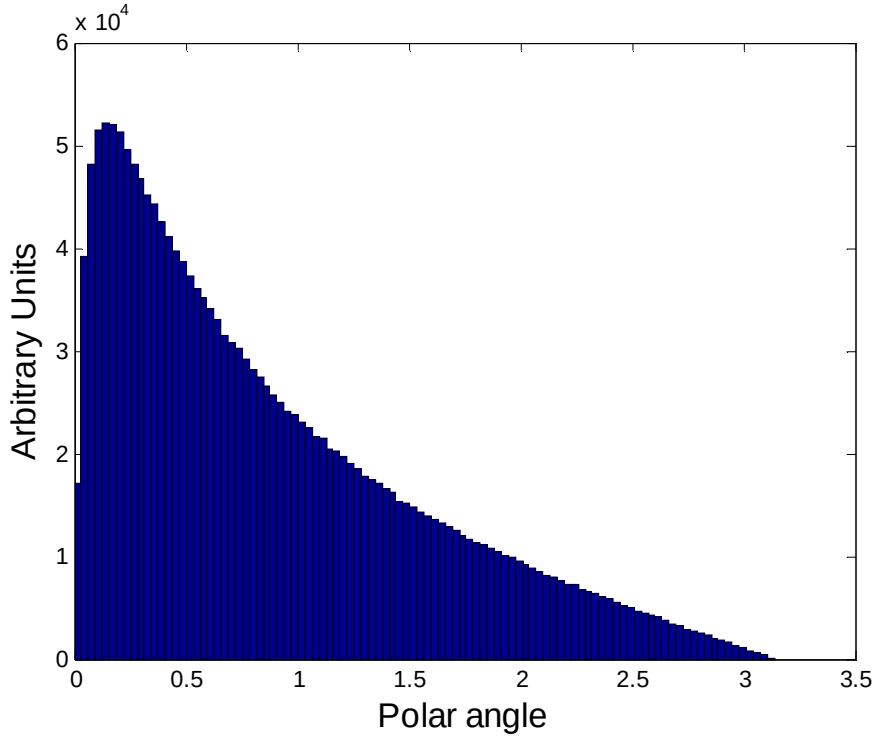
Step 4:

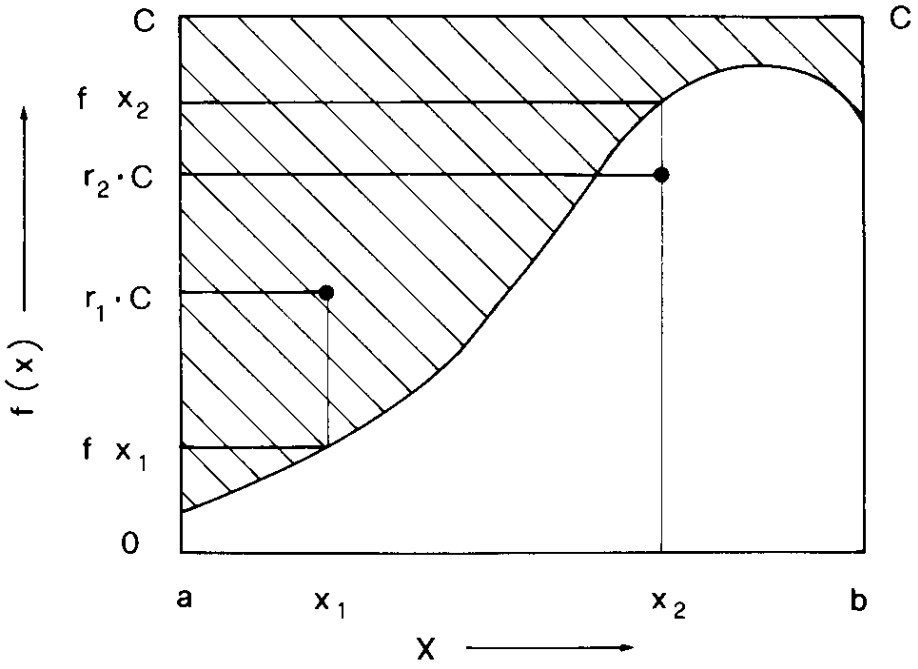
$k_{xp} = k'\sin\theta\cos\varphi$, $k_{yp} = k'\sin\theta*\sin\varphi$, $k_{zp} = k'\cos\theta$

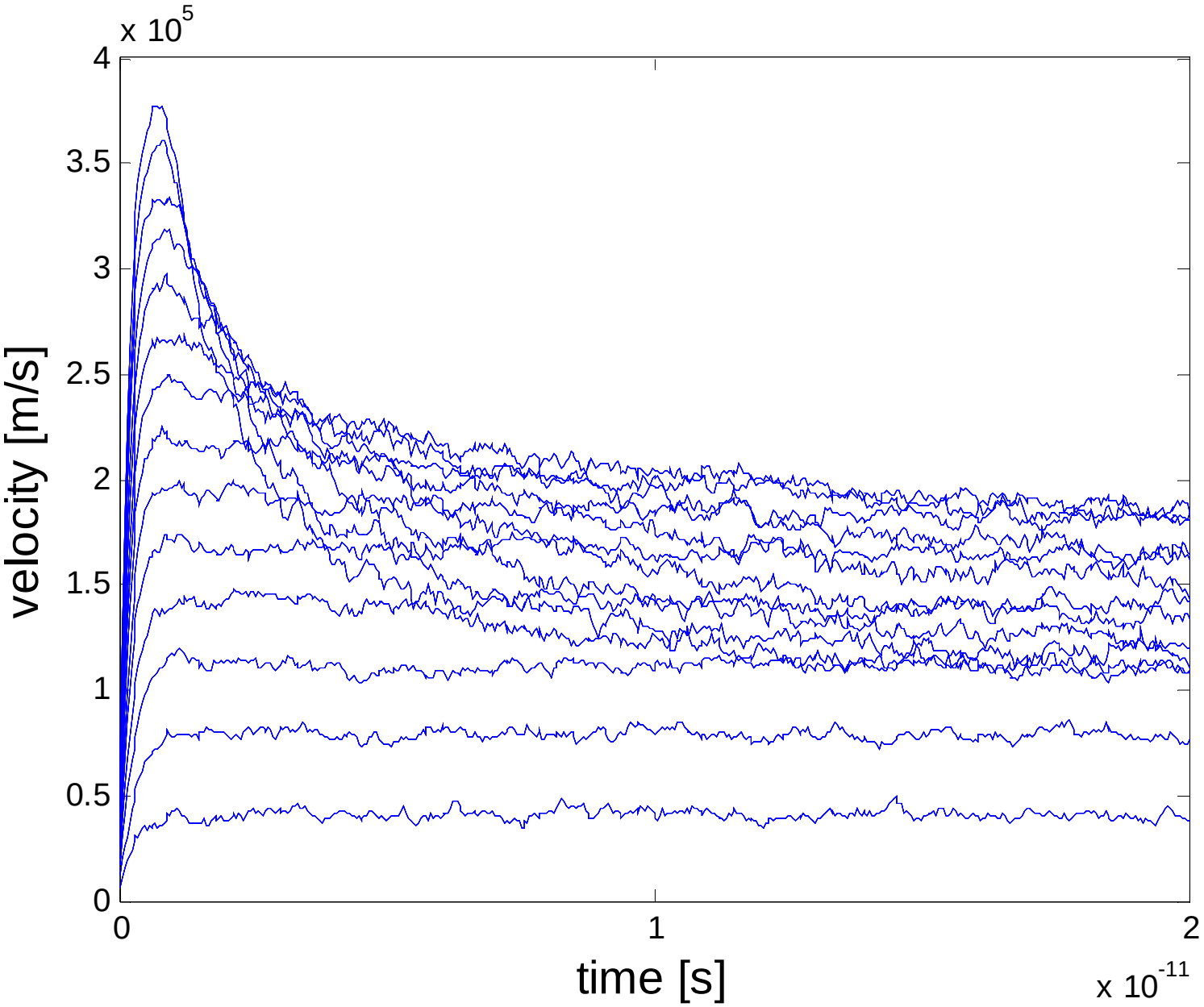
Return back to the original coordinate system:

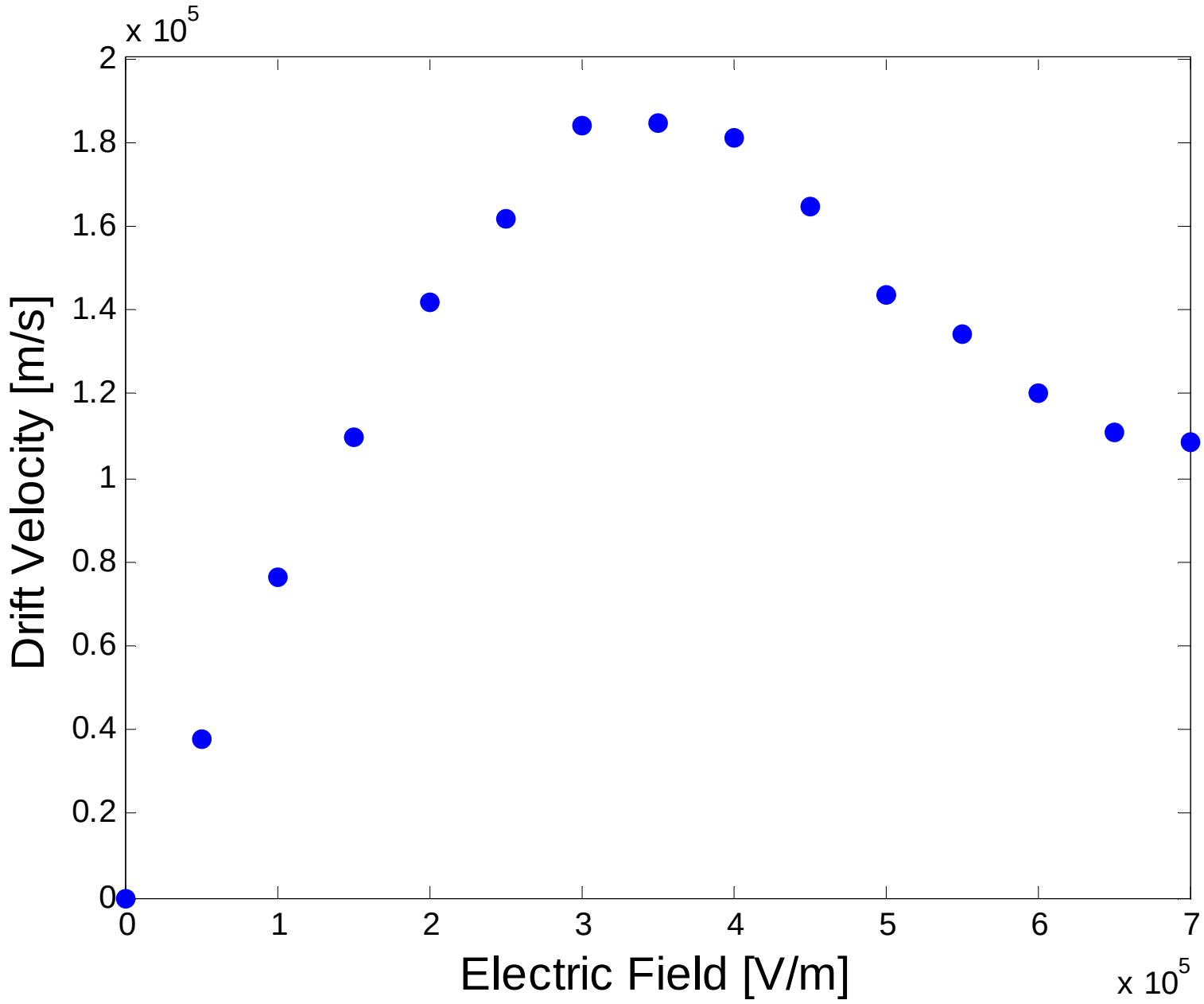
$k_x = k_{xp}\cos\varphi_o\cos\theta_o - k_{yp}\sin\varphi_o + k_{zp}\cos\varphi_o\sin\theta_o$
$k_y = k_{xp}\sin\varphi_o\cos\theta_o + k_{yp}\cos\varphi_o + k_{zp}\sin\varphi_o\sin\theta_o$
$k_z = -k_{xp}\sin\theta_o + k_{zp}\cos\theta_o$

