Quantum-quasiclassical analysis of CM nonseparability in atom due to relativistic effects stimulated by laser field

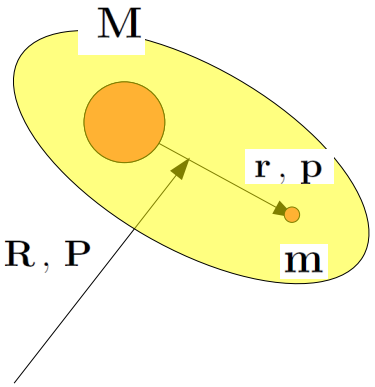
Vladimir S. Melezhik

Bogoliubov Laboratory of Theoretical Physics JINR, Dubna

supported by Grant of Russian Science Foundation No. 20-11-20257

MQFTP-22, St-Petersburg, 10-14 October 2022

quantum-quasiclassical approach - idea



$$\mathbf{M} \gg \mathbf{m}$$

$$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$$

$$i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{r}, t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r}, \mathbf{R}(t))] |\psi(\mathbf{r}, t)\rangle$$

$$H_{cl}(\mathbf{P}, \mathbf{R}, t) = \frac{\mathbf{P}^2}{2M} + \langle \psi(\mathbf{r}, t) | V(\mathbf{r}, \mathbf{R}(t)) | \psi(\mathbf{r}, t) \rangle$$

$$\frac{d}{dt}\mathbf{P} = -\frac{\partial}{\partial \mathbf{R}} H_{cl}(\mathbf{P}, \mathbf{R}, t)$$

$$\frac{d}{dt}\mathbf{R} = \frac{\partial}{\partial \mathbf{P}} H_{cl}(\mathbf{P}, \mathbf{R}, t)$$

VOLUME 84, NUMBER 9 PHYSICAL REVIEW LETTERS 28 FEBRUARY 2000

Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields

V. S. Melezhik[1,*] and P. Schmelcher[2]

K. J. McCann and M. R. Flannery, Chem. Phys. Lett. **35**, 124 (1975); J. Chem. Phys. **63**, 4695 (1975).
G. D. Billing, Chem. Phys. **9**, 359 (1975).

quantum-quasiclassical approach - results

VOLUME 84, NUMBER 9 PHYSICAL REVIEW LETTERS 28 FEBRUARY 2000

Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields

V. S. Melezhik[1,*] and P. Schmelcher[2]

PHYSICAL REVIEW A **69**, 032709 (2004)

Stripping and excitation in collisions between p and $He^+(n \leq 3)$ calculated by a quantum time-dependent approach with semiclassical trajectories

Vladimir S. Melezhik,[1,*] James S. Cohen,[2] and Chi-Yu Hu[1]

quantum-quasiclassical approach - results

VOLUME 84, NUMBER 9 PHYSICAL REVIEW LETTERS 28 FEBRUARY 2000

Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields

V. S. Melezhik[1,*] and P. Schmelcher[2]

PHYSICAL REVIEW A **69**, 032709 (2004)

Stripping and excitation in collisions between p and $He^+(n \leq 3)$ calculated by a quantum time-dependent approach with semiclassical trajectories

Vladimir S. Melezhik,[1,*] James S. Cohen,[2] and Chi-Yu Hu[1]

Hyperfine Interactions **138:** 351–354, 2001.

Recent Progress in Treatment of Sticking and Stripping with Time-Dependent Approach

VLADIMIR S. MELEZHIK[1,2]

quantum-quasiclassical approach - results

VOLUME 84, NUMBER 9 PHYSICAL REVIEW LETTERS 28 FEBRUARY 2000

Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields

V. S. Melezhik[1,*] and P. Schmelcher[2]

PHYSICAL REVIEW A **69**, 032709 (2004)

Stripping and excitation in collisions between p and $He^+(n \leqslant 3)$ calculated by a quantum time-dependent approach with semiclassical trajectories

Vladimir S. Melezhik,[1,*] James S. Cohen,[2] and Chi-Yu Hu[1]

Hyperfine Interactions **138:** 351–354, 2001.

Recent Progress in Treatment of Sticking and Stripping with Time-Dependent Approach

VLADIMIR S. MELEZHIK[1,2]

PHYSICAL REVIEW A **103**, 053109 (2021)

Improving efficiency of sympathetic cooling in atom-ion and atom-atom confined collisions

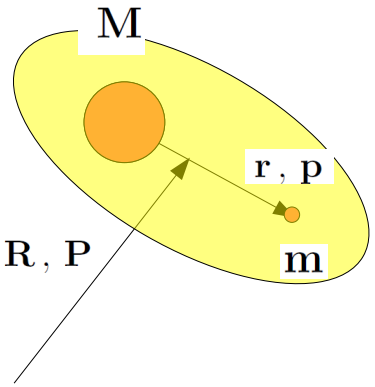
Vladimir S. Melezhik[*]

Eur. Phys. J. A (2022) 58:34
https://doi.org/10.1140/epja/s10050-022-00684-z
THE EUROPEAN PHYSICAL JOURNAL A

Investigation of low-lying resonances in breakup of halo nuclei within the time-dependent approach

Dinara Valiolda[1,2,3], Daniyar Janseitov[1,2,3,a], Vladimir Melezhik[3,4,b]

hydrogen atom in strong laser field



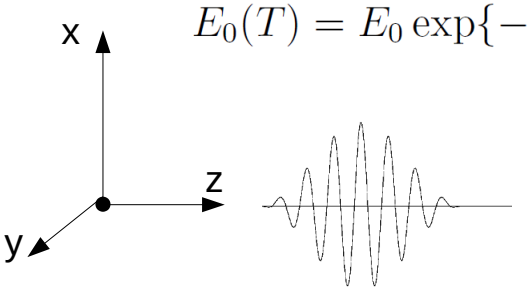
$$\mathbf{M} \gg \mathbf{m}$$

$$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},\mathbf{R},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},\mathbf{R},t)\rangle$$

