# SIMULATIONS OF NONIDEAL PLASMAS BY THE METHOD OF MOLECULAR DYNAMICS WITH WAVEPACKET SPLITTING


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## Classical and Wave Packet MD

The method of classical molecular dynamics (MD) is widely used to study equilibrium and nonequilibrium nonideal plasmas [1,2]. At the same time the applicability of MD is restricted to non-degenerate and fully ionized plasmas. The main problems of the classical MD approach are as follows:

– **choice of electron-ion interaction pseudopotential;**

– **dependence of the pseudopotentials on temperature which restricts to the systems close to equilibrium;**

– **presence of the bound states of electrons and ions with incorrect binding energy;**

– **missing of the antisymmetrization effects except some corrections to the pseudo-potentials which reproduce the Pauli blocking.**

One can improve the method of MD without loosing its performance benefits by considering **electrons as wave packets (WP)** [3,4]. The exchange interaction between electrons in the Hartree-Fock limit can be taken into accounts using **antisymmetrized wave packets** [5]. This method was named as **Wave Packet Molecular Dynamics (WPMD)**. However, it causes new problems [6]:

– **spreading of wave packet for a weakly bound electron;**

– **poor accuracy for a bound state of electron and ion when using simple Gaussian wavepackets.**

## Split WPMD Technique

We propose expansion of the wave function for each electron in the bases of multiple Gaussians. Advantages:

➢ **accuracy for bound states is greatly improved;**

➢ **quantum effects related to the wave function splitting are reproduced (tunnel ionization);**

➢ **simultaneous description of bound electrons by WPMD and free electrons by the classical MD becomes possible.**

## Model Description

**Parametrization of an electron wavefunction:**

$$\phi_k(\mathbf{x}) = n_k^{-1/2}\sum_{\alpha=1}^{M_k} c_{k\alpha}\varphi_{k\alpha}(\mathbf{x})$$

*k*-th electron wavefunction; normalizing factor for $\phi_k$: $n_k = \sum_{\alpha,\beta} c_\alpha^* c_\beta \int \varphi_{k\alpha}^*\varphi_{k\beta} d^3x$; complex coefficient $c_{k\alpha}$; Gaussian wavepacket:

$$\varphi_{k\alpha}(\mathbf{x}) = \left(\frac{3}{2\pi s_{k\alpha}^2}\right)^{3/4} e^{-\left(\frac{3}{4s_{k\alpha}^2} - \frac{ip_{s_{k\alpha}}}{2\hbar s_{k\alpha}}\right)(\mathbf{x}-\mathbf{r}_{k\alpha})^2 + \frac{i}{\hbar}\mathbf{p}_{k\alpha}(\mathbf{x}-\mathbf{r}_{k\alpha})}$$

**Dynamical variables** (10 real numbers per wavepacket):

| | |
|---|---|
| $(\mathbf{r}, \mathbf{p})$ | classical-like coordinate and momentum |
| $s$ | width of the packet ( $\gamma > 0$) |
| $p_s$ | "momentum" of the width |
| $c$ | complex coefficient |

**Hamiltonian:** (electron kinetic energy; electron-ion Coulomb interaction; electron-electron Coulomb repulsion; external field potential)

$$\hat H = \hat K^e + \hat V^{ei} + \hat V^{ee} + \hat H_{\rm ext} = -\sum_k \frac{\hbar^2\Delta_k}{2m} - \sum_{k,i}\frac{eq_i}{|\hat{\mathbf{x}}_k - \mathbf{R}_i|} + \sum_{k<m}\frac{e^2}{|\hat{\mathbf{x}}_k - \hat{\mathbf{x}}_m|} + \hat H_{\rm ext}$$

**The total energy for both Hartree and UHF cases in the Split WPMD model:**

$$\begin{aligned} H = &\sum_{\text{same spin }(k,l)} (n_k n_l)^{-\frac12} y_{kl} \sum_{\alpha,\beta} (c_{k\alpha}^* o_{k\alpha l\beta} c_{l\beta})(K^e_{k\alpha l\beta} + V^{ei}_{k\alpha l\beta}) \\ &+ \sum_{\substack{\text{same spin }(k,m),\\ \text{same spin }(l,n)}} (n_k n_l n_m n_n)^{-\frac12} y_{mk} y_{nl} \sum_{\alpha,\beta,\gamma,\delta} (c_{k\alpha}^* o_{k\alpha m\gamma} c_{m\gamma})(c_{l\beta}^* o_{l\beta n\delta} c_{n\delta}) V^{ee}_{k\alpha l\beta m\gamma n\delta} \\ &- k_{exch} \sum_{\substack{\text{same spin}\\ (k,l,m,n)}} (n_k n_l n_m n_n)^{-\frac12} y_{ml} y_{nk} \sum_{\alpha,\beta,\gamma,\delta} (c_{k\alpha}^* o_{k\alpha m\gamma} c_{m\gamma})(c_{l\beta}^* o_{l\beta n\delta} c_{n\delta}) V^{ee}_{k\alpha l\beta m\gamma n\delta} \end{aligned}$$

