The Multi-Dimensional Transient Challenge: The Wigner Particle Approach

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The Wigner equation is a full quantum mechanical, time dependent, multi-dimensional transport model which can include, in a natural way, the effects due to elastic, inelastic, and diffusive scattering centers [1]. The first attempts to simulate quantum transport by means of the Wigner formalism were built on finite difference methods and, as such, introduced serious problems in the numerical treatment [2]. This eventually resulted in lost interest in the model. During the last decade Monte Carlo (MC) particle methods which avoid the mentioned problems were developed, which are based, respectively, on quantum affinities [3] and signed particles [4]. We focus on the signed particle MC method which exploits the boundedness of the domain to impose momentum quantization. In a semi-discrete space the Wigner equation reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*}\mathbf{M}\Delta\mathbf{k}\cdot\nabla_{\mathbf{x}} f_W = \\ = \sum_{\mathbf{N}=-\infty}^{+\infty} V_W\left(\mathbf{x},(\mathbf{M}-\mathbf{N}),t\right) f_W(\mathbf{x},\mathbf{N},t)$$

where $f_W = f_W(\mathbf{x},\mathbf{M},t)$ is the unknown pseudo-distribution function, and $V_W = V_W(\mathbf{x},\mathbf{M},t)$ is the semi-discrete Wigner potential. Thus a particle l is characterized by discrete momentum values $\mathbf{n}_l = \mathbf{n}\pi/\mathbf{L}$ with n integer and $\mathbf{L}$ the coherence box. The problem is reformulated as an integral equation [5], whose iterative expansion forks at each application of the kernel into three terms. These can be interpreted as three signed particles - the original one and two newly generated, one of them with opposite sign. The created pair, in turn, generates new pairs, etc. and the mean value of a general macroscopic quantity is provided by $\langle A\rangle = \sum_k A(\mathbf{r}_k,\mathbf{n}_k)sign(k)$, where $\mathbf{r}_k$ is the position of the k-th one. Two particles k and k' with opposite $sign$ and equal $\mathbf{n}$ do not have a net contribution in the limit $\mathbf{r}_k \to \mathbf{r}_{k'}$, thus, they annihilate. The Markovian dynamics allows to reduce the total number of particles to be considered by recording at consecutive time steps. We note the fieldless character of the evolution: In all existing models part of the Wigner potential is used as a force, changing the particle momentum according to Newton's law. It is interesting to see that generation and annihilation of signed particles is an asymptotic alternative to Newton's acceleration [4]. Fig. 1 shows a comparison between Schrödinger and Wigner solutions for a Gaussian packet tunneling trough a barrier. In Fig. 2 a study of the decoherence role for different surface types is shown. Fig. 3 shows a fully three-dimensional Wigner MC simulations with single dopant interactions. Fig. 4 and Fig. 5 represent ab initio calculations of the time-dependent process of bonding creation in a H_2 molecule. Fig. 6 shows a study of charge capture by oxide traps and scattering by single dopants in the channel of a realistic MOSFET.

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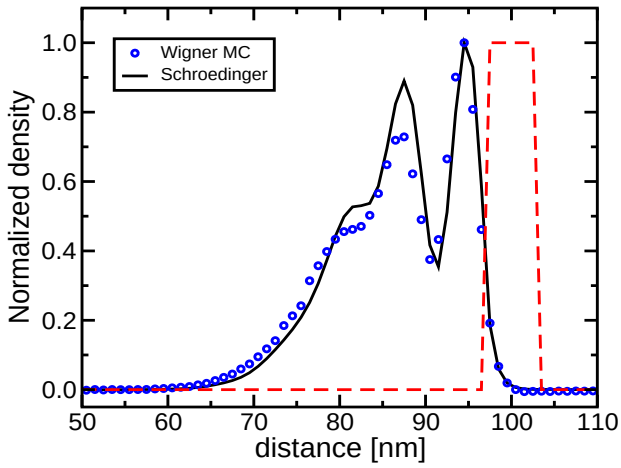

Fig. 1. Comparison at 40fs of Schrödinger and Wigner solutions. An initially Gaussian wave packet evolves in proximity of a potential barrier. The agreement is quantitatively excellent in contrast to alternative approaches which demonstrate only qualitative ressemblance.

