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THE CRF-METHOD FOR SEMICONDUCTORS' INTRAVALLEY COLLISION KERNELS: I - the 2D case

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If the collisions are redefined as a flux a kinetic conservation law can be written in divergence form. This can be handled numerically, in the framework of Finite Particle Approximation, using the CRF-method. In the present paper the relevant quantities needed for computer implementation of the CRF-method are derived in the case of a 2D momentum space for the semiconductors' intravalley collision kernels.

1. Introduction.

Semiconductors' kinetic transport equation has been usually treated numerically using the Monte Carlo methods [4] [5]. For a few years Deterministic Particles Methods have been proposed as an alternative scheme for this class of problems [2] [3] [8] [10] [11] [13]. In this framework the CRF-method for kinetic equations has been recently presented [1] [12]. The idea of this method is to write a conservation law in divergence form. This can be done easily by introducing a flux equivalent to the inhomogeneity. In a classical frame, the reciprocal of the desired function multiplied by the flux gives a velocity field. However, in the finite point approximation a reciprocal does not exist. Since the velocity field can also be interpreted as the Radon-Nikodym derivative of the flux, we use the latter for a numerical approximation. This gives a scheme where the numerical

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effort depends only on the desired accuracy and not directly on the dimension of the phase space. In the present paper we apply the method to intravalley collision kernels for semiconductors in a 2D momentum space. The scattering rate in semiconductors depends on the energy of the carriers. In the parabolic approximation, the collision integral is spherically symmetric (spherical energy-wavevector relationship). The ellipsoidal case can be reduced to the spherical one using the Herring-Vogt transformation [5]. For this purpose it is useful to use the method recast in spherical coordinates. In [1] the method was recast in general coordinates and it was shown that the method can be used efficiently for numerical computation of the semiconductor kernels. Examples involving more than one kernel will need the analytical computation of the relevant quantities for each kernel. Semiconductors' intravalley kernels show similarities that one can use in order to optimize the analytical work and to reduce the implementation effort. Keeping in mind these similarities, all kernels may be derived from three model kernels. In this paper we present a derivation of the relevant quantities for the CRF-method for these model kernels. The plan of the paper is the following: in §2 we recall the CRF-method; in §3 we analyze the intravalley collision kernels for semiconductors and we identify the relevant model kernels; in §4 we compute analytically the relevant quantities needed for computer implementation of the CRF-method using polar coordinates. Finally, we make some concluding remarks.

2. Description of the CRF-method.

The CRF-method has been widely described in [1] [12]. In the interest of clarity the derivation of the method is presented once again in the following. Kinetic equations usually split in the transport and the collision part. The transport part can be written easily in divergence form,

$$\frac{\partial}{\partial t} f_{trans} = -div_{space}(fv) - div_{momentum}(fK)$$

In the CRF-method one wants to write the collision part also in this form. For this purpose one considers the equation

$$f_t = Q(f) \tag{1}$$

where $\Omega = \Omega_x \times \Omega_\xi \subset \mathbf{R}^3 \times \mathbf{R}^3$, $z = (x, \xi) \in \Omega$, $f : [0, \infty) \times \Omega \to \mathbf{R}$ and

$$\int_{\Omega_\xi} Q(f)\, d\xi = 0\,.$$

The initial condition $f_0 : \Omega \to \mathbf{R}$ should be a given non-negative function with

$$\int_\Omega f_0(z)\,dz = 1\,. \tag{2}$$

Let ψ be a vector field such that

$$div_\xi \psi = -Q(f) \tag{3}$$

$$\psi(t,x,\xi) = 0 \qquad \text{for } \xi \in \partial\Omega_\xi \tag{4}$$

This means the collision $Q(f)$ is expressed as a flux ψ and there is no flux across the boundary of Ω_ξ, which guarantees that the conservation property is satisfied. The associated velocity field g is given according to

$$\int_B gf\,d\xi = \int_B \psi\,d\xi \tag{5}$$

for all Borel sets $B \subset \Omega_\xi$. Then the equation (1) becomes

$$f_t + div_\xi(fg) = 0\,. \tag{6}$$

The full kinetic equation then reads

$$f_t + div_x(fv) + div_\xi(f(K+g)) = 0$$

and the equation of motion is given by

$$\dot{z} = (v, K+g)^T\,.$$

Since the components of g are added to the given vector field, the only need is the computation of g itself. For this purpose one introduces the set