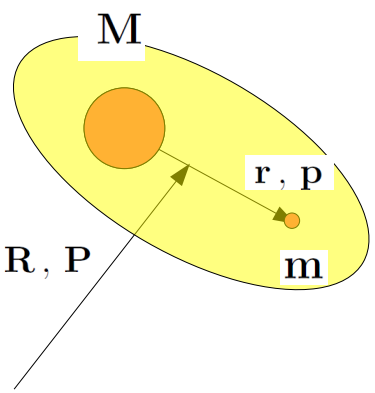
$$H_0(\mathbf{r}) = \frac{p^2}{2\mu} - \frac{1}{r} - E_0(T)\cos(\omega t)x + \alpha[...]$$

$$E_0(T) = E_0 \exp\{-\frac{t^2}{T^2}\}$$



$$\alpha = \frac{1}{c} = \frac{1}{137}$$

hydrogen atom in strong laser field



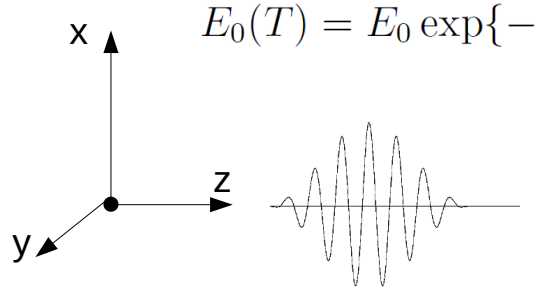
$$\mathbf{M} \gg \mathbf{m}$$

$$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},\mathbf{R},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},\mathbf{R},t)\rangle$$

$$H_0(\mathbf{r}) = \frac{p^2}{2\mu} - \frac{1}{r} - E_0(T)\cos(\omega t)x + \alpha[...]$$

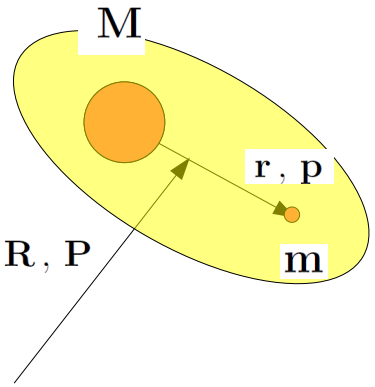
$$E_0(T) = E_0 \exp\{-\frac{t^2}{T^2}\}$$



$$\alpha = \frac{1}{c} = \frac{1}{137}$$

$$V(\mathbf{r},\mathbf{R}) = -\alpha\omega E_0(T)\sin(\omega t)[xZ(t) + zX(t)] - \alpha E_0(T)\cos(\omega t)X(t)p_z$$

hydrogen atom in strong laser field



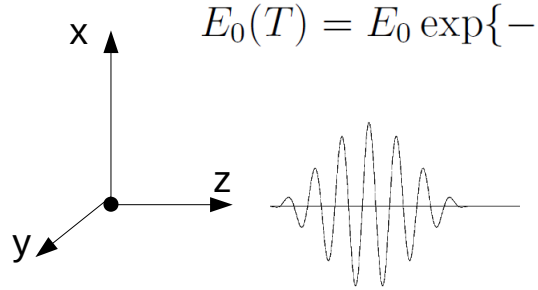
$\mathbf{M} \gg \mathbf{m}$

$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$

$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},\mathbf{R},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},\mathbf{R},t)\rangle$$

$$H_0(\mathbf{r}) = \frac{p^2}{2\mu} - \frac{1}{r} - E_0(T)\cos(\omega t)x + \alpha[...]$$

$$E_0(T) = E_0 \exp\{-\frac{t^2}{T^2}\}$$

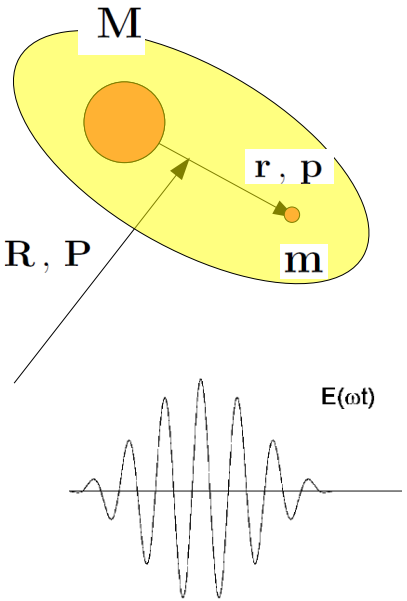


$$\alpha = \frac{1}{c} = \frac{1}{137}$$

$$V(\mathbf{r},\mathbf{R}) = -\alpha\omega E_0(T)\sin(\omega t)[xZ(t) + zX(t)] - \alpha E_0(T)\cos(\omega t)X(t)p_z$$

how integrate 6D TDSE ? !!!

hydrogen atom in strong laser field



how integrate 6D TDSE ? !!!

