

Combination of the final element and quantum trajectory methods for numerical solution of the wave equation

V.A. Khodyrev¹

Institute of Nuclear Physics, Moscow State University, Moscow 119991, Russia

Synopsis For description of ion-atom collisions the final elements approach is applied in regions close to the nuclei and in the quantum trajectory method is applied in the outer region. Applicability of the quasi-classics at the boundary provide a possibility to join two solutions. The method is computationally efficient and also provides detailed insight into the phenomenon.

Low-energy ion-atom collisions require non-perturbative method of description. However, in these conditions where the phenomenon is developing in a large volume the direct numerical solution of the wave equation is also non-practicable. As is well known the purely classical description, CMTC, often provides realistic results though, seemingly, the applicability of classical mechanics is not guarantied at all.

In the picture of quantum trajectories [1], the wave function is supplemented by a flux of deterministic trajectories. Such interpretation is inspired by the fact that, with the unipolar amplitude-phase ansatz for the wave function $\Psi(\mathbf{r}, t) = R(\mathbf{r}, t)e^{iS(\mathbf{r}, t)/\hbar}$, the Schrödinger equation can be transformed to the classical-like continuity and Hamilton-Jacoby equations. The latter

$$\frac{\partial S}{\partial t} = -\frac{(\nabla S)^2}{2m} - (U + Q)$$

includes all quantum effects by an additional potential term

$$Q = -\frac{1}{2} \frac{\Delta R}{R},$$

the "quantum potential" depending on the derivative of the amplitude $R(\mathbf{r})$.

The idea of the respective computation approach is to follow simultaneously many Bohmian particles according to the classical definition of velocities $\mathbf{v} = \nabla S/m$ with on-the-fly determination of their density. Then, knowing R and S one can reconstruct the wave function. However, realization of this method also encounters with a number of specific problems. Among them are the necessity to approximate the second derivatives of R and coping with the node problem, Q diverges where the amplitude R tends to zero. Additional problem in our case is the singularity of the Coulomb potential.

To cope with these problems we consider the following possibilities. First, quantum effects are localized near the nuclei [2]. Thus, a direct nu-

merical solution is here valuable. For relatively small region this is not a difficult problem, also the effect of Coulomb singularities can be excluded by separation of factors in the wave functions which shape reproduces the Kato cusps. On the other hand, the method of trajectories is well applicable in the outer region. Moreover, assuming that here the amplitude R does not display significant wiggles we may totally disregard the quantum potential Q (proportional to \hbar^2). The only quantum feature left is the phase S , here coinciding with the classical action described by the Lagrange mechanics.

The two solutions should be joined at the boundary of the internal region. Specifically, we need to define how Ψ is evolved in the boundary layer, the boundary conditions for the internal region, and the intensity of emission of the Bohmian particles outward. A clear procedure is constructed when the right-hand part of the Schrödinger equation is presented as follows:

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2}\nabla(\nabla\Psi) + U\Psi,$$

that is the first term as divergence of the "wave function flux" $\nabla\Psi$. Assuming that the quasi-classics works also at the boundary we may use the corresponding expression for the flux

$$\nabla\Psi = iR\mathbf{v}\exp(iS/\hbar).$$

From this ansatz the recipe of solution of the boundary problem immediately follows.

Illustrations of usage of this method will be presented to the Conference.

References

- [1] Wyatt R E 2005 *Quantum Dynamics with Trajectories: Introduction to Quantum Hydrodynamics* (New York: Springer)
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¹E-mail: khodyrev@anna19.sinp.msu.ru

