Electron scattering and ionization processes in strong laser fields

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Overview

1. Introduction

2. Simulation Method
   - Numerical solution of the time-dependent Schrödinger equation

3. Ionization and scattering processes in strong laser fields
   - Ionization in strong fields
     - Angle-resolved electron spectra
   - Electron–Ion collisions in strong laser fields
     - Angle-resolved scattering

4. Conclusions
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Matter–light interaction

- active field of research: strong field interactions
- quantum nature of particles important
- simplification: consider only basic processes
- focus on fundamental effective one-particle processes:
Introduction

Matter–light interaction

- active field of research: strong field interactions
- quantum nature of particles important
- simplification: consider only basic processes
- focus on fundamental effective one-particle processes:
  - ionization phenomena of atoms in strong fields
  - electron scattering in presence of a strong laser field
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Simulation method: one-particle TDSE

Time-dependent Schrödinger equation (TDSE)

\[ i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m_e} \Delta + V(r, t) \right) \psi(r, t) \]

\[ V(r, t) = -\frac{Ze^2}{\sqrt{r^2 + \kappa^2}} + E_0 ex \sin(\omega t) \]

- exact numerical treatment of quantum effects in single-active electron approximation
- the exact many-body problem is computationally impossible to solve, approximative methods are given in K. Balzers talk
- laser field is treated classically within the dipole approximation
- num. important: regularization of Coulomb potential by \( \kappa \)
**Simulation method: one-particle TDSE**

Time-dependent Schrödinger equation (TDSE)

\[
i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left( -\frac{\hbar^2}{2m_e} \Delta + V(r, t) \right) \Psi(r, t)
\]

General solution given by

\[
\Psi(r, t) = \hat{U}(t, t_0) \Psi(r, t_0)
\]

with time evolution operator

\[
\hat{U} = \exp(-i\hat{H}t)
\]
Numerical solution of the time-dependent Schrödinger equation

Numerical solution of the TDSE

Discretization of time...

\[ e^{-i\hat{H}\Delta t} \approx \frac{1 - \frac{1}{2}i\hat{H}\Delta t}{1 + \frac{1}{2}i\hat{H}\Delta t} \]

Cayley's form of \( \hat{U} \)
Numerical solution of the time-dependent Schrödinger equation

**Numerical solution of the TDSE**

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**Cayley's form of \( \hat{U} \)**

**...and space**

\[
\frac{d^2}{dx^2}\psi \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{(\Delta x)^2}
\]

**Finite-difference approx.**
Numerical solution of the TDSE

**Discretization of time...**

\[ e^{-i\hat{H}\Delta t} \approx 1 - \frac{1}{2}i\hat{H}\Delta t \]

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*Cayleys* form of \( \hat{U} \)

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\[ \frac{d^2}{dx^2}\psi \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{(\Delta x)^2} \]

**Finite-difference** approx.

- this scheme gives the *Crank-Nicolson* procedure for
diffusive-like initial value problems
- \( \Delta t \) and \( \Delta x \) numerical parameters (convergence!)
- leads to a tridiagonal system of linear equations which are
very efficiently solvable
- generalization to two-dimensional systems by the
*operator-splitting* technique possible
Numerical solution of the time-dependent Schrödinger equation

**Numerical solution of the TDSE**

**Discretization of time...**

\[ e^{-i\hat{H}\Delta t} \approx 1 - \frac{1}{2}i\hat{H}\Delta t \]

...and space

\[ \frac{d^2}{dx^2}\psi \approx \psi_{i+1}^{n} - 2\psi_{i}^{n} + \psi_{i-1}^{n} \]

Tridiagonal system of \( N_x \) linear equations

\[
\begin{pmatrix}
    b_1 & c_1 & 0 & 0 \\
    a_2 & b_2 & c_2 & 0 \\
    \vdots & \vdots & \vdots & \vdots \\
    0 & 0 & a_N & b_N \\
\end{pmatrix} \cdot
\begin{pmatrix}
    \psi_{1}^{n+1} \\
    \psi_{2}^{n+1} \\
    \vdots \\
    \psi_{N}^{n+1} \\
\end{pmatrix} =
\begin{pmatrix}
    r_1^{n} \\
    r_2^{n} \\
    \vdots \\
    r_N^{n} \\
\end{pmatrix}
\]

leads to a tridiagonal system of linear equations which are very efficiently solvable

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Numerical solution of the time-dependent Schrödinger equation

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Propagation scheme

- set up numerical grids with spatial step size $\Delta x$ and time step size $\Delta t$
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- set up numerical grids with spatial step size $\Delta x$ and time step size $\Delta t$
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Propagation scheme

**Numerical scheme**

- set up numerical grids with spatial step size $\Delta x$ and time step size $\Delta t$
- set initial conditions $\psi_0$
- define boundary conditions $\psi(x = 0, x = n)$
Numerical solution of the time-dependent Schrödinger equation

**Propagation scheme**

- set up numerical grids with spatial step size $\Delta x$ and time step size $\Delta t$
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- set initial conditions $\psi_0$
- define boundary conditions $\psi(x = 0, x = n)$
- advance time by successive application of time evolution operator $\hat{U}(t, t + \Delta)$ onto $\psi$
- analyze final solution $\psi(t_0 + n_t \cdot \Delta t)$
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Ionization in strong fields: two different mechanisms

