A Zero Field Monte Carlo Algorithm Accounting for the Pauli Exclusion Principle

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A generalized Monte Carlo algorithm is presented which allows calculation of the whole carrier mobility tensor at zero electric field for both nondegenerate and degenerate bulk semiconductors. This algorithm represents a limiting case of a small-signal algorithm when the stationary distribution function is replaced by the Fermi-Dirac distribution at zero electric field.

As a starting point we use the transient Boltzmann transport equation with a scattering operator including the Pauli blocking factor. As we only consider bulk semiconductors, the space dependence of the distribution function and of the differential scattering rates is neglected. We also suppose the scattering rate to be time invariant.

After linearization and transformation of the Boltzmann equation to integral form and assuming impulse-like excitation for $\mathbf{E}_1(t)$, we derive the following equation for the perturbation $f_1(\mathbf{k},t)$ of the distribution function:

$$f_1(\mathbf{k},t) = \int_0^t dt' \int d\mathbf{k}' \, f_1(\mathbf{k}',t) \cdot \widetilde{S}\left(\mathbf{k}', \mathbf{K}(t')\right) \cdot \exp\left[-\int_{t'}^t \widetilde{\lambda}\left(\mathbf{K}(y)\right) \, dy\right] + \\ + G(\mathbf{K}(0)) \cdot \exp\left[-\int_0^t \widetilde{\lambda}\left(\mathbf{K}(y)\right) \, dy\right]. \tag{1}$$

The differential scattering rate $\widetilde{S}(\mathbf{k}',\mathbf{k})$ and the total scattering rate $\widetilde{\lambda}(\mathbf{k})$ are defined by the following expressions:

$$\begin{aligned} \widetilde{S}(\mathbf{k}',\mathbf{k}) &= [1 - f_s(\mathbf{k})] \cdot S(\mathbf{k}',\mathbf{k}) + f_s(\mathbf{k}) \cdot S(\mathbf{k},\mathbf{k}') \\ \widetilde{\lambda}(\mathbf{k}) &= \int \tilde{S}(\mathbf{k},\mathbf{k}') \, d\mathbf{k}', \end{aligned} \tag{2}$$

where $f_s(\mathbf{k})$ is the stationary distribution function, $S(\mathbf{k}',\mathbf{k})\, d\mathbf{k}'$ is the scattering rate from $d\mathbf{k}'$ to state with wave vector $\mathbf{k}$, which must not be occupied. Employing the δ-function of the Fermi golden rule the expression for $\widetilde{\lambda}(\mathbf{k})$ can be rewritten in the following manner:

$$\widetilde{\lambda}(\mathbf{k}) = [1 - f_s(\epsilon_f)] \cdot \lambda(\mathbf{k}) + f_s(\epsilon_f) \cdot \lambda^*(\mathbf{k}), \tag{3}$$

where ϵ_f is the final energy, $\lambda(\mathbf{k}) = \int S(\mathbf{k},\mathbf{k}')\, d\mathbf{k}'$ is the total scattering rate, $\lambda^*(\mathbf{k}) = \int S(\mathbf{k}',\mathbf{k})\, d\mathbf{k}'$ is the backward total scattering rate. The new variables $\widetilde{S}(\mathbf{k}',\mathbf{k})$ and $\widetilde{\lambda}(\mathbf{k})$ introduced above are used to construct the Monte Carlo algorithm. It should be also noted that for nondegenerate statistics ($f_s \ll 1$) this algorithm gives the method described previously. For intermediate doping levels there is a mixture of the total scattering rate $\lambda(\mathbf{k})$ and the backward scattering rate $\lambda^*(\mathbf{k})$ (see (3)) while for the degenerate case ($f_s \lesssim 1$) the kinetic properties are predominantly determined by the backward scattering rate $\lambda^*(\mathbf{k})$.