$$I^i_{[\alpha_i,\gamma_i]} = \{\xi \in \Omega_\xi : \alpha_i \leq \xi_i \leq \gamma_i\} \tag{7}$$

for $i = 1,2,3$ and considers the integrals of the relation (5) over this set. For the r.h.s. one finds

$$\Psi^i(\gamma_i) = \int_{I^i_{[\alpha_i,\gamma_i]}} \psi^i(t,x,\xi)\,d\xi = -\int_{I^i_{[\alpha_i,\gamma_i]}} \Big(\int_{\alpha_i}^{\xi_i} Q(f)\,d\xi_i'\Big)\,d\xi \tag{8}$$

The numerical calculation of the left integral in (5) can be performed, as shown in [12], by

$$\int_{I^i_{[\alpha_i,\gamma_i]}} g^i f\, d\xi = \sum_{j=1}^{n} \omega_j \chi_{[\xi_{i,r},\xi_{i,r+k}]}(\xi_j) g^i_j + R$$

where R indicates the remainder. In [12] the Simpson rule has been choosen, where $k = 2$. This leads to a linear system of order N

$$Ag^i = \Psi^i \tag{9}$$

where A is a diagonal dominant matrix independent of f.
Moreover in the numerical process the distribution function f will be approximated by a discrete measure [12]

$$f(t,z) = \frac{1}{N}\sum_{j=1}^{N} \delta(z - z_j(t))$$

The extension of the method to general coordinates can be obtained by coordinate transformations [1]. Let T be a regular coordinate transformation, $\{\xi\} \to \{\eta\}$ and $|T|$ denotes its Jacobian. Then

$$Q(f) = Q((f \circ T)\,|T|)\,. \tag{10}$$

Since T is time independent one gets

$$\partial_t f \circ T = \partial_t (f \circ T) = Q((f \circ T)\,|T|) \circ T\,. \tag{11}$$

But $f \circ T$ must be multiplied by $|T|$ to be a density function. Letting $\widetilde{f} = (f \circ T)\,|T|$ and $\widetilde{Q}(\widetilde{f}) = (Q((f \circ T)\,|T|) \circ T)\,|T|$ one finds

$$\partial_t \widetilde{f} = \widetilde{Q}(\widetilde{f})\,. \tag{12}$$

Suppose in the choosen coordinate system Ω_η can be represented as a Cartesian product of three intervals

$$\Omega_\eta = [\alpha_1, \beta_1] \times [\alpha_2, \beta_2] \times [\alpha_3, \beta_3]$$

and one chooses the set

$$I^i_{[\alpha_i,\gamma_i]} = \{\eta \in \Omega_\eta : \alpha_i \le \eta_i \le \gamma_i\} \tag{13}$$

for $i = 1, 2, 3$. Then instead of (8) one gets [1]

$$\Psi^i(\gamma_i) = \int_{I^i_{[\alpha_i,\gamma_i]}} \psi^i(t, x, \eta)\, d\eta = -\int_{I^i_{[\alpha_i,\gamma_i]}} \left(\int_{\alpha_i}^{\eta_i} \widetilde{Q}(\widetilde{f})\, d\eta_i' \right) d\eta \tag{14}$$

and

$$\int_{I_{[\alpha_i,\gamma_i]}} g^i \widetilde{f}\, d\eta = \Psi^i(\gamma_i)\,. \tag{15}$$

3. Semiconductors' Intravalley Model Kernels.

In the semiclassical approach the collision term for semiconductors can be expressed as the difference between the electrons scattered in and out of the state k

$$Q(f) = \int_\Omega (S(k', k)f(k')(1 - f(k)) - S(k, k')f(k)(1 - f(k')))\, dk' \tag{16}$$

where $S(k, k')$ represents the probability per unit time of an electron transition from a state k into an empty state k', induced by the lattice imperfections. The $(1 - f)$ coefficients accounts for the Pauli exclusion principle. In many cases these factors do not contribute since it is always assumed $f \ll 1$ [5].
The transition probability $S(k, k')$ from the initial state k to the final state k', having energies ϵ and ϵ', due to a given interaction mechanism, is given [5] [14]

$$S(k, k') = \frac{V_0}{(2\pi)^3} \frac{2\pi}{\hbar} |V(k - k')|^2 G(k, k') \delta(\epsilon' - \epsilon)$$

where V_0 is the volume of the crystal, $G(k', k)$ is the overlap integral and $|V(k - k')|^2$ is the square of the matrix element of the interaction mechanism. For electrons intravalley transition process G is equal to unity [5].
We note here that most of the relevant intravalley interaction mechanism can be described - by suitably changing the meaning and the values of the constants - through model kernels. We list here three examples of the model kernels.

