Nonseparable Schrödinger equation in Discrete Variable Representation

Sara Shadmehri

JINR, Dubna

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Overview

1. Discrete Variable Representation Method
   - hydrogen atom in crossed static electric and magnetic fields
   - hydrogen atom in elliptically polarized strong laser field
   - Laser-atom interaction beyond dipole approximation

Discrete Variable Representation Method

The solution of the Schrödinger equation associated with a particle of mass m under the interaction $V(\mathbf{r}, t)$

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)\right]\Psi(\mathbf{r}, t) \tag{1}$$

is expressed as

$$\psi(r, \Omega, t) = \frac{1}{r}\sum_{j=1}^{N_\Omega} f_j(\Omega)u_j(r, t) \tag{2}$$

$f_j(\Omega)$: basis defined on the 2D angular grid $\Omega_j = (\theta_j, \phi_j)$

Orthogonality Condition

$$\int Y_\nu{}^*(\Omega)Y_{\nu'}(\Omega) \approx \sum_j w_j Y_\nu{}^*(\Omega_j)Y_{\nu'}(\Omega_j) = \delta_{\nu\nu'} \quad , \quad \nu = (l, m)$$

Quadratures on Unit Sphere

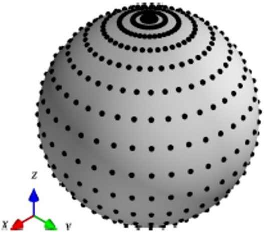
$$\int_{\mathbb{S}^2} f(\theta,\phi)d\Omega \approx \sum_{j=1}^{N_\Omega} w_j f(\theta_j,\phi_j) \equiv Q(f)$$

- By solving a simultaneous set of nonlinear equations, the nodes (θ_j, ϕ_j) and weights w_j of a quadrature rule $Q(f)$ is determined.
- Lebedev (and Popov) quadratures invariant under specific rotation groups [Sobolev,1962]
- Accuracy order of $Q(f)$: p - maximum degree of the polynomial f which can be integrated exactly
- Quadrature efficiency : $\frac{(p+1)^2}{3N_\Omega}$

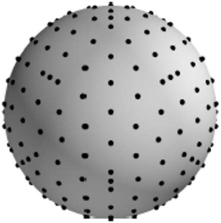
	1D×1D Gaussian	**2D Popov** or **Lebedev**
$Q(f)$	$\sum_{i=1}^{N_\theta} w_i \sum_{i'=1}^{N_\phi} w_{i'} f(\theta_i,\phi_{i'})$	$\sum_{j=1}^{N_\Omega} w_j f(\theta_j,\phi_j)$
N_Ω	$= N_\theta \times N_\phi$	$= N_\theta = N_\phi$
efficiency	2/3	$\simeq 1$

S. L. Sobolev *Sibirsk. Math* **3**, 769 (1962)

Quadratures on Unit Sphere



(A) Gaussian Product grid with $N_\Omega = 800$



(B) Lebedev grid with $N_\Omega = 266$

Constructing DVR basis function

$$\psi(r,\Omega,t) = \frac{1}{r}\sum_{j=1}^{N_\Omega} f_j(\Omega) u_j(r,t)$$

Gaussian	Lebedev or Popov
$f_j(\Omega) = \sum_{\nu=1}^{N_\Omega} \bar{Y}_\nu(\Omega)[Y^{-1}]_{\nu j}$	$f_j(\Omega) = \sum_{\nu=1}^{N_\Omega} \sqrt{4\pi w_j}\Phi_\nu(\Omega)\Phi^*_\nu(\Omega_j)$
$Y_{j\nu} = \sqrt{w_j}\bar{Y}_\nu(\Omega_j)$	
$\bar{Y}_\nu(\Omega) = \bar{Y}_{lm}(\Omega) = e^{im\phi}\sum_{l'} c_l^{l'} P_{l'}^m(\theta)$	$\Phi_\nu(\Omega) = \sum_\mu S_{\nu\mu} Y_\mu(\Omega)$

Gaus $\bar{Y}_\nu$ coinsides with the spherical harmonics except the largest incorporated l values which are orthonalized by the the Gram-Schmidt method

Leb $\hat{S}$: a matrix which makes a set of N_Ω basis functions Φ_ν orthonormal over the Lebedev (or Popov) grid points Ω_j .