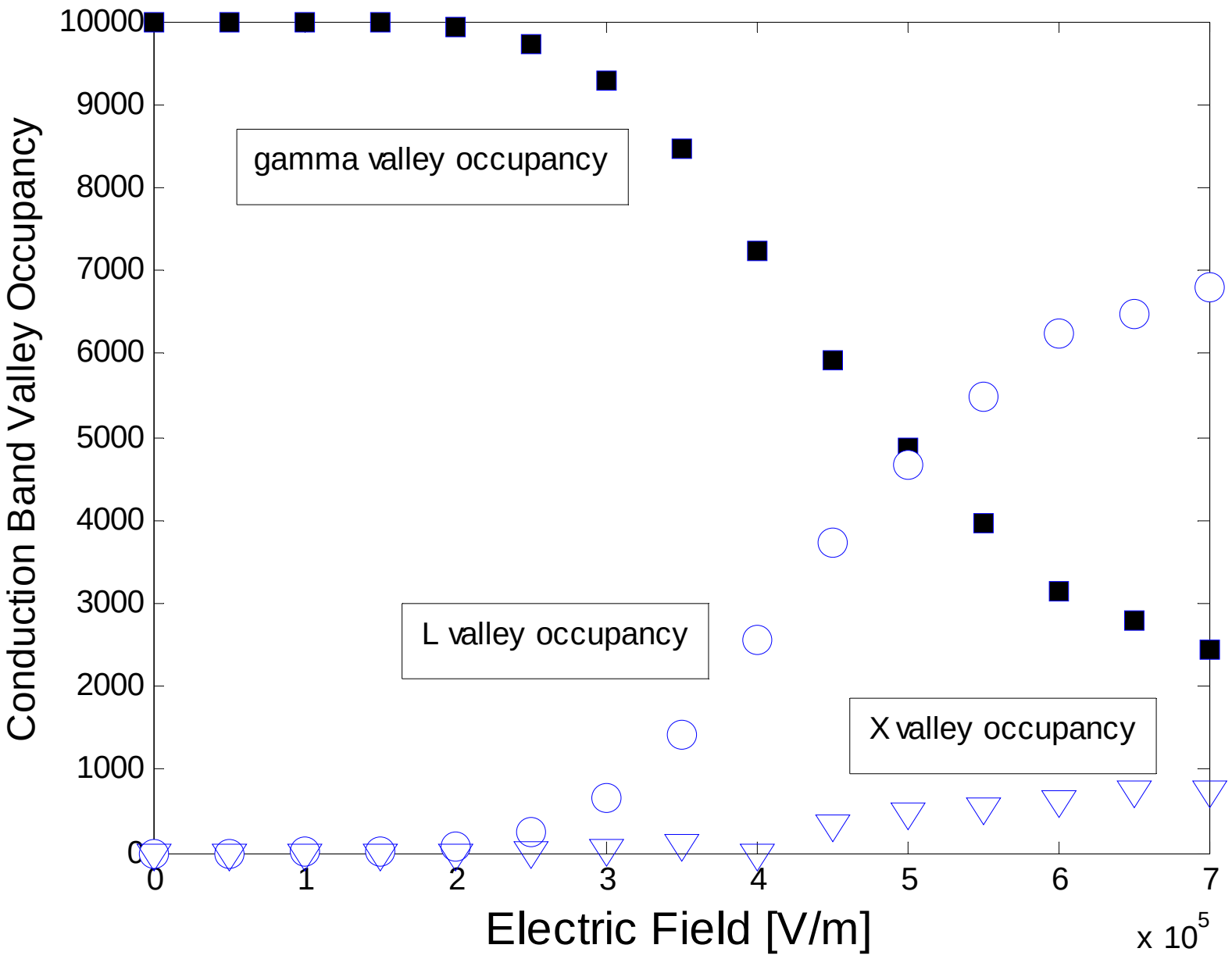
Rejection technique for final angle selection



