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:

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

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:

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

The easiest way to generate the duration of the carrier free-flights is to use random numbers with uniform probability density $p(r)=1$ in the interval between 0 and 1. For this purpose, we can do random variables transformation,

$$p(r)dr = p(t)dt = \Gamma e^{-\Gamma t} dt$$

Then:

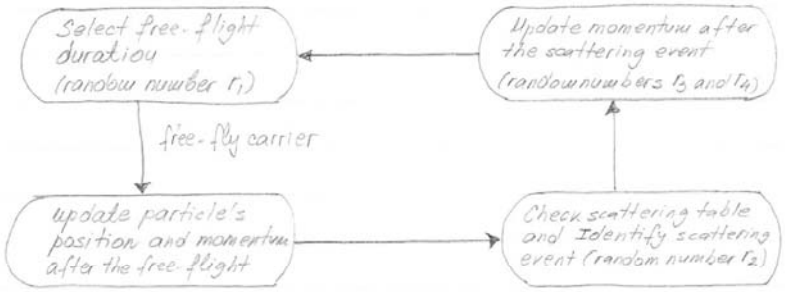
$$\int_0^{r_c} p(r)dr = \int_0^{t_c} \Gamma e^{-\Gamma t} dt = -e^{-\Gamma t}\Big|_0^{t_c} = 1 - e^{-\Gamma t_c} = r_c$$

or: $e^{-\Gamma t_c} = 1 - r_c$ which gives $t_c = -\frac{1}{\Gamma} ln(1-r_c) = -\frac{1}{\Gamma} ln(r_c')$.

Hence, the duration of the carrier free-flights is calculated using:

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

The generic algorithm for a single particle Monte carlo simulation of the carrier transport is shown schematically on the figure bellow:



(b) Momentum and position update after free-flight.

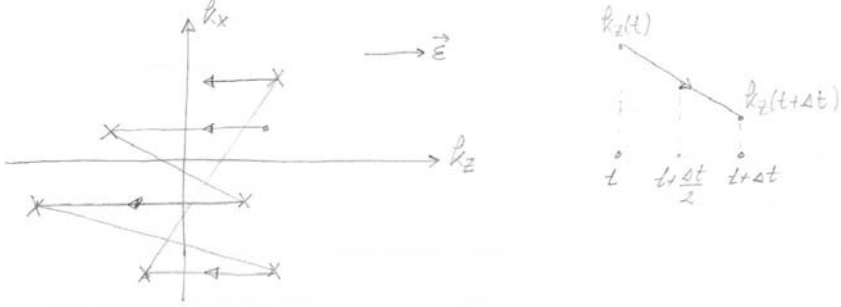
The particle's position and momentum after the free-flight are updated using:

$$\vec{F} = -e\vec{\mathcal{E}} = \hbar \frac{d\vec{k}}{dt} \quad \text{and} \quad \vec{v} = \frac{\hbar \vec{k}}{m^*} = \frac{d\vec{r}}{dt}$$

For the case when the electric field is along the z-direction, we have:

$$k_x(t) = k_x(0)$$
$$k_y(t) = k_y(0)$$
$$k_z(t) = k_z(0) - \frac{e}{\hbar}\mathcal{E}_z t$$

The particle trajectory in k-space is thus:



Since the momentum increases/decreases linearly in time, one has to be really careful when calculating the position update, for which we use: $d\vec{r} = \frac{\hbar}{m^*}\vec{k}(t)\,dt$. Rather accurate result can be obtained if we substitute for $\vec{k}(t)$, to get:

$$x(t) = \frac{\hbar}{m^*}k_x(0)t + x(0)$$

$$y(t) = \frac{\hbar}{m^*}k_y(0)t + y(0)$$

$$dz = \frac{\hbar}{m^*}\left[k_z(0) - \frac{e}{\hbar}\mathcal{E}_z t\right]dt$$

$$z(t) = z(0) + \frac{\hbar}{m^*}k_z(0)t - \frac{e}{m^*}\mathcal{E}_z\frac{t^2}{2}$$