S. Shadmehri, S. Saeidian and V. S. Melezhik *J. Phys. B: At. Mol. Opt. Phys.* **53**, 085001 (2020)

Applying DVR to the main Hamiltonian

The problem is reduced to a system of Schrödinger-type equations which should be solved for the unknown N_Ω-dimensional vector $\mathbf{u}(r,t) = \{\sqrt{w_j} u_j(r,t)\}_1^{N_\Omega} = \{\sqrt{w_j} r\psi(r,\Omega_j,t)\}_1^{N_\Omega}$,

$$i\frac{\partial}{\partial t}\mathbf{u}(r,t) = \left[\hat{H}_0(r) + \hat{V}(r,t)\right]\mathbf{u}(r,t) \tag{3}$$

where the elements of the $N_\Omega \times N_\Omega$ matrices $\hat{H}^{(0)}(r)$ and $\hat{V}(r,t)$ are represented as

$$H^{(0)}_{jj'}(r) = -\frac{1}{2}(\delta_{jj'}\frac{d^2}{dr^2} - \frac{L^2_{jj'}}{r^2}) - \frac{1}{r}\delta_{jj'}\,, \tag{4}$$

$$V_{jj'}(r,t) = V(r,\Omega_j,t)\delta_{jj'}\,. \tag{5}$$

Gaus $L^2_{jj'} = \sum_{\nu=1}^{N_\Omega} \sqrt{w_j w_{j'}}\,\bar{Y}_\nu(\Omega_j) l(l+1)\bar{Y}^*_\nu(\Omega_{j'})$

Leb $L^2_{jj'} = 4\pi \sum_{\nu=1}^{N_\Omega} \sqrt{w_j w_{j'}} \sum_{\mu=1}^{\bar{N}_\Omega} S_{\nu\mu} l_\mu(l_\mu+1) Y_\mu(\Omega_j)\Phi^*_\nu(\Omega_{j'})$

Propagating the wavefunction in time $t_n \to t_{n+1} = t_n + \Delta t$

The component-by-component split-operator method is applied as

$$\mathbf{u}(r, t_n + \Delta t) = \exp[-\frac{i}{2}\Delta t \hat{V}(r, t_n)] \exp[-i\Delta t \hat{H}_0(r)] \exp[-\frac{i}{2}\Delta t \hat{V}(r, t_n)]\mathbf{u}(r, t_n) \tag{6}$$

Operators $\hat{M}$ and $\hat{W}$ diagonalizing $\hat{L}^2$ in $\hat{H}_0$

Gaus $M_{j\nu} = \sqrt{w_j}\bar{Y}_\nu(\Omega_j)$, $\bar{\mathbf{u}} = \hat{M}\mathbf{u}$

$$\hat{A}_{\nu\nu'} = \left(\hat{M}\hat{H}_0\hat{M}^\dagger\right)_{\nu\nu'} = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{1}{r}\right]\delta_{\nu\nu'}$$

Leb $\hat{W}^{-1}\hat{L}^2\hat{W} = \hat{J}$, $\bar{\mathbf{u}} = \hat{W}^{-1}\mathbf{u}$, $\hat{W}$: numerically

$$\hat{A}_{\nu\nu'} = \left(\hat{W}^{-1}\hat{H}_0\hat{W}\right)_{\nu\nu'} = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{J_\nu}{2r^2} - \frac{1}{r}\right]\delta_{\nu\nu'}$$

The total number of operations at each time step (6) in our algorithm: $N_r(2N_\Omega^2 + \alpha N_\Omega)$

$\alpha = (2 \times 7)^2 \simeq 200$

Hydrogen atom in crossed static electric **F** and magnetic **B** fields

The interaction potential is expressed as

$$\hat{V}(\mathbf{r}) = -\frac{1}{r} + (\mathbf{F} \cdot \mathbf{r}) + \frac{1}{2}(\mathbf{B} \cdot \mathbf{L}) + \frac{1}{8}[\mathbf{B} \times \mathbf{r}]^2 \qquad (7)$$

The vectors **B** and **F**, which form an arbitrary angle α, are placed in the xz-plane,

$$\mathbf{B} = \beta \mathbf{n}_z \quad , \quad \mathbf{F} = \gamma(\sin\alpha \mathbf{n}_x + \cos\alpha \mathbf{n}_z) \,. \qquad (8)$$

The strengths γ and β of the electric and magnetic field are expressed in atomic units $F_0 = e^5 m_e^2/\hbar^4 \approx 5.14 \times 10^9$ V/cm and $B_0 = (e/\hbar)^3 m_e^2 c \approx 2.35 \times 10^9$ G ($\hbar = e = m_e = 1$).

