Superposed States and the Wigner Approach

J. Cervenka, J. Weinbub

During the development of modern electronic devices quantum-mechanical effects of the carrier transport processes have to be increasingly accounted for. A convenient way of description can be achieved by the Wigner formalism through distribution functions in phase-space. In contrast to classical probability distributions, the distributions in the Wigner picture may also take negative values. Currently, there are stochastic and deterministic approaches in use. In our deterministic method, the critical discretization of the diffusion term is done through the utilization of an integral formulation of the Wigner equation. This deterministic method was studied in the context of superposed quantum states as a precursor to simulations of entangled states.

A superposition of two Schrödinger wave states transforms to Wigner phase-space into a system of two particular states plus an additional term, called the correlation state. Whereas the two particular states show the usual behavior, the correlation term reveals oscillatory behavior with respect to the wave vector and/or the spatial direction. This oscillation holds the phase information of the two base states and its period in x (or k), depending on the distance of those states in k or x, respectively. During time evolution, the particular state packets move according to their k-value and the setup of the applied potentials.

Especially the oscillatory behavior represents a challenge in discretization and calculation of the transport model. The density of the underlying grid has to properly resolve the periods of the distributions. On the other hand, the memory and simulation-time demands have to be feasible. Additional improvements in the performance can be achieved by parallelization. Analysis of the parallelization methods is performed to optimize the communication overhead between the computational units.

Subspace Descent Method

L. Chen, X. Hu, H. Wu

In this work, we propose an optimization algorithm based on subspace decomposition. Our subspace descent (SD) method is inspired by the method of subspace corrections. Under the standard assumptions on the objective function, search directions, and space decomposition, we derive the convergence analysis for both cyclic and random ordering SD. Moreover, accelerated SD is developed based on either Nesterov acceleration or catalyst acceleration. Finally, we show that (block) coordinate descent method from the optimization community and full approximation storage scheme from numerical PDE community can be analyzed under the SD framework.