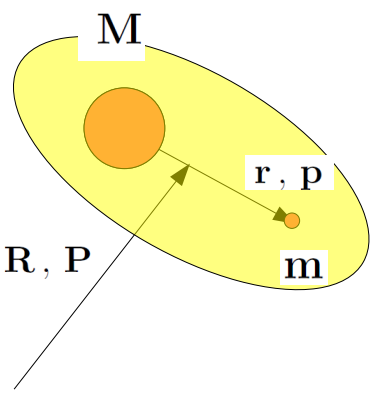
$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},\mathbf{R},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},\mathbf{R},t)\rangle$$

A. Bray, U. Eichmann, S. Patchkovskii, PRL 124 (2020)

With additional artificial trapping potential the problem was reduced to effective 3D

They proposed to use CM-velosity spectroscopy as a «build-in» classical monitoring devise for observing internal quantum dynamics in strong external laser fields

hydrogen atom in strong laser field



$$\mathbf{M} \gg \mathbf{m}$$

$$\mathbf{P} = \mathbf{M}\mathbf{V} \gg \mathbf{p} = \mathbf{m}\mathbf{v}$$

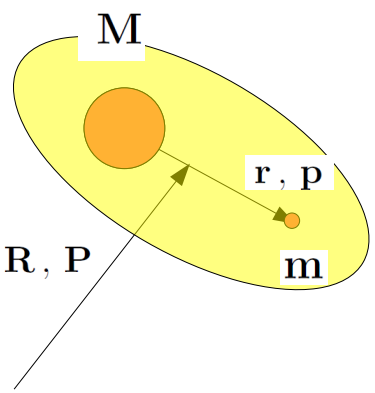
$$i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{r}, t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r}, \mathbf{R}(t))] |\psi(\mathbf{r}, t)\rangle$$

$$H_{cl}(\mathbf{P}, \mathbf{R}, t) = \frac{\mathbf{P}^2}{2M} + \langle \psi(\mathbf{r}, t) | V(\mathbf{r}, \mathbf{R}(t)) | \psi(\mathbf{r}, t) \rangle$$

$$\frac{d}{dt}\mathbf{P} = -\frac{\partial}{\partial \mathbf{R}} H_{cl}(\mathbf{P}, \mathbf{R}, t)$$

$$\frac{d}{dt}\mathbf{R} = \frac{\partial}{\partial \mathbf{P}} H_{cl}(\mathbf{P}, \mathbf{R}, t)$$

hydrogen atom in strong laser field



$$\mathbf{M} \gg \mathbf{m}$$

$$\mathbf{P} = \mathbf{MV} \gg \mathbf{p} = \mathbf{mv}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(\mathbf{r},t)\rangle = [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))]|\psi(\mathbf{r},t)\rangle$$

$$H_{cl}(\mathbf{P},\mathbf{R},t) = \frac{\mathbf{P}^2}{2M} + \langle\psi(\mathbf{r},t)|V(\mathbf{r},\mathbf{R}(t))|\psi(\mathbf{r},t)\rangle$$

$$\frac{d}{dt}\mathbf{P} = -\frac{\partial}{\partial\mathbf{R}}H_{cl}(\mathbf{P},\mathbf{R},t)$$

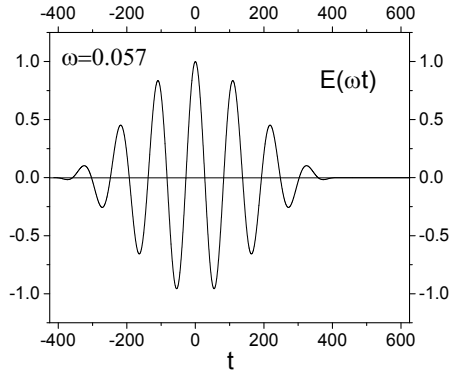
$$\frac{d}{dt}\mathbf{R} = \frac{\partial}{\partial\mathbf{P}}H_{cl}(\mathbf{P},\mathbf{R},t)$$

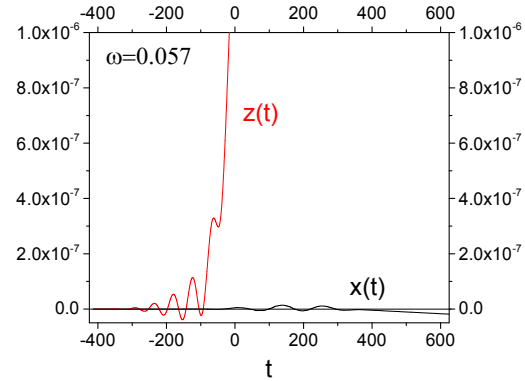
$$\langle\psi(\mathbf{r},t)|\mathbf{r}(t)|\psi(\mathbf{r}),t)\rangle \quad \langle\psi(\mathbf{r},t)|\mathbf{p}(t)|\psi(\mathbf{r},t)\rangle \qquad \mathbf{R}(t) \quad \mathbf{P}(t)$$

$$\langle|E_{kin}(t)|\rangle = \frac{1}{2T}\int_{-T}^{T}\frac{P^2(t)}{2M}dt \sim \int|P(\omega)|^2dt \sim \int\{|P_x(\omega)|^2+|P_y(\omega)|^2+|P_z(\omega)|^2\}dt$$

$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

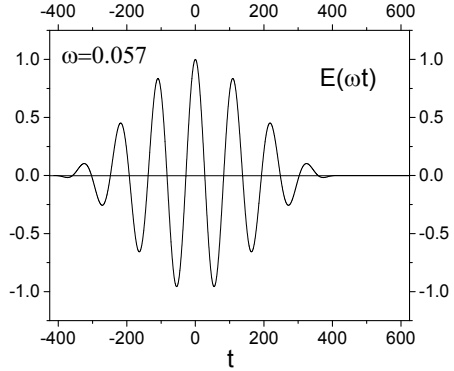
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$

