

On the Characteristic Neumann Equation and the Wigner Equation

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For a density matrix $\rho(x_1, x_2)$, the Wigner function $w(r, k)$ is defined as the result of two consecutive transformations:

1. Introduce characteristic coordinates

$$r = (x_1 + x_2)/2$$

$$s = x_1 - x_2$$

and define the sigma function

$$\sigma(r, s) = \rho(r + s/2, r - s/2). \quad (1)$$

2. Fourier transformation of $\sigma(r, s)$ with respect to s gives $w(r, k)$.

In this work we study properties of the sigma function as defined in (1) and its numerical application to quantum transport problems. Our first goal is a comparison with the finite difference Wigner method [2].

Using coordinates (r, s) the von Neumann-Liouville equation with potential energy V takes on its characteristic form:

$$\frac{\partial \sigma}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial}{\partial r} \frac{\partial}{\partial s} \sigma + U \sigma \quad (2)$$

Here the potential term U is defined as $U(r, s) = V(r + s/2) - V(r - s/2)$. Scattering can be included in a relaxation time approximation using the same model as in the finite difference Wigner method.

Differential equation (2) can be transformed into a two-dimensional integral equation of Volterra type, see [5].

$$\sigma(R, S) = \sigma_0(R, S) + \iint_{00}^{RS} U(r, s) dr ds \quad (3)$$

Here the stationary case is assumed and constants have been absorbed into U . The term $\sigma_0(R, S)$ is a solution to the homogeneous equation and is given by boundary conditions (Goursat or Darboux problem). Existence and uniqueness of the solution to (3) can be proved similarly to the ordinary differential case (expand into a Neumann series and check convergence).

In typical quantum transport problems inflow conditions on left and right boundaries are given. We can impose these boundary conditions through a local Fourier transform. The appropriate choice of boundary conditions for upper and lower boundaries is anti-periodic:

$$\sigma(r, s_{max}) = -\sigma(r, -s_{max})$$

This is consistent with Frenslley's discretization as the shifted Fourier transform used in [2] for the Wigner function implies anti-periodic boundary conditions in s -space and periodic boundary conditions in k -space according to Martucci's classification of discrete Fourier transforms [4].

From (2) we can derive the continuity equation $\frac{\partial n}{\partial t} + \frac{\partial j}{\partial r} = 0$, where local carrier density and current density are given by

$$n(r) = \sigma(r, 0), \quad j(r) = \frac{-i\hbar}{m} \frac{\partial \sigma}{\partial s}(r, 0).$$

Frensley's discretization in [2] is based on the use of an equispaced k -mesh. This is necessary to guarantee conservation of mass which, in the Wigner formulation, is a condition non-local in k . In contrast for the sigma equation conservation of mass is a condition local to $s = 0$. Consequently global meshing constraints are less stringent and we are not restricted to the use of an equispaced mesh in s . Discontinuities in U resulting from potential steps can be dealt with by using exact matching conditions.

All operators in (2) can be sparsely discretized. In the stationary case (2) can be solved by a shooting method. No big system matrix needs to be stored and the method can easily be parallelized. Sparsity of operators can be exploited which is a major numerical advantage in comparison with the finite difference Wigner method.

There is a large body of knowledge on the numerical solution of hyperbolic equations and on Volterra integral equations [1] [3]. These methods need to be adapted and specialized for use with (2). A further research topic is incorporation of scattering models beyond the relaxation time approximation.

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1. H. Brunner. "Collocation methods for Volterra integral and related functional equations." Cambridge University Press, 2004.
2. W. R. Frensley. "Boundary conditions for open quantum systems driven far from equilibrium." In: Reviews of Modern Physics **62.3** (1990), pp. 745–791.
3. J. S. Hesthaven and T. Warburton. "Nodal discontinuous Galerkin methods." Springer, 2008.
4. S. A. Martucci. "Symmetric convolution and the discrete sine and cosine transforms." In: IEEE Trans. Sig. Processing SP-**42** (1994), pp. 1038–1051.
5. M. B. Suryanarayana. "On multidimensional integral equations of Volterra type." In: Pacific Journal of Mathematics **41.3** (1972), pp. 809–828.