a) The optical non polar interaction. Kernel is given by:

$$S(k, k') = \frac{\hbar D_0^2}{8\pi^2 \rho_0 \hbar\omega_p} \binom{N_0 + 1}{N_0} \delta(\epsilon' - \epsilon \pm \hbar\omega_p)$$

where $\hbar\omega_p$ is the constant energy of the optical non polar phonon; D_0 is the optical deformation potential and ρ_0 is the density of the material.

b) The optical polar interaction. Kernel is given by:

$$S(k,k') = \frac{q^2\hbar\omega_p}{8\pi^2\hbar\epsilon_0}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_r}\right)\frac{1}{\|k-k'\|^2}\binom{N_0+1}{N_0}\delta(\epsilon' - \epsilon \pm \hbar\omega_p)$$

where $\hbar\omega_p$ is the constant energy of the optical polar phonon; ϵ_0 is the vacuum permittivity; ϵ_r is the low frequency relative permittivity and ϵ_∞ is the high frequency relative permittivity.

c) The interaction with ionized impurity. Kernel is given by:

$$S(k,k') = \frac{q^4 N_I Z_I^2}{4\pi^2\hbar(\epsilon_0\epsilon_r)^2}\frac{1}{(\|k-k'\|^2+\beta^2)^2}\delta(\epsilon' - \epsilon)$$

where N_I is the impurity density; Z_I is the number of charge units of the impurity; β^{-1} is the screening length.

All the other relevant kernels have similar forms [3] [5]. Seeking to produce a numerical code one would like to emphasize similarities and differences among the various kernels to optimize the writing of the code, i.e. minimizing the necessary subroutines. The above examples show that, by suitably changing the meaning and the numerical values of the parameters, all the previous kernels can be described by using the following three types of model kernels

$$S(k,k') = A\delta(k'^2 - k^2 + \varphi) \tag{17}$$

$$S(k,k') = \frac{A}{\|k-k'\|^2}\delta(k'^2 - k^2 + \varphi) \tag{18}$$

$$S(k,k') = \frac{A}{(\|k-k'\|^2+\beta^2)^2}\delta(k'^2 - k^2)\,. \tag{19}$$

Here we have used the parabolic approximation $\epsilon = \hbar k^2/2m^*$. The constant φ is obviously suitably defined.

4. The Ψ^i evaluation.

As shown in section 2 the solution of the equation of motion reduces to the computation of the velocity field g. We are then involved in computing the r.h.s of (15), i.e. the Ψ^i. Here we want to use polar coordinates. For this purpose let (ξ_1, ξ_2), (k_1, k_2) respectively the Cartesian and the polar coordinates, $\Omega_k = [\alpha_1, \beta_1] \times [0, 2\pi]$, and denote by T the coordinate transformation from $\{\xi\} \to \{k\}$ and by $|T| = k_1$ its Jacobian. The collision term for semiconductors can be expressed as the difference between a gain term G and a lost term L. Then in the new coordinate system we have

$$\widetilde{Q}(\widetilde{f}(k_1, k_2)) = \widetilde{G}(k_1, k_2) - \widetilde{L}(k_1, k_2)$$

where $\widetilde{G}$ and $\widetilde{L}$ are given by

$$\widetilde{G}(k_1, k_2) = \int_{\Omega_\mu} S(\mu_1, \mu_2, k_1, k_2)\widetilde{f}(\mu_1, \mu_2) k_1 \, d\mu \tag{20}$$

$$\widetilde{L}(k_1, k_2) = \widetilde{f}(k_1, k_2)\, \widetilde{C}(k_1, k_2) \tag{21}$$

with

$$\widetilde{C}(k_1, k_2) = \int_{\Omega_\mu} S(k_1, k_2, \mu_1, \mu_2)\mu_1 \, d\mu \tag{22}$$

where $\mu = (\mu_1, \mu_2)$. Then (14) can be written in the form

$$\Psi^i(\gamma_i) = -\Psi^i_{\widetilde{G}}(\gamma_i) + \Psi^i_{\widetilde{L}}(\gamma_i) \tag{23}$$