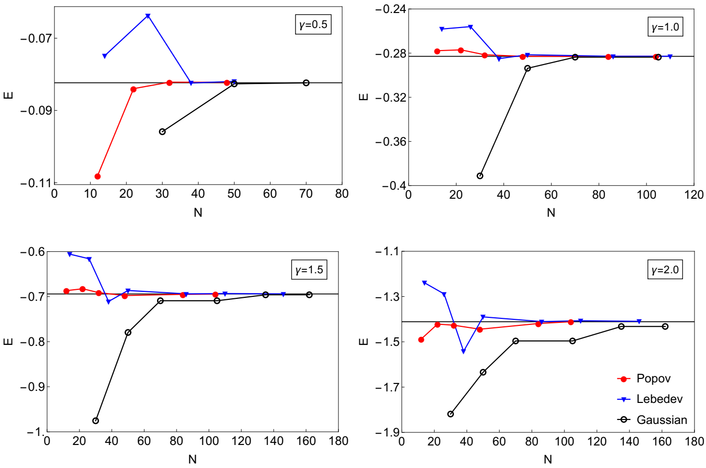


Figure: The ground-state energies of a hydrogen atom in the external magnetic $\beta = 2.0$ and electric $\gamma = 0.5, 1.0, 1.5, 2.0$ fields perpendicular to one another ($\alpha = \pi/2$). The thin horizontal black lines show the most accurate value obtained for each case.

S. Shadmehri, S. Saeidian and V. S. Melezhik *J. Phys. B: At. Mol. Opt. Phys.* **53**, 085001 (2020)

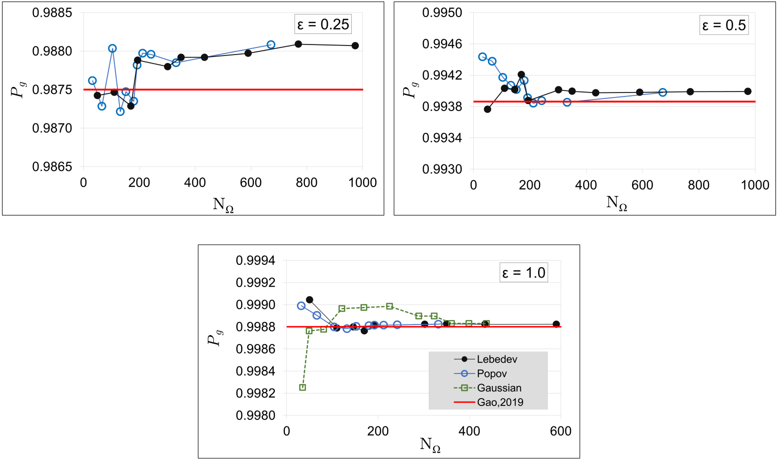
Hydrogen atom in elliptically polarized strong laser field

