Dominant interaction hamiltonians DIH

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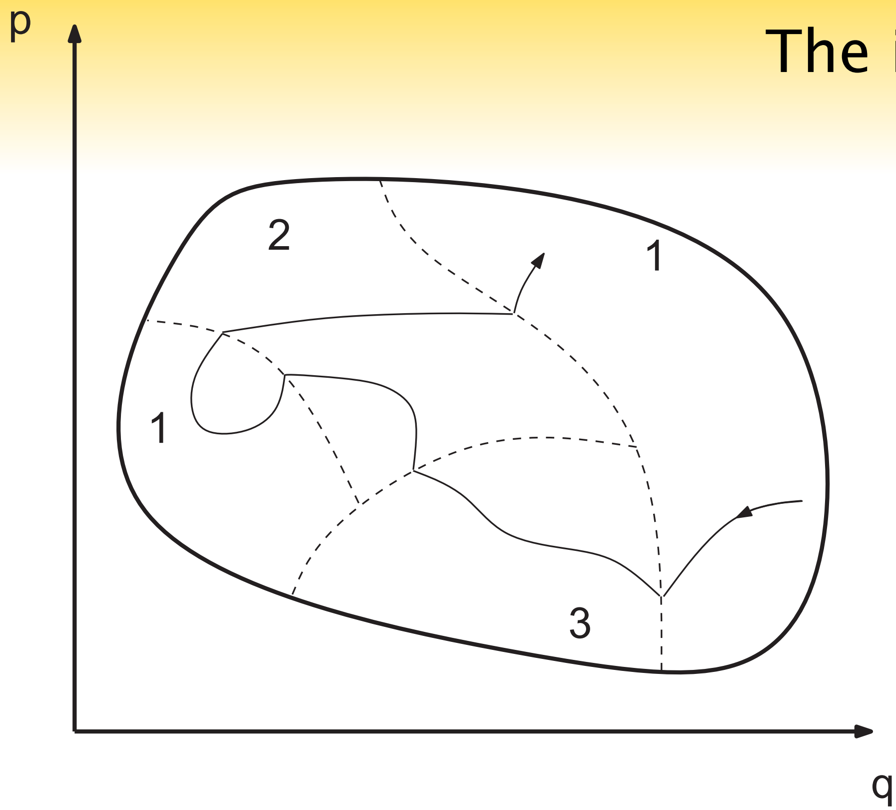
Motivation

- full semiclassical continuous (propagator based) methods are quite expensive and suffer from instabilities due to non-linear classical dynamics
- often, *locally*, (classical) dynamics is regular
- from other methods (e.g. TDDFT) one knows that correlations can develop in time
- can one formulate an approximation where the system evolves along trajectories which visit a sequence of phase space regions (may be repeatedly) ruled by different approximate Hamiltonians ?

➜ (ab-)using adiabaticity: *Fix* the hamiltonian within an interval of parameters (phase space) and then *jump* to a new fixed H.

The idea



- Different regions of phase space are dominated by different hamiltonians (DIH)
- DIHs are simpler (may be even integrable) than the full H

goals:

- Better handling of large systems
- Better understanding of dynamics (trajectories classified through DIH sequence, example 132121)
- Can shift chaotic dynamics for H to regular dynamics for the DIH but chaotic discrete meta dynamics in the DIH sequences
- classical-quantum interface:
  - DIH are local and therefore classical
  - immediate connection to semiclassics through concatenation of propagators under the different DIH

Overview

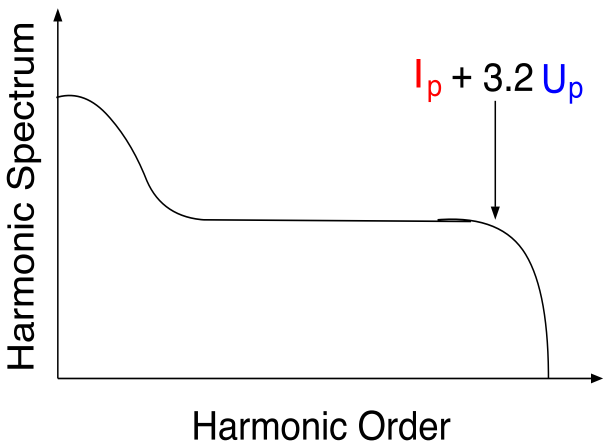
- 1.5 *degrees of freedom* example: e- - ion scattering under laser pulse (HHG)

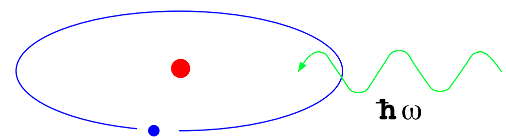
- *5 degrees of freedom* example: planar e- He^+ scattering

➜ electronic problems

High harmonic generation
(the drossophila of strong field physics)

atom in a strong laser field: $H_{atom} = \frac{p^2}{2} + V(x) + xf(t)\cos\omega t$





spectrum:

$$\sigma(\omega) = \int e^{i\omega t} a(t)\ dt$$

with dipole acceleration

$$a(t) = -\left\langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \right\rangle$$