To evaluate the $\Psi^i(\gamma_i)$ for $i = 1, 2$ we can proceed as follows:

1. We approximate the density function $\widetilde{f}(t, k)$ by a discrete measure

$$\widetilde{f}(t, k_1, k_2) = f(t, k_1, k_2)\,|T| = \frac{1}{N}\sum_{j=1}^{N} \delta(k_1 - k_{1,j})\, \delta(k_2 - k_{2,j});$$

2. Compute $\widetilde{G}(k)$ and $\widetilde{L}(k)$;
3. Compute $\Psi^1(\gamma_1)$ and $\Psi^2(\gamma_2)$ separately for $\widetilde{G}(k)$ and $\widetilde{L}(k)$.

In performing the above analytical calculations one should be aware of the proper treatment of the " δ-function " [6] [7] [9]. Then, after some algebra, variable transformations and appropriate use of the Heaviside function $H(\cdot)$ one gets the following results.

1. Model kernel (17)

$$\widetilde{G}(k_1, k_2) = \frac{1}{N}\sum_{j=1}^{N} \widetilde{S}(k_j, k_1, k_2) \tag{24}$$

$$\widetilde{C}(k_1, k_2) = \pi A H[(k_1^2 - \varphi - \alpha_1^2)(\beta_1^2 - k_1^2 + \varphi)] \tag{25}$$

Using the above results in the definition of $\Psi^i(\gamma_i)$ for the first component we get

$$\Psi^1_{\widetilde{G}}(\gamma_1) = \frac{\pi A}{N}\sum_{j=1}^{N}(\gamma_1 - \sqrt{a_j})H[(a_j - \alpha_1^2)(\gamma_1^2 - a_j)] \tag{26}$$

$$\Psi^1_{\widetilde{L}}(\gamma_1) = \frac{\pi A}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j})\widetilde{C}(k_{1,j}, k_{2,j})H(\gamma_1 - k_{1,j}) \tag{27}$$

where $a_j = k_{1,j}^2 - \varphi$.
For the second component we get

$$\Psi^2_{\widetilde{G}}(\gamma_2) = \frac{A\gamma_2^2}{4N}\sum_{j=1}^{N} H[(a_j - \alpha_1^2)(\beta_1^2 - a_j)] \tag{28}$$

$$\Psi^2_{\widetilde{L}}(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2 - k_{2,j})\widetilde{C}(k_{1,j}, k_{2,j})H(\gamma_2 - k_{2,j}) \tag{29}$$

One can perform, at least for the Ψ^1 term, an easy check of the previous formulae using the elastic limit. In this limit the energy is conserved so the radial component of the momentum should not change, i.e. the g^1 should be identically zero for all particles. As the matrix A is not singular, this implies that the Ψ^1 on the r.h.s. are identically zero. In the elastic limit $\varphi = 0$ so $a_j = k_{1,j}$. Then after some algebra, using the definition of the Heaviside function, we get

$$\Psi^1_{\widetilde{G}}(\gamma_1) = \Psi^1_{\widetilde{L}}(\gamma_1) = \frac{\pi A}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j})H(\gamma_1 - k_{1,j})$$

as required.

2. Model kernel (18)

$$\widetilde{G}(k_1,k_2) = \frac{1}{N}\sum_{j=1}^{N} \widetilde{S}(k_j,k_1,k_2) \tag{30}$$

$$\widetilde{C}(k_1,k_2) = \frac{A}{2}F(k_1,k_2)H[(k_1^2-\varphi-\alpha_1^2)(\beta_1^2-k_1^2+\varphi)] \tag{31}$$

where

$$F(k_1,k_2) = \int_0^{2\pi} \frac{dk_2'}{2k_1^2-\varphi-2k_1(k_1^2-\varphi)^{\frac{1}{2}}\cos(k_2-k_2')}\,. \tag{32}$$