- interaction potential: length gauge, dipole approximation,

$$V(\mathbf{r}, t) = -\mathbf{r} \cdot \mathbf{E}(t)$$

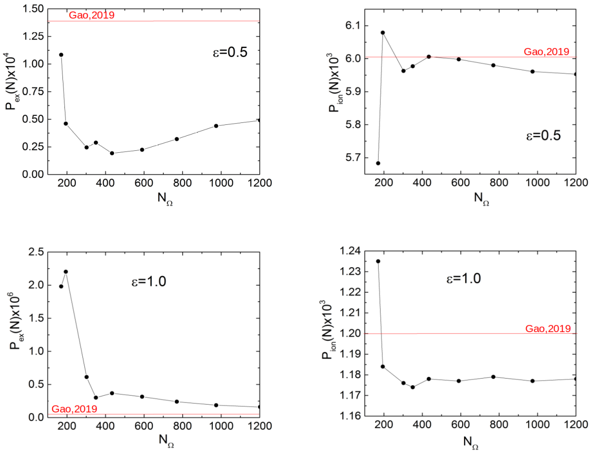
- $\mathbf{E}(t) = \frac{f(t)}{\sqrt{1+\varepsilon^2}} E_0 \left(\hat{\mathbf{x}} \cos \omega t + \hat{\mathbf{y}} \varepsilon \sin \omega t\right)$
- Laser Parameters :
  $\lambda = 800$ nm , $I = 10^{14}$ W/cm^2 , $N = 7.5$ optical cycles of period $T = 2\pi/\omega$ with pulse envelope function,
  $$f(t) = \cos^2\left(\frac{\pi t}{NT}\right) \quad , \quad -NT/2 < t < NT/2$$
- initial state of the system: ground state of the hydrogen atom

$$P_g = |\langle \psi | \phi_{100} \rangle|^2 = |\int \psi(\mathbf{r}, t = t_{out}) \phi_{100}(\mathbf{r}) d\mathbf{r}|^2$$



X. Gao and X -M Tong, PRA **100**, 063424 (2019)

$$P_{nlm} = \mid \langle \psi | \phi_{nlm} \rangle \mid^2 = \mid \int \psi(\mathbf{r}, t = t_{out}) \phi_{nlm}(\mathbf{r}) d\mathbf{r} \mid^2$$



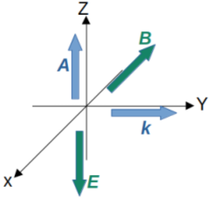
S. Shadmehri and V.S. Melezhik, Laser Phys. **33**, 026001 (2023)

Laser-atom interaction beyond dipole approximation

Laser-atom interaction beyond dipole approximation

Assume a strong laser field linearly polarized along the z-axis and propagating along the y-axis,

$$\mathbf{A}(\mathbf{r},t) = \hat{\mathbf{z}}\frac{E_0}{\omega}\sin^2(\frac{\pi t}{NT})\sin(\omega t - \mathbf{k}\cdot\mathbf{r}) \quad (9)$$



Dipole Approximation: $\mathbf{A}(\mathbf{r},t) \approx \mathbf{A}(t) \;\rightarrow\; V(\mathbf{r},t) = \mathbf{r}\cdot\mathbf{E}(t)$

Beyond dipole approximation

expanding $\mathbf{A}(\mathbf{r},t)$ to the first order of $\mathbf{k}\cdot\mathbf{r}$,

$\sin(\mathbf{k}\cdot\mathbf{r}) \approx \mathbf{k}\cdot\mathbf{r}$, $\cos(\mathbf{k}\cdot\mathbf{r}) \approx 1.0$

$$\mathbf{A}(\mathbf{r},t) = \hat{\mathbf{z}}\frac{E_0}{\omega}\sin^2(\frac{\pi t}{NT})\left[\sin(\omega t) - \frac{\omega}{c}y\cos(\omega t)\right] \quad (10)$$

The electric $\mathbf{E} = -\frac{d\mathbf{A}}{dt}$ and magnetic $\mathbf{B} = \nabla\times\mathbf{A}$ fields can be calculated accordingly.

The Lorentz force acting on each constituent particle of the hydrogen atom (with charge $q_i = \pm e$, mass m_i and momentum $\mathbf{p}_i$) is of the form $\mathbf{F}_i = q_i \mathbf{E} + \frac{q_i}{m_i} (\mathbf{p}_i \times \mathbf{B})$

Passing to the coordinates of CM, the interaction potential U between the atom and the electromagnetic field follows

$$\begin{aligned} U &= -E_0 \left[\sin^2(\frac{\pi t}{NT}) \cos(\omega t) + \frac{1}{2N} \sin(\frac{2\pi t}{NT}) \sin(\omega t) \right] z \\ &- E_0 \frac{\omega}{c} \left[\sin^2(\frac{\pi t}{NT}) \sin(\omega t) - \frac{1}{2N} \sin(\frac{2\pi t}{NT}) \cos(\omega t) \right] (yz + yZ + Yz) \\ &- \frac{E_0}{c} \sin^2(\frac{\pi t}{NT}) \cos(\omega t) \left(\frac{yp_z - zp_y}{\tilde{\mu}} + \frac{Yp_z - Zp_y}{\mu} + \frac{yP_z - zP_y}{M} \right) \end{aligned} \quad (11)$$

