Quantum-quasiclassical method for fewbody processes in atomic and nuclear physics

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quantum-quasiclassical approach -> FBS

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PHYSICAL REVIEW LETTERS

28 February 2000

Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields

V.S. Melezhik^{1,*} and P. Schmelcher²

PHYSICAL REVIEW A 69, 032709 (2004)

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

Vladimir S. Melezhik,^{1,*} James S. Cohen,² and Chi-Yu Hu¹

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	THE EUROPEAN
https://doi.org/10.1140/epja/s10050-022-00684-z	Physical Journal
Investigation of low-lying resonances in breakup of halo nuclei within the time-dependent approach	
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hydrogen atom + EM pulse

- Nondipole effects (NDE) in interaction of atoms with short-wave EM radiation
- NDE nonseparability of CM and electron variables _____ acceleration
- Mechanisms for acceleration of neutral atoms by EM pulses
- Acceleration and «twisting» of atoms by circularly polarized EM pulse

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 Image: Constraint of a study: chirality, magnetization mapping, transpher of angular momentum to nanoparticls ...

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several proposals to create vortex beams of composite particles (neutrons, protons and atoms)

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several proposals to create vortex beams of composite particles (neutrons, protons and atoms)

Conclusion & perspectives

electromagnetic wave + atom

$$\mathbf{x} \quad E(\omega t, z) = E_0 \cos(\omega t - kz) = E_0 \cos(\omega t - \frac{\omega}{c}z)$$

$$\mathbf{x} \quad \mathbf{x} \quad \mathbf{x}$$

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$$\mathbf{$$

optical range

 $\lambda \sim 500$ nm $\omega \sim 10^{-1}a.u.$

$$\frac{\omega}{c} \simeq \frac{10^{-1}}{137} \to 0$$

electromagnetic wave + atom

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$$\mathbf{k} \quad z$$

$$\mathbf{y} \quad B(\omega t, z) = \frac{1}{c}E(\omega t, z) \qquad \qquad \frac{1}{c} = \alpha = \frac{1}{137}$$

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 dipole approximation

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X-ray
$$\lambda \sim (10^2 - 10^{-3}) nm \ \omega \sim (1 - 10^4) a.u. \ \frac{\omega}{c} \sim \frac{1}{137} - 10^2$$

electromagnetic wave + atom

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optical range
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 $\frac{\omega}{c} \simeq \frac{10^{-1}}{137} \rightarrow 0$ dipole approximation
X-ray $\lambda \sim (10^2 - 10^{-3})nm \quad \omega \sim (1 - 10^4)a.u.$ $\frac{\omega}{c} \sim \frac{1}{137} - 10^2$



$$V_2(\mathbf{r},\mathbf{R}) = \frac{1}{c} E_0 f(t) \{\cos(\omega t) [Z\hat{p}_x - X\hat{p}_z] + \omega \sin(\omega t) [xZ + zX]\}$$



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

$$H(\mathbf{r}, \mathbf{R}, t) = \frac{\mathbf{P}^2}{2M} + h_0(\mathbf{r}) + V_1(\mathbf{r}, t) + \frac{V_2(\mathbf{r}, \mathbf{R}, t)}{h_0(\mathbf{r})} = \frac{\hat{\mathbf{p}}^2}{2\mu} - \frac{1}{r}$$

PHYSICAL REVIEW LETTERS 124, 233202 (2020)

Dissecting Strong-Field Excitation Dynamics with Atomic-Momentum Spectroscopy

A. W. Bray,^{1,2,*} U. Eichmann,^{2,†} and S. Patchkovskii^{2,‡} ¹Australian National University, Canberra ACT 2601, Australia ²Max-Born-Institute, 12489 Berlin, Germany

$$H(\mathbf{r}, \mathbf{R}, t) \rightarrow H_{eff}(\mathbf{r}, t) = h_0(\mathbf{r}) + V_{eff}(\mathbf{r}, t)$$
 3D !!

We propose using the c.m. degrees of freedom of atoms and molecules as a "built-in" monitoring device for observing their internal dynamics in nonperturbative laser fields.

detection of the internal electron quantum dynamics with CM-velocity spectroscopy.