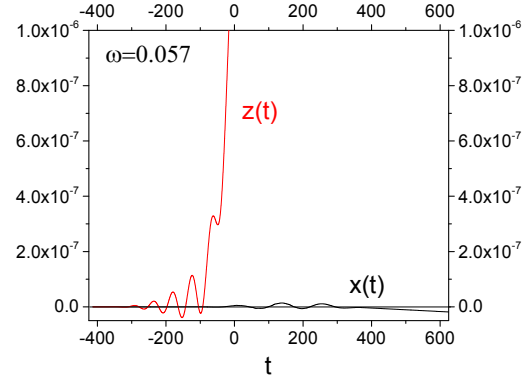


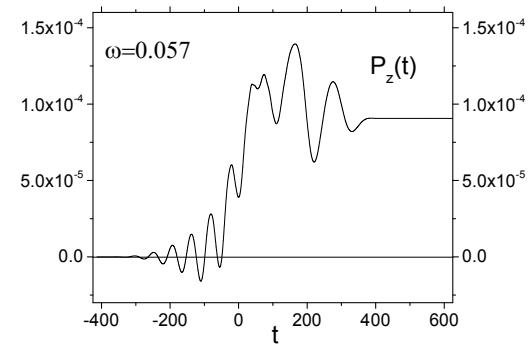


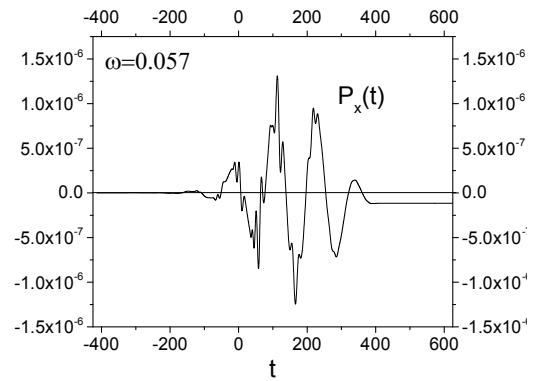
$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



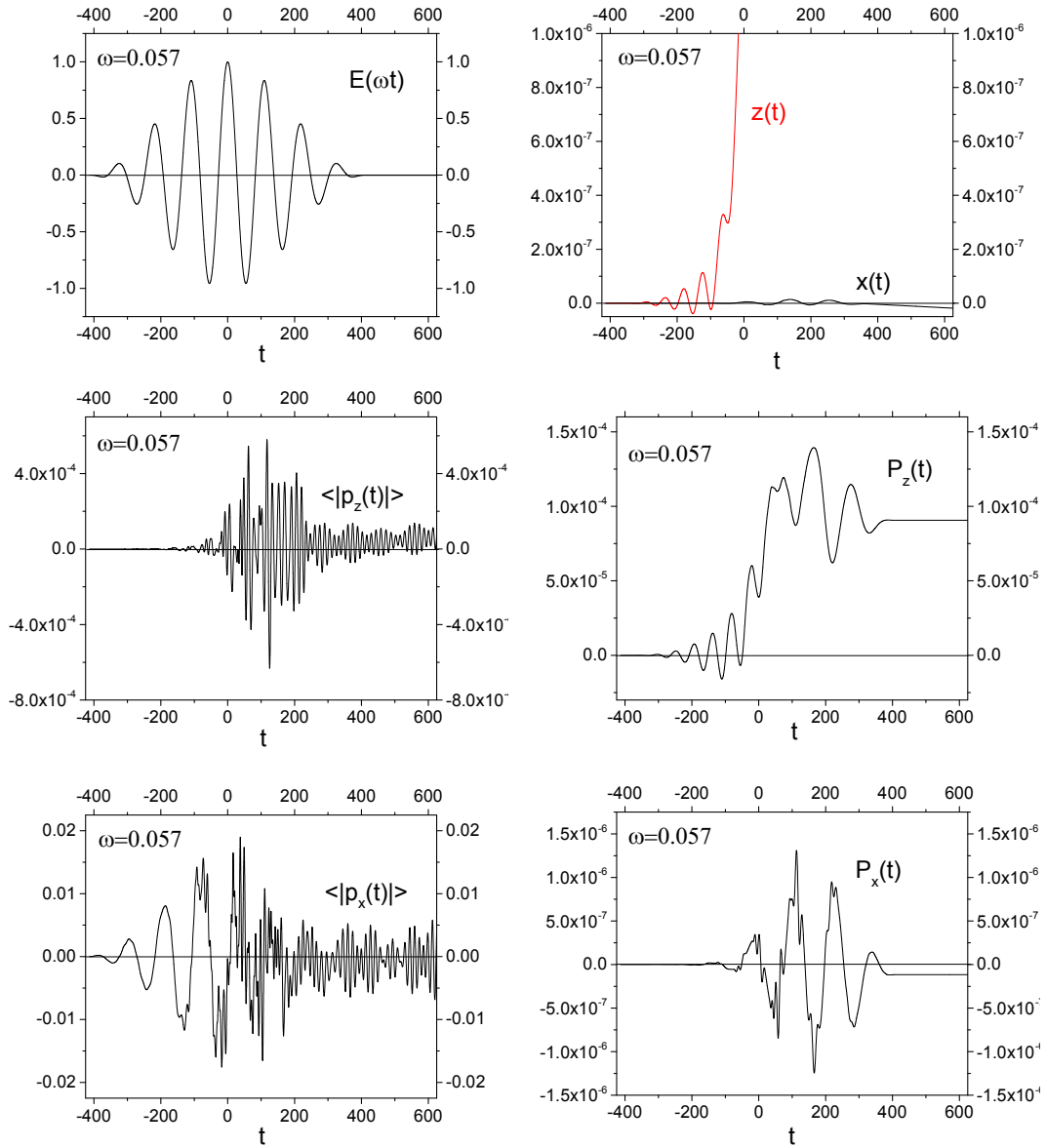






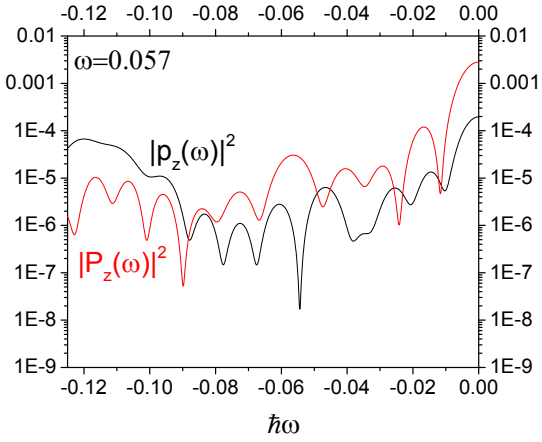
$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