- ionisation potential I_p
- ponderomotive potential $U_p = \frac{F^2}{4\omega^2}$, $F = f(t) = const.$

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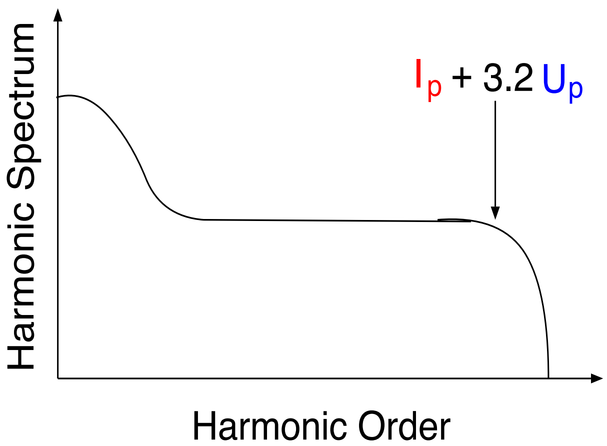

separable DIH approach:

switch between Coulomb potential only and laser field only (large distances)

spectrum:

$$\sigma(\omega) = \int \mathrm{e}^{i\omega t} a(t)\ dt$$

with dipole acceleration

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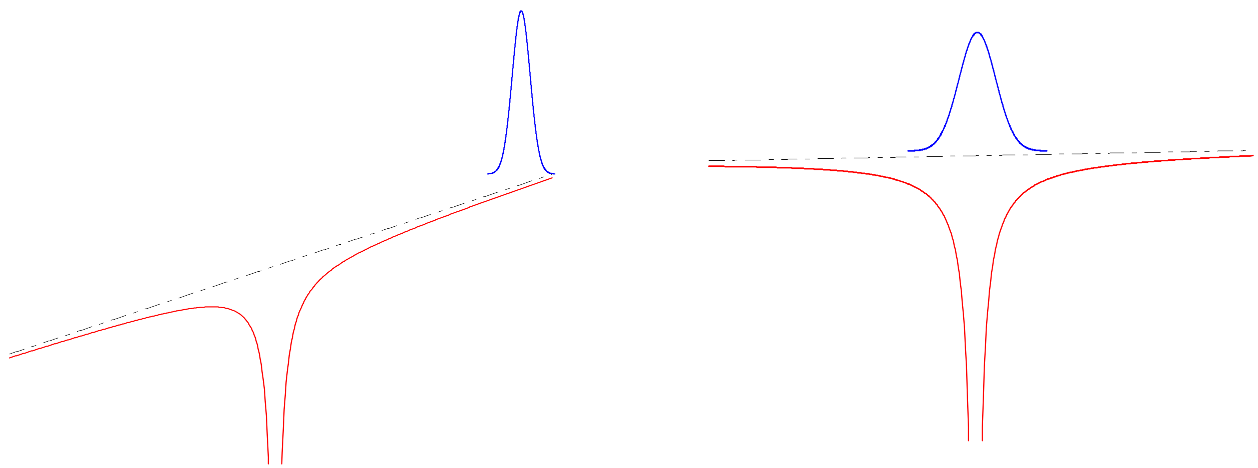
high harmonics in laser assisted electron-ion scattering

$$\Psi_\alpha(x',0) = \left(\frac{\gamma}{\pi}\right)^{1/4} \exp\left\{-\frac{\gamma}{2}(x'-q_\alpha)^2 + \mathrm{i}\,p_\alpha(x'-q_\alpha)\right\}$$



