THE CRF-METHOD FOR SEMICONDUCTORS' INTRAVALLY COLLISION KERNELS: II - The 3D 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 this paper we use the CRF-method for the semiconductors' intravalley collision kernels. We extend the results obtained in a previous paper to the case of a 3D momentum space.

1. Introduction.

Semiconductors kinetic transport equation has been usually treated numerically using the Monte Carlo methods [5], [6]. For a few years Deterministic Particles Methods have been proposed as an alternative scheme for this class of problems [3], [4], [10], [11], [13]. In this framework the CRF-method for kinetic equations has been recently presented [2], [12]. The idea of the 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

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the numerical effort depends only on the desired accuracy and not directly on
the dimension of the phase space. In a previous paper [1] we have derived the
relevant quantities needed for the numerical scheme in a 2D momentum space
for the intravalley semiconductors kernels. In this paper we present the same
analysis in a 3D momentum space.

We assume that the energy-momentum relationship can be treated in the parabolic
approximation. Under this assumption the natural coordinate system for the
problem is the spherical one. Then one should use the CRF-method formulation
in generalized coordinates [2]. As shown in [1] one can use the existing similari-
ties between the semiconductors' intravalley collision kernels to identify three
different model kernels. This will optimize the analytical work and reduce the
implementation effort.

2. 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

\[ Q(f) = \int_{\Omega} \left( S(k', k) f(k') (1 - f(k)) - S(k, k') f(k) (1 - f(k')) \right) \, dk' \]

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 case
these factors do not contributes since it is always assumed \( f \ll 1 \) [6].

The transition probability \( S(k, k') \) from the initial state \( k \) to the final state
\( k' \), having energies \( \varepsilon \) and \( \varepsilon' \), due to a given interaction mechanisms, is given [6],
[14]

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

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 [6].

In the previous paper [1] we have pointed out that most of the relevant
intvalley interaction mechanism can be described – by suitably changing the
meaning and the values of the constants – through three model kernels

\[ S(k, k') = A\delta(k'^2 - k^2 + \varphi) \]
\[ S(k, k') = \frac{A}{||k - k'||^2} \delta(k'^2 - k^2 + \varphi) \]

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

Here we have used the parabolic approximation \( \varepsilon = \hbar k^2/2m^* \). The constant \( \varphi \) is obviously suitably defined.

All the other relevant kernels can then be derived from these [4] and one can minimize both the analytical effort and the code writing.

As shown in section 2 of [1] the solution of the equation of motion reduces to the computation of the vector field \( g \). We are involved in computing the r.h.s. of the equation (15) of [1], i.e. the \( \Psi^i \). Here we want to use spherical coordinates. For this purpose let \((\xi_1, \xi_2, \xi_3), (k_1, k_2, k_3)\) respectively the Cartesian and the spherical coordinates, \( \Omega_k = [\alpha_1, \beta_1] \times [0, \pi] \times [0, 2\pi] \), and denote by \( T \) the coordinate transformation from \( \{\xi\} \rightarrow \{k\} \) and by \( |T| = k_1^2 \sin k_2 \) 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

\[ \tilde{Q}(\tilde{f}(k_1, k_2, k_3)) = \tilde{G}(k_1, k_2, k_3) - \tilde{L}(k_1, k_2, k_3) \]

where \( \tilde{G} \) and \( \tilde{L} \) are given by

\[ \tilde{G}(k_1, k_2, k_3) = \int_{\Omega_{\mu}} S(\mu_1, \mu_2, \mu_3, k_1, k_2, k_3) \tilde{f}(\mu_1, \mu_2, \mu_3) k_1^2 \sin k_2 \, d\mu \]

\[ \tilde{L}(k_1, k_2, k_3) = \tilde{f}(k_1, k_2, k_3) \tilde{C}(k_1, k_2, k_3) \]

with

\[ \tilde{C}(k_1, k_2, k_3) = \int_{\Omega_{\mu}} S(k_1, k_2, k_3, \mu_1, \mu_2, \mu_3) \mu_1^2 \sin \mu_2 \, d\mu \]

where \( \mu = (\mu_1, \mu_2, \mu_3) \). Then the \( \Psi^i(\gamma_i) \) can be written in the form

\[ \Psi^i(\gamma_i) = -\Psi_G^i(\gamma_i) + \Psi_L^i(\gamma_i). \]

To evaluate the \( \Psi^i(\gamma_i) \) for \( i = 1, 2, 3 \) we can proceed as in [1]:

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

\[ \tilde{f}(t, k_1, k_2, k_3) = f(t, k_1, k_2, k_3) |T| = \]

\[ = \frac{1}{N} \sum_{j=1}^{N} \delta(k_1 - k_{1,j}) \delta(k_2 - k_{2,j}) \delta(k_3 - k_{3,j}); \]

2. Compute \( \tilde{G}(k) \) and \( \tilde{L}(k) \);

3. Compute \( \Psi^i(\gamma_i), i = 1, 2, 3, \) separately for \( \tilde{G}(k) \) and \( \tilde{L}(k) \).

After some algebra, variable transformations and appropriate use of the Heaviside function \( H(\cdot) \) we get the following results.
1. MODEL KERNEL (2).

\[ \tilde{G}(k) = \frac{1}{N} \sum_{j=1}^{N} S(k_j, k) \]

\[ \tilde{C}(k) = 2\pi A \sqrt{k_1^2 - \varphi} H \left[ (k_1^2 - \varphi - \alpha_1^2)(\beta_1^2 - k_1^2 + \varphi) \right]. \]

Then we compute the \( \Psi \) components. Setting \( a_j = k_{1,j}^2 - \varphi \) for the first component we get

\[ \Psi^1_G(\gamma_1) = \frac{2\pi A}{N} \sum_{j=1}^{N} (\gamma_1 - \sqrt{a_j}) \sqrt{a_j} H[(a_j - \alpha_1^2)(\gamma_1^2 - a_j)] \]

\[ \Psi^1_L(\gamma_1) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_1 - k_{1,j}) \tilde{C}(k_j) H(\gamma_1 - k_{1,j}). \]

For the second component we get

\[ \Psi^2_G(\gamma_2) = \frac{\pi A(\gamma_2 - \sin \gamma_2)}{N} \sum_{j=1}^{N} \sqrt{a_j} H[(a_j - \alpha_1^2)(\beta_1^2 - a_j)] \]

\[ \Psi^2_L(\gamma_2) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_2 - k_{2,j}) \tilde{C}(k_j) H(\gamma_2 - k_{2,j}). \]

For the third component we get

\[ \Psi^3_G(\gamma_3) = \frac{A\gamma_3^2}{2N} \sum_{j=1}^{N} \sqrt{a_j} H[(a_j - \alpha_1^2)(\beta_1^2 - a_j)] \]

\[ \Psi^3_L(\gamma_3) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_3 - k_{3,j}) \tilde{C}(k_j) H(\gamma_3 - k_{3,j}). \]

We note that in the elastic limit we get \( \Psi^1_G(\gamma_1) = \Psi^1_L(\gamma_1) \) as required.
2. MODEL KERNEL (3).

\begin{equation}
\widetilde{G}(k) = \frac{1}{N} \sum_{j=1}^{N} \tilde{S}(k_j, k) \tag{17}
\end{equation}

\begin{equation}
\widetilde{C}(k) = \frac{A}{2} \sqrt{k_i^2 - \varphi F(k) H \left[ (k_i^2 - \varphi - \alpha_1^2)(\beta_1^2 - k_1^2 + \varphi) \right]} \tag{18}
\end{equation}

where

\begin{equation}
F(k) = \int_0^{\pi} \int_0^{2\pi} \frac{\sin k'_2 \, dk'_2 \, dk'_3}{2k_i^2 - \varphi - 2k_1 \sqrt{k_1^2 - \varphi} \left[ \sin k_2 \sin k'_2 \cos(k_3 - k'_3) + \cos k_2 \cos k_3 \right]} \tag{19}
\end{equation}

Then we compute the \( \Psi \) components. Setting \( a_j = k_{1,j}^2 - \varphi \) for the first component we get

\begin{equation}
\Psi_1^L(\gamma_1) = \frac{A}{2N} \sum_{j=1}^{N} (\gamma_1 - \sqrt{a_j}) \sqrt{a_j} F_1(\sqrt{a_j}, k_j) H \left[ (a_j - \alpha_1^2)(\gamma_1^2 - a_j) \right] \tag{20}
\end{equation}

\begin{equation}
\Psi_1^L(\gamma_1) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_1 - k_{1,j}) \widetilde{C}(k_j) H(\gamma_1 - k_{1,j}) \tag{21}
\end{equation}

where

\begin{equation}
F_1(k'_1, k_j) = \int_0^{\pi} \int_0^{2\pi} \frac{\sin k_2 \, dk_2 \, dk_3}{k_{1,j}^2 + k_1^2 - 2k_{1,j}k_1' \left[ \sin k_{2,j} \sin k_2 \cos(k_{3,j} - k_3) + \cos k_{2,j} \cos k_2 \right]} \tag{22}
\end{equation}