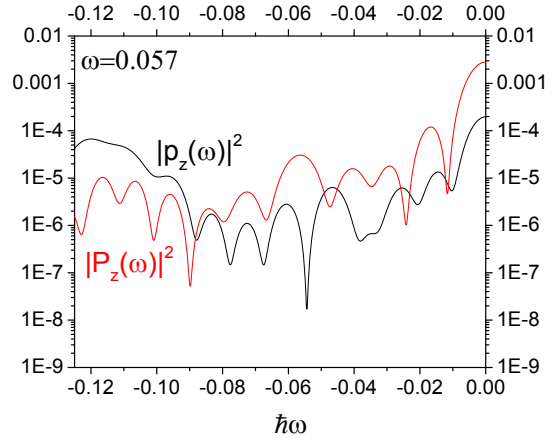
$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

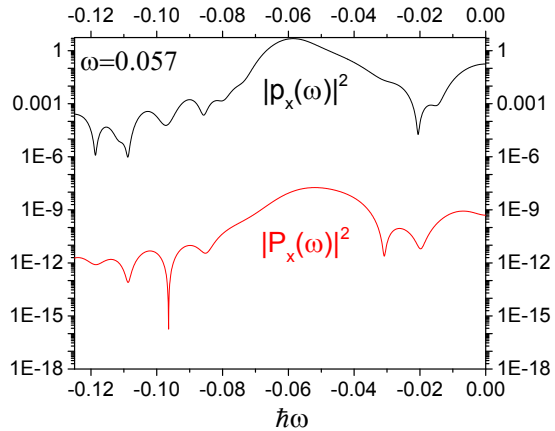
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

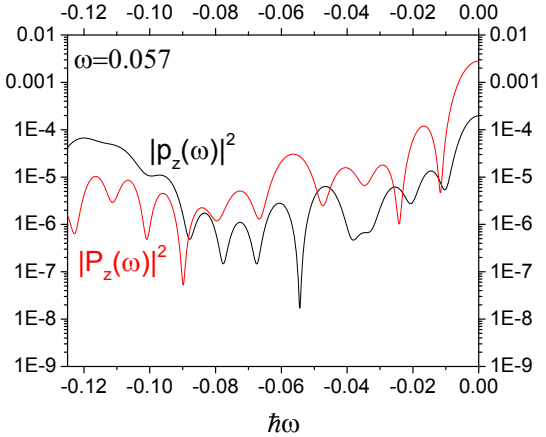
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$