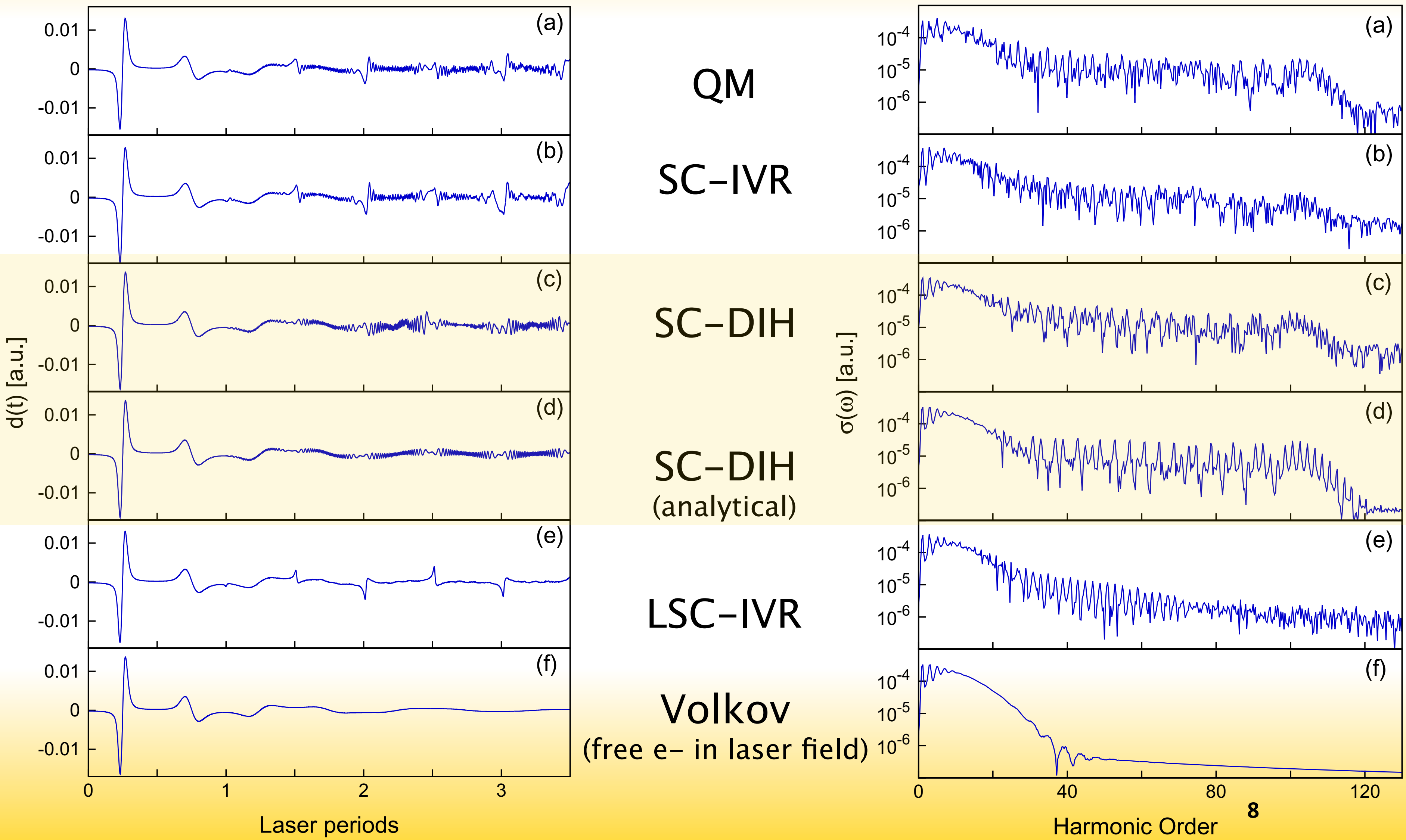
- Gaussian wave packet

  (initiated at 70 a.u. distance from the nucleus):

  laser assisted electron-ion scattering

laser field: $F = 0.1\,au$, $\omega = 0.038\,au$, γ = 0.05 au

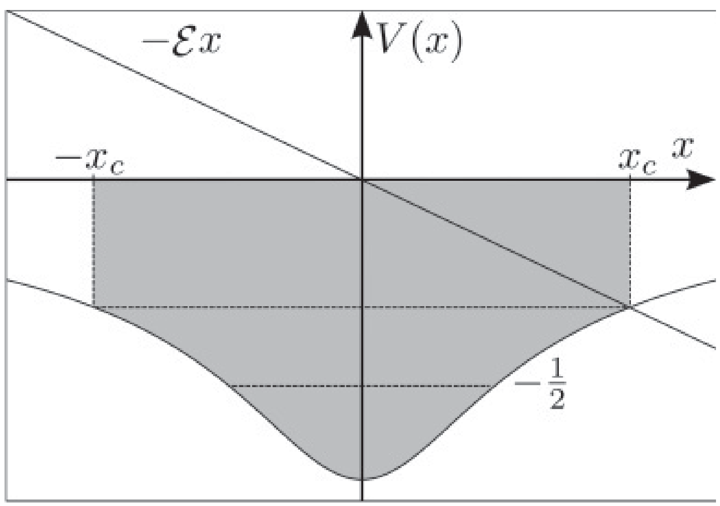
$$a(t) = -\left\langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \right\rangle \qquad \sigma(\omega) = \int \mathrm{e}^{i\omega t} a(t)\; dt$$



Switching condition for HHG

(when does an electron, floating with the laser field, get trapped by the ion ?)

$$H_{atom} = \frac{p^2}{2} + V(x) + x f(t) \cos \omega t$$



$V_{ion}(x) < V_{laser}(x)$

→ maximal $x = x_c$

trapping should occur when the electron is slow:

