Modeling Coulomb Interaction with a 'Wigner-Poisson' Coupling Scheme

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Entangled quantum particles, for which operating on one particle instantaneously influences the state of the associated particle, are attractive for carrying quantum information at the nanoscale. However, describing entanglement in traditional time-dependent quantum transport simulations requires doubling the degrees of freedom, involving an almost prohibitive computational effort. Considering electrons, one approach to analyze their entanglement is through modeling the Coulomb interaction (Coulomb Entangler) via the Wigner formalism. We showed that the computational complexity of the time evolution of two interacting electrons is reduced by approximating the Wigner equation in the two-particle phase space by two equations, each defined in a single-particle phase space [1]. In particular, we replace the non-local Wigner potential operator of the electron-electron interaction by an electrostatic field which is introduced through the spectral decomposition of the potential. The coupling between the two equations, based on a consecutive update of the electric field, establishes the entanglement. It is demonstrated that for some particular configurations of an electron-electron system, the introduced approximations are feasible. Purity, identified as the maximal coherence for a quantum state, is analyzed and it is consequently demonstrated that entanglement due to Coulomb interaction is well-accounted for by the introduced local approximation. Fig.1(a) shows the purity of two electrons without Coulomb interaction. The first electron is injected into the simulation region within 60 fs. After the complete injection of the electron the uncertainty rule is satisfied and the purity stabilizes at the perfect value one, which prevails, until the electron starts to exit the simulation region after about 190 fs. The injection of the second electron begins 70 fs after the first one, indicated by the blue curve. In the time interval between $t = 140$ fs and $t = 190$ fs, highlighted by the dashed red lines, both electrons evolve quantum mechanically, without interaction as two independent pure states. Fig.1(b) focuses on this time interval and shows the purity being perfectly equal to one. Fig.2(a) demonstrates the effect of Coulomb repulsion. To better highlight the influence, the charge of each electron is increased by an order of magnitude. Accordingly, at $t = 140$ fs the purity starts to drop at the beginning of the interaction. The level of entanglement due to the Coulomb interaction increases during the evolution, which is well-demonstrated by the continuous decline of the purity. As can be seen in Fig.2(b), the purity evolves equally for both electrons as expected.

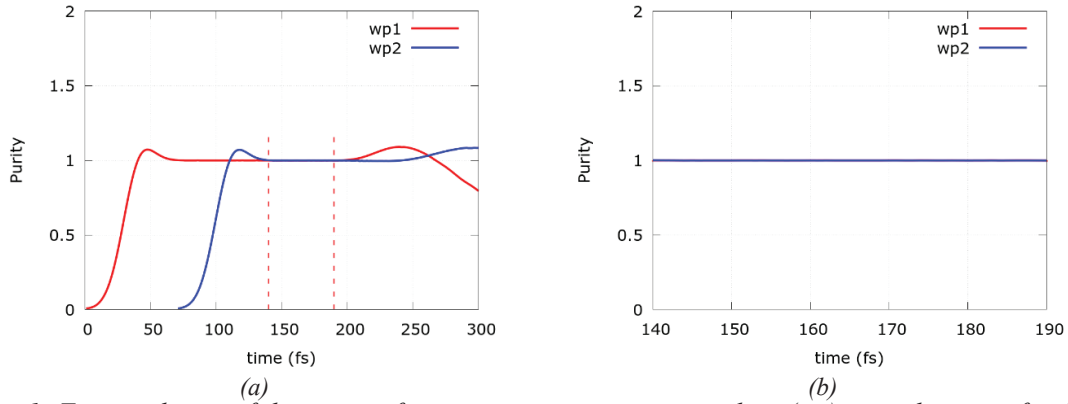[1] M. Benam *et al.*, J. Comput. Electron. 20, 775-784 (2021)

Fig.1: Time evolution of the purity of two non-interacting wavepackets (wp), i.e., electrons, for (a) the entire evolution time (dashed red lines indicate time interval shown in (b)), and (b) the time interval from $t = 140\,fs$ to $t = 190\,fs$. Reprinted with permission from [1]. Copyright 2021 Author(s), licensed under Creative Commons Attribution 4.0 International.
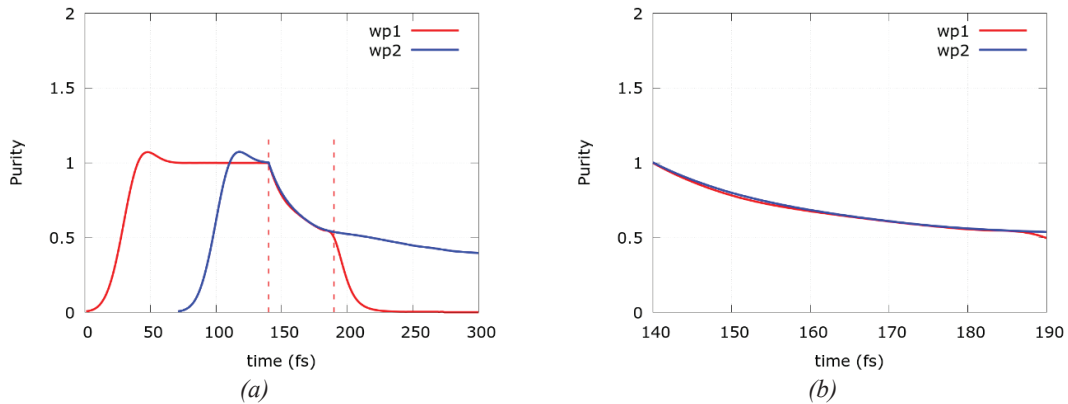

Fig.2: Time evolution of the purity of the two states in the Coulomb Entangler for (a) the entire evolution time (dashed red lines indicate time interval shown in (b)), and (b) the time interval from $t = 140\,fs$ to $t = 190\,fs$. Reprinted with permission from [1]. Copyright 2021 Author(s), licensed under Creative Commons Attribution 4.0 International.