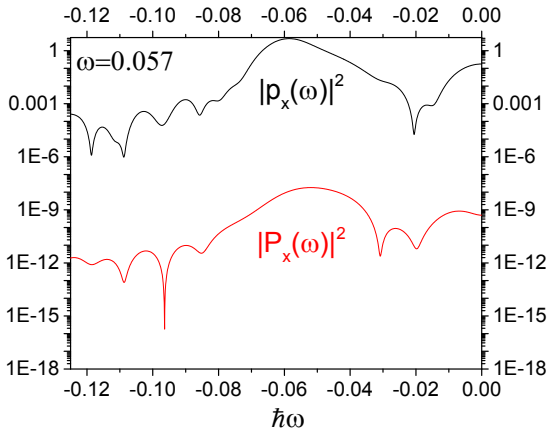


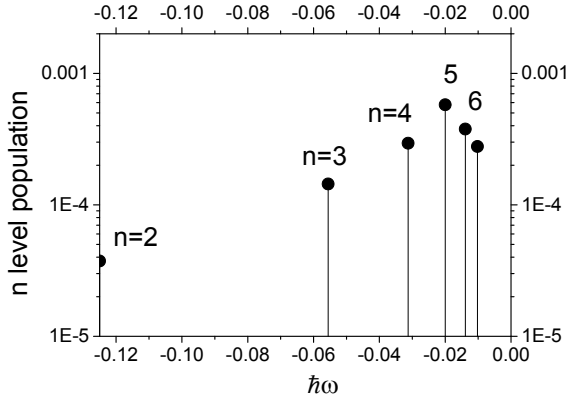


$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



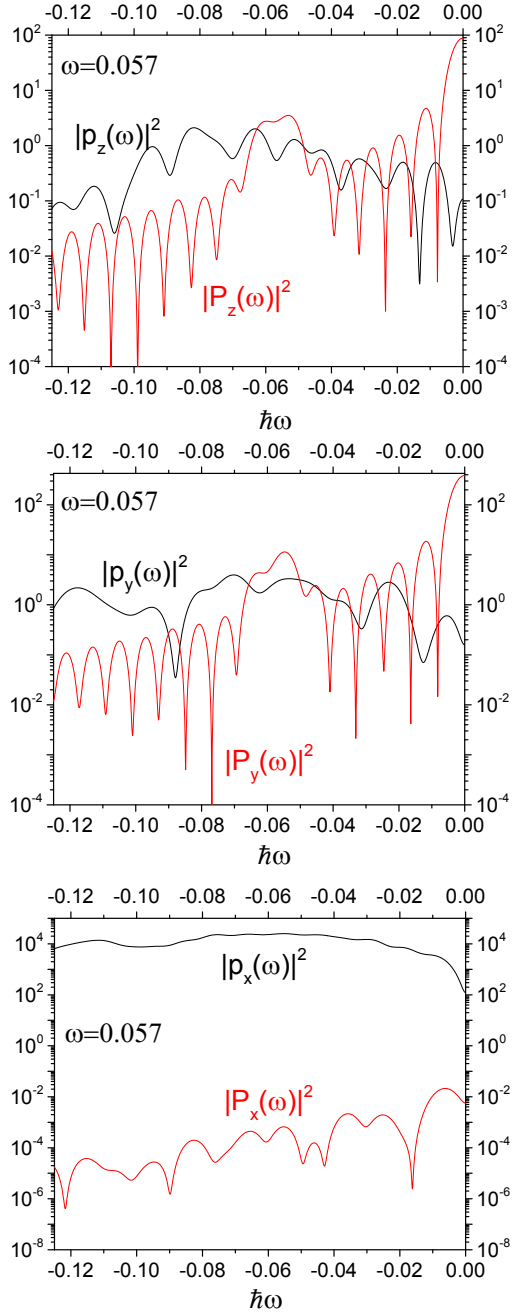




$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

$$X(-T) = Z(-T) = 0\ ,\ Y(-T) = \frac{w_0}{2}$$

$$\mathbf{P}(-T) = 0$$

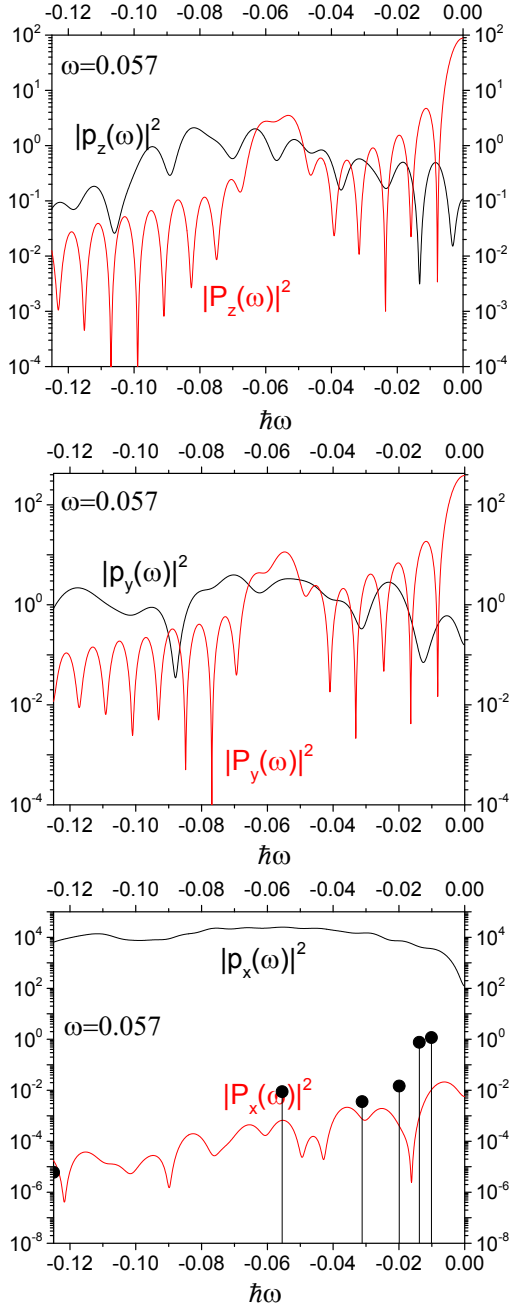


$$E_0(T) = E_0 \exp\{-\frac{t^2}{T^2}\} \exp\{-\frac{\rho^2}{w_0^2}\}$$

$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 800nm\ T = 5.3fs$$

$$X(-T) = Z(-T) = 0\ ,\ Y(-T) = \frac{w_0}{2}$$

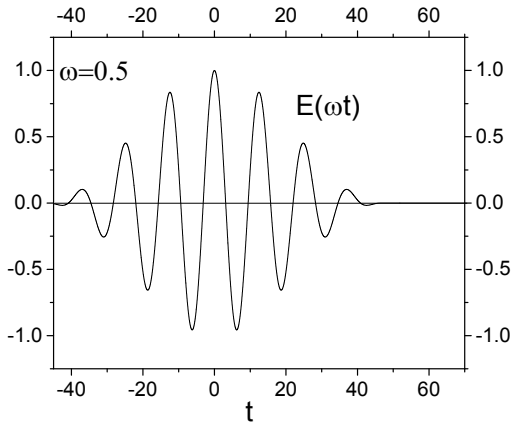
$$\mathbf{P}(-T) = 0$$

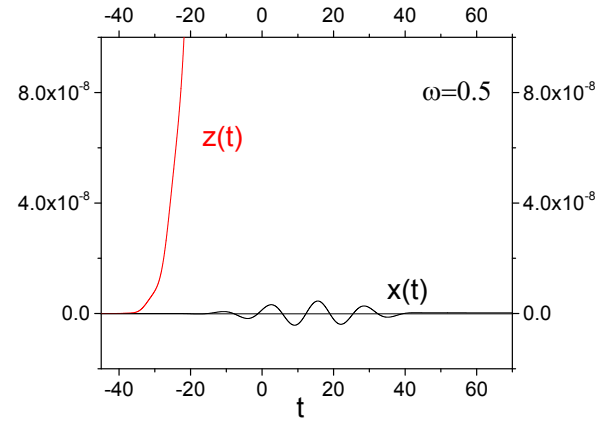


$$E_0(T) = E_0 \exp\{-\frac{t^2}{T^2}\} \exp\{-\frac{\rho^2}{w_0^2}\}$$

$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 80nm\ T = 0.52fs$$

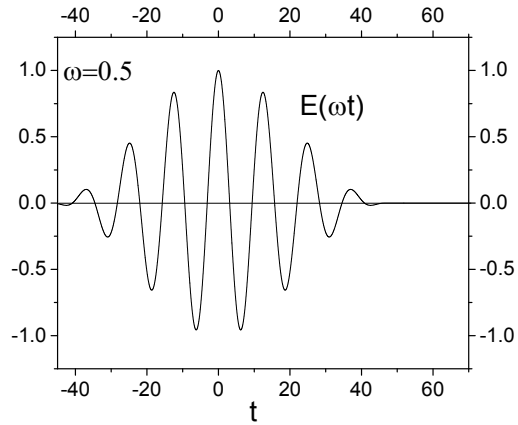
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$