$M = m_1 + m_2$, $\mu = \frac{m_1 m_2}{M}$, $\tilde{\mu} = \frac{m_1 m_2}{m_2 - m_1}$

The total Hamiltonian of the system turns into

$$H(\mathbf{r},\mathbf{R},t)=\frac{\mathbf{P}^2}{2M}+h_0(\mathbf{r})+U_1(\mathbf{r},t)+U_2(\mathbf{r},\mathbf{R},t), \tag{12}$$

$c = 137$ a.u.
$\omega = 0.2, ..., 1.0$ a.u.

$$h_0(\mathbf{r}) = \frac{\mathbf{p}^2}{2\mu}-\frac{1}{r} \tag{13}$$

$$\begin{aligned} U_1(\mathbf{r},t) &= -E_0\left[\sin^2\left(\frac{\pi t}{NT}\right)\cos(\omega t)+\frac{1}{2N}\sin\left(\frac{2\pi t}{NT}\right)\sin(\omega t)\right]z \\ &- E_0\frac{\omega}{c}\left[\sin^2\left(\frac{\pi t}{NT}\right)\sin(\omega t)-\frac{1}{2N}\sin\left(\frac{2\pi t}{NT}\right)\cos(\omega t)\right]yz \\ &- \frac{E_0}{c}\sin^2\left(\frac{\pi t}{NT}\right)\cos(\omega t)\hat{L}_x \end{aligned} \tag{14}$$

$$\begin{aligned} U_2(\mathbf{r},\mathbf{R},t) &= -E_0\frac{\omega}{c}\left[\sin^2\left(\frac{\pi t}{NT}\right)\sin(\omega t)-\frac{1}{2N}\sin\left(\frac{2\pi t}{NT}\right)\cos(\omega t)\right] \\ &\times (yZ+zY) \\ &- \frac{E_0}{c}\sin^2\left(\frac{\pi t}{NT}\right)\cos(\omega t)\,(Yp_z-Zp_y) \end{aligned} \tag{15}$$

The problem is reduced to the simultaneous integration of a system of coupled equations:

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[h_0(\mathbf{r}) + U_1(\mathbf{r},t) + U_2(\mathbf{r},\mathbf{R},t)\right]\psi(\mathbf{r},t) \qquad (16)$$

$$\frac{d}{dt}\mathbf{P} = -\frac{\partial}{\partial \mathbf{R}} H_{eff}\left(\mathbf{R}(t),\mathbf{P}(t)\right) \qquad (17)$$

$$\frac{d}{dt}\mathbf{R} = +\frac{\partial}{\partial \mathbf{P}} H_{eff}\left(\mathbf{R}(t),\mathbf{P}(t)\right) \qquad (18)$$

$$H_{eff}\left(\mathbf{R},\mathbf{P}\right) = \frac{\mathbf{P}^2}{2M} + \langle\psi(\mathbf{r},t)|U_2(\mathbf{r},\mathbf{R},t)|\psi(\mathbf{r},t)\rangle$$

The initial conditions :

$$\psi(\mathbf{r},t=0) = \phi_{100}(\mathbf{r})$$
$$\mathbf{R}(t=0) = 0 \quad , \quad \mathbf{P}(t=0) = 0$$

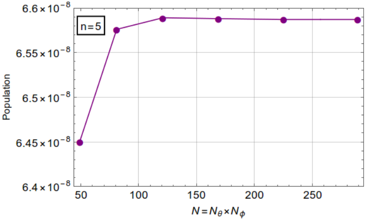
Applying DVR to the time-dependent 3D Schrödinger equation
and
simultaneously integrating the Hamilton equations of motion with the Störmer-Verlet method:

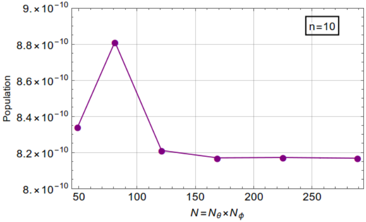
$$
\begin{aligned}
\mathbf{P}(t_n+\frac{\Delta t}{2}) &= \mathbf{P}(t_n) - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{R}} H_{eff}\left(\mathbf{R}(t_n), \mathbf{P}(t_n+\frac{\Delta t}{2})\right) \ , \\
\mathbf{R}(t_n+\Delta t) &= \mathbf{R}(t_n) + \frac{\Delta t}{2}\{\frac{\partial}{\partial \mathbf{P}} H_{eff}\left(\mathbf{R}(t_n), \mathbf{P}(t_n+\frac{\Delta t}{2})\right) \\
&\quad + \frac{\partial}{\partial \mathbf{P}} H_{eff}\left(\mathbf{R}(t_n+\Delta t), \mathbf{P}(t_n+\frac{\Delta t}{2})\right)\} \ , \\
\mathbf{P}(t_n+\Delta t) &= \mathbf{P}(t_n+\frac{\Delta t}{2}) - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{R}} H_{eff}\left(\mathbf{R}(t_n+\Delta t), \mathbf{P}(t_n+\frac{\Delta t}{2})\right) \ .
\end{aligned}
\tag{19}
$$

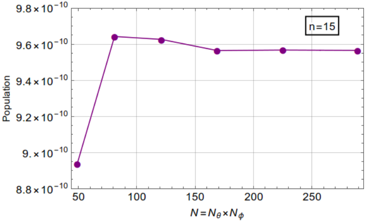
Once the wave-packet $\psi(\mathbf{r}, t)$ and $\mathbf{R}(t)$ and $\mathbf{P}(t)$ of the CM are found during the time interval $0 \leq t \leq t_{out}$ of the laser pulse action, we can calculate the ionization and excitation probabilities, and analyse the acceleration of the atom.

Convergence Test

$I = 10^{14}\ W/cm^2 \quad , \quad \tau = NT = 7.6\ fs$
$\omega = 0.3\ a.u.\ (\lambda = 152\ nm)$

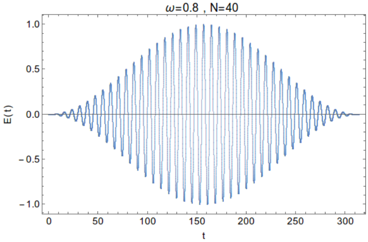


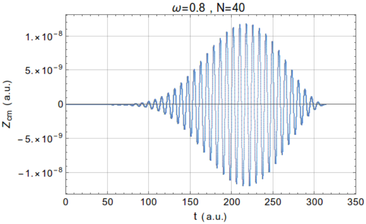


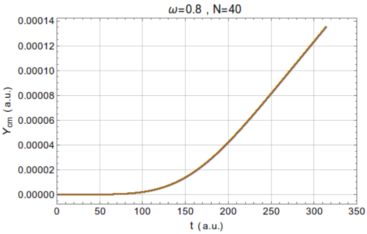


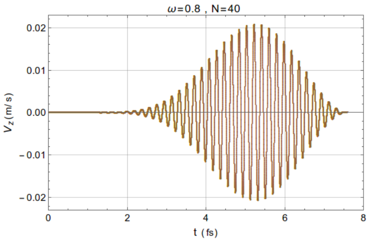
Hydrogen atom interacting with a laser pulse intensity of $I = 10^{14}\ W/cm^2$ and duration $\tau = NT = 7.6\ fs$

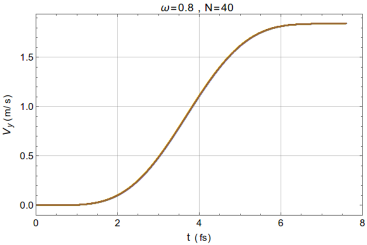
$\omega = 0.8\ a.u.\ (\lambda = 57\ nm)$

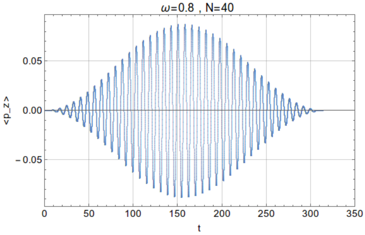







ω=0.8 , N=40
0.02
0.01
0.00
- 0.01
- 0.02
V_z (m/s)
0
2
4
6
8
t (fs)