Using the above results in the definition of $\Psi^i(\gamma_i)$ for the first component we get

$$\Psi^1_{\widetilde{G}}(\gamma_1) = \frac{A}{2N}\sum_{j=1}^{N}(\gamma_1-\sqrt{a_j})F_1(\sqrt{a_j},k_j)H[(a_j-\alpha_1^2)(\gamma_1^2-a_j)] \tag{33}$$

$$\Psi^1_{\widetilde{L}}(\gamma_1) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_1-k_{1,j})\widetilde{C}(k_{1,j},k_{2,j})H(\gamma_1-k_{1,j}) \tag{34}$$

where

$$F_1(k_1',k_j) = \int_0^{2\pi} \frac{dk_2}{k_{1,j}^2+k_1'^2-2k_{1,j}k_1'\cos(k_{2,j}-k_2)} \tag{35}$$

and $a_j = k_{1,j}^2-\varphi$.
For the second component we get

$$\Psi^2_{\widetilde{G}}(\gamma_2) = \frac{A}{2N}\sum_{j=1}^{N} H[(a_j-\alpha_1^2)(\beta_1^2-a_j)]\int_{\alpha_2}^{\gamma_2} F_2(k_2,k_j)\,dk_2 \tag{36}$$

$$\Psi^2_{\widetilde{L}}(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2-k_{2,j})\widetilde{C}(k_{1,j},k_{2,j})H(\gamma_2-k_{2,j}) \tag{37}$$

where

$$F_2(k_2, k_j) = \int_0^{k_2} \frac{dk_2'}{k_{1,j}^2 + a_j - 2k_{1,j}\sqrt{a_j}\cos(k_{2,j} - k_2')} . \tag{38}$$

We note that the integral functions defined by equations (32) (35) and (38) can be computed analytically (see appendix A), while the r.h.s. integral in (36) must be computed numerically.
Furthermore we note that in the elastic limit we get $\Psi^1_{\widetilde{G}}(\gamma_1) = \Psi^1_{\widetilde{L}}(\gamma_1)$ as required.

3. Model kernel (19)

$$\widetilde{G}(k_1, k_2) = \frac{1}{N}\sum_{j=1}^{N} \widetilde{S}(k_j, k_1, k_2) \tag{39}$$

$$\widetilde{C}(k_1, k_2) = \frac{A}{2} F(k_1, k_2) H[(k_1^2 - \alpha_1^2)(\beta_1^2 - k_1^2)] \tag{40}$$

where

$$F(k_1, k_2) = \int_0^{2\pi} \frac{dk_2'}{[2k_1^2 + \beta^2 - 2k_1^2\cos(k_2 - k_2')]^2} . \tag{41}$$

Using the above results in the definition of $\Psi^i(\gamma_i)$ for the first component we get

$$\Psi^1_{\widetilde{G}}(\gamma_1) = \frac{A}{2N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j}) F_1(k_{1,j}, k_j) H(\gamma_1 - k_{1,j}) \tag{42}$$

$$\Psi^1_{\widetilde{L}}(\gamma_1) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j}) \widetilde{C}(k_{1,j}, k_{2,j}) H(\gamma_1 - k_{1,j}) \tag{43}$$

where

$$F_1(k_1', k_j) = \int_0^{2\pi} \frac{dk_2}{[k_{1,j}^2 + k_1'^2 + \beta^2 - 2k_{1,j}k_1'\cos(k_{2,j} - k_2)]^2} . \tag{44}$$

For the second component we get

$$\Psi^2_{\underset{\sim}{G}}(\gamma_2) = \frac{A}{2N}\sum_{j=1}^{N}\int_{\alpha_2}^{\gamma_2} F_2(k_2, k_j)\, dk_2 \tag{45}$$

$$\Psi^2_{\underset{\sim}{L}}(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2 - k_{2,j})\widetilde{C}(k_{1,j}, k_{2,j})H(\gamma_2 - k_{2,j}) \tag{46}$$

where

$$F_2(k_2, k_j) = \int_0^{k_2} \frac{dk'_2}{[2k^2_{1,j} + \beta^2 - 2k^2_{1,j}\cos(k_{2,j} - k'_2)]^2}\,. \tag{47}$$

We note that the integral functions defined by equations (41) (44) and (47) can be computed analytically (see appendix A), while the r.h.s. integral in (45) must be computed numerically.
This model kernel is already elastic. This property is conserved by the CRF-method as can be seen, with simple algebra, from (42) and (43).