For the second component we get

\begin{equation}
\Psi_2^L(\gamma_2) = \frac{A}{2N} \sum_{j=1}^{N} \sqrt{a_j} H \left[ (a_j - \alpha_1^2)(\beta_1^2 - a_j) \right] \int_0^{\gamma_2} F_2(k_2, k_j) \, dk_2 \tag{23}
\end{equation}

\begin{equation}
\Psi_2^L(\gamma_2) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_2 - k_{2,j}) \widetilde{C}(k_j) H(\gamma_2 - k_{2,j}) \tag{24}
\end{equation}
where

\[ F_2(k_2, k_j) = \int_0^{2\pi} \int_0^{k_2} \frac{\sin k'_2 \, dk'_2 \, dk_3}{k^2_{1,j} + a_j - 2k_{1,j} \sqrt{a_j} \left[ \sin k_{2,j} \sin k'_2 \cos (k_{3,j} - k_3) + \cos k_{2,j} \cos k'_2 \right]} \]

For the third component we get

\[ \Psi^3_G(\gamma_3) = \frac{A}{2N} \sum_{j=1}^{N} \sqrt{a_j} H \left[ (a_j - \alpha_1^2)(\beta_1^2 - a_j) \right] \int_0^{\gamma_3} F_3(k_3, k_j) \, dk_3 \]

\[ \Psi^3_L(\gamma_3) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_3 - k_{3,j}) \tilde{C}(k_j) H(\gamma_3 - k_{3,j}) \]

where

\[ F_3(k_3, k_j) = \int_0^{\pi} \int_0^{k_3} \frac{\sin k_2 \, dk_2 \, dk'_2}{k^2_{1,j} + a_j - 2k_{1,j} \sqrt{a_j} \left[ \sin k_{2,j} \sin k_2 \cos (k_{3,j} - k'_3) + \cos k_{2,j} \cos k'_2 \right]} \]

The calculation of the integral functions defined by equations (22), (25) and g is presented in appendix A, while the r.h.s. integrals in (23) and (26) must be computed numerically.

Furthermore we note that in the elastic limit we get \( \Psi^1_G(\gamma_1) = \Psi^1_L(\gamma_1) \) as required.

3. MODEL KERNEL (4).

\[ \tilde{G}(k) = \frac{1}{N} \sum_{j=1}^{N} \tilde{S}(k_j, k) \]

\[ \tilde{C}(k) = \frac{A}{2} k_1 F(k) H \left[ (k^2_1 - \alpha_1^2)(\beta_1^2 - k_1^2) \right] \]

where

\[ F(k) = \int_0^{\pi} \int_0^{2\pi} \frac{\sin k'_2 \, dk'_2 \, dk'_3}{\left[ 2k_1^2 - 2k_1^2 (\sin k_2 \sin k'_2 \cos (k - k'_3) + \cos k_2 \cos k'_2) + \beta^2 \right]^2} \]
Then we compute the $\Psi$ components. For the first component we get

\begin{equation}
\Psi^1_G(\gamma_1) = \frac{A}{2N} \sum_{j=1}^{N} k_{1,j}(\gamma_1 - k_{1,j}) F_1(k_{1,j}, k_j) H(\gamma_1^2 - k_{1,j})
\end{equation}

\begin{equation}
\Psi^1_L(\gamma_1) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_1 - k_{1,j}) \tilde{C}(k_j) H(\gamma_1 - k_{1,j})
\end{equation}

where

\begin{equation}
F_1(k_{1}', k_j) = \int_0^\pi \int_0^{2\pi} \frac{\sin k_2 \, dk_2 \, dk_3}{\left[ \alpha - 2k_{1,j}k_1' \left( \sin k_2 \sin k_2 \cos(k_{3,j} - k_3) + \cos k_{2,j} \cos k_2 \right) \right]^2}
\end{equation}

with $\alpha = k_{1,j}^2 + k_1'^2 + \beta^2$.

