MATHEMATICAL ASPECTS OF THE SCATTERING MATRIX APPROACH

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ABSTRACT

In this paper, we formulate the Boltzmann equation in terms of scattering matrices and examine the uniqueness and convergence of the solution of the reformulated equations. We also study the properties of orthogonal transformation of scattering matrices and prescribe a device simulation algorithm using Hermite polynomials.

1. INTRODUCTION:

In recent years there have been considerable interest in different techniques for directly solving the space dependent Boltzmann equation. These techniques include the Monte Carlo method [1], the hydrodynamic approach [2], the spectral technique [3], the Scattering Matrix Approach (SMA)[4] etc. The Scattering matrix approach was originally developed as a physically based extension of McKelvey's flux method [5]. In this paper, we give a brief derivation of the SMA from the Boltzmann equation, formally prove the algorithm for device simulation using the SMA with an emphasis on convergence and uniqueness of the solution. Details of this work will appear in ref. [6]. We also present an algorithm for device simulation using orthogonal polynomials which is expected to reduce the memory requirement of the SMA.

2. THE BOLTZMANN EQUATION AND SMA:

The steady state path integral formulation of the Boltzmann equation is given by:

$$g(x,k) = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} d^3k' \frac{1}{8\pi^3} S(k_1,k',x') e^{-\int_{x'}^{x} \frac{dx''}{L_m(x'',k'')}} g(x',k'), \tag{1}$$

where $g(x,k)$ is the distribution function, L_m is the steady state mean free path between collisions, $S(k,k',x)$ is the scattering rate as computed from Golden rule divided by local velocity $v_x(k)$. The wavevector k_1 is given by

$$k_1 = k - \frac{eE}{\hbar} \int_{x'}^{x} \frac{dx''}{v_x(k'')}, \tag{2}$$

where the electric field is assumed to be constant. If we define positive flux to be the number of electrons crossing a surface at x, per unit time, from the left to the right, we have

$$J^+(x, k_x > 0, k_t) \Delta k_x \Delta^2 k_t = g(x, k_x, k_t) \Delta k_x \Delta^2 k_t v_x(k) \tag{3}$$

$$J^+(x,k_x,k_t) = \int_{-\infty}^{\infty} d^2k'_t \int_{-\infty}^{\infty} dk'_x \int_{-\infty}^{x} \frac{dx'}{8\pi^3} S(k_1,k',x') e^{-\int_{x'}^{x} \frac{dx''}{L_m(x'',k'')}} v_x(k') g(x',k'). \tag{4}$$

and negative flux is

$$J^-(x, k_x < 0, k_t)\Delta k_x \Delta^2 k_t = g(x, k_x, k_t)\Delta k_x \Delta^2 k_t \mid v_x(k) \mid \tag{5}$$

$$J^-(x, k_x, k_t) = \int_{-\infty}^{\infty} d^2k'_t \int_{-\infty}^{\infty} dk'_x \int_x^{\infty} \frac{dx'}{8\pi^3} S(k_1, k', x') e^{-\int_{x'}^{x} \frac{dx''}{L_m(x'', k'')}} \mid v_x(k') \mid g(x', k'). \tag{6}$$

Differentiating eq. (4,6) and discretizing both real and momentum space, we obtain following set of matrix equations:

$$\begin{aligned} J^+(x + dx, k) = \; & J^+(x, k)(1 - \frac{dx}{L_m(x, k)}) + \sum_{k'_x > 0, k'_t} S(k, k', x) J^+(x, k') dx \\ & + \sum_{k'_x < 0, k'_t} S(k, k', x) J^-(x + dx, k') dx \end{aligned} \tag{7}$$

$$\begin{aligned} J^-(x, k) = \; & J^-(x + dx, k)(1 - \frac{dx}{L_m(x, k)}) + \sum_{k_x > 0, k_t} S(k, k', x) J^+(x, k') dx \\ & + \sum_{k_x < 0, k_t} S(k, k', x) J^-(x + dx, k') dx. \end{aligned} \tag{8}$$

For each wavevector k characterizing a bin in momentum space, there will be two such equations. These equations can be put into a scattering matrix form:

$$\begin{bmatrix} J^+(x+dx,1) \\ J^+(x+dx,2) \\ \vdots \\ J^+(x+dx,n) \\ J^-(x,1) \\ J^-(x,2) \\ \vdots \\ J^-(x,n) \end{bmatrix} = \begin{bmatrix} t^+_{11} & t^+_{12} & \cdots & r^+_{11} & r^+_{12} & \cdots \\ t^+_{21} & t^+_{22} & \cdots & r^+_{21} & r^+_{22} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \\ r^-_{11} & r^-_{12} & \cdots & t^-_{11} & t^-_{12} & \cdots \\ r^-_{21} & r^-_{22} & \cdots & t^-_{21} & t^-_{22} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} J^+(x,1) \\ J^+(x,2) \\ \vdots \\ J^+(x,n) \\ J^-(x+dx,1) \\ J^-(x+dx,2) \\ \vdots \\ J^-(x+dx,n) \end{bmatrix} \tag{9}$$