Hydrogen atom in strong laser field (quantum-quasiclassical method)



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

classical ideal gas perfectly describes gas laws

$$\lambda_{dB} = \frac{h}{MV} \to 0$$

$$\begin{split} i\hbar \frac{\partial}{\partial t} |\psi(\mathbf{r},t)\rangle &= [H_0(\mathbf{r}) + V(\mathbf{r},\mathbf{R}(t))] |\psi(\mathbf{r},t)\rangle \\ H_{cl}(\mathbf{P},\mathbf{R},t) &= \frac{\mathbf{P}^2}{2M} + \langle \psi(\mathbf{r},t) | V(\mathbf{r},\mathbf{R}(t)) |\psi(\mathbf{r},t)\rangle \\ &\frac{d}{dt} \mathbf{P} = -\frac{\partial}{\partial \mathbf{R}} H_{cl}(\mathbf{P},\mathbf{R},t) \\ &\frac{d}{dt} \mathbf{R} = \frac{\partial}{\partial \mathbf{P}} H_{cl}(\mathbf{P},\mathbf{R},t) \end{split}$$

$$\psi(\mathbf{r}, t = -n_T T/2) = \phi_{nlm}(\mathbf{r}),$$

 $\mathbf{R}(t = -n_T T/2) = \mathbf{R}_0, \ \mathbf{P}(t = -n_T T/2) = \mathbf{P}_0,$

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Quantum-quasiclassical analysis of center-of-mass nonseparability in hydrogen atom stimulated by strong laser fields*

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Abstract

We have developed a quantum-quasiclassical computational scheme for quantitative treating of the nonseparable quantum-classical dynamics of the 6D hydrogen atom in a strong laser pulse. In this approach, the electron is treated

Hydrogen atom in strong laser field (quantum-quasiclassical method)



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

classical ideal gas perfectly describes gas laws

$$\lambda_{dB} = \frac{h}{MV} \to 0$$

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

splitting method + DVR for angular variables

V. Melezhik, Phys Lett A230, 203 (1997)

V. Melezhik, EPJ Web Conf 108, 01008 (2016)

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

Hydrogen atom in strong laser field (quantum-quasiclassical method)



 $P=MV\gg p=mv \\$

classical ideal gas perfectly describes gas laws

$$\lambda_{dB} = \frac{h}{MV} \to 0$$

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

modified Stormer-Verlet method

V. Melezhik, Phys Rev A103, 053109 (2021)

Hydrogen atom in strong laser field (results of calculations)



 $\lambda = 800 \text{ nm} (\omega = 0.057 \text{ a.u.})$

Hydrogen atom in strong laser field (results of calculations)

 $\lambda = 800 \text{ nm} (\omega = 0.057 \text{ a.u.})$

$$\langle E_{kin} \rangle = \frac{1}{T_{out} - T_{in}} \int_{T_{in}}^{T_{out}} \frac{\boldsymbol{P}^2(t)}{2M} dt \sim \int_{-\infty}^{\infty} \left[\sum_{s=x,y,z} |\boldsymbol{P}_s(\omega)|^2 \right] d\omega,$$

$$\langle E_{kin}^{(el)} \rangle = \frac{1}{T_{out} - T_{in}} \int_{T_{in}}^{T_{out}} \frac{\boldsymbol{p}^2(t)}{2\mu} dt \sim \int_{-\infty}^{\infty} \left[\sum_{s=x,y,z} |p_s(\omega)|^2 \right] d\omega$$

$$P_s(\omega) = \int_{T_{in}}^{T_{out}} P_s(t) e^{i\omega t} dt$$

$$p_s(\omega) = \int_{T_{in}}^{T_{out}} \langle |p_s(t)| \rangle e^{i\omega t} dt$$

$$\langle |p_s(t)| \rangle = \int \psi^*(\mathbf{r}, t) \hat{p}_s \psi(\mathbf{r}, t) d\mathbf{r}.$$



Hydrogen atom in strong laser field (results of calculations)



 $\lambda = 400 \text{ nm} (\omega = 0.114 \text{ a.u.})$

Promising tasks: acceleration of atoms by strong EM pulses



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nature

Acceleration of neutral atoms in strong short-pulse laser fields

U. Eichmann^{1,2}, T. Nubbemeyer¹, H. Rottke¹ & W. Sandner^{1,2}

 $a_{exp} \sim 10^{14} q$

 $8 \times 10^{15} \frac{W}{cm^2}$, (700 - 1100) nm, (40 - 100) fs, He, Ne atoms

Mechanisms of acceleration of atoms by EM pulses





Article

Acceleration of Neutral Atoms by Strong Short-Wavelength Short-Range Electromagnetic Pulses

Vladimir S. Melezhik ^{1,2,*} and Sara Shadmehri ^{1,*}

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Citation: Melezhik, V.S.; Shadmehri,

S. Acceleration of Neutral Atoms by

Strong Short-Wavelength

Short-Range Electromagnetic Pulses.