For the second component we get

\begin{equation}
\Psi^2_G(\gamma_2) = \frac{A}{2N} \sum_{j=1}^{N} k_{1,j}^2 \int_0^{\gamma_2} F_2(k_2, k_j) \, dk_2
\end{equation}

\begin{equation}
\Psi^2_L(\gamma_2) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_2 - k_{2,j}) \tilde{C}(k_j) H(\gamma_2 - k_{2,j})
\end{equation}

where

\begin{equation}
F_2(k_2, k_j) = \int_0^{2\pi} \int_0^{k_2} \frac{\sin k_2' \, dk_2' \, dk_3}{\left[ 2k_{1,j}^2 - 2k_{1,j}' \left( \sin k_2 \sin k_2' \cos(k_{3,j} - k_3) + \cos k_{2,j} \cos k_2' \right) + \beta^2 \right]^2}
\end{equation}

For the third component we get

\begin{equation}
\Psi^3_G(\gamma_3) = \frac{A}{2N} \sum_{j=1}^{N} k_{1,j} \int_0^{\gamma_3} F_3(k_3, k_j) \, dk_3
\end{equation}
\[ \Psi^3_L(\gamma_3) = \frac{1}{N} \sum_{j=1}^{N} (\gamma_3 - k_{3,j}) \tilde{C}(k_j) H(\gamma_3 - k_{3,j}) \]

where

\[ F_3(k_3, k_j) = \int_0^{\pi} \int_0^{k_3} \frac{\sin k_2 \, dk_2 \, dk'_3}{\left[ 2k_{1,j}^2 - 2k_{1,j}' \sin k_2 \cos(k_3,j - k'_3) + \cos k_2 \cos k_2 + \beta^2 \right]^2} \]

The calculation of the integral functions defined by equations (34), (37) and (40) is presented in appendix A, while the r.h.s. integrals in (35) and (38) 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 (32) and (33).

3. 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 [2]. For this we have computed the relevant quantities for the application of the method to intravalley model kernels in a 3D momentum space.

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Appendix A.

In this appendix we compute the integral functions defined by equations (22), (25), (28), (34), (37) and (28).

We consider first the integral functions (22), (25), (28). These can be written in the following equivalent ways

\[ F_1(k'_1, k_j) = \int_0^{\pi} \tilde{F}_1(k'_1, k_2, k_j) \sin k_2 \, dk_2 \]

\[ = \int_0^{2\pi} \tilde{F}_1(k'_1, k_3, k_j) \, dk_3 \]
\[ F_2(k_2, k_j) = \int_0^{k_2} F_2(\tilde{k}_2', k_j) \sin \tilde{k}_2' \, d\tilde{k}_2' \]
\[ = \int_0^{2\pi} \tilde{F}_2(k_2, k_3, k_j) \, dk_3 \]
\[ F_3(k_3, k_j) = \int_0^{k_3} \tilde{F}_3(k_3', k_j) \, dk_3 \]
\[ = \int_0^{\pi} \tilde{F}_3(k_2, k_3, k_j) \sin k_2 \, dk_2 \]

where

\[ \tilde{F}_1(k_1', k_2, k_j) = \int_0^{2\pi} \frac{dk_3}{\bar{a}_1 - \bar{b}_1 \cos(k_3 - k_3')} \]
\[ \tilde{F}_1(k_1', k_3, k_j) = \int_0^{\pi} \frac{\sin k_2}{\bar{a}_1 + \bar{b}_1 \sin k_2 + \bar{c}_1 \cos k_2} \, dk_2 \]
\[ \tilde{F}_2(k_2', k_j) = \int_0^{2\pi} \frac{dk_3}{\bar{a}_2 - \bar{b}_2 \cos(k_3 - k_3')} \]
\[ \tilde{F}_2(k_2, k_3, k_j) = \int_0^{k_2} \frac{\sin \tilde{k}_2'}{\bar{a}_2 + \bar{b}_2 \sin \tilde{k}_2' + \bar{c}_2 \cos \tilde{k}_2'} \, d\tilde{k}_2' \]
\[ \tilde{F}_3(k_3', k_j) \, dk_3 = \int_0^{\pi} \frac{\sin k_2}{\bar{a}_3 + \bar{b}_3 \sin k_2 + \bar{c}_3 \cos k_2} \, dk_2 \]
\[ \tilde{F}_3(k_2, k_3, k_j) = \int_0^{k_3} \frac{dk_3'}{\bar{a}_3 - \bar{b}_3 \cos(k_3' - k_3')} \]