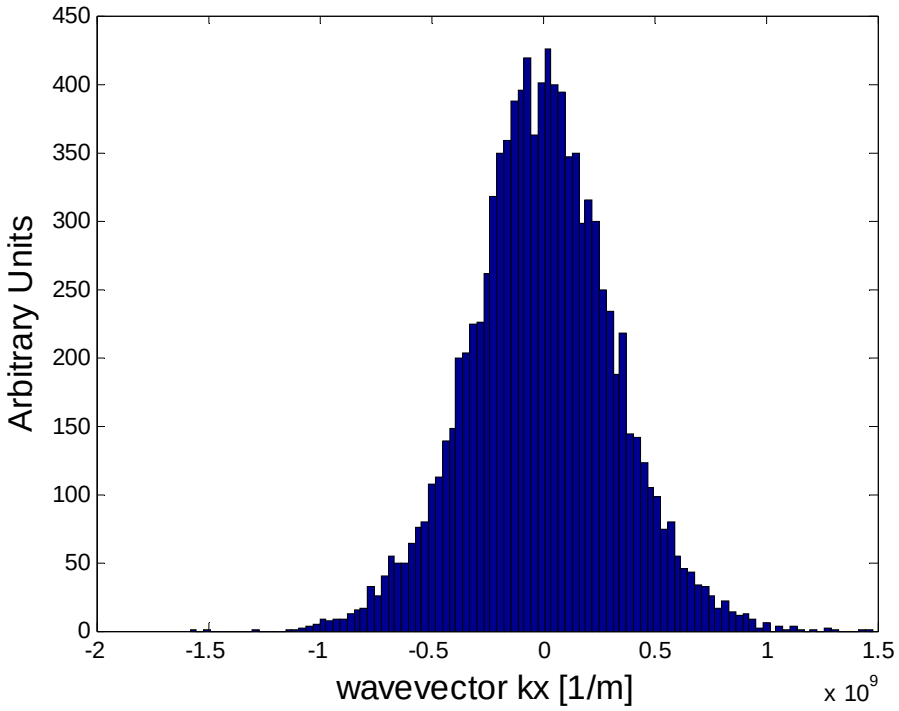


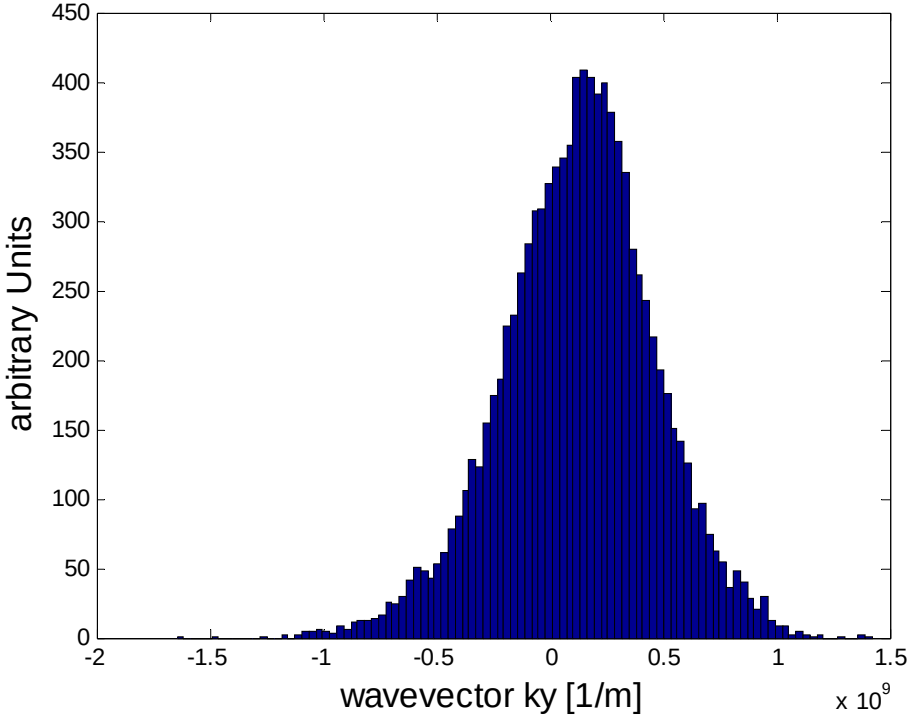

x 10^5
4
3.5
3
2.5
2
1.5
1
0.5
0
velocity [m/s]
0
1
2
time [s]
x 10^-11

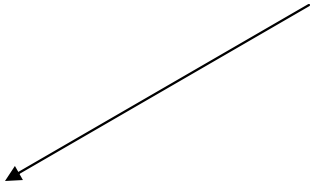

x 10^5
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Drift Velocity [m/s]
0
1
2
3
4
5
6
7
Electric Field [V/m]
x 10^5


Conduction Band Valley Occupancy
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
gamma valley occupancy
L valley occupancy
X valley occupancy
0
1
2
3
4
5
6
7
Electric Field [V/m]
x 10^5

Initial and final wavevector along the field

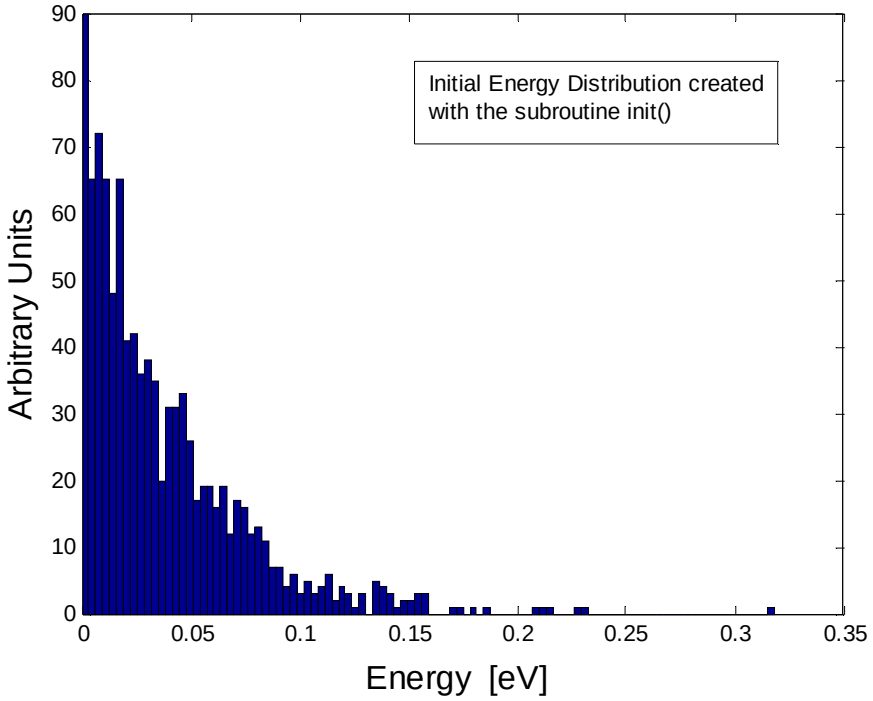


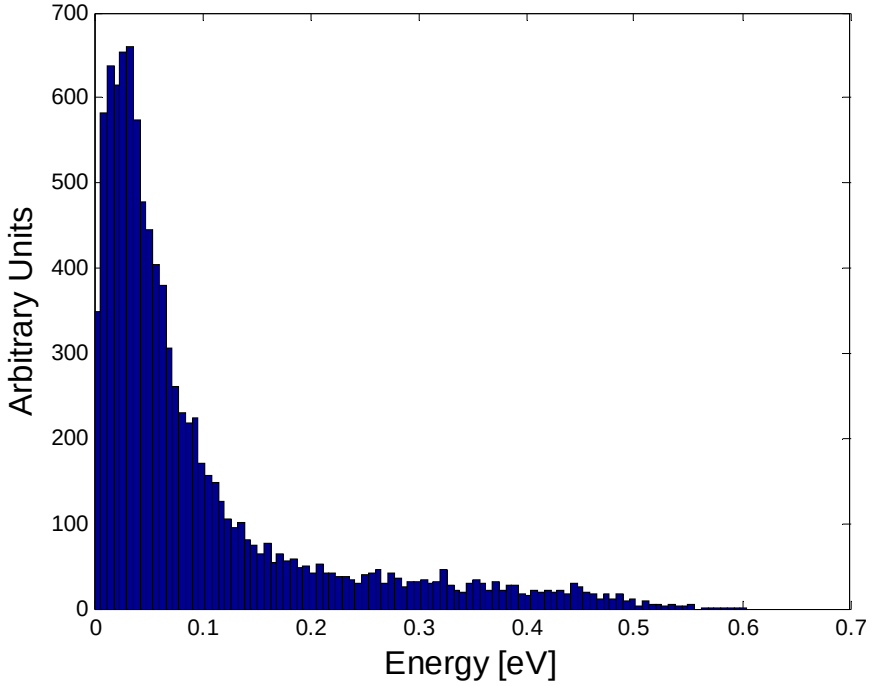


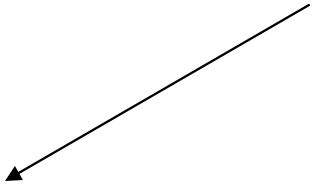


Shift in the distribution due to application of electric field.