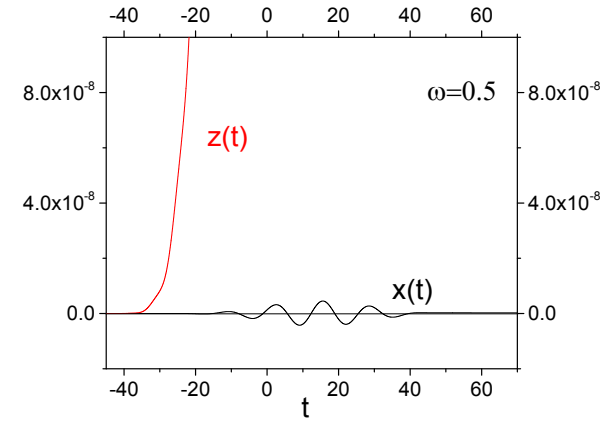


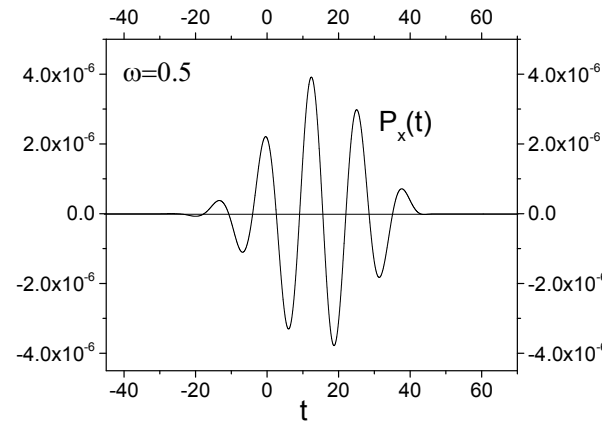


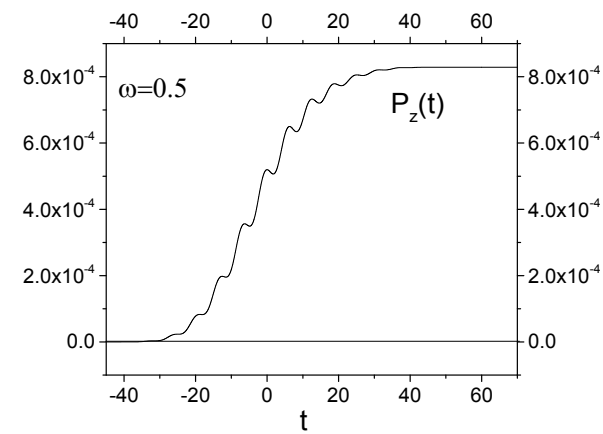
$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 80nm\ T = 0.52fs$$