with

\[ \bar{a}_1 = \bar{k}_{1,j}^2 + k_1' - 2k_{1,j}k_1' \cos k_{2,j} \cos k_2 \]
\[ \bar{b}_1 = 2k_{1,j}k_1' \sin k_{2,j} \sin k_2 \]
\[ \bar{a}_2 = \bar{k}_{1,j}^2 + a_j - 2k_{1,j} \sqrt{\bar{a}_1} \cos k_{2,j} \cos k_2' \]
\[ \bar{b}_2 = 2k_{1,j} \sqrt{\bar{a}_1} \sin k_{2,j} \sin k_2' \]
\[ \bar{a}_3 = \bar{k}_{1,j}^2 + a_j - 2k_{1,j} \sqrt{\bar{a}_1} \cos k_{2,j} \cos k_2 \]
\[ \bar{b}_3 = 2k_{1,j} \sqrt{\bar{a}_1} \sin k_{2,j} \sin k_2 \]
and

\[ \tilde{a}_1 = k_{1,j}^2 + k_1' \]
\[ \tilde{b}_1 = -2k_{1,j}k_1' \sin k_{2,j} \cos (k_{3,j} - k_3) \]
\[ \tilde{c}_1 = -2k_{1,j}k_1' \cos k_{2,j} \]
\[ \tilde{a}_2 = k_{1,j}^2 + a_j \]
\[ \tilde{b}_2 = -2k_{1,j} \sqrt{a_j} \sin k_{2,j} \cos (k_{3,j} - k_3) \]
\[ \tilde{c}_2 = -2k_{1,j} \sqrt{a_j} \cos k_{2,j} \]
\[ \tilde{a}_3 = k_{1,j}^2 + a_j \]
\[ \tilde{b}_3 = -2k_{1,j} \sqrt{a_j} \sin k_{2,j} \cos (k_{3,j} - k_3') \]
\[ \tilde{c}_3 = -2k_{1,j} \sqrt{a_j} \cos k_{2,j} \]

We note that the integral functions defined by equations (44), (45), (46), (47), (48) and (49) can be computed analytically (see appendix B and appendix A of [1]), while the integrals on the r.h.s. of the equations (41), (42) and (43) must be computed numerically. Moreover, as pointed out, there are two equivalent ways to compute the integral functions \( F_1 \), \( F_2 \) and \( F_3 \). The choice of the most convenient way needs to be carefully evaluated.

We now consider the integral functions (34), (37), (40). These can also be written in the forms (41), (42) and (43) respectively, where

\[ \tilde{F}_1(k_1', k_2, k_j) = \int_0^{2\pi} \frac{dk_3}{[\tilde{a}_1 - \tilde{b}_1 \cos (k_{3,j} - k_3)]^2} \]  
\[ \tilde{F}_1(k_1', k_3, k_j) = \int_0^{2\pi} \frac{cos k_2}{[\tilde{a}_1 + \tilde{b}_1 \sin k_2 + \tilde{c}_1 \cos k_2]^2} \]  
\[ \tilde{F}_2(k_2', k_j) = \int_0^{2\pi} \frac{dk_3}{[\tilde{a}_2 - \tilde{b}_2 \cos (k_{3,j} - k_3)]^2} \]  
\[ \tilde{F}_2(k_2, k_3, k_j) = \int_0^{k_2} \frac{cos k_2'}{[\tilde{a}_2 + \tilde{b}_2 \sin k_2' + \tilde{c}_2 \cos k_2']^2} \]  
\[ \tilde{F}_3(k_3', k_j) = \int_0^{2\pi} \frac{cos k_2}{[\tilde{a}_3 + \tilde{b}_3 \sin k_2 + \tilde{c}_3 \cos k_2]^2} \]
\[
F_3(k_2, k_3, k_j) = \int_0^{k_3} \frac{dk_3'}{[\bar{a}_3 - \bar{b}_3 \cos(k_{3,j} - k_3')]^2}
\]

with
\[
\bar{a}_1 = k_{1,j}^2 + k_1' + \beta^2 - 2k_{1,j}k_1' \cos k_{2,j} \cos k_2,
\bar{b}_1 = 2k_{1,j}k_1' \sin k_{2,j} \sin k_2,
\bar{a}_2 = 2k_{1,j}^2 + \beta^2 - 2k_{1,j}^2 \cos k_{2,j} \cos k_2,
\bar{b}_2 = 2k_{1,j}^2 \sin k_{2,j} \sin k_2,
\bar{a}_3 = 2k_{1,j}^2 + \beta^2 - 2k_{1,j}^2 \cos k_{2,j} \cos k_2,
\bar{b}_3 = 2k_{1,j}^2 \sin k_{2,j} \sin k_2
\]