→ $p_c=0$

$$p(t) = p_0 - \frac{\mathcal{E}}{\omega} \sin(\omega t),$$

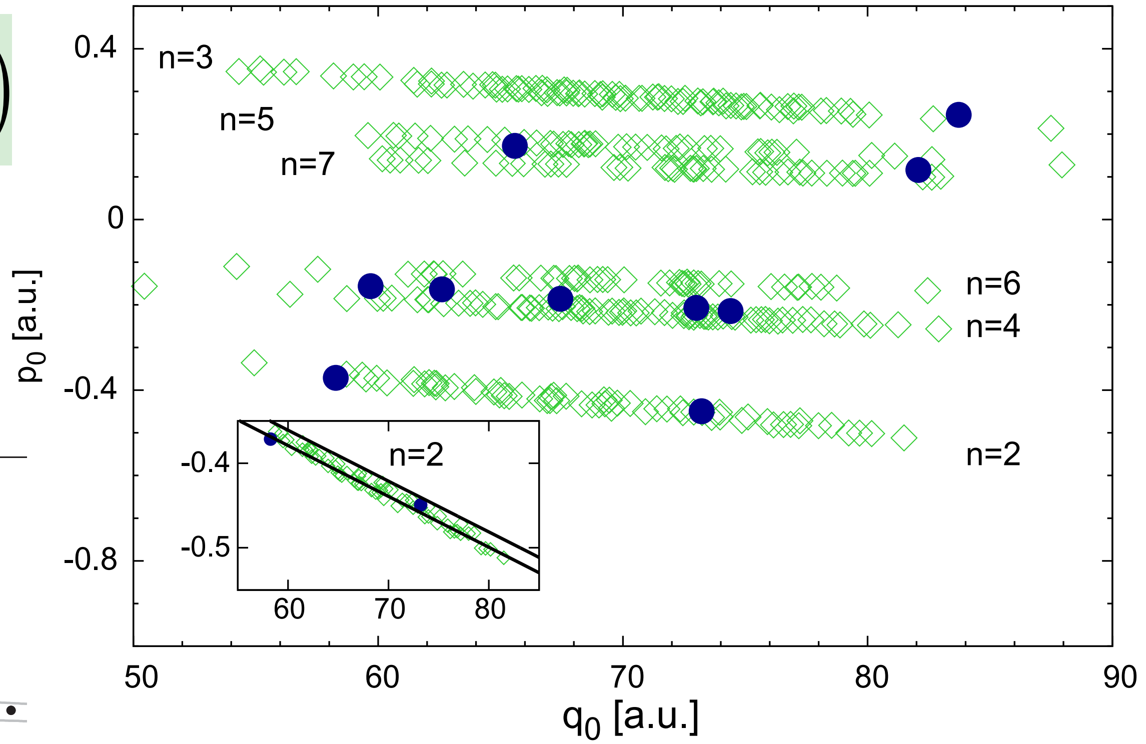
$$q(t) = q_0 + p_0 t + \frac{\mathcal{E}}{\omega^2} [\cos(\omega t) - 1].$$

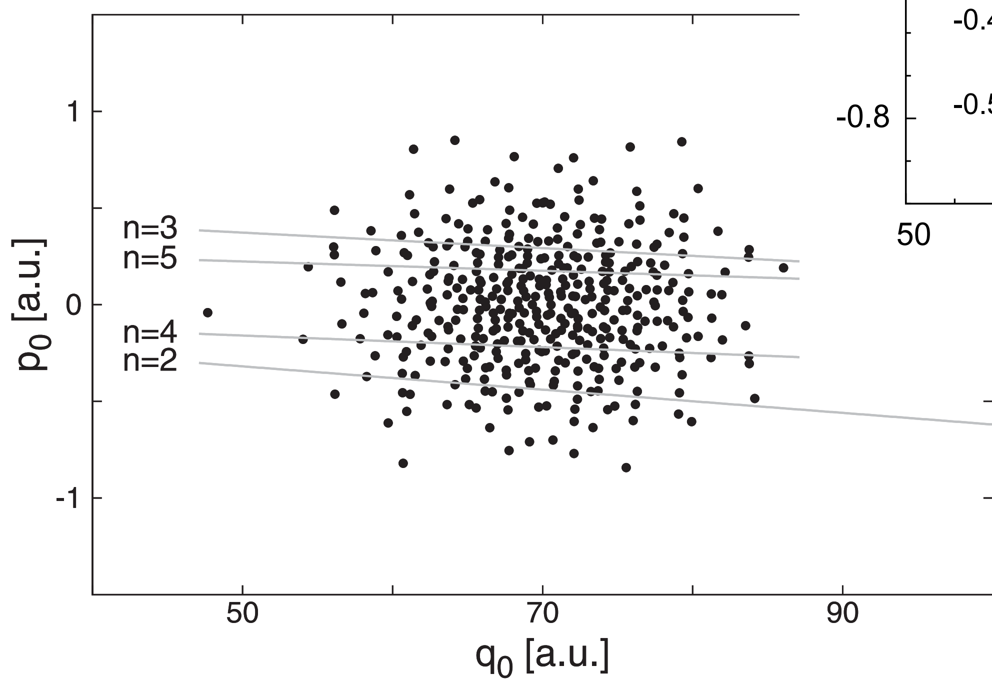
Setting $p(t_c) = 0$ leads to switching times

$$\omega t_c = n\pi + \arcsin\left(\frac{\omega p_0}{\mathcal{E}}\right),$$

Initial conditions for trapped trajectories

$$p_0^{(n)}(q_0) = -\frac{\omega}{n\pi}\left(q_0 - \frac{1-(-1)^n}{2}\frac{2\mathcal{E}}{\omega^2}\right)$$