$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



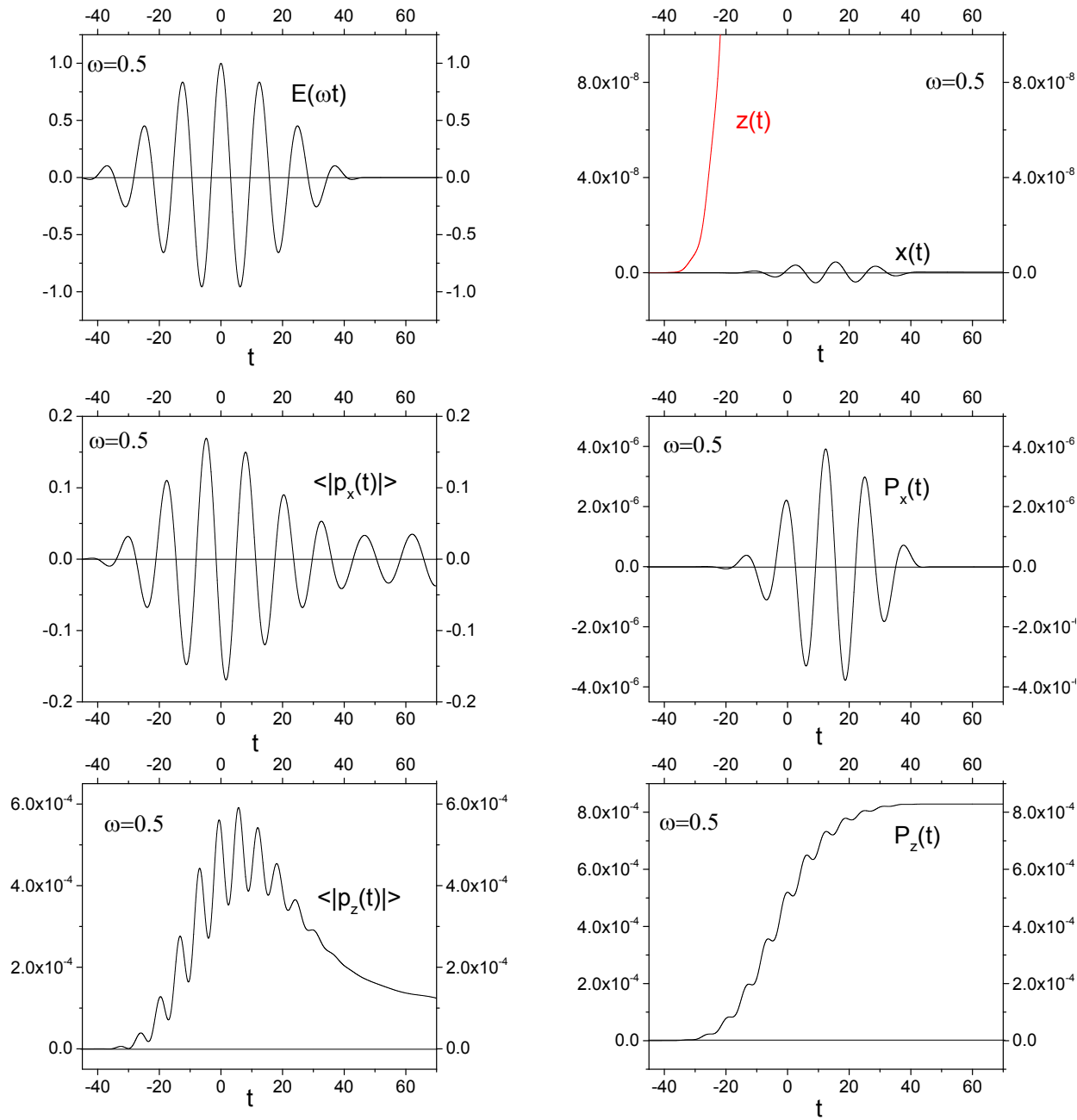






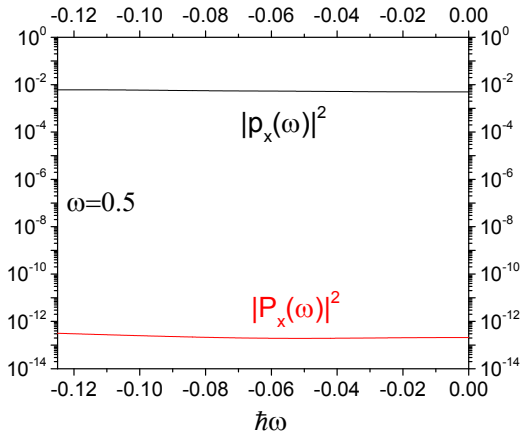
$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 80nm\ T = 0.52fs$$

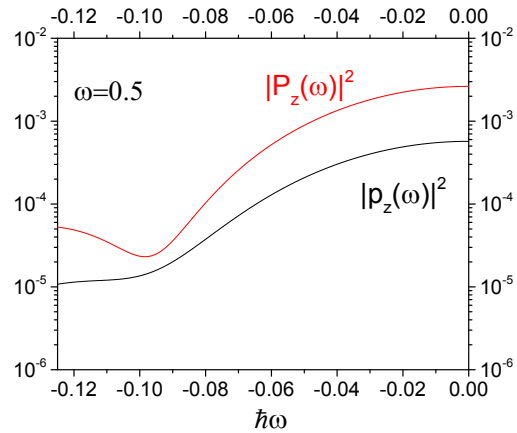
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$



$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 80nm\ T = 0.52fs$$

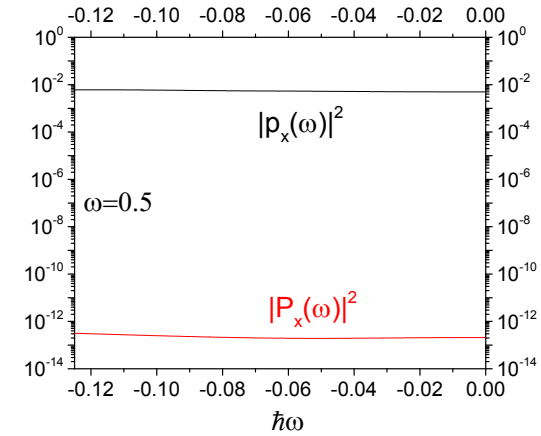
$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$

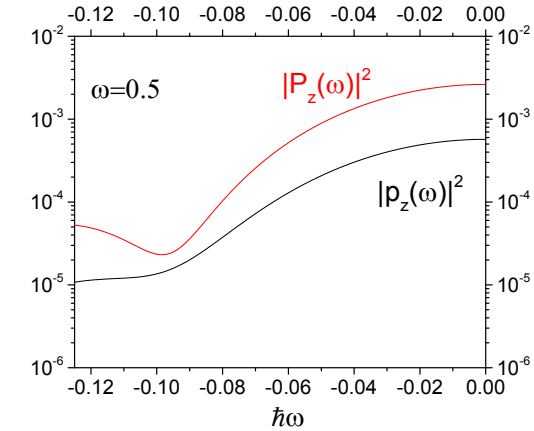


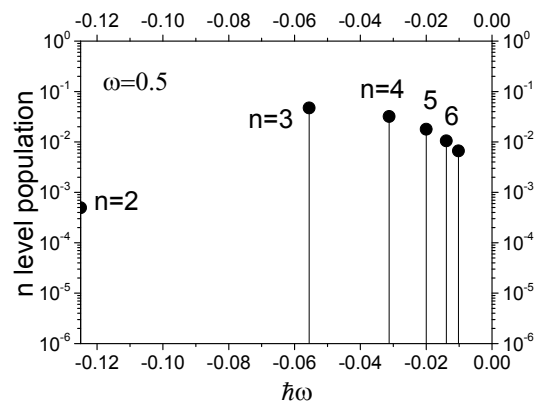


$$I = 10^{14}\frac{W}{cm^2}\ \lambda = 80nm\ T = 0.52fs$$

$$\mathbf{R}(-T) = \mathbf{P}(-T) = 0$$







Conclusion & Outlook

- ***it was confirmed with quantum-quasicalassical approach***

  the correlation between internal and CM dynamics

  in hydrogen atom in strong laser fiels

- ***by using CM-velocity spectroscopy as the «build-up» classical set up***

  we obtain information about internal quantum dynamics of atoms

  in intense laser fields