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

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

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.

In other words, the scattering rate for binary collision processes, of the form:

$$\frac{1}{\tau(\vec{k})} = \frac{nm^* e^4 L_D^2}{4\pi\hbar^3 \varepsilon_\infty^2} \sum_{\vec{k}_1} f(\vec{k}_1) \frac{|\vec{k}-\vec{k}_1|}{|\vec{k}-\vec{k}_1|^2 + 1/L_D^2}$$

is replaced with a sum over all the carriers in the ensemble of the form:

$$\frac{1}{\tau(\vec{k})} = \frac{nm^* e^4 L_D^2}{4\pi\hbar^3 \varepsilon_\infty^2} \sum_{i=1}^{N} \frac{|\vec{k}-\vec{k}_i|}{|\vec{k}-\vec{k}_i|^2 + 1/L_D^2}$$

→ The advantages of this method are the following ones:

- The scattering rate defined from the ensemble average does not require any assumption on the form of the distribution function.
- The method is not limited to steady-state situations, but it is also applicable for transient phenomena, such as femto-second laser excitations.

→ The main limitation of this method is the computational cost since it involves 3D-sums over all carriers and the rate depends on $\vec{k}$ rather than its magnitude.

Method 2: A second method for k-space treatment of the electron-electron interactions is based on a rejection algorithm. A self-scattering mechanism, internal to the interparticle scattering is introduced by substituting the term:

$$\frac{|\vec{k}-\vec{k}_i|}{|\vec{k}-\vec{k}_i|^2 + 1/L_D^2}$$

with a maximum value $1/(2L_D)$. When carrier-carrier collision event is selected during the simulation, the

counterpart electron is chosen at random from the ensemble. Internal rejection is performed by comparing the random number 'r' between 0 and 1 with:

$$\frac{|\vec{k}-\vec{k}_0|}{|\vec{k}-\vec{k}_0|^2+1/L_D^2} \longrightarrow \begin{array}{l}\vec{k} \text{ - wavevector of initial electron}\\ \vec{k}_0 \text{ - wavevector of target electron}\end{array}$$

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

$$\cos\theta_r = 1 - \frac{2r}{1+g^2(1-r)L_D^2}, \qquad \theta_r = \measuredangle(\vec{g},\vec{g}')$$

where $\vec{g} = \vec{k} - \vec{k}_0$ and $\vec{g}' = \vec{k}' - \vec{k}_0'$ ($\vec{k}'$ and $\vec{k}_0'$ are final state values). The azimuthal angle is taken at random between 0 and 2π. The final states are then calculated using:

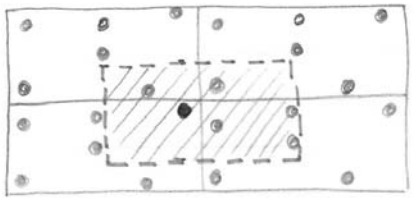
$$\begin{cases} \vec{k}_0' = \vec{k}_0 - \frac{1}{2}(\vec{g}' - \vec{g}) \\ \vec{k}' = \vec{k}_0 + \frac{1}{2}(\vec{g}' - \vec{g}) \end{cases}$$

METHOD 3: An alternative to the above-described k-space methods is the real space molecular dynamics treatment of the carrier-carrier interactions, which has been proposed by Jacoboni. According to this method, at the observation time instants $t_i = i\Delta t$, 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.

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 the simulation volume equals $V = N/n$.

(2) Periodic boundary conditions imposed on this volume for homogeneous systems. Care must be taken, however, that the simulated volume and the number of particles are sufficiently large that artifacts from periodic replication of this volume do not appear in the calculation results.



For a given carrier, a second volume is defined that is centered around the carrier when the interparticle forces are being calculated. Then:

$$\vec{F} = -\frac{e^2}{4\pi\varepsilon(0)} \sum_{i=1}^{N} \frac{\vec{a}_{ri}}{r_i^2}$$

, $\vec{a}_{ri}$ unit vector between target electron and the other electrons in the system.