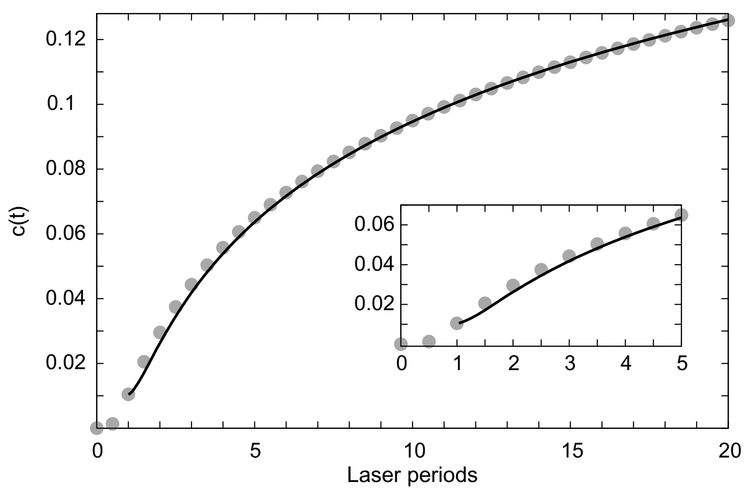


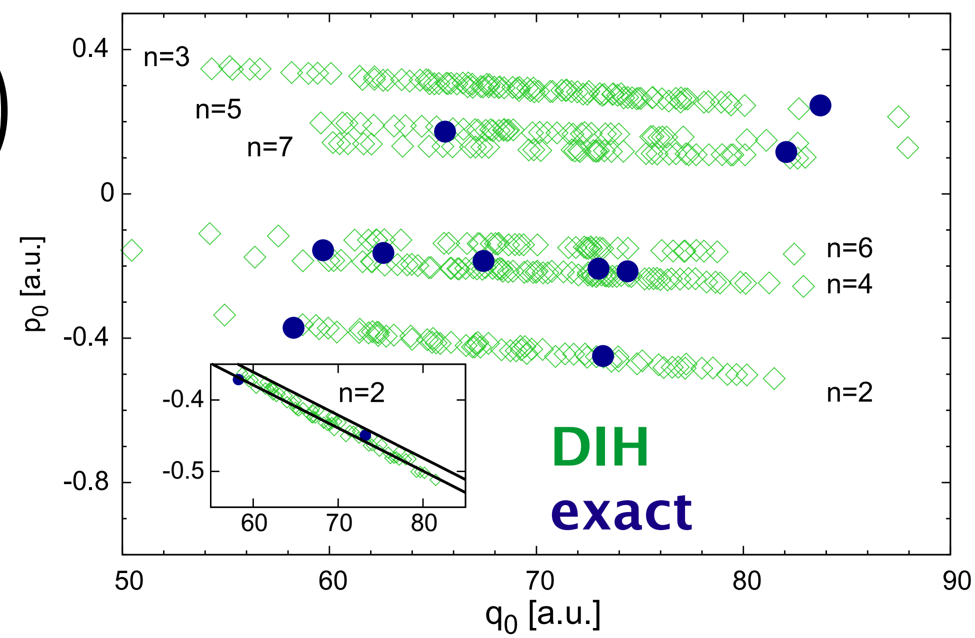
SC-DIH
full SC-IVR

analytical wave function for HH

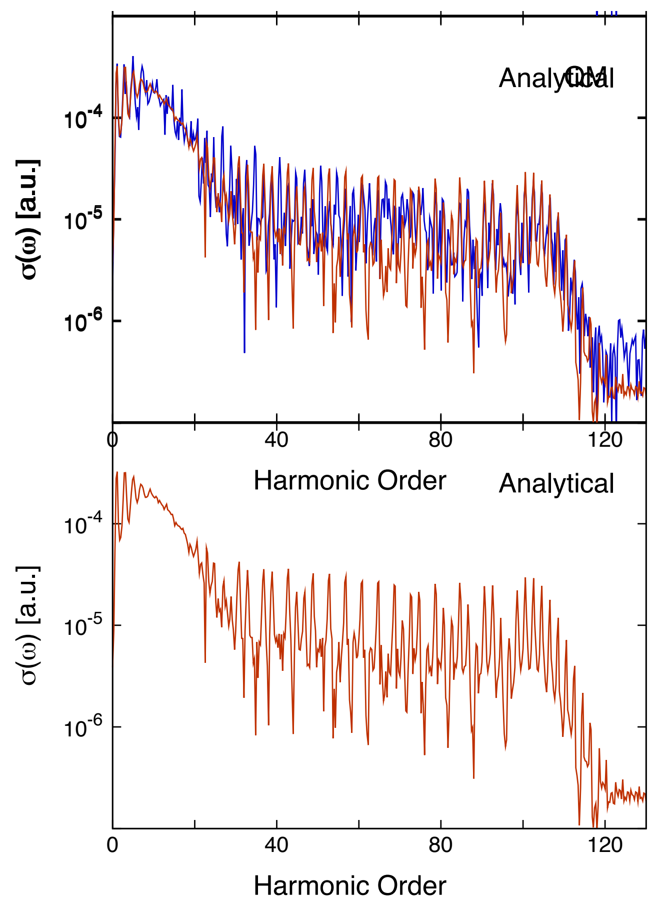
$$|\Psi(t)\rangle = N(t)(|\Psi_V\rangle + c(t)|\Psi_0\rangle) \qquad c(t) = \sum_{n=1}^{2N} \Theta(t - nT/2)c_n$$

