Recent Advances of the Wigner Signed-Particle Approach

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The signed-sarticle (SP) interpretation [1] of Wigner quantum mechanics provides a fundamental approach to model a wide range of phenomena, from fully coherent problems, such as interference, to scattering dominated processes, such as Brownian motion. The standard formulation of the latter considers near electrostatic conditions presented by the scalar potential V defining the electric field $\mathbf{E} = -\nabla V$. Generalizations including the magnetic field $\mathbf{B}$ are derived in terms of pseudo-differential operators, where the position dependence of $\mathbf{E}$ and $\mathbf{B}$ is replaced by an operator containing $\nabla_{\mathbf{p}}$. Thus the order of the equation with respect to the momentum derivatives varies with the position dependence of the electromagnetic field. We derive an equation for general, inhomogeneous, and time-dependent electromagnetic conditions, which has an explicit mathematical structure in the sense that the differential and integral operations are fixed and independent on $\mathbf{E}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$. In the case of a homogeneous magnetic field the equation for the Wigner function $f_w(\mathbf{r}, \mathbf{p})$ of the phase space position and momentum variables is:

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{r}} + e\frac{\mathbf{p}}{m} \times \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{p}}\right] f_w(\mathbf{r}, \mathbf{p}, t) = \int d\mathbf{p}' V_w(\mathbf{p} - \mathbf{p}', \mathbf{r}) f_w(\mathbf{r}, \mathbf{p}', t)\,. \qquad (1)$$

Here, V_w is the standard Wigner potential obtained by the Fourier transform $e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}$ of the potential difference $V(\mathbf{r} + \mathbf{s}/2) - V(\mathbf{r} - \mathbf{s}/2)$.

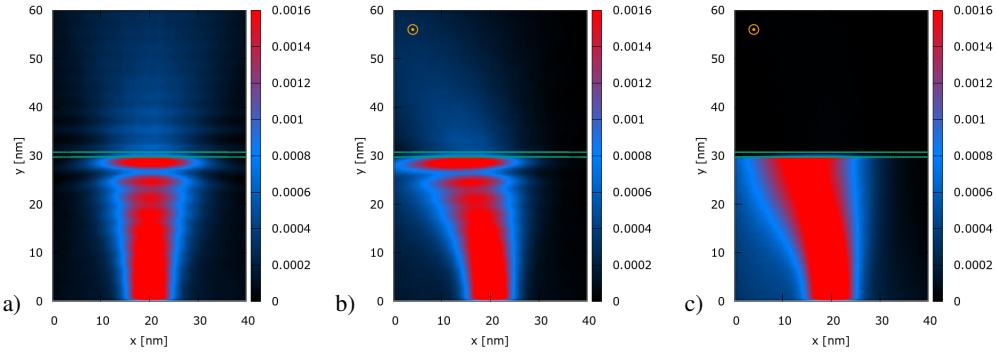

Figure 1: Electron evolution around a $0.2\,\mathrm{eV}$ potential barrier: a) quantum density (a.u.) for $\mathbf{B} = 0$, b) quantum density for $\mathbf{B} = 6\mathrm{T}$, c) classical density for $\mathbf{B} = 6\mathrm{T}$.

The SP concepts have been developed (for a recent review see [1]), by applying the numerical Monte Carlo theory to the integral form of the electrostatic ($\mathbf{B} = 0$) form of Equation 1. The corresponding Neumann series is convergent [2], but the kernel gives rise to a branching Markov chain with ± 1 weight factor of each branch. The stochastic process of construction of the numerical trajectories can be interpreted as a process of generation of positive and negative particles - the SPs, which evolve over fieldless Newtonian trajectories. The Wigner function in a phase space cell is given by the sum of the sign of the particles inside which corresponds to the opposite process of annihilation. A stochastic analysis shows that the numerical approach is generalized for $\mathbf{B} \neq 0$ by a SP evolution over

magnetic force governed Newtonian trajectories. Furthermore, apart from the processes of generation and annihilation, the stochastic evolution is the same as for the classical ballistic Boltzmann equation. The latter can thus be conveniently used as a reference frame to outline quantum processes. We note that magnetic field aware problems are utterly multidimensional and currently only the SP model allows multidimensional computations. As a generic application we demonstrate the effect of the magnetic field on the process of electron tunneling through a potential barrier. In the numerical experiment coherent electrons are injected from the bottom boundary towards the barrier marked by the green line in the middle of the simulation domain, Figure 1. The left picture shows the symmetry of the $\mathbf{B} = 0$ problem. Two important quantum properties are demonstrated: (i) interference effects reveal the wave nature of the evolution, in particular the finite density after the barrier is due to tunneling; (ii) the non-locality of the potential, which affects the electron density far before the barrier. In contrast, classical electrons with energies less than 0.2 eV (the here presented case) are back scattered locally. The magnetic field breaks the symmetry by bending the electron trajectory. Even if the electric field action is still non-local the coherence of the transport is affected. Fig. 1c) shows the density obtained by the solution of the corresponding Boltzmann equation under the action of the same magnetic field. In this case there is no wave-like transport and no tunneling as all particles are reflected back from the barrier. The SP approach has been recently applied also to the study of the quantum coherence effects induced by a single repulsive dopant in the center of a nanowire [3]. The physical setup is the same as in 1a), but the barrier is replaced by a dopant and the lateral boundary conditions are set to reflecting. Due to the reflection the shape of the current resembles a *tulip*, which is much more *closed* in the quantum case, Figure 2a). The reasons for the manifesting current density in the classically *shadowed* region - (i.e., the white area behind the dopant) on Fig. 2b), are twofold: (i) processes of tunneling, and (ii) nonlocal action of the potential, where reflected particles appear close to after the dopant due to the repulsion, occurring further before the dopant. These effects enhance the current as compared to the classical counterpart. *This talk highlights the role of the Monte Carlo SP approach as a powerful method for investigating quantum phenomena in nanoelectronics and physics.*

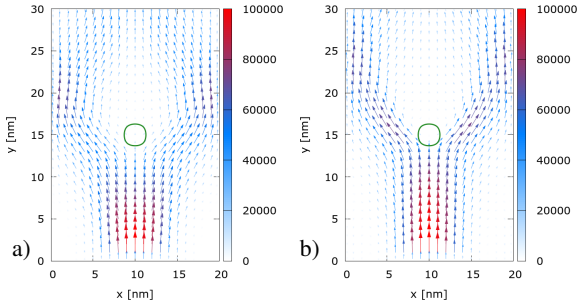

Figure 2: Quantum, (a) and classical (b), current density [a.u.] around a dopant indicated by a green $0.15\,\mathrm{eV}$ isoline.

References

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[3] M. Ballicchia, J. Weinbub, and M. Nedjalkov, *Nanoscale*, 2018, doi:10.1039/c8nr06933.