The matrix elements may be obtained by comparing the above three equations:

$$\begin{aligned} t^+_{ii} &= 1 - \frac{dx}{L_m(i)} \\ t^+_{ij} &= S(ij)dx \\ r^+_{ij} &= S(ij)dx. \end{aligned} \tag{10}$$

In presence of electric field, these matrix elements are modified as:

$$\begin{aligned} t^+_{ii} &= (1 - \frac{dx}{L_m(i)} - \frac{eEdx}{\hbar v_x(i) dk_x}) \\ t^+_{i,i-1} &= S(i, i-1)dx + \frac{eEdx}{\hbar v_x(i) dk_x} \\ r^+_{ij} &= S(ij)dx. \end{aligned} \tag{11}$$

In eq. (11) t^+_{ii} stands for transmission of a incident mode to the same mode at the output. This term equals incident flux less the flux lost to other streams due to scattering within a distance Δx plus contribution due electron drifting from the lower momentum state to the state under consideration. Other terms have similar interpretation.

The above equations proves that Boltzmann equation can be reformulated in terms of scattering matrices, thus establishing the basic assumption of the SMA.

3. ITERATIVE CASCADING OF SCATTERING MATRIX APPROACH:

The cascading technique used to simulate bulk properties in ref.[4] can be formally established by noting that scattering matrices constructed above in Markovian, i.e. the elements are nonnegative and the column sum equals 1. For such a matrix $[M]$, there is unique probability vector with eigenvalue 1, and for an arbitrary vector J_0 that satisfies the relation $J_{n+1} = [M]J_n$, the sequence $J_0, J_1, J_2 \ldots$ converges to eigenvector J_∞ corresponding to eigenvalue 1. In ref. [4], it was assumed that if one injects arbitrary fluxes in different bins of momentum space and repeatedly feeds back the scattered fluxes as incident fluxes, the final solution would correspond to the steady state eigenvector with eigenvalue 1. Repeated feeding back the outscattered fluxes as input is formally equivalent to repeatedly multiplying a vector by the scattering matrix. The above theorem establishes that the procedure is uniquely and absolutely convergent with eigenvalue 1. This proof can be extended to device simulation as well, since that cascading rules used for device simulation join two Markov matrices to form a Markov matrix. Therefore, the entire device can be considered to be one Markov matrix and the above theorem applies to devices. As a consequence, we may conclude that regardless the initial guess, the simulation procedure is uniquely and absolutely convergent for devices with arbitrary field profile.

4. ORTHOGONAL POLYNOMIALS:

A large computer memory requirement is one of the basic limitations of the scattering matrix approach and limits its application to one spatial dimension at the present time. One of the ways to reduce the memory requirement would be to use orthogonal polynomials as basis functions for fluxes. If the distribution functions of the chosen set closely resemble the distribution of fluxes over momentum space, one can, in principle retain only a few coefficients to accurately describe the scattering matrix.

Since flux functions are defined over semi-infinite momentum space along z direction, we chose a set of even order Hermite polynomials as the basis functions. This set can be shown to be both orthogonal and complete for all flux functions.

Let $[M]$ be the scattering matrix computed using rectangular basis. Transforming this matrix to the new basis, we have:

$$[M'] = [B]^{-1}[M][B], \tag{12}$$

where $[B]$ is the orthogonal matrix. The matrix $[M']$ is presumably smaller than the original scattering matrix for comparable accuracy; hence the memory requirement is reduced. However, the transformed matrix $[M']$ is no longer Markovian and as such, is not suitable for device simulation. One can transform the matrix $[M']$ into a Markov matrix $[\tilde{M}]$ by following transformation:

$$[\tilde{m}_{ij}] = [m'_{ij}\frac{w_i}{w_j}], \tag{13}$$

where w_i and w_j are the areas under the curves for the i-th and j-th 2-D Hermite polynomials. Once these matrices are obtained , the device simulation rules prescribed in ref. [4] can be applied to cascade matrices and compute internal fluxes. The relation between coefficient of the internal fluxes computed this way and that of the internal fluxes computed using $[M']$ are related to each other by following relation:

$$\tilde{c}_l = c'_l \frac{w_l}{w_1}. \tag{14}$$

With these known coefficients of Hermite polynomials, we can obtain the flux functions over momentum space and compute all relevant physical parameters using the algorithm of ref. [4].

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