$$c_n \approx \frac{x_c}{\sqrt{\gamma\pi}} \frac{1}{nT}\left(1 - \frac{(q_\alpha + x_c/2)^2}{\gamma\, n^2 T^2}\right)$$





harmonic spectrum



analytical
DIH

Zagoya, Goletz, Grossmann & Rost, New J. Phys. 14, 093050 (2012);
Phys Rev. A 85, 041401 (2012)

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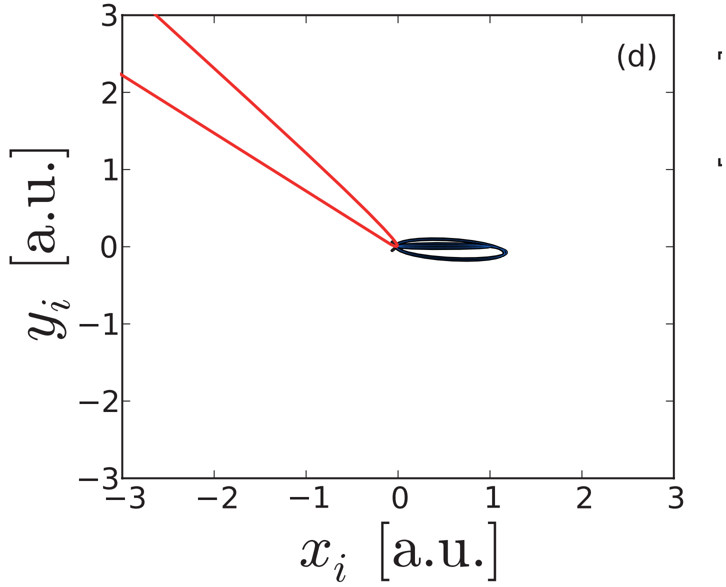
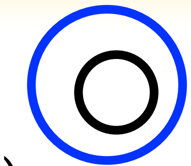


How to identify DIH and criteria for switching between them ?
symmetry arguments, physical intuition, trial & error…

- try to concentrate interactions to instants in time



- approximate Hamiltonian: $H_{FF} = (p_1^2+p_2^2)/2 - 1/r_1 - 2/r_2$ $(r_1 > r_2)$

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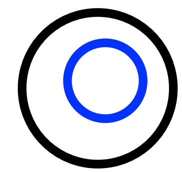

Temkin – Poet model

A Temkin, Phys Rev 126, 130 (1962);
R. Poet, J Phys B 11, 3081 (1978)

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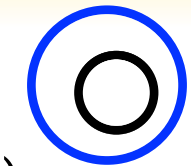

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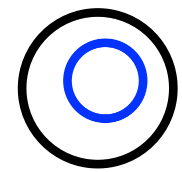

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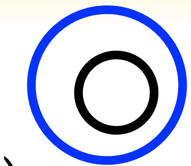

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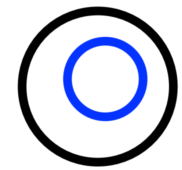
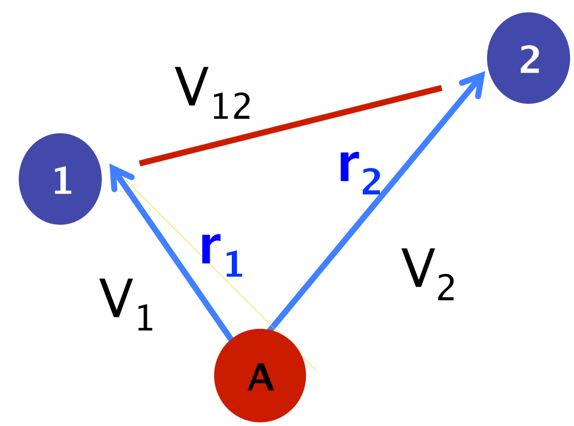


- interaction event '1': $F \equiv \left|\frac{2V_{12}}{V_1+V_2}\right|$ = 1, then $\mathbf{p}'_{12} = K\, \mathbf{p}_{12}$
- approximate Hamiltonian: $H_{NF} = p_{12}^2 + 1/r_{12}$
  [$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 = \mathbf{R}$, $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$]
- transformation K uniquely defined by respecting constants of motion and locality:

H, **p, L** and since the $\mathbf{r}_i$ are fixed for the momentum kick:

P^2, $\mathbf{l}_{12}$



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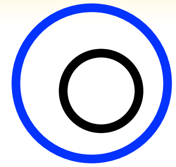

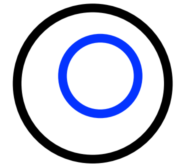

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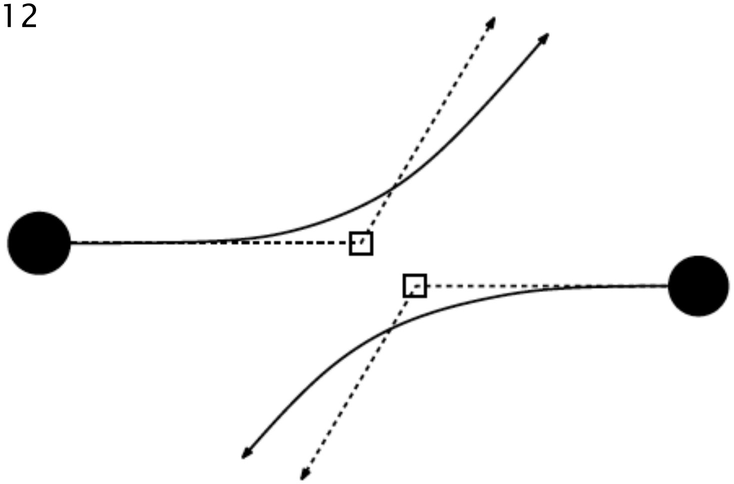


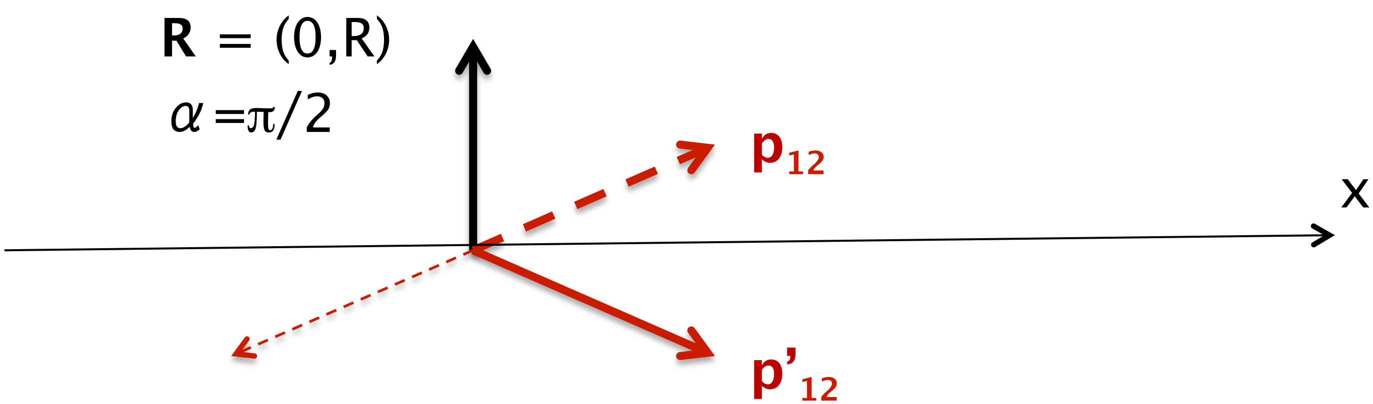
How to identify DIH and criteria for switching between them ?
symmetry arguments, physical intuition, trial & error…

- interaction event '1': if $F = 1$, then $\mathbf{p}'_{12} = K\,\mathbf{p}_{12}$

let $\mathbf{r}_{12} = \mathbf{R} = \mathbf{r}_2 - \mathbf{r}_1$ be in the x-y plane with $\tan\alpha = y_{12}/x_{12}$

then $K = \mathrm{In}_X\, D(-2\alpha)$ with a rotation by -2α and an

inversion in x: $$\mathrm{In}_X = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$ $$F \equiv \left| \frac{2V_{12}}{V_1 + V_2} \right|$$