ω=0.8 , N=40
1.5
1.0
0.5
0.0
V_y (m/s)
0
2
4
6
8
t (fs)


ω=0.8 , N=40
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0.00
- 0.05
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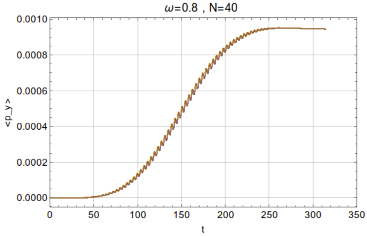
100
150
200
250
300
350
t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0.0002
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0
50
100
150
200
250
300
350
t

Influence of Nondipole Effects

Table: The probabilities of the population of the ground state P_g and total excitation P_{ex} calculated in the dipole and nondipole approaches for a few laser frequencies with intensity 10^{14} W/cm^2 and 7.6 fs pulse duration.

	P_g			P_{ex}		
ω	**Dipole**	**Nondipole**	$\lvert\Delta P\rvert$ [1]	**Dipole**	**Nondipole**	$\lvert\Delta P\rvert$ [1]
0.30	0.896815	0.896805	1.05E-05	6.3410E-05	6.3414E-05	6.59E-05
0.40	0.987600	0.987599	1.34E-06	2.3058E-03	2.3052E-03	2.51E-04
0.48	0.382308	0.382294	3.54E-05	5.8582E-01	5.8568E-01	2.37E-04
0.52	0.488483	0.488465	3.74E-05	1.9974E-02	1.9984E-02	4.84E-04
0.80	0.867150	0.867131	2.20E-05	4.6748E-07	4.6756E-07	1.64E-04
1.00	0.941058	0.941045	1.39E-05	4.8210E-07	4.8218E-07	1.68E-04

[1] $$|\Delta P| = \left|\frac{P_{Dipole} - P_{Nondipole}}{P_{Dipole}}\right|$$

V. S. Melezhik and S. Shadmehri, *Photonics* **10**, 1290 (2023)

Conclusion

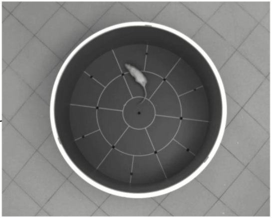
1. An efficient computational scheme based on 2D DVR for integration of the Schrödinger equation with nonseparable angular part is developed.
2. With this approach, we demonstrate computational advantages in description of hydrogen atom in strong crossed electric and magnetic fields and in strong elliptically polarized laser fields.
3. New opening in analysing the nondipole effects in laser-atom interaction

Automation the Analysis of Video Data for the “Open Field” Behavioral Test

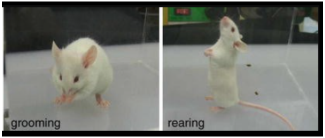
(MLIT)

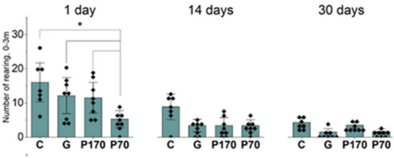
BIOHLIT (MLIT and LRB): Behavioral Test System

«Open Field» maze



Objective: Counting the number of specific behaviors of the animal pre and post-radiation

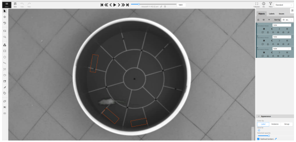


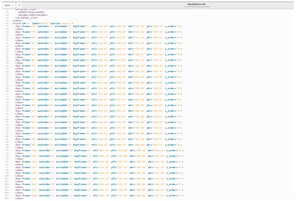


BIOHLIT: Video Data Analysis

- Video Annotation for Activity Recognition

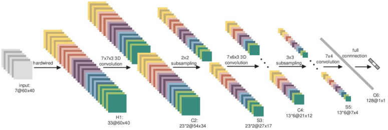
Behavioral Indicators
- crossed sectors
- center entries
- hole dipping
- rearing
- grooming
- freezes





- Using Neural Networks and Learning Algorithms for Classification

Video Classification Methods
- Single Frame CNN
- Late Fusion
- Early Fusion
- CNN with LSTM
- Pose Detection and LSTM
- Optical Flow and CNN
- 3D CNN



Thanks for Your Attention