Atoms in strong laser fields

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Lecture 2: Theoretical methods I

- Classical methods
- Perturbative methods
  - Low-intensity perturbation theory
  - Gordon-Volkov series
  - Strong-field approximation (KFR theories)

References

- M. Gavrila, Atoms in Strong Laser Fields, Academic Press, 1992
- C.F.M.F, Ph.D. thesis (TU-Berlin, 1999)
- A. Fring, V. Kostrykin and R. Schrader, J. Phys. B 29, 5651 (1996)
- W. Becker, A. Lohr, M. Kleber and M. Lewenstein, PRA 56, 645 (1997)

Classical methods

Classical electron in a laser field

- Electron propagation in the continuum:

$$\ddot{\mathbf{r}}(t) = \underbrace{-\nabla V}_{neglected} - \mathbf{E}(t)$$

- Initial conditions:
  - $\mathbf{v}(t_0) = 0$ (vanishing drift velocity)
  - $\mathbf{r}(t_0) = 0$ (electron released from the origin)

$$\mathbf{v}(t) = \mathbf{A}(t) - \mathbf{A}(t_0)$$

$$\mathbf{r}(t) = \int_{t_0}^{t} \mathbf{A}(\tau) d\tau - (t - t_0)\mathbf{A}(t_0)$$

- return time t_1: $\mathbf{r}(t_1) = 0$

- High-harmonic generation: $\Omega = |\varepsilon_0| + E_{kin}(t_1, t_0)$
- High-order above-threshold ionization: $\frac{1}{2}\left[\mathbf{p} - \mathbf{A}(t_0)\right]^2 = E_{kin}(t_1, t_0)$
- Nonsequential double ionization:

$$\sum \left[\mathbf{p}_i - \mathbf{A}(t_0)\right]^2 = E_{kin}(t_1, t_0) - \underbrace{|\varepsilon_{02}|}_{2^{nd}\text{ ionization potential}}$$

with $E_{kin}(t_1, t_0) = \frac{1}{2}[A(t_1) - A(t_0)]^2$ (kinetic energy upon return)

Tangent construction

- Graphical method for finding t_1
  (see, e.g., G.G. Paulus et al, PRA 52, 4043 (1995))
- Pre-requisite: linear polarization

Return condition

- $x(t_1) = 0 \Rightarrow \int_{t_0}^{t_1} \mathbf{A}(\tau) d\tau = (t_1 - t_0)\mathbf{A}(t_0)$
- Defining $F(t) = \int^t A(\tau) d\tau$ we have

$$F(t_1) = F(t_0) + (t_1 - t_0)F'(t_0)$$

Intersection of F(t) with its tangent at t_0

Cutoff condition

- $\partial E_{kin}(t_1, t_0)/\partial t_0 = 0$

$$A(t_0) = A(t_1) - (t_1 - t_0)E(t_1)$$

Intersection of A(t) with its tangent at t_1

Perturbative methods

Time evolution operator

$$|\psi(t)\rangle = U(t,t')\,|\psi(t')\rangle$$

- Makes the system evolve from t' to t
- Obeys:
  - Time-dependent Schrödinger equation
  - $U(t,t') = U^{-1}(t',t); U(t,t) = 1;\ U(t,t')U(t',t'') = U(t,t'')$

DuHamel (or Dyson) equation:

$$\begin{aligned} U_a(t,t') &= U_b(t,t') - i\int_{t'}^{t} U_a(t,s)(H_a(s) - H_b(s))U_b(s,t')ds \\ &= U_b(t,t') - i\int_{t'}^{t} U_b(t,s)(H_a(s) - H_b(s))U_a(s,t')ds \end{aligned}$$

with

- $U_j(t,t')(j = a,b)$ time evolution operators
- $H_j(t)(j = a,b)$ time-dependent Hamiltonians

Perturbation theory: DuHamel equation is iterated

$$\begin{aligned} U_a(t,t') &= U_b(t,t') - i\int_{t'}^{t} U_b(t,s)H_{a,b}(s)U_b(s,t')ds \\ &\quad - \int_{t'}^{t} ds \int_{t'}^{s} U_b(t,s)\underbrace{H_{a,b}(s)}_{H_a - H_b}U_b(s,s')H_{a,b}(s')U_b(s',t')ds' + \ldots \end{aligned}$$

Standard ("low-intensity") perturbation theory:

- $H_a \equiv H = p^2/2 + V + H_{int}(t)$(“full” Hamiltonian)
- $H_b \equiv H_0 = p^2/2 + V$ (field-free Hamiltonian)

Gordon-Volkov (GV) series:

(Volkov, Zeit. für Physik 94, 250 (1935); Gordon, ibid. 40, 117 (1926).)