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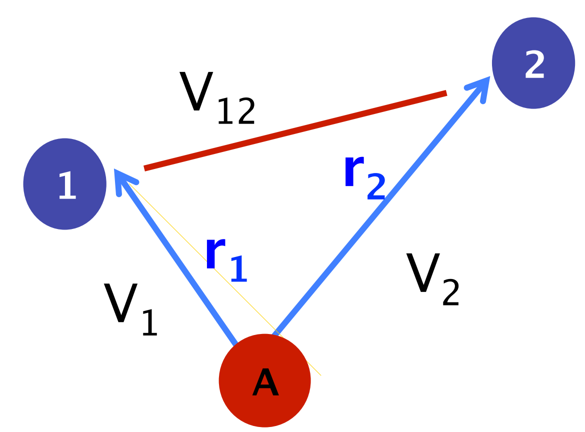
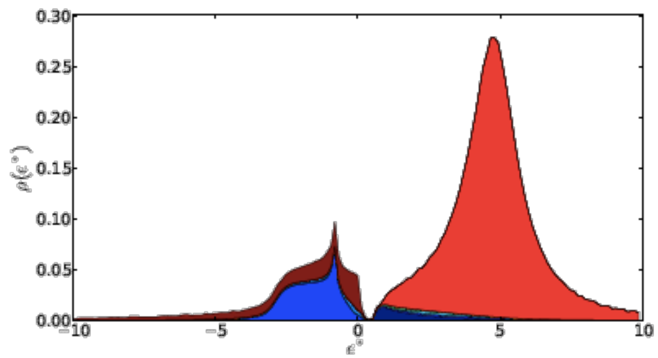
event	'1'	'2'
condition	$F=1$	$r_1=r_2$
action	$\mathbf{p}'_2-\mathbf{p}'_1 = K_{\mathrm{NF}}(\mathbf{p}_2-\mathbf{p}_1)$	$r_1 \leftrightarrow r_2$
effect	$\Delta l_i \neq 0, \Delta E_i \neq 0$	$\Delta E_i \neq 0$



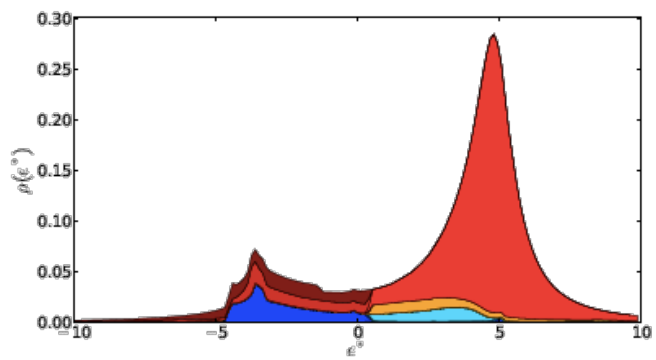
DIH qualitative – collision sequences of $2e^-$

'1': kick (near field)
'2': switch (far field)

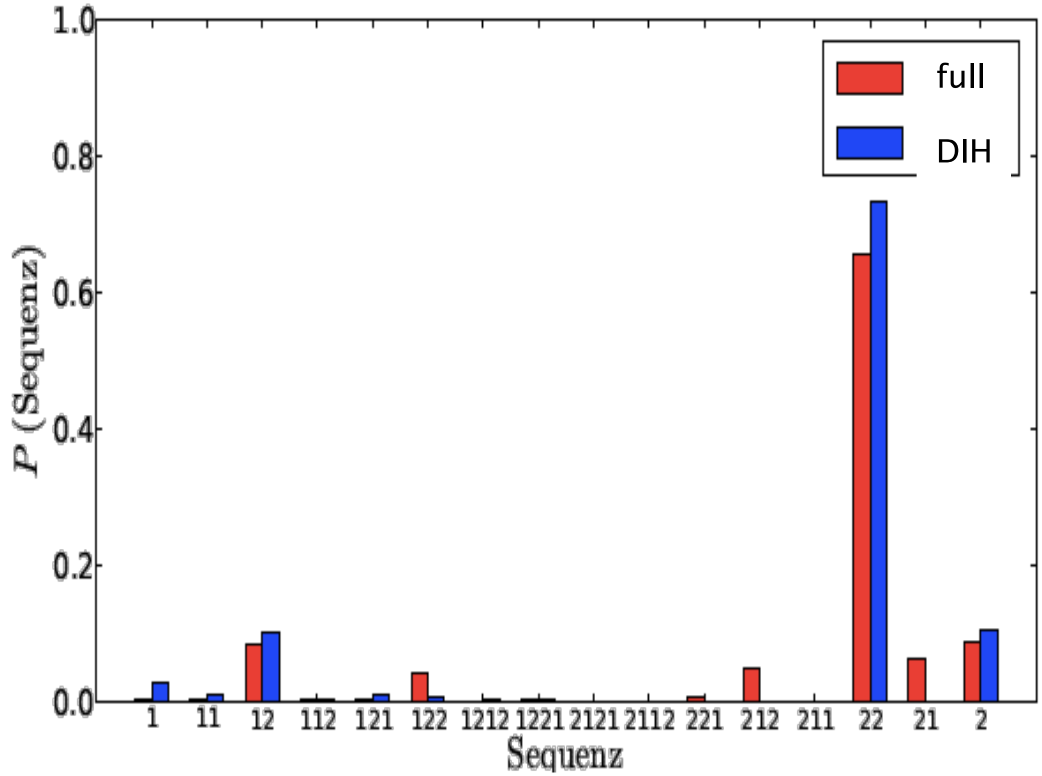
DIH



full