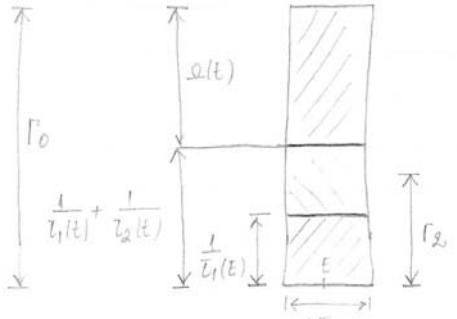
$$= z(0) + \frac{\hbar}{2m^*}k_z(0)t + \frac{\hbar}{2m^*}k_z(0)t - \frac{e\mathcal{E}_z}{2m^*}t^2$$

$$= z(0) + \frac{\hbar}{2m^*}k_z(0)t + \frac{\hbar}{2m^*}t\left[k_z(0) - \frac{e\mathcal{E}_z}{\hbar}t\right]$$

$$= z(0) + \frac{\hbar}{2m^*}k_z(0)t + \frac{\hbar}{2m^*}k_z(t)\,t = z(0) + \frac{\hbar}{m^*}\underbrace{\frac{k_z(0)+k_z(t)}{2}}_{k_{z\text{av}}}t$$

(c) Identification of scattering events

Before a simulation starts, a scattering table is generated which describes the cumulative scattering rates for all the scattering mechanisms included in the model. One line of this scattering table is shown below:



To be able to use random numbers uniformly distributed between 0 and 1, all cumulative rates are renormalized with Γ_0. Then, a particular scattering mechanism is selected when:

$$\frac{\sum_{m=1}^{l-1} \frac{1}{\tau_m(t)}}{\Gamma_0} \leq \Gamma_2 < \frac{\sum_{m=1}^{l} \frac{1}{\tau_m(t)}}{\Gamma_0}$$

Since most of the time self-scattering is selected for low energy electrons, it will speed up the selection process if the self-scattering mechanism is checked first.

(d) Selection of final state after scattering

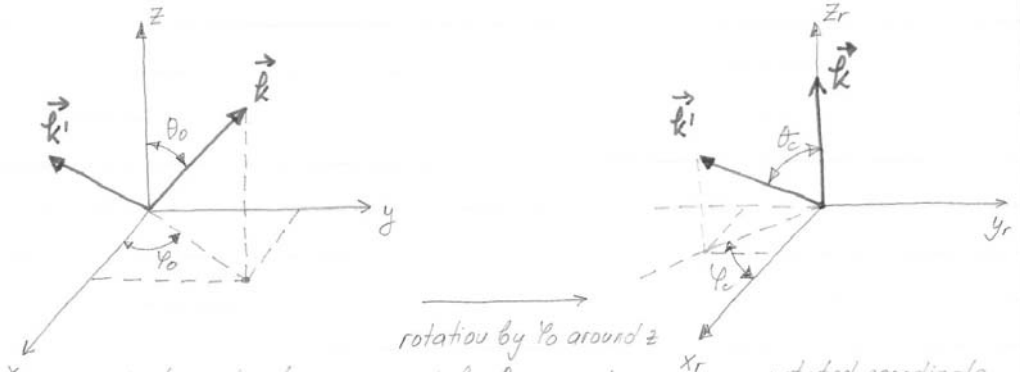
- Both the carrier momentum and energy are affected by the scattering event. If we take, for example intervalley scattering, the carrier energy after the scattering event is given by:

$$E(k^+) = E(k') = E(k) \pm \hbar\omega_{iv}$$

where the top sign is for absorption and the bottom sign is for the phonon emission process.

- The carrier momentum after the scattering event is given by:

$$k' = \sqrt{\frac{2m^* E(k')}{\hbar^2}} \quad \text{for parabolic band structure.}$$



→ In the rotated coordinate system, for isotropic scattering processes (for which the matrix element is q-independent), the probability that $\vec{k}'$ lies between azimuthal angles φ and $\varphi + d\varphi$ is:

$$P(\varphi)d\varphi = \frac{d\varphi \int_0^\infty k'^2 dk' \int_{-1}^{1} d(\cos\theta)\, S(\vec{k},\vec{k}')}{\int_0^{2\pi} d\varphi \int_0^\infty k'^2 dk' \int_{-1}^{1} d(\cos\theta)\, S(\vec{k},\vec{k}')} = \frac{d\varphi}{2\pi} = P(r)dr$$

Hence: $$\int_0^{r_3} P(r)dr = \int_0^{\varphi_c} P(\varphi)d\varphi \Rightarrow r_3 = \frac{\varphi_c}{2\pi} \Rightarrow \boxed{\varphi_c = 2\pi r_3}$$

Since r_3 is uniformly distributed between 0 and 1, φ_c is uniformly distributed between 0 and 2π.