Photonics 2023, 10, 1290. https://

doi.org/10.3390/photonics10121290



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

$$P_{ex} = \sum_{n=2}^{\infty} P_n = \sum_{n=2}^{N'} P_n + \sum_{n=N'+1}^{\infty} P_n$$
$$P_{ion} = \int_0^{+\infty} \frac{dP}{dE} dE$$

$$\sum_{n=1}^{\infty} P_n + \int_0^{+\infty} \frac{dP}{dE} dE = 1$$

Shadmehri, S.; Melezhik, V.S. *Laser Phys.* **2023**, *33*, 026001.





$$\hbar\omega = \frac{1}{2n^2} - \frac{1}{2n'^2}$$
 $\omega = 0.38, 0.44, 0.47$ (a.u.)

 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



 $H_{n=1} + \hbar \omega \rightarrow H_{n'}$, n' = 2,

 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$





 $H_{n=1} + \hbar \omega \rightarrow H_{n'}$ n' = 3.

 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



 $H_{n=1} + \hbar \omega \rightarrow H_{n'}$ n' = 4





two-photon transition $2\hbar\omega \approx 0.47$ a.u. for n = 1 and n' = 4peak in $P_{ex}(\omega)$ at $\omega = 0.24$ a.u.

 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



two-photon transition $2\hbar\omega \approx 0.47$ a.u. for n = 1 and n' = 4



 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



 $P_n(\omega,t) \xrightarrow{t \to T_{out}} P_n(\omega)$



non-resonant mechanism







strong correlation between $P_{ex} + P_{ion}$ and V_y (CM momentum = MV_y)



strong correlation between $P_{ex} + P_{ion}$ and V_y (CM momentum = MV_y)

mechanism of CM acceleration:

generation of nonzero dipole between proton and electron cloud transferred either to excited states of atom or to its continuum



 $\omega = 0.48$ a.u. one-photon resonant transition $n = 1 \rightarrow n' = 4$

 $\omega = 0.24$ a.u. two-photon resonant transition $n = 1 \rightarrow n' = 4$

 $\omega=0.8a.u.$ non-resonant mechanism



areas promising for accelerating atoms where ionization is suppressed

Vortex beams of atoms and molecules

Alon Luski¹[†], Yair Segev¹[†][‡], Rea David¹, Ora Bitton¹, Hila Nadler¹, A. Ronny Barnea², Alexey Gorlach³, Ori Cheshnovsky², Ido Kaminer³, Edvardas Narevicius¹*

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ig. 2. Experimental setup for the production and detection of atomic and molecular vortex beams.

Fig. 4. Comparison of intensity measured in the experiment to theory, with simulated contribution of only the atoms.

 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

Linear polarization (ε =0)

 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

Linear polarization (ε =0)

 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

Circular polarization (ϵ =1)

 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

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 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

Elliptical polarization (ϵ =0-1)

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Elliptical polarization (ϵ =0-1)

 10^{14} BT/CM^2 , ~10¢c, $hv \sim 133B \sim 0.48a.u.$

Circular polarization (ϵ =1)

- acceleration of atom due to non-dipole corrections kr in EM wave and magnetic component B/c in it was invastigated
- strong correlation was found between V (MV) and P_{ex}+ P_{ion}
- two resonant mechanisms of atom acceleration were found: through single-photon and two-photon excitation of atom

single-photon $V \sim I$

two-photone $V \sim I^2$

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single-photon $V \sim I$

two-photone $V \sim I^2$

three-photone $V \sim I^3$?

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- strong correlation was found between V (MV) and P_{ex} + P_{ion}
- two resonant mechanisms of atom acceleration were found: through single-photon and two-photon excitation of atom
- potential applications:

accelerated atoms — lithography of micro-chips for microelectronics, plasma diagnostics in TOKAMAK, ... «twisted» atoms — modification of fundamental interactions, new «tool» for investigation of atomic collisions, ...

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- non-dipole effects (accounting nuclei motion) in atomic int. with EM pulse $V_2(r, R, t) = \frac{\omega}{c} E_0(....)$: influence on high harmonic generation, stabilization of atoms, ... groundwork was created for study of non-dipole effects: different atoms, accounting of spatial inhomogeneity of EM pulse, different polarizations, twisted atoms, ...

hybrid quantum-quasiclassical approach + DVR

- S Shadmehri, V S Melezhik, Laser Phys. 33, 026001 (2023)
- V Melezhik, J. Phys. A56, 154003 (2023)
- V S Melezhik, S Shadmehri, Photonics 10(12), 1290 (2023)
- V S Melezhik, S Shadmehri, arXiv: 2408.08613