Initial and final carrier energy







Shift in the distribution due to application of electric field.

Monte Carlo Method Described

7. Higher-order effects

Inclusion of the Pauli Exclusion Principle

- The influence of the final state on the scattering rate is important at low temperatures and high carrier densities.
- This effect may be included via a self-scattering rejection method (Bosi and Jacoboni, *J. Phys. C*9, 315 (1976); Lugli and Ferry, *IEEE Trans. Elec. Dev.* 32, 2431 (1985)).
- The electron (hole) distribution function $f(k_x,k_y,k_z)$ is updated in k-space (on a 2D or a 3D grid).
- Once the final state has been selected, a new random number is generated:
  - If $0 < r < f(\mathrm{k})$, then self-scattering is assumed to occur with no change of momentum or energy
  - If $f(\mathrm{k}) < r < 1$, then accept the scattering event

Simulation size:

$$Let \quad \frac{N}{n_{2d}} = A = L^2$$

The area per state in *k*-space is

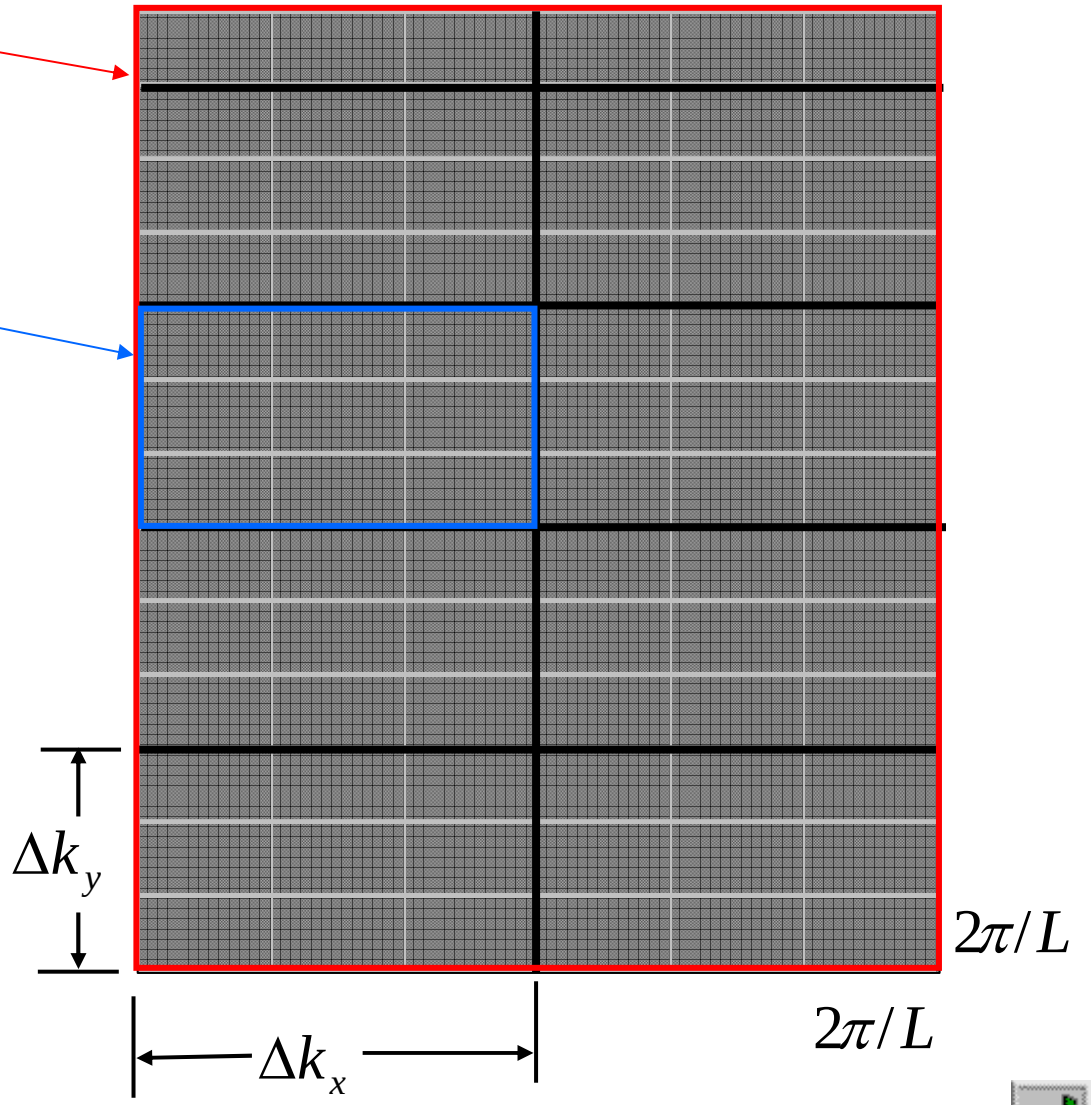
cell size $A_k = \left(\frac{2\pi}{L}\right)^2$

Upon scattering, we increase or decrease the population in the cell, and the latter gives *f(k)*

Some important notes:

- **The size of the grid in k-space determines how many electrons may occupy the grid.**
- **The accuracy improves as the number of particles increases.**