**Symmetry effects:**

$k_{exch} = 0$ Hatree approximation

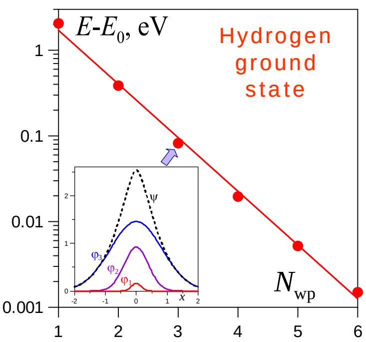
$k_{exch} = 1$ Unrestricted Hartree-Fock with $y_{km}$ are elements of the inverse overlap matrix $\mathbf{Y} = \mathbf{O}^{-1}$: $O_{km} = \sum_{\alpha,\beta} c_{k\alpha}^* o_{k\alpha m\beta} c_{m\beta}$

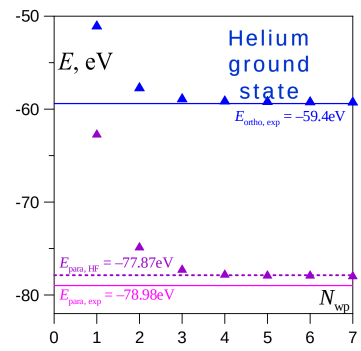
**Equations of motion**

**Split WPMD:** $\frac{dq_i}{dt} = \sum_j \left(\mathbf{N}^{-1}\right)_{ij}\frac{\partial H}{\partial q_j}$, $q_i = \{\mathbf{r}, \mathbf{p}, s, p_s, c\}$, $N_{ij} = \frac{\partial}{\partial q_i^*}\frac{\partial}{\partial q_j}\ln\langle\Psi(\mathbf{q}^*)|\Psi(\mathbf{q})\rangle$

**Original WPMD:** $\dot{\mathbf{r}}_k(t) = \frac{\partial H}{\partial \mathbf{p}_k}$, $\dot{\mathbf{p}}_k(t) = -\frac{\partial H}{\partial \mathbf{r}_k}$, $\dot s_k(t) = \frac{\partial H}{\partial p_{s_k}}$, $\dot p_{s_k}(t) = -\frac{\partial H}{\partial s_k}$

## Ground States for Simple Atoms



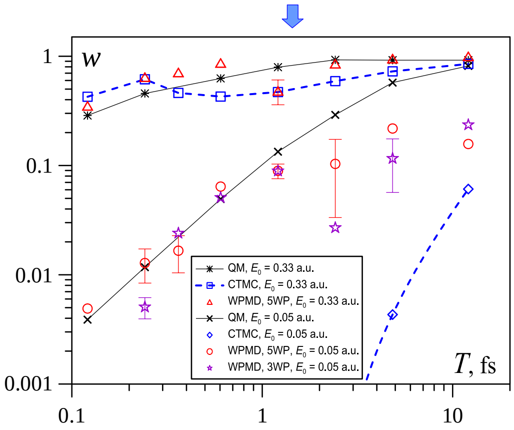




Ground state energies for Hydrogen and Helium depending on the number of wavepackets per electron $N_{wp}$.

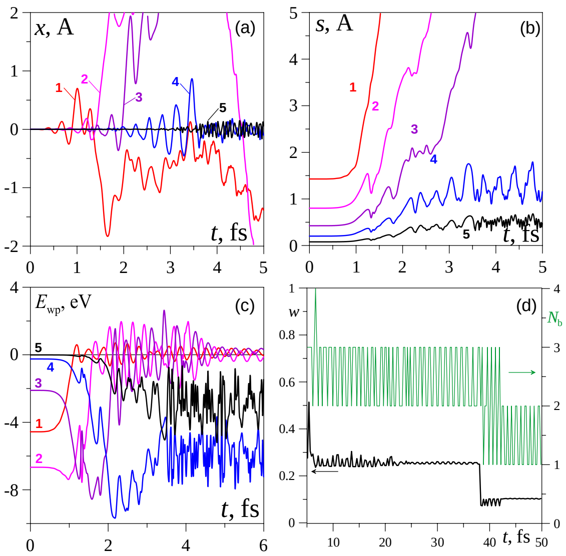
## Test Problem: Ionization of a Hydrogen Atom in a Short Laser Pulse

**Definition of the ionization rate:**

$$\psi = \psi_{\rm bound} + \psi_{\rm free}, \quad w = \frac{\langle\psi_{\rm free}|\psi_{\rm free}\rangle}{\langle\psi|\psi\rangle}$$




Ionization probability as function of pulse length $T$ for two different intensities $E_0$: **QM** – quantum mechanical calculations [7], **CTMC** – Classical Trajectory Monte Carlo, **WPMD** – present results for five and three WPs per electron




(a) – (c) Evolution of the main parameters of five WPs in a strong laser pulse; (d) Instant ionization probability $w$ (left axis) and the number of bound WPs $N_b$ (right axis) depending on time

## References


1. Morozov I.V., Norman G.E., JETP, 2005, v. **100**, No. 2, p. 370.
2. T. Raitza, H. Reinholz, G. Röpke, I. Morozov, E. Suraud, Contrib. Plasma Phys. **49**, 496 (2009).
3. D. Klakow, C. Toepffer, P. G. Reinhard, J. Chem. Phys. **101**, 10766 (1994).
4. J. T. Su and W. A. Goddard III, Phys. Rev. Lett. **99**, 185003 (2007).
5. B. Jakob, P. G. Reinhard, C. Toepffer, G. Zwicknagel, J. Phys. A **42**, 214055 (2009).
6. I.V. Morozov and I. A. Valuev, J. Phys. A **42**, 214044 (2009).
7. J. P. Hansen, J. Lu, L. B. Madsen, and H. M. Nilsen, J. Phys. A **64**, 033418 (2001).



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