Posedness of Stationary Wigner Equation

Mihail Nedjalkov[1] and Josef Weinbub[1,2], Mauro Ballicchia[1],
Siegfried Selberherr[1], Ivan Dimov[3], David K. Ferry[4], and Karl Rupp[1]
[1] *Institute for Microelectronics, TU Wien, Austria*
[2] *Christian Doppler Laboratory for High Performance TCAD at the Institute for Microelectronics, TU Wien, Austria*
[3] *IICT Bulgarian Academy of Sciences, Sofia, Bulgaria*
[4] *School of Electrical Computer and Energy Engineering, Arizona State University, USA*
nedjalkov@iue.tuwien.ac.at

The problem about the existence and uniqueness of the Wigner equation solution is directly related to physical and computational aspects of actual quantum transport problems. In the case of evolution problems in presence of initial and boundary conditions, it can be shown that there is a unique solution. However, if we consider the long time limit, giving rise to a stationary Wigner picture, it appears that the equation becomes ill-defined: This is associated to the loss of the time derivative and thus the specific evolution role played by the equation in the set of notions needed to define a phase space quantum mechanics. The Weyl map defines an isomorphism from the algebra of the position and the momentum operators $\hat{x}$, $\hat{y}$ with a product and a commutator $[.,.]_c$ to the algebra of the phase space functions $A(x,p)$ with a non-commutative star ($*$)-product and Moyal bracket $[.,.]_M$. In particular the evolution of the density operator, the von Neumann equation involving the commutator with the Hamiltonian, gives rise via the Moyal bracket to the equation for the Wigner function. The latter carries the information about the evolution of the physical system, but is not sufficient to define independently phase space quantum mechanics: The $*$-product is needed to determine the eigenfunctions to provide a physically admissible initial condition. It has been shown that the Wigner equation in presence of the initial and boundary conditions is well posed, i.e. it has a solution which is unique [1]. The proof is based on the resolvent expansion of the integral form of the equation:

$$f(x,k,t) = \int_0^t dt' \int dk' \, V_w(x(t'), k(t') - k') f(x(t'), k', t) \; + \; f_0(x,k) \tag{1}$$

with $f_0 = f_i\big(x(0), k(0)\big)\theta_\Omega\big(x(0)\big) + f_b\big(x(t_b), k(t_b)\big)\theta_\Omega(t_b)$ and the field-less Newton trajectories $x(t') = x - v(k)(t - t'), k(t') = k$ initialized by x, k, t determine the time crossing the boundary, the time t_B by moving backwards in time, $t' < t$ and f_i and f_b provide two complementary contributions from the initial condition and the boundaries. The equation is of Volterra type with respect to the time variable (Markovian evolution) which allows one to prove convergence of the resolvent series under the very general assumption that the potential is absolutely integrable function. The stationary Wigner equation is obtained by the long time limit of (1), using the change $-\tau = t - t'$: $x(\tau) = x + v(k)(\tau)$; $k(\tau) = k$.

$$f(x,k) = \int_{-t=-\infty}^{0} dt' \int dk' \, V_w(x(\tau), k(t') - k') f(x(\tau), k') \; + \; f_b(x(\tau_b), k) \tag{2}$$

$-\infty < \tau_b < 0$ is now the time for a trajectory initialized by point x at time 0 to reach the boundary moving backwards.

The limit $f(x,k) = \lim_{t'\to\infty} f(x,k,t') = \lim_{t\to\infty} f(x,k,t+\tau)$ defines the stationary solution. Without loss of generality we assumed that the initial condition vanishes in the long time limit. Now we analyze if the existence of the free term f_b in (2) guarantees an unique solution. Or if we formally write the equation as: $(I - \hat{V}_w)f = f_b$, we need to show that the operator $I - \hat{V}_w$ has an inverse operator. This is equivalent to showing that the only solution of the homogeneous equation (2) is the function $f = 0$. We consider the Fourier transform $\tilde{f}(q,k) = 1/2\pi \int dx\, e^{-iqx} f(x,k)$ and use the change $y = x + v(k)\tau$ to obtain:

$$\tilde{f}(q,k) = \frac{1}{2\pi} \int_{-\infty}^{0} d\tau \int dy\, e^{-iqy} e^{-iqv(k)\tau} \int dk'\, V_w(y,k') f(y,k-k') \tag{4}$$

The time integral of the exponent can be evaluated in terms of generalized functions to finally give:

$$\hbar q v(k) \tilde{f}(q,k) = \int dq''\, \tilde{V}(q'') \left(\tilde{f}\left(q - q'', k + \frac{q''}{2}\right) - \tilde{f}\left(q - q'', k - \frac{q''}{2}\right) \right) \tag{5}$$

with $\tilde{V}(q) = 1/2\pi \int dy\, e^{-iqy}\, V(y)$. This equation must be analyzed for existence of non-trivial solutions. Such solutions can be constructed from the stationary Schrödinger equation in momentum space,

$$\big(E - \epsilon(k)\big)\psi(k) = \int dq\, \tilde{V}(q)\psi(k-q); \qquad \epsilon(k) = \frac{\hbar^2 k^2}{2m} \tag{6}$$

As observed by Carruthers et al. [2] in their study of quantum collisions, the function f(q,k) = ψ*(k-q/2) ψ(k+q/2) is a solution of (5). Hence the null space of the operator $I - \hat{V}_w$ contains any stationary solution obtained by (6) and we cannot expect a unique solution corresponding to given boundary conditions. This is in accordance with the results presented in [3].

We associate this problem with the loss of the evolution character of the equation: For eigenstates of the Hamiltonian the stationary Wigner equation reduces to $v(k)\, \partial f(x,k)/\partial x = 0$ with a solution $f(x,k) = \psi(k)$ given by an arbitrary function of k. On the contrary, the evolution problem determined by the time derivative

$$v(k)\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} = \frac{d\, f(x(t),k,t)}{dt} = 0 \tag{7}$$

has a solution $f(x.k,t) = f(x(0),k,0)$ so that a correct physical picture can be obtained by a relevant initial condition $f(x(0),k,0)$ which obeys the uncertainty relations. In conclusion, both the Wigner equation and the $*$ eigenvalue problem are necessary notions of the phase space quantum mechanics. The stationary limit of the former of the former cannot replace the latter and actually lacks physical argumentation.

Acknowledgments: The financial support by the Austrian Science Fund (FWF) through the projects P29406-N30 and P29119-N30, by the Bulgarian National Science Fund (NSF) through the project DN 12/5-2017 and National Scientific Program ICT-SDM-SES, by the Austrian Federal Ministry of Science, Research and Economy, and by the National Foundation for Research, Technology and Development are gratefully acknowledged.

[1] I. Dimov, *et al.*, J. Comput. Electron. **14**, 859 (2015)

[2] P. Carruthers and F. Zachariasen, Rev. Mod. Phys. **55**, 245 (1983)

[3] R. Rosati *et al.*, Phys. Rev. B **88**, 035401 (2013)