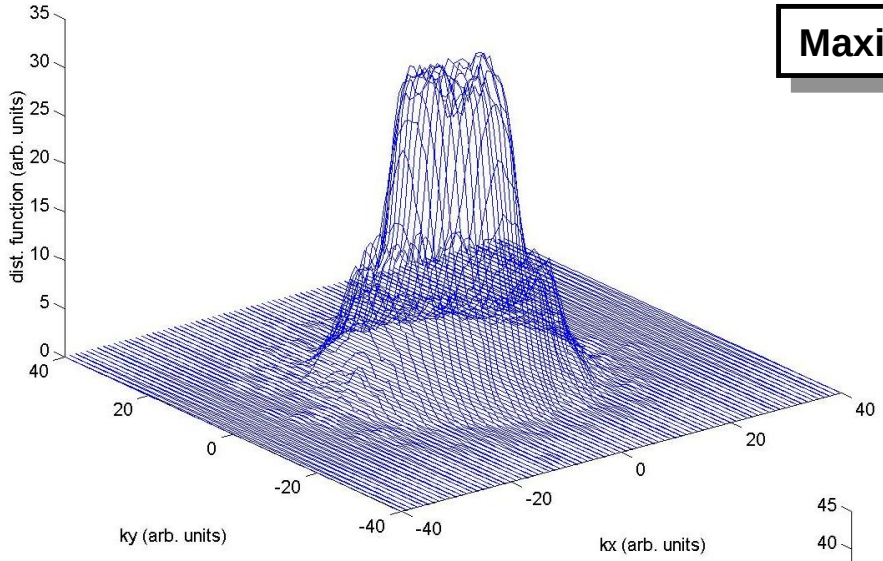
Two-Dimensional System Example



Number of states that can be occupied
Within one cell is:

$$\frac{\Delta k_x \Delta k_y}{\left(2\pi / L\right)^2}$$

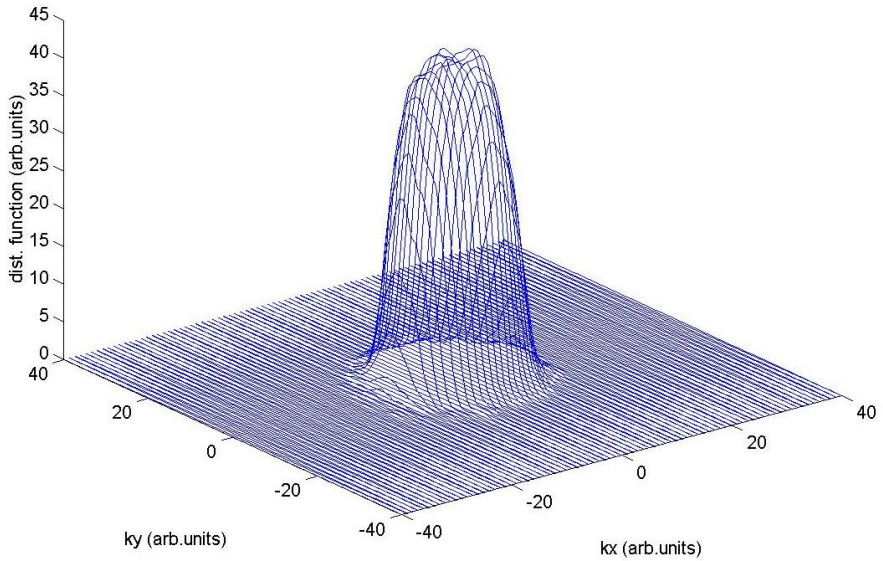
Maximum number of states per cell = 40



Non-degenerate statistics

$N_S = 4.75\times10^{13}$ cm^{-2}

$E_{eff} = 1.04\times10^{6}$ V/cm

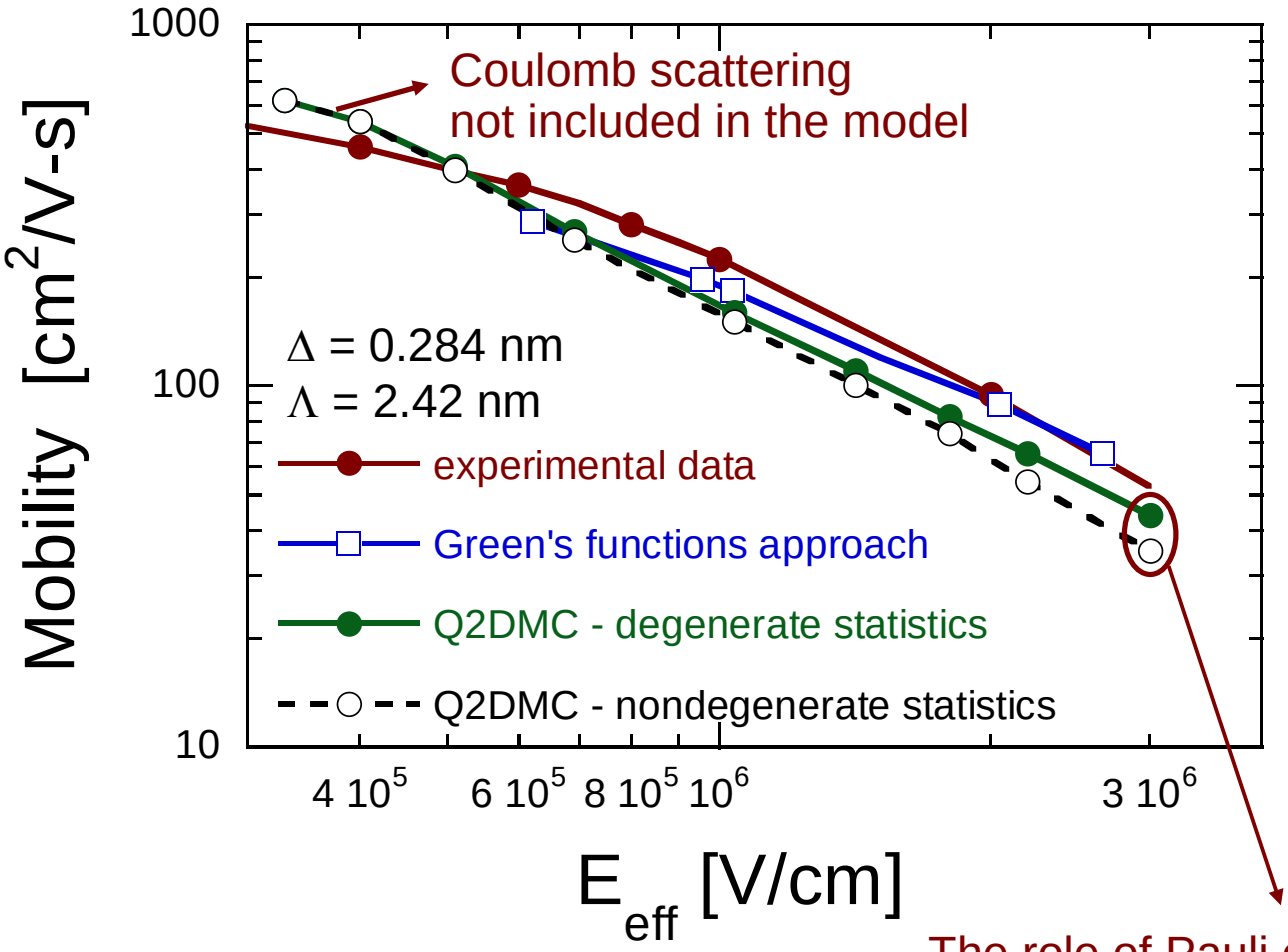


Degenerate statistics

$N_S = 2.71\times10^{13}$ cm^{-2}

$E_{eff} = 3.01\times10^{6}$ V/cm

Mobility vs. Experimental Data



The role of Pauli exclusion principle (screening not included)

