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Wave Packet Molecular Dynamics to study atom electrons in strong fields

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Abstract

In order to study the dynamical behavior of atomic electrons interacting with strong fields, a semi-classical model is built from the Wave Packet Molecular Dynamic model. In our calculations, the Gaussian Wave Packets approach has been improved by introducing Hermite–Gaussian functions. Results are presented for laser–atom interaction at intensities where tunnel ionization plays an important role.

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1. Introduction

For several applications related to high energy density in matter, one has to get an accurate description of the dynamics of atomic electrons interacting with strong fields. One case concerns laser–atom interaction as for example when considering soft X-ray laser sources produced by focusing an intense laser beam inside a Xenon gas in Ref. [1]. Another case is related to high energy collisions between partially ionized heavy ions as encountered in heavy ion fusion [2]. In both cases the strength and the duration of the time dependent fields are so large that perturbative theories cannot yield accurate results, therefore non-perturbative models are required. Several non-perturbative calculations have been proposed in which the time dependent Schrödinger equation (TDSE) is solved either using a grid in real or in Fourier space or also by using an atomic basis. In our calculations the starting point has been the semi-classical approximation in which the perturbation potential can be large but its space variation on a scale length given by the wave function is assumed to be small. When considering only first and second order derivative of the potentials, Gaussian Wave Packet (GWP) become exact solution of the TDSE. In Ref. [3], thermodynamic properties of dense plasmas were studied using a time dependent variational principle (TDVP) [4] together with GWP leading to Wave Packet Molecular Dynamic (WPMD) calculations. The objective of the present work is to apply WPMD for studying dynamical properties of atomic electrons. Results presented below show that WPMD with GWP yield realistic results when the semi-classical approximation is valid, as expected. It corresponds to very strong perturbation, for which the energy gain by the electron is large. To extend the validity domain of the GWPMD calculations we have introduced a sum of Hermite–Gaussian functions. In the general case WPMD with Hermite Gaussian Wave Packet (HGWP) lead to calculations that are difficult to solve. We show that the numerical complexity can be strongly reduced by considering only a reduced ensemble of HGWP (R-HGWP). In the present work we will compare the results obtained using either spherical GWP (S-GWP), GWP or R-HGWP for calculating ground state properties of atom and molecules and their dynamical evolution when interaction with a high intensity laser field or with an energetic ion. Atomic units will be used, excepted when specified.

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2. Time dependent variational principle

Let us consider a physical system characterized by a Hamiltonian $\hat{H}$ and a wave function φ, that depends on several parameters $\{q_i\}$. Following Ref. [4] we define a Lagrangian through

$$\mathscr{L}(q_j,\dot{q}_j)=\sum_j p_j(q_j)\dot{q}_j-\mathscr{H}(q_j) \tag{1}$$

where $p_j=\langle\varphi|\mathrm{i}\partial/\partial q_j|\varphi\rangle$ is the conjugated momentum of the introduced parameter q_j, and $\mathscr{H}=\langle\varphi|\hat{H}|\varphi\rangle$ is the semi-classical Hamiltonian. Our quantum problem originally driven by the TDSE could now be treated by classical Lagrange equations on $\mathscr{L}(q,\dot{q})$.

From the Lagrange equations on $\mathscr{L}$, one gets the dynamical equations of the coordinates $\{q_j\}$ with the help of the so-called *norm-matrix* $\mathscr{N}$ defined by $\mathscr{N}_{j,k}=\partial p_j/\partial q_k-\partial p_k/\partial q_j$:

$$\sum_j \mathscr{N}_{j,k}\dot{q}_j=\frac{\partial\mathscr{H}}{\partial q_k}\Rightarrow\dot{q}_j=\sum_k \mathscr{N}^{-1}_{k,j}\frac{\partial\mathscr{H}}{\partial q_k}. \tag{2}$$

$\mathscr{N}$ invertibility depends on φ choice. If $\mathscr{N}$ is invertible, we obtain a set of coupled differential equations. $\mathscr{N}$ is easily invertible when conjugated moments are by construction parameters, which is the case with GWP φ_{G}:

$$\varphi_{\mathrm{G}}(\vec{q};\vec{x})=\prod_{j=x,y,z}\left(\frac{\omega_j}{\pi}\right)^{1/4}\mathrm{e}^{-(\omega_j/2+\mathrm{i}\gamma_j)(x_j-r_j)^2}\mathrm{e}^{\mathrm{i}p_j(x_j-r_j)}. \tag{3}$$

We have studied the different following shapes:

- SGWP: Width variations are identical in each direction. $\forall j,\omega_j=\omega,\gamma_j=\gamma$. We have 8 degrees of freedom. This shape was precedently used in Refs. [3,5].
- GWP, φ_{G} as written above in Eq. (3). The problem dimension is 12.
- HGWP: φ_{HG}. The wave function φ_{HG} is written as a linear combination of Hermite–Gauss functions:

$$\varphi_{\mathrm{HG}}(c_{i,j,k},\vec{q};\vec{x})=\sum_{i,j,k\in A}c_{i,j,k}\psi_{i,j,k}(\vec{q};\vec{x}) \tag{4}$$

where the Hermite–Gauss functions ψ_{n_x,n_y,n_z} are

$$\psi_{n_x,n_y,n_z}(\vec{q},\vec{x})=\prod_{j=x,y,z}h_{n_j}(\sqrt{\omega_j}(x_j-r_j))\times\mathrm{e}^{-(\omega_j/2+\mathrm{i}\gamma_j)(x_j-r_j)^2}\mathrm{e}^{\mathrm{i}p_j(x_j-r_j)}. \tag{5}$$

The h_{n_j} are the normalized Hermite polynomials of degree n_j and A the set of allowed integer triplet (i,j,k). In most of the presented results we have use a reduce ensemble of $c_{i,j,k}$ in order to reduce the numerical effort in the $\mathscr{N}$ inversion. The basic idea is to limit the dependency of the conjugated moments of $\vec{r}$, $\vec{p}$, γ_{x_i} and ω_{x_i} on the coefficients $c_{i,j,k}$. It has been obtained by choosing the set A such that

$$\begin{aligned}c_{i,j,k}c_{i\pm1,j,k}&=c_{i,j,k}c_{i\pm2,j,k}=0\\ c_{i,j,k}c_{i,j\pm1,k}&=c_{i,j,k}c_{i,j\pm2,k}=0\\ c_{i,j,k}c_{i,j,k\pm1}&=c_{i,j,k}c_{i,j,k\pm2}=0.\end{aligned} \tag{6}$$

For example, for $(i,j,k)\in[0,2]^3$, the following table lists the triplet for the non-zero coefficient:

i	j	k	i	j	k
0	0	0	2	2	0
1	1	0	2	0	2
1	0	1	0	2	2
0	1	1			

When condition (6) is satisfied, the norm-matrix becomes easily invertible. The problem dimension for the HGWP calculations becomes 12+ card(A).

3. Ground state properties

Let us first consider the case of a spherical atomic potential. The difference in the results obtained by the different models are nearly independent of the specific form of the atomic potential so that we choose the simple one corresponding to atomic hydrogen. The stationary state of the hydrogen atom is studied from semi-classical Hamiltonian $\mathscr{H}(q_j)$ written as

$$\mathscr{H}(q_j)=\left\langle\varphi(q_j;\vec{x})\left|-\frac{1}{2}\frac{\partial^2}{\partial\vec{x}^2}-\frac{1}{|\vec{x}|}\right|\varphi(q_j;\vec{x})\right\rangle. \tag{7}$$

Minimization of $\mathscr{H}(q_j)$ yields the (1s) ground state, which has been calculated using either the GWP or the HGWP representation. Fig. 1. shows the minimum energy vs. the wave function width ω obtained with HGWP for different sets $A_n=\{(i,j,k)|i+j+k\leqslant n\}$.

From this figure, we can observe that GWP ($n=0$) yields a minimum energy of -0.424 obtained at $\omega\sim0.57$, i.e. 16% higher than the exact value. By adding HGWP of higher degrees, we get closer to the exact result of -0.5.

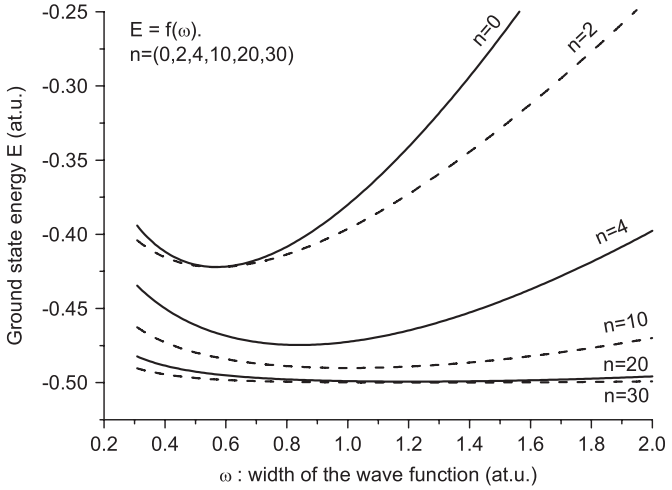

Fig. 1. Minimum energy by minimization of $\mathscr{H}$ obtained with HGWP wave function ansatz. The wave function is written as a linear combination of $\psi_{i,j,k}$ where $i+j+k\leqslant n$. Note that with $n=0$ we retrieve the GWP assertion.