5. Conclusions.

The numerical experiments performed using the CRF-method, performed for a 2D model using the Polar Optical Scattering collision kernel, show that the method can be used for numerical computations [1]. For this we have computed the relevant quantities for the application of the method to intravalley model kernels in a 2D momentum space. The formulation of the CRF-method in spherical coordinates is particularly suitable in the parabolic approximation. In a subsequent paper we will present the analytical computations, for the same model kernels, in a 3D momentum space.

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Appendix A.

In this appendix we recall the results of two well known generalized integrals which we have used in the previous calculations.

We consider first the r.h.s. integrals in (32) (35) and (38). These can be written in the form

$$I(x) = \int \frac{dx}{a - b\cos x}$$

where a, b are two real constants with $a^2 > b^2$ and $a \neq b$.
The primitive $I(x)$ of $(a - b\cos x)^{-1}$ can be computed analytically and we get

$$I(x) = \frac{2}{\sqrt{a^2 - b^2}} \arctan\left(\frac{a+b}{\sqrt{a^2 - b^2}} \tan\frac{x}{2}\right).$$

We note that if $\pi \in [\alpha, \beta]$ we have

$$\int_\alpha^\beta \frac{dx}{a - b\cos x} = I(\pi^-) - I(\alpha) + I(\beta) - I(\pi^+).$$

We now consider the r.h.s. integrals in (41) (44) and (47). These can be written in the form

$$J(x) = \int \frac{dx}{(a - b\cos x)^2}$$

where a, b are two real constants with $a^2 > b^2$ and $a \neq b$.
Again the primitive can be computed analytically and we get

$$J(x) = \frac{2}{a^2 - b^2}\left[\frac{1}{2c} \arctan\frac{t}{c} + \frac{t}{2(t^2 + c^2)}\right]$$

where $t = \tan\frac{x}{2}$ and $c = \frac{\sqrt{a^2 - b^2}}{a + b}$.
Also in this case if $\pi \in [\alpha, \beta]$ we have

$$\int_\alpha^\beta \frac{dx}{(a - b\cos x)^2} = J(\pi^-) - J(\alpha) + J(\beta) - J(\pi^+).$$

REFERENCES

[1] R. Burkhard - S. Motta - J. Wick, *The CRF-method in general coordinates,* Preprint, 1992.

[2] P. Degond - F. Guyot-Delaurens - F.J. Mustieles - F. Nier, *Simulation Particulaire du trasport bidimensionnel d'electrons parallele a l'interface d'une heterojonction,* rapport interne n.189, Ecole Polytechnique, Palaiseau (1989).

[3] P. Degond - F.J. Mustieles, *Le Logicien SPADES-1 Version 2,* Documentation Scientifique, Centre de Mathematiques Appliquees, Ecole Polytechnique, Palaiseau (1990).

[4] R.W. Hockney - J.W. Eastwood, *Computer simulation Using Particles,* Adam Hilger, Bristol (1988).

[5] C. Jacoboni - P. Lugli, *The MonteCarlo Method for Semiconductor Device simulation,* Springer-Verlag, Berlin (1989).

[6] L.D. Landau - E.M. Lifshitz, *Quantum Mechanics,* Pergamon Press (1964).

[7] A. Messiah, *Mecanique Quantique,* Dunod, Paris (1965).

[8] H. Moock, *Ein deterministisches Teilchenverfahren zur Simulation der Boltzmann Vlasov Gleichung für Halbleiter,* Ph.D. Thesis, University of Kaiserslautern, 1992.

[9] P.M. Morse - H. Feshbach, *Methods of Theoretical Physics,* McGraw-Hill, New-York (1953).

[10] S. Motta - G. Russo - H. Moock - J. Wick, *A Number-theoretical Convergence Proof of a Point Approximation of a Space Homogeneous Transport Equation,* Le Matematiche XLI (1986), pp. 161-178.

[11] S. Motta - G. Russo - H. Moock - J. Wick, *Point Approximation of a Space Homogeneous Transport Equation,* Numer. Math. 56 (1990), pp. 763-774.

[12] S. Motta - J. Wick, *A New Numerical Method for Kinetic Equations in Several Dimensions,* Computing 46 (1991), pp. 223-232.

[13] B. Niclot - P. Degond - F. Poupaud, *Deterministic Particle Simulation of the Boltzmann transport equation of semiconductors,* J. Comp. Phys 78 (1988), pp. 313-349.

[14] L. Reggiani (Ed.), *Hot-Electron Transport in Semiconductors,* Springer Verlag, Berlin (1985).

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