and
\[
\bar{c}_1 = -2k_{1,j}k_1' \sin k_{2,j} \cos (k_{3,j} - k_3),
\bar{c}_1 = -2k_{1,j}k_1' \cos k_{2,j},
\bar{c}_2 = 2k_{1,j}^2 + \beta^2,
\bar{c}_2 = -2k_{1,j}^2 \sin k_{2,j} \cos (k_{3,j} - k_3),
\bar{c}_3 = 2k_{1,j}^2 + \beta^2,
\bar{c}_3 = -2k_{1,j}^2 \sin k_{2,j} \cos (k_{3,j} - k_3),
\bar{c}_3 = -2k_{1,j}^2 \cos k_{2,j}.
\]

Also in this case the integral functions defined by equations (50), (51), (52), (53), (54) and (55) can be computed analytically (see appendix B and appendix A of [1]), while the integrals on the r.h.s. of the equations (41), (42) and (43) must be computed numerically. Again the choice of the most convenient way to perform the integration needs to be carefully evaluated.

Appendix B.

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 integral
\[
I(x) = \int \frac{\sin x}{a + b \sin x + c \cos x} \, dx
\]
where \( a, b, c \) are real constants with \( a^2 > b^2 + c^2 \) and \( a \neq c \). The primitive \( I(x) \) can be computed analytically. Let

\[
p = \frac{2b}{a-c},
\]

\[
q = \frac{a+c}{a-c},
\]

\[
t = \tan \frac{x}{2}.
\]

Then we get

\[
I(x) = \frac{4}{a-c} \int \frac{t}{(1+t^2)(t^2+pt+q)} \, dt.
\]

The r.h.s. integral of the equation (57) can be split in the following way

\[
\int \frac{t}{(1+t^2)(t^2+pt+q)} \, dt = \int \frac{At+B}{1+t^2} \, dt + \int \frac{Ct+D}{t^2+pt+q} \, dt
\]

where \( A, B, C, D \) are the following constants

\[
A = \frac{q-1}{p^2 + (q-1)^2},
\]

\[
B = \frac{p}{p^2 + (q-1)^2},
\]

\[
C = -A
\]

\[
D = -qB.
\]

The integrals on the r.h.s. of the equation (58) can be easily calculated and we have

\[
\int \frac{At+B}{1+t^2} \, dt = \frac{A}{2} \log(1+t^2) + B \arctan t
\]

\[
\int \frac{Ct+D}{t^2+pt+q} \, dt = \frac{C}{2} \log(t^2+pt+q) + \left( D - \frac{pC}{2} \right) \frac{2}{\sqrt{4q-p^2}} \arctan \frac{2t+p}{\sqrt{4q-p^2}}.
\]
We note that, if \( \pi \in [\alpha, \beta] \), we have

\[
\int_{\alpha}^{\beta} \frac{\sin x}{a + b \sin x + c \cos x} \, dx = I(\pi^-) - I(\alpha) + I(\beta) - I(\pi^+).
\]

We now consider the integral

\[
(59) \quad J(x) = \int \frac{\sin x}{(a + b \sin x + c \cos x)^2} \, dx
\]

where \( a, b, c \) are real constants with \( a^2 > b^2 + c^2 \) and \( a \neq c \). Again the primitive can be obtained in a closed form

\[
(60) \quad J(x) = -\frac{1}{2(a - c)(t^2 + pt + q)} - \frac{8p\sqrt{4q - p^2}}{2(a - c)(4q - p^2)} \left\{ \frac{1}{2} \arctan y + \frac{y}{2(1 + y^2)} \right\}.
\]

where

\[
p = \frac{2b}{a - c}
\]

\[
q = \frac{a + c}{a - c}
\]

\[
t = \tan \frac{x}{2}
\]

\[
y = 2t + p\sqrt{4q - p^2}.
\]

Also in this case, if \( \pi \in [\alpha, \beta] \), we have

\[
\int_{\alpha}^{\beta} \frac{\sin x}{(a + b \sin x + c \cos x)^2} \, dx = J(\pi^-) - J(\alpha) + J(\beta) - J(\pi^+).
\]
REFERENCES


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