- $H_a = p^2/2 + V + H_{int}(t)$
- $H_b \equiv H^{(GV)} = p^2/2 + H_{int}(t)$ (GV Hamiltonian)

Strong-field approximation (KFR theories)

L. V. Keldysh, Sov. Phys. JETP 20, 1307 (1965); F.H.M. Faisal, J. Phys. B 6, L89 (1973); H. R. Reiss, PRA 22, 1786 (1980).

- Formally:
  - Both series are mixed
  - Referred to as perturbation theory with a modified basis
- Physical idea:
  - Neglect H_{int} when the e^- is bound
  - Neglect V when the e^- is in the continuum

Which of these approximations breaks the Gauge invariance?

Different formulations: difference between K F and R

(context: ionization probabilities)

- Initial state: field-free bound state
- Final state: continuum state

Transition amplitude:

$$M = \lim_{t_\pm \to \pm\infty} \left\langle \psi_p(t_+) \right| S(t_+, t_-) \left| \phi_0(t_-) \right\rangle$$

with

$$S = \lim_{t_\pm \to \pm\infty} \exp(it_+ H_+) \cdot U(t_+, t_-) \cdot \exp(-it_- H_-)$$

and
$H_\pm = \lim_{t\pm \to \pm\infty} H(t)$

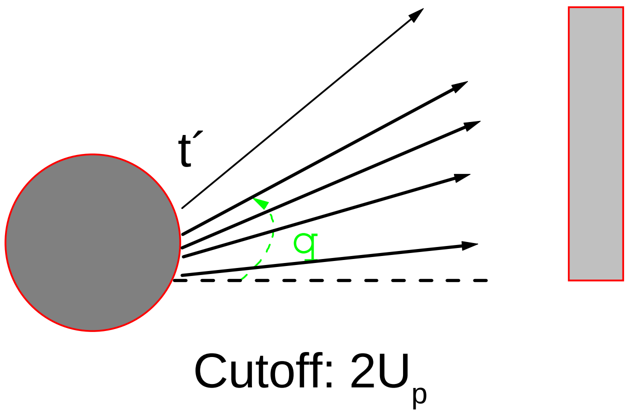
Strong-field approximation:

$$U(t, t') \simeq U_0(t, t') - i \int_{t''}^{t} dt'' U^{(GV)}(t, t'') H_{int}(t'') U_0(t'', t')$$

Keldysh	Faisal-Reiss
Length gauge:	Velocity gauge
$H_{int}(t) = \mathbf{r}.\mathbf{E}(t)$	$H_{int}(t) = -\mathbf{p}.\mathbf{A}(t) + \mathbf{A}^2(t)$

Application: above-threshold ionization

Direct electrons



Transition amplitude:

Becker et al: $M = -i \lim_{t\pm\to\pm\infty} \int_{t_-}^{t_+} \left\langle \psi_p^{(GV)}(t) \right| V \left|\psi_0(t')\right\rangle dt'$

This formulation is equivalent to

$$M = -i \lim_{t\pm\to\pm\infty} \int_{t_-}^{t_+} \left\langle \psi_p^{(GV)}(t) \right| H_{int}(t) \left|\psi_0(t)\right\rangle dt$$

How to prove it ?

- We take

$$H_{int}(t) = \underbrace{H_{int}(t) + p^2/2}_{H^{(GV)}(t)} - \underbrace{(p^2/2 + V)}_{H_0(t)} + V$$

- and use

$$i\partial_t U^{(*)}(t,t') = H^{(*)}(t)U^{(*)}(t,t')$$

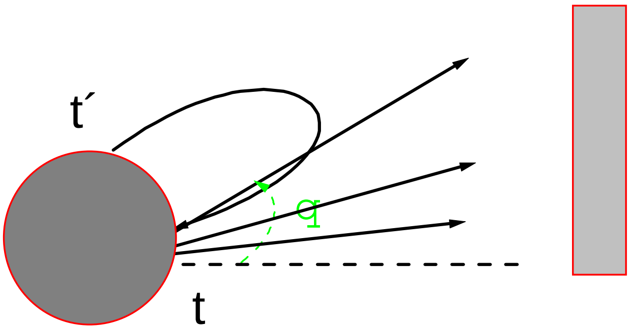
$$-i\partial_{t'} U^{(*)}(t,t') = U^{(*)}(t,t')H^{(*)}(t')$$

with $(*) = (GV)$ or (0)

and

$$\partial_t (ABC) = \partial_t(A)BC + A\partial_t(B)C + AB\partial_t(C)$$

Rescattered electrons



Cutoff: $10U_p$

Generalized KFR theory:

$$U(t,t') \simeq U_0(t,t') - i\int_{t'}^{t} dt'' U^{(GV)}(t,t'')H_{int}(t'')U_0(t'',t')$$
$$-\int_{t'}^{t} dt'' \int_{t'}^{t''} dt''' U^{(GV)}(t,t'')VU^{(GV)}(t'',t''')H_{int}(t''')U_0(t''',t')$$

