A High Order Local Solver for Wigner Equation [1]

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In the modeling of nanoscale heterogeneous structure, quantum effects must be included. Several approaches have been suggested such as density matrix, non-equilibrium Green's function and phase space Wigner formalism. Among them Wigner function formalism is suitable for describing time dependent dynamics and connecting quantum and semi-classical regimes.
A few numerical solvers have been proposed in [1, 2, 3, 4]. The major difficulty comes from the global and highly oscillatory nature of the Wigner integral term. Most of the proposed solvers introduce excessive numerical diffusion that overcomes the physical dispersive effects: as a result these solvers have poor agreement with Schrodinger solvers for the pure state simulations. Therefore, the dynamical behavior of the numerical simulation is often strongly dictated by numerical spurious modes.
We present here a new deterministic solver for Wigner equations. High order numerical discretization is employed in order to minimize the spurious numerical dissipation and dispersion. Semi-classical boundary condition is enforced thanks to suitable localization of the Wigner integral kernel. The accurate quantum interference is captured when compared with the corresponding Schrodinger simulation.
In Figs.(1-3), the Gaussian wave packet tunneling process of a single potential barrier is simulated. The height of the potential barrier equals the initial mean energy hence there is a metastable resonant state in the barrier. Fig.1 is the exact solution computed from Schrodinger equation. Fig.2 is the simulation from traditional low order Wigner solver. Fig.3 is the simulation from our newly proposed high order Wigner solver. It is clear from the picture that the high order solver captures accurately quantum interference and the dispersive nature of the process while the numerical dissipation in the low order solver destroys it.

References

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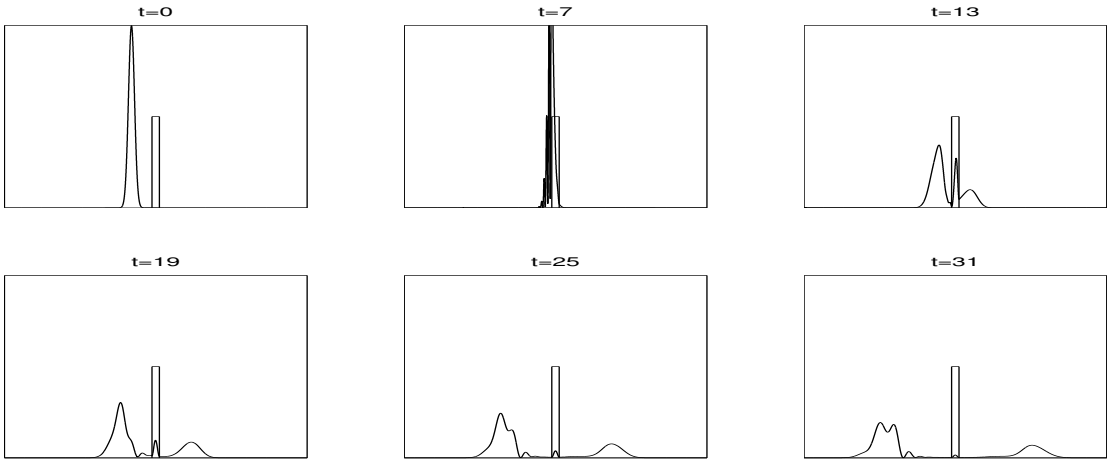

Figure 1: exact solution

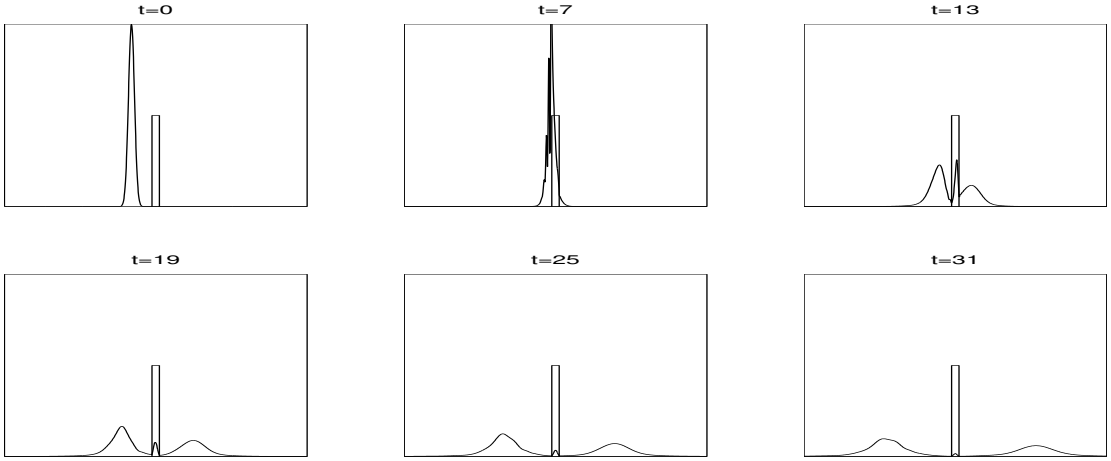

Figure 2: low order solver

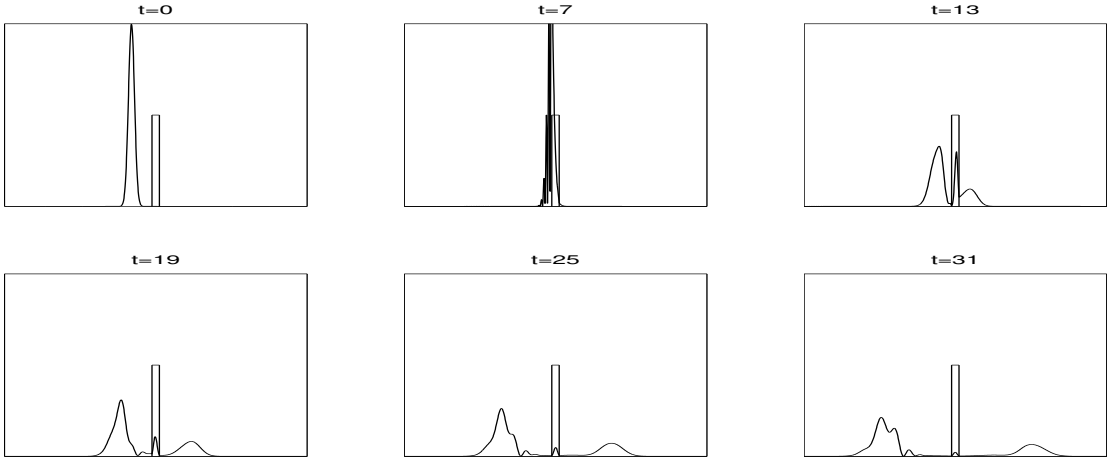

Figure 3: high order solver