Carrier-Carrier Scattering

For two-particle interactions, the electron-electron (hole-hole, electron-hole) scattering rate may be treated as a screened Coulomb interaction (impurity scattering in a relative coordinate system). The total scattering rate depends on the instantaneous distribution function, and is of the form:

$$\Gamma_{ee}(\mathbf{k}_0) = \frac{m^* e^4}{\hbar^3 V \varepsilon_\infty^2} \sum_{\mathbf{k}} f(\mathbf{k}) \frac{|\mathbf{k}-\mathbf{k}_0|}{\beta^2 \left(|\mathbf{k}-\mathbf{k}_0|^2 + \beta^2 \right)}$$

screening constant

There are three methods commonly used for the treatment of the electron-electron interaction:

A. **Method due to Lugli and Ferry**
B. **Rejection algorithm**
C. **Real-space molecular dynamics**

All are complicated!

Method due to Lugli and Ferry

- This method starts form the assumption that the sum over the distribution function is simply an ensemble average of a given quantity.
- In other words, the scattering rate is defined to be of the form:

$$\Gamma_{ee}(\mathrm{k}_0) = \frac{n m_n e^4 L_D^2}{4\pi\hbar^3 \varepsilon_\infty^2} \sum_{i=1}^{N} \frac{|\mathrm{k} - \mathrm{k}_i|}{|\mathrm{k} - \mathrm{k}_i|^2 + 1/L_D^2}$$

- The advantages of this method are:

  1. The scattering rate does not require any assumption on the form of the distribution function

  2. The method is not limited to steady-state situations, but it is also applicable for transient phenomena, such as femtosecond laser excitations

- The main limitation of the method is the computational cost, since it involves 3D sums over all carriers and the rate depends on **k** rather on its magnitude.

Rejection Algorithm

Within this algorithm, a self-scattering mechanism, internal to the interparticle scattering is introduced by the following substitution:

$$\frac{\left|\mathrm{k}-\mathrm{k}_0\right|}{\left|\mathrm{k}-\mathrm{k}_0\right|^2+1/L_D^2} \rightarrow \frac{1}{2L_D}$$

- When carrier-carrier collision is selected, a counterpart electron is chosen at random from the ensemble.
- Internal rejection is performed by comparing the random number with:

$$\frac{\left|\mathrm{k}-\mathrm{k}_0\right|}{\left|\mathrm{k}-\mathrm{k}_0\right|^2+1/L_D^2}$$

Rejection Algorithm (cont'd)

- If the collision is accepted, then the final state is calculated using:

$$\cos\theta_r = 1 - \frac{2r}{1 + g^2(1-r)L_D^2}, \quad \textit{where} \quad \theta_r = \textit{angle}(\mathbf{g}, \mathbf{g}')$$

where:

$$\mathbf{g} = \mathbf{k} - \mathbf{k}_0; \quad \mathbf{g}' = \mathbf{k}' - \mathbf{k}_0'$$

The azimuthal angle is then taken at random between 0 and 2π.

- The final states of the two particles are then calculated using:

$$\mathbf{k}_0' = \mathbf{k}_0 - \frac{1}{2}(\mathbf{g}' - \mathbf{g})$$

$$\mathbf{k}' = \mathbf{k}_0 + \frac{1}{2}(\mathbf{g}' - \mathbf{g})$$

Real-Space Molecular Dynamics

- An alternative to the previously described methods is the real-space treatment proposed by Jacoboni.

- According to this method, at the observation time instant $t_i = i\Delta t$, the total force on the electron equals the sum of the interparticle coulomb interaction between a particular electron and the other (N-1) electrons in the ensemble.

Real-Space Molecular Dynamics

- When implementing this method, several things need to be taken into account:
  1. The fact that N electrons are used to represent a carrier density $n = N/V$ means that a simulation volume equals $V = N/n$.
  2. Periodic boundary conditions are imposed on this volume, and because of that, care must be taken that the simulated volume and the number of particles are sufficiently large that artificial application from periodic replication of this volume do not appear in the calculation results.

Real-Space Molecular Dynamics

- Using Newtonian kinematics, the real-space trajectories of each particle are represented as:

$$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}\Delta t + \frac{1}{2}\frac{\mathbf{F}(t)}{m^*}\Delta t^2$$

and:

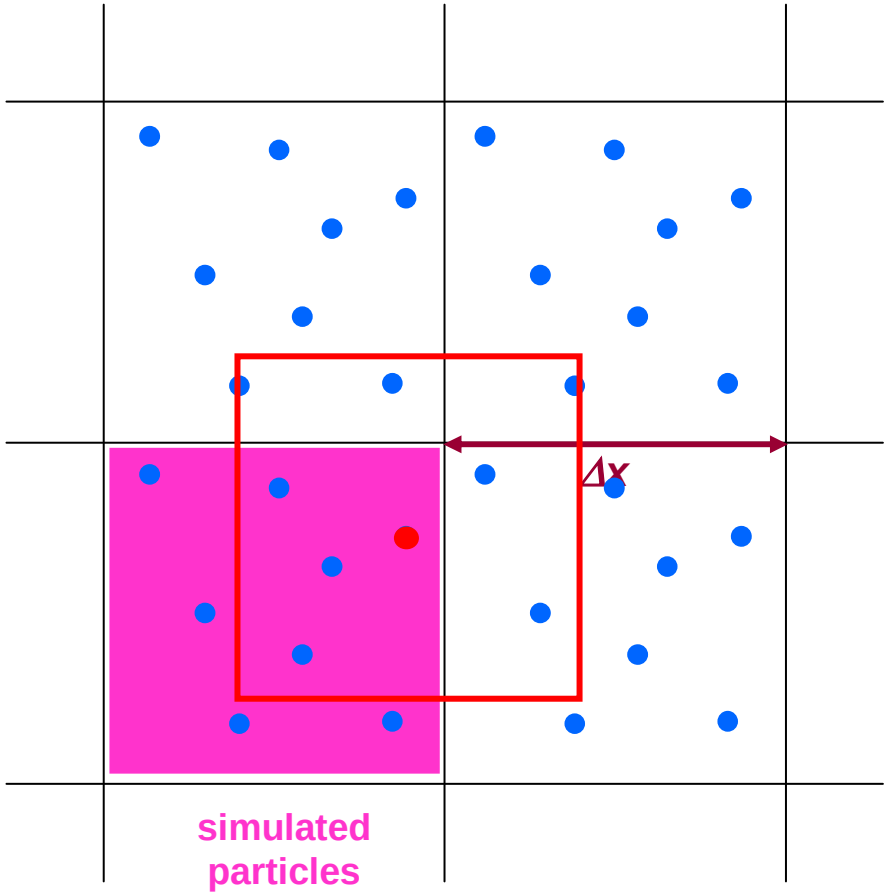
$$\mathbf{v}(t+\Delta t) = \mathbf{v}(t) + \frac{\mathbf{F}(t)}{m^*}\Delta t$$