Transition amplitude:

$$M = -i \lim_{t\pm\rightarrow\pm\infty} \int_{t_-}^{t_+} dt \int_{t_-}^{t} dt' \left\langle \psi_p^{(GV)}(t) \right| VU^{(GV)}(t,t')V \left|\psi_0(t')\right\rangle$$

Gauge-equivalent Hamiltonians

$$H_i(t) = i\partial_t T_{j\leftarrow i}(t) T_{j\leftarrow i}(t)^{-1} + T_{j\leftarrow i}(t) H_j(t) T_{j\leftarrow i}(t)^{-1}$$

- Length gauge

$$H_l(t) = -\frac{\Delta}{2} + V + \mathbf{r}\cdot\mathbf{E}(t)$$

$$T_{v\leftarrow l}(t) = e^{i\mathbf{A}(t).\mathbf{r}}$$

- Velocity gauge

$$H_v(t) = \frac{1}{2}(-i\nabla - \mathbf{A}(t))^2 + V$$

$$T_{v\leftarrow KH}(t) \; = e^{-ia(t)} e^{i\mathbf{c}(t).\mathbf{p}}$$

- Kramers-Henneberger gauge

$$T_{l\leftarrow KH}(t) = e^{-ia(t)} e^{-i\mathbf{A}(t).\mathbf{r}} e^{i\mathbf{c}(t).\mathbf{p}}$$

$$H_{KH}(t) = -\frac{\Delta}{2} + V(\mathbf{r} - \mathbf{c}(t))$$

- $a(t) = \frac{1}{2}\int^t A^2(s)ds$
- $\mathbf{c}(t) = \int^t \mathbf{A}(s)ds$

Time evolution operators

$$U_i(t,t') = T_{j\leftarrow i}(t) U_j(t,t') T_{j\leftarrow i}(t')^{-1}$$

Gordon-Volkov time-evolution operator

- Kramers-Henneberger gauge

$$U_{KH}^{(GV)}(t,t') = \exp[-ip^2(t-t')/2]$$

- Length gauge

$$T_{l\leftarrow KH} = \exp[-ia(t) - i\mathbf{A}(t).\mathbf{r} + i\mathbf{c}(t).\mathbf{p}]$$

$$U_l^{(GV)}(t,t') = T_{l\leftarrow KH}(t) \exp[-ip^2(t-t')/2] T_{l\leftarrow KH}^{-1}(t')$$

- Velocity gauge

$$T_{v\leftarrow KH} = \exp[-ia(t) + i\mathbf{c}(t).\mathbf{p}]$$

$$U_v^{(GV)}(t,t') = T_{v\leftarrow KH}(t) \exp[-ip^2(t-t')/2] T_{v\leftarrow KH}^{-1}(t')$$

Momentum space

Amplitude

$$M_{\rm resc} = -\int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt' \int d^3\mathbf{k}\, e^{iS_{\mathbf{p}}(t,t',\mathbf{k})} V_{\mathbf{pk}} V_{\mathbf{k}0}$$

with

$$S_{\mathbf{p}}(t,t',\mathbf{k}) = -\tfrac{1}{2}\int_t^{\infty} d\tau\ [\mathbf{p}-\mathbf{A}(\tau)]^2 - \tfrac{1}{2}\int_{t'}^{t} d\tau\ [\mathbf{k}-\mathbf{A}(\tau)]^2 + |E_0|t'$$

- $V_{\mathbf{pk}} = \langle \mathbf{p}|\, V\, |\mathbf{k}\rangle$
- $V_{\mathbf{k0}} = \langle \mathbf{k}-\mathbf{A}(t')|\, V\, |0\rangle$

Derivation: one needs

$$\langle \mathbf{p}'|\, U_l^{(GV)}(t,t')\, |\mathbf{p}\rangle = \exp[-i\int_{t'}^{t} [\mathbf{p}-\mathbf{A}(s)]^2 ds \delta(\mathbf{p}-\mathbf{p}'-\mathbf{A}(t))]$$