→ For the polar angle, again working in the rotated coordinate system, and assuming isotropic scattering processes, we have:

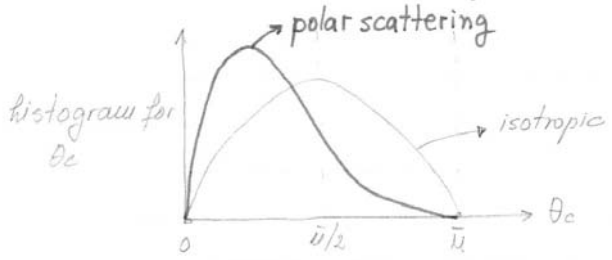
$$P(\theta)d\theta = \frac{\sin\theta d\theta \int_0^{2\pi} d\varphi \int_0^\infty k'^2 dk'\, S(\vec{k},\vec{k}')}{\int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\varphi \int_0^\infty k'^2 dk'\, S(\vec{k},\vec{k}')} = \frac{\sin\theta d\theta}{2} = P(r)dr$$

Then: $$\int_0^{r_4} P(r)dr = \int_0^{\theta_c} \frac{1}{2}\sin\theta\, d\theta \Rightarrow r_4 = -\frac{1}{2}\cos\theta \Big|_0^{\theta_c} = -\frac{1}{2}\cos\theta_c + \frac{1}{2}$$

or $\quad 1-\cos\theta_c = 2r_4 \quad \Rightarrow \cos\theta_c = 1-2r_4$

$$\boxed{\theta_c = \cos^{-1}(1-2r_4)}$$

Note that θ_c is not going to be uniformly distributed between 0 and $\bar{\pi}$. It is $\cos\theta_c$ that will be uniformly distributed between -1 and 1.



For polar optical phonon scattering and for ionized impurity scattering, where small angle scattering is prefered the weight will shift towards $\theta_c = 0$.

- Having determined θ_c and φ_c, we can calculate the components of $\vec{k}'_r$ in the rotated coordinate system using:

$$\vec{k}'_r = \begin{cases} k' \cos\varphi_c \cdot \sin\theta_c \\ k' \sin\varphi_c \cdot \sin\theta_c \\ k' \cos\theta_c \end{cases}$$

To find the components of this vector in the original coordinate system we need to do the inverse rotation procedure, i.e. used to perform rotation by $(-\theta_c)$ around y_r, and then by $(-\varphi_c)$ about z_r.

(e) Estimators

After sufficient time has elapsed, the average carrier velocity is calculated using:

$$v_{d,est} = \frac{1}{t_{total}} \sum_i \int_{t_{i-1}}^{t_i} v(t)\,dt = \frac{1}{t_{total}} \sum_i \int_{t_{i-1}}^{t_i} \frac{dx}{dt}\,dt = \frac{1}{t_{total}} \sum_i (x_i - x_{i-1}) = \frac{x_{final} - x_{initial}}{t_{total}}$$

For this average to be valid, the distribution function has to be in steady state. This limitation prevents, for example, the single particle Monte Carlo for being used in examination of transients, i.e. when we have non-ergodic processes.

Note on stationary and ergodic processes:

- A process is stationary if all probability distributions of any order are time independent, i.e.

$$P(t_i) = P(t_{i-1}) = P(t_0)$$

- If a process is ergodic, then the time average equals the ensemble average, i.e.

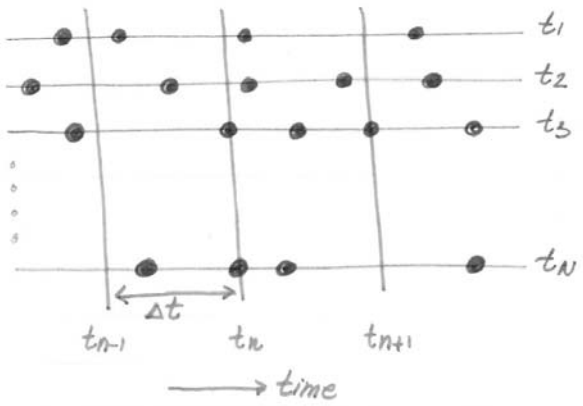
$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} X_i = E(X_i) = E(X_0) .$$

ENSEMBLE MONTE CARLO METHOD

More commonly used approach in simulations is the ensemble Monte Carlo technique, in which rather than following a single particle over time, one follows ensemble of particles. Note that the time coordinate for each electron must be maintained during the simulation. There are two different time scales involved in an Ensemble Monte Carlo method:

- free-flight duration time
- observation time steps, at the end of which the ensemble averages are computed and, if necessary, the molecular dynamics forces are updated.

The different time scales in an ensemble Monte carlo method are illustrated on the figure on the next page.



- The drift velocity in this case is calculated using:

$$\bar{v}_d(t) = \langle v_d(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} v_{di}(t)$$

where N is the number of particles in the ensemble. Note that the Ensemble Monte Carlo does not require the stationary conditions, which means that it is suitable for investigating transients in devices. Non-stationary transport is always observed in ultra-small devices. The equation for $\bar{v}_d(t)$ represents an estimate of the true velocity, which has a standard error of $\sigma/\sqrt{N}$, where σ^2 is the variance that is estimated from:

$$\sigma^2 \approx \frac{N}{N-1} \left\{ \frac{1}{N} \sum_{j=1}^{N} (v_{dj}^2) - \bar{v}_d^{\,2} \right\}$$

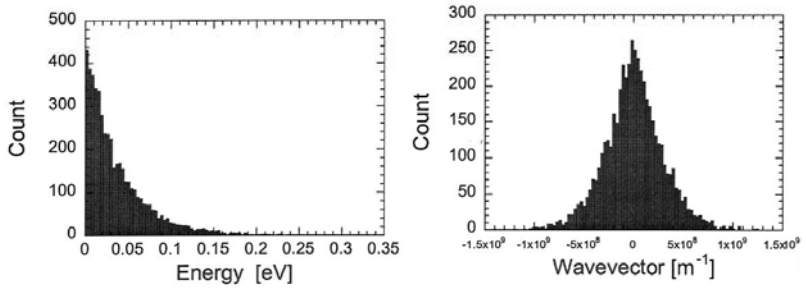
Typical ensemble sizes for good statistics are in the range $10^4 \div 10^5$ particles.

- To initialize carrier energy, one assumes non-degenerate statistics, for which the probability that a state is occupied by an electron is given by the Maxwell-Boltzmann statistics, i.e.

$$P(E)dE = \frac{1}{E_0} e^{-E/E_0} \quad \text{, where } E_0 = \frac{3}{2} k_B T.$$

Then: $E = -\frac{3}{2} k_B T \ln(r)$, where r is a random number uniformly distributed

in the interval [0,1]. An example for the initial carrier distribution (histogram) for an ensemble of 5,000 electrons is given in the figure below.



• Note on the time evolution of the distribution function:

(1) The steady-state distribution function is proportional to the number of electrons $n(\vec{k})\Delta\vec{k}$ that at time t are found to be in a cell of fixed volume $\Delta\vec{k}$, around $\vec{k}$. Then, the expectation value, or the average value of a quantity $\langle A\rangle$, can also be evaluated using:

$$\langle A\rangle = C\sum_{k} n(\vec{k})A(\vec{k}),$$

where C is a normalization constant, and $n(\vec{k})$ is proportional to the probability of finding any given electron in state $\vec{k}$.

(2) The 'before scattering' distribution function $n_b(\vec{k})$ is proportional to the probability that an electron is found in $\vec{k}$ immediately before a scattering event. Therefore, the steady-state distribution function is given by:

$$n(\vec{k}) = n_b(\vec{k})\frac{\tau(\vec{k})}{\tau_0}, \quad \text{where } \tau_0 \text{ is a normalization constant}$$

$n_b(\vec{k})$: before scattering

$\frac{\tau(\vec{k})}{\tau_0}$: change of the distribution function due to scattering out of state $\vec{k}$

If $\gamma(\vec{k})$ is chosen to be constant by introducing self-scattering, then: $n(\vec{k}) \propto n_e(\vec{k})$. In this case:

$$\langle A \rangle = C' \sum_{\vec{k}} n_e(\vec{k}) A_b(\vec{k}) = \frac{1}{N} \sum_i A_{bi}$$

where the sum covers all electron free-flights, and A_{bi} indicates the value of the quantity A evaluated at the end of the free-flight, immediately before the i-th scattering event.

MANY-PARTICLE EFFECTS

In describing the electron-electron interaction Hamiltonian, we have separated it into:

- short-range contribution → Screened two-body interaction
- long-range contribution → collective behavior described in terms of plasmons. Treated as the other scattering mechanisms.

More difficult task is the inclusion of the screened Coulomb interaction into the standard algorithm, since it depends upon the distribution function that is one of the outputs of the monte carlo method! The use of the Ensemble Monte Carlo technique simplifies considerably the treatment of the carrier-carrier scattering because the distribution function is built in the simulated ensemble of carriers. Three alternative methods have been proposed for including carrier-carrier scattering in Ensemble Monte Carlo simulations.

Method 1: The first method, due to Lugli and Ferry, starts from the assumption that a sum over the distribution function is simply an ensemble average of a given quantity.