**Fig:** Multi-photon ionization: $\gamma < 1$

**Fig:** Tunnel ionization $\gamma > 1$

- relevant quantity: Keldysh parameter $\gamma = \sqrt{I_p/2U_p}$
- connects ionization potential $I_p$ and ponderomotive potential $U_p$
- separates tunneling and multi-photon regime
- corresponds to a classification in terms of the laser intensity
Ionization in strong fields: two different mechanisms

Overview: field intensity regimes

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**Above Threshold Ionization**

- \( \gamma > 1 \)
- Optical field ionization
- \( \gamma < 1 \)
- tunnel ionization

**Ionization Potential**

- Multi-photon ionization
- 2nd order processes
- 3rd order processes
- 4th order processes

**Electric Field**

- Modified Coulomb potential
- ground state
- ionic potential

**Overview Diagram**

- Log (Intensity [W/cm²])
- 11, 12, 13, 14, 15, 16, 17, 18, 19
Ionization in strong fields: two different mechanisms

- Above Threshold Ionization
- Multiphoton Ionization
- Tunnel ionization

Overview: field intensity regimes

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Fig: Multi-photon ionization ($\gamma < 1$)

Fig: Tunnel ionization ($\gamma > 1$)
Ionization in strong fields

A simple single-atom model system

\[ V(x, y) = -\frac{1}{\sqrt{x^2 + y^2 + \kappa^2}} \]

Model for a two-dimensional hydrogen atom

- potential: Coulomb with regularization
- initial condition: eigenstate (bound electron)
- ionization with strong linearly polarized laser field
- up to X-FEL radiation (\( \lambda = 13.2\text{nm} \) with \( I = 10^{15} \text{ W/cm}^2 \))
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Spherical detector
Ionization in strong fields

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→ Angle- and energy-resolved photoelectron spectra
Angle-resolved multi-photon ionization spectra

Absorption of $\hbar \omega$

Absorption of $2\hbar \omega$

Ionization in strong fields

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Absorption of $\hbar \omega$

(b) $\omega = 1.0$

(a) $\omega = 0.5$

laser polarization

φ

0.0001 0.01 1

intensity [arbitrary units]
Angle-resolved multi-photon ionization spectra

(b) $\omega = 1.0$

(a) $\omega = 0.5$

Absorption of $\hbar \omega$

Ekin
Angle-resolved multi-photon ionization spectra

Absorption of $\hbar \omega$

Absorption of $2\hbar \omega$

(b) $\omega = 1.0$

(a) $\omega = 0.5$
laser polarization

$\varphi$

Intensity [arbitrary units]
Angle-resolved multi-photon ionization spectra

- clear evidence of multi-photon absorption
- unexpected angular distributions
Explanation: scattering features in electron spectra

Angular-resolved photoelectron spectra depending on $\hbar \omega$

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**Ionization in strong fields**

**Explanation: scattering features in electron spectra**

Angular-resolved photoelectron spectra depending on $\hbar \omega$

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Electron–Ion collisions in strong laser fields

**Electron–Ion collisions: One-dimensional model system**

- electron represented by free Gaussian wave packet
- initial momentum $k_0$
- ion represented by (regularized) Coulomb potential
- forward and backward scattered parts of electronic wave function are detected
Electron–Ion collisions in strong laser fields

Electron–Ion collisions: One-dimensional model system

Generation of a distribution of fast electrons
- during scattering on the ion the electron gains energy
- absorbs \textit{many} photons as in the case of strong field ionization
- additional $E_{\text{kin}}$ originates from ponderomotive motion of $e^-$
Electron–Ion collisions in strong laser fields

Correlated scattering: fast electron generation

Acceleration of electrons by scattering

- variation of distance: resonance behavior
- depending on period of laser field, ion distance and electron velocity
- plasmas: density adjusts average ion distance
- non-trivial, resonant acceleration of electrons

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Correlated scattering: fast electron generation

Electron spectra of electron–ion pair scattering

- back scattered
- forward scattered

Energy [a.u.]

Electron–ion collisions in strong laser fields

Angle-resolved scattering processes

Two-dimensional Coulomb scattering

- Additional degree of freedom: direction of scattered electron
- Classical picture: distribution of initial conditions
- Quantum case: interference of many classical trajectories
Electron–ion collisions in strong laser fields

Angle-resolved scattering processes

Angle-resolved spectrum of scattered electrons

Two-dimensional Coulomb scattering

- Additional degree of freedom: direction of scattered electron
- Classical picture: distribution of initial conditions
- Quantum case: interference of many classical trajectories
Overview

1. Introduction

2. Simulation Method
   - Numerical solution of the time-dependent Schrödinger equation

3. Ionization and scattering processes in strong laser fields
   - Ionization in strong fields
     - Angle-resolved electron spectra
   - Electron–Ion collisions in strong laser fields
     - Angle-resolved scattering

4. Conclusions
Conclusions: Fundamental processes in strong laser fields

Numerical method: TDSE solution
- implementation of the Crank-Nicolson scheme
- fast and efficient method for the solution on spatial grids
- exact treatment of quantum nature within one-particle picture

Strong field ionization
- multi-photon absorption
- non-trivial angular distributions of $e^-$
- explanation: rescattering of photoionized electron

Electron scattering in strong fields
- Scattering increases $E_{\text{kin}}$ by absorption of photons
- possibility of resonant acceleration
- strong angular dependence
Thank you for your attention!