Here, **F**(*t*) is the force arising from the applied field as well as that of the Coulomb interaction:

$$\mathbf{F}(t) = q\left[\mathbf{E} - \sum_i \nabla\varphi(\mathbf{r}(t)_i)\right]$$

- The contributions due to the periodic replication of the particles inside *V* in cells outside is represented with the Ewald sum:

$$\mathbf{F}(t) = -\frac{e^2}{4\pi\varepsilon}\sum_{i=1}^{N}\left(\frac{1}{\mathbf{r}_i^2}\mathbf{a}_i + \frac{2\pi}{3V}\mathbf{r}_i\right)$$



$$\Delta x = \left(\frac{N}{n} \right)^{1/3}$$

The actual force calculation must be done on a centered box, to avoid artificial drift forces.

So, this requires two boxes in practice: (1) the real box, and (2) a box around each particle.

The remaining particles are “replicas”

$$\sum_{all} \frac{1}{r} = \sum_{N} \frac{1}{r} + \sum_{replicas} \frac{1}{r}$$

$$= \sum_{\mathbf{R}_{cell}} \sum_{N} \frac{1}{|\mathbf{r} + \mathbf{R}_{cell}|}$$

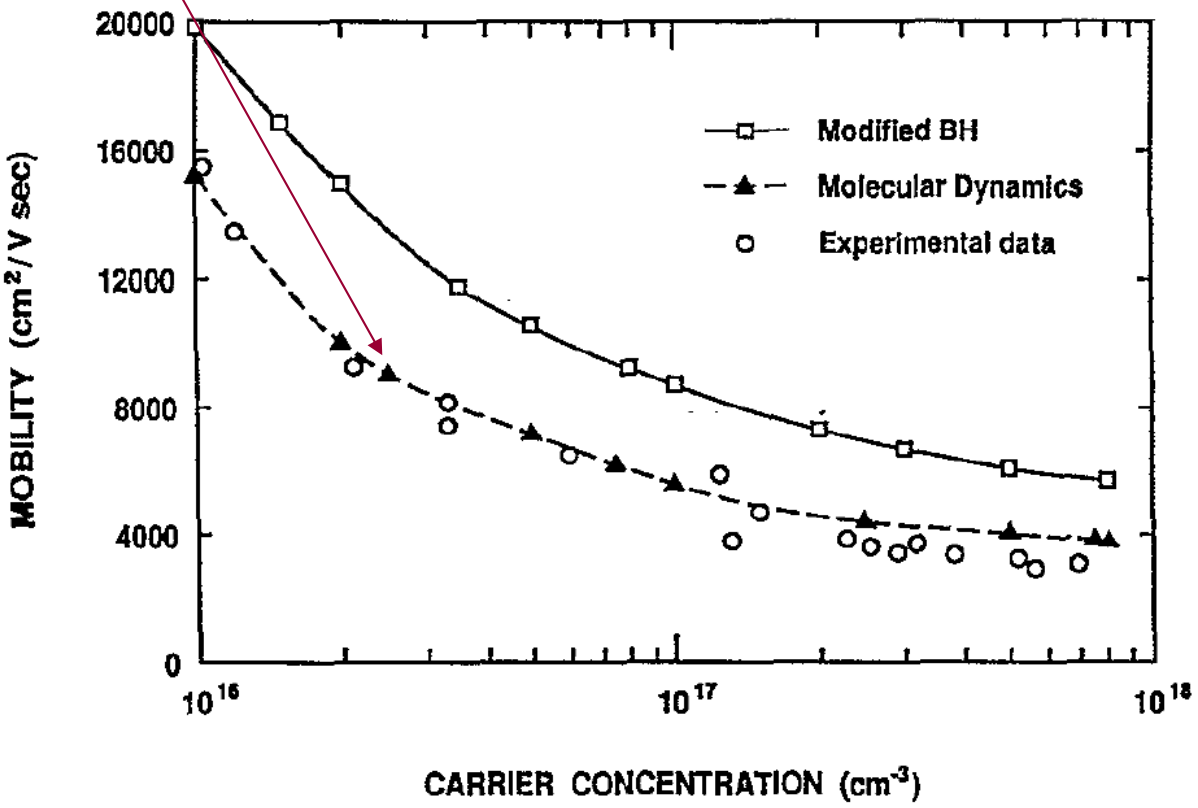
$$\cong \sum_{N} \frac{1}{r} \left[1 + \sum_{\mathbf{R}_{cell} > 0} \frac{1}{R_{cell}} - r \sum_{\mathbf{R}_{cell} > 0} \frac{1}{R_{cell}^2} + \ldots \right]$$

$$\sim f(r)$$

This can be made to be quite small, if enough particles are used.

This becomes even more exact when only the short-range part is kept (discussed later).

Role of an improved treatment of impurity scattering using MD approach in GaAs: only with this correct method can the mobility be made to match the data over two orders of magnitude in heavy doping.



Here, the impurities were put in randomly in the sample to simulate real doping. Each electron is, on average, interacting with *three* impurities at any one time!

Simulation Example

- The effect of the e-e scattering allows equilibrium distribution function to approach Fermi-Dirac or Maxwell Boltzmann distribution.
- Without e-e, there is a phonon ‘kink’ due to the finite energy of the phonon