The reason for using this super-cell model is to eliminate any bias in the force that would arise if N electrons are used to represent the whole crystal. Then, the total potential arising from the interparticle force is:

$$\phi = \frac{e^2}{4\pi\varepsilon(0)} \frac{1}{2} \sum_{i \neq j} \frac{1}{r_{ij}}$$

where (1/2) factor prevents from double counting each pairwise force. The sum can also be written as:

$$\sum_{i \neq j} \frac{1}{r_{ij}} = \sum_{\vec{L}} \sum_{i \neq j} \frac{1}{|\vec{L} + \vec{r}_{ij}|} = \sum_{i \neq j} \frac{1}{r_{ij}} + \sum_{L>0} \sum_{i \neq j} \frac{1}{|\vec{L} + \vec{r}_{ij}|}$$

- $\vec{L}$: Lattice translation vector
- $i \neq j$ within cell: summation over the particles in the basic centered cell
- $L>0$ $i \neq j$: summation over the particles that lie outside this cell.

Now Looking at the second term, we have:

$\sum_{L>0} \frac{1}{|\vec{L}+\vec{r}_{ij}|}$ → use analogy of scalars:

$$\sum_L \frac{1}{(L+r)} = \sum_L \frac{1}{L}\frac{1}{1+r/L} = \sum_L \frac{1}{L}\left[1 - \frac{r}{L} + \frac{1}{2}\left(\frac{r}{L}\right)^2 + \cdots\right]$$

$$= \sum_L \frac{1}{L} - r\sum_L \frac{1}{L^2} + \frac{r^2}{2}\sum_L \frac{1}{L^3} + \cdots$$

Therefore,

$$\sum_{i\neq j} \frac{1}{r_{ij}} = \sum_{i\neq j} \frac{1}{r_{ij}} + \sum_{i\neq j}\left[\sum_{L>0}\frac{1}{L} - r_{ij}\sum_{L>0}\frac{1}{L^2} + \frac{r_{ij}^2}{2}\sum_{L>0}\frac{1}{L^3} + \cdots\right]$$

all particles in crystal — particles in centered cell — particles in cell

The summations over the lattice vectors are known as EWALD SUMS that account for the long-range portion of the force. If the number of particles is small (100), these correction forces are large.

An important parameter to calculate in the description of the molecular dynamics calculation is the radial distribution function that describes the probability of finding a carrier at a distance r from a carrier (test particle) centered at $\vec{r}=0$. It can also be described as the number of particles in a shell with radius r and a thickness Δr, i.e.

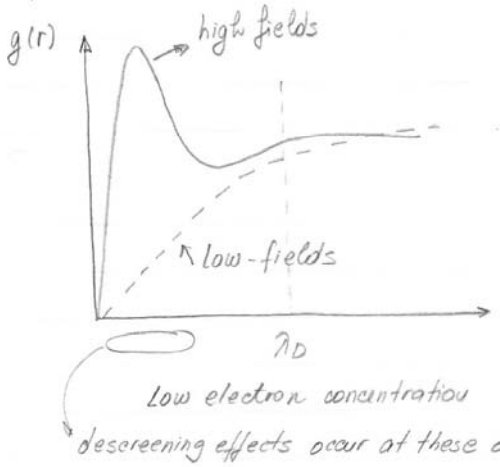
$$g(r) = \frac{1}{4\bar{\nu}r^2}\int_0^{2\bar{\nu}} d\varphi \int_{-1}^{1} d(\cos\theta) \int_r^{r+\Delta r} r^2 \rho(\vec{r})\, dr$$

Now using: $\rho(\vec{r}) = \sum_{i=1}^{N-1} \delta(\vec{r}-\vec{r}_k)$, we finally arrive at:

$$g(r) = \frac{1}{4\bar{\nu}} \cdot 2\bar{\nu} \cdot 2 \cdot \sum_{r\le r_k<r+\Delta r} \frac{r_k^2}{r^2} = \sum_{r\le r_k<r+\Delta r} \left(\frac{r_k}{r}\right)^2$$

where $\vec{r}_k$ is the vector that describes the position of arbitrary particle in the ensemble with respect to the test particle that is centered at $\vec{r}=0$.

When g(r) is calculated for each particle and averaged over all particles in the ensemble, we get:



- At low fields, no drift or heating effects are present and g(r) approaches its asymptotic value corresponding to a Debye-screened interparticle potential.
- At higher electric fields, reduced screening effect takes place since the particles can not redistribute rapidly, and g(r) approaches its asymptotic value more rapidly.

The advantages of using the real space molecular dynamics approach come from the fact that:

(1) it avoids simplifying assumptions on the form of the distribution function and on the form of the dielectric function involved in the screening process.

(2) Real-space fluctuations of the carrier gas are naturally included in the model.

(3) Interaction between several carriers at the same time is also included in the model, rather than the simple binary collisions approach used in the k-space treatments.

(4) g(r) can give accurate description of the two particle correlations.

DEGENERACY AND FERHI-DIRAC STATISTICS

- The Ensemble Monte Carlo method is a semiclassical technique, in that it simulates electrons as classical particles that undergo a sequence of free-flight and scattering events. The transition probability is calculated using Fermi's golden rule. The probability of an electronic transition from a state $\vec{k}$ to a state $\vec{k}'$ is, in general, proportional to:

$$f(\vec{k})\, S(\vec{k},\vec{k}')\, [1-f(\vec{k}')]$$

$f(\vec{k})$: probability that state $\vec{k}$ is occupied

$S(\vec{k},\vec{k}')$: transition probability

$[1-f(\vec{k}')]$: probability that state $\vec{k}'$ is empty

- Standard monte carlo works with the assumption that $f(\vec{k}')=0$. In other words, it is assumed that all final states are empty, which is a reasonable approximation for non-degenerate semiconductors only. If $f(\vec{k}')$ is used, then as the distribution function evolves towards its steady-state value, constant re-evaluation of the scattering rates is needed. Powerful method has been proposed by Bosi and Jacoboni and extended to EMC (Ensemble Monte Carlo) by Lugli and Ferry.
- In the EMC code the implementation works as follows. After the scattering event is determined and final carrier momentum has been calculated, a random number is generated. Then, if the final carrier wavevector is $\vec{k}_2$ and if

$$r < 1 - f(\vec{k}_2, t)$$

then the scattering process is accepted. This means that as the carrier states fill, most scattering events into the state are rejected and treated as self-scattering.

An important issue in this approach is the normalization of the distribution function and how it is generated.

(a) Generation of the distribution function

A grid in momentum space is defined so that the number of electrons (particles) in each state can be tracked.

(b) Renormalization

- In the EMC simulation, N electrons are simulated to describe density $n = N/V$, which leads to a simulation volume in real space equal to $V = N/n$.
- The volume associated with a single-spin state in the momentum space is then given by $(2\pi)^3/V$.
- When setting the grid in the three-dimensional k-space, the elementary cell volume is defined as: $\Omega_c = \Delta k_x \cdot \Delta k_y \cdot \Delta k_z$. Therefore, each cell can accomodate

$$N_c = 2 \Omega_c \frac{V}{(2\pi)^3} = \frac{2V\Omega_c}{(2\pi)^3}$$

electrons, where a factor of 2 has been included for spin degeneracy.

- Now, if the initial distribution $f'(k_x, k_y, k_z)$ is calculated by counting the number of electrons in each cell, the normalized distribution $f(k_x, k_y, k_z)$ is obtained by dividing by N_c. This renormalization allows usage of random numbers that are uniformly-distributed between 0 and 1.

The inclusion of the Pauli exclusion principle leads to hotter electrons. In the degenerate EMC calculation, a very large number of transitions (more than 80%) are prevented by the Pauli exclusion principle.