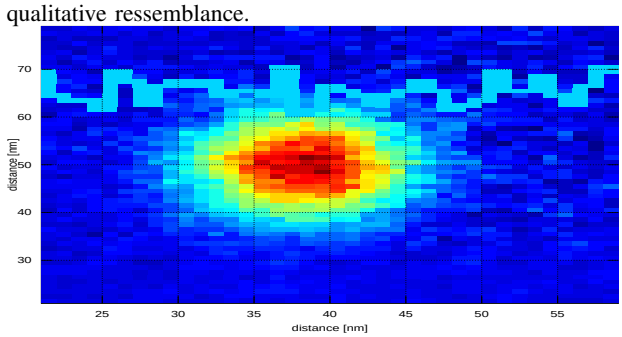

Fig. 2. A rough surface with specular reflection of the incident electron state does not cause decoherence. Au contraire, a random type of reflection causes loss of quantum information.

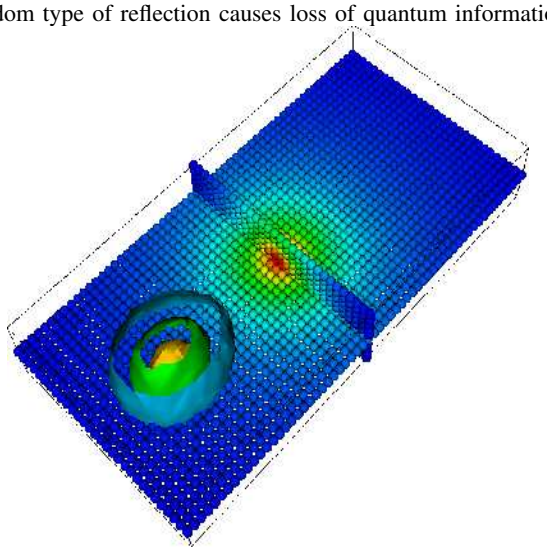

Fig. 3. Three-dimensional electron density in proximity of a Phosphorus dopant. A channel dopant may block an area larger than its geometric characteristics due to the nonlocality of the quantum interaction.

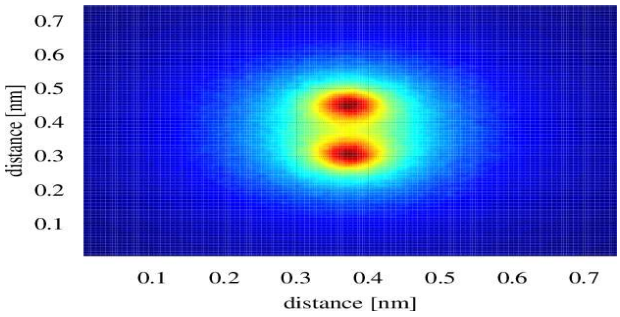

Fig. 4. Electron density in a hydrogenic diatomic molecule. These results are a combination of Wigner Monte Carlo and DFT methods recently developed. The exchange-correlation effects are taken into account by a proper choice of the density functional.

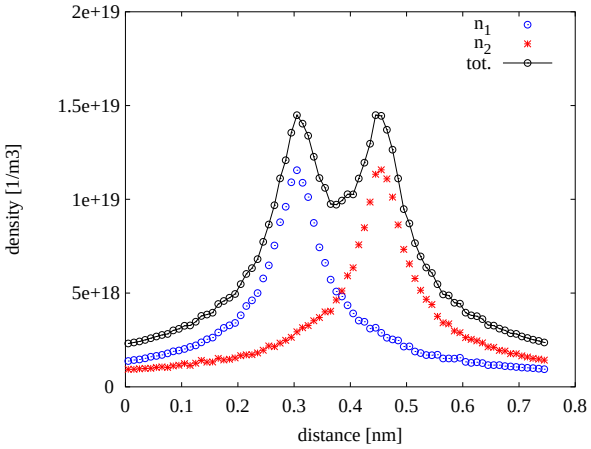

Fig. 5. Cut of the total electron density in a hydrogenic biatomic molecule. A stationary state is reached after about 5 attoseconds. The creaton of a bond (electron density) between the two nuclei is clearly observable.

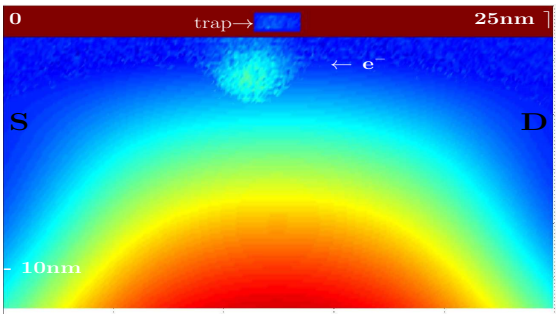

Fig. 6. The electron state moves in a MOSFET potential and charges the trap into the oxide by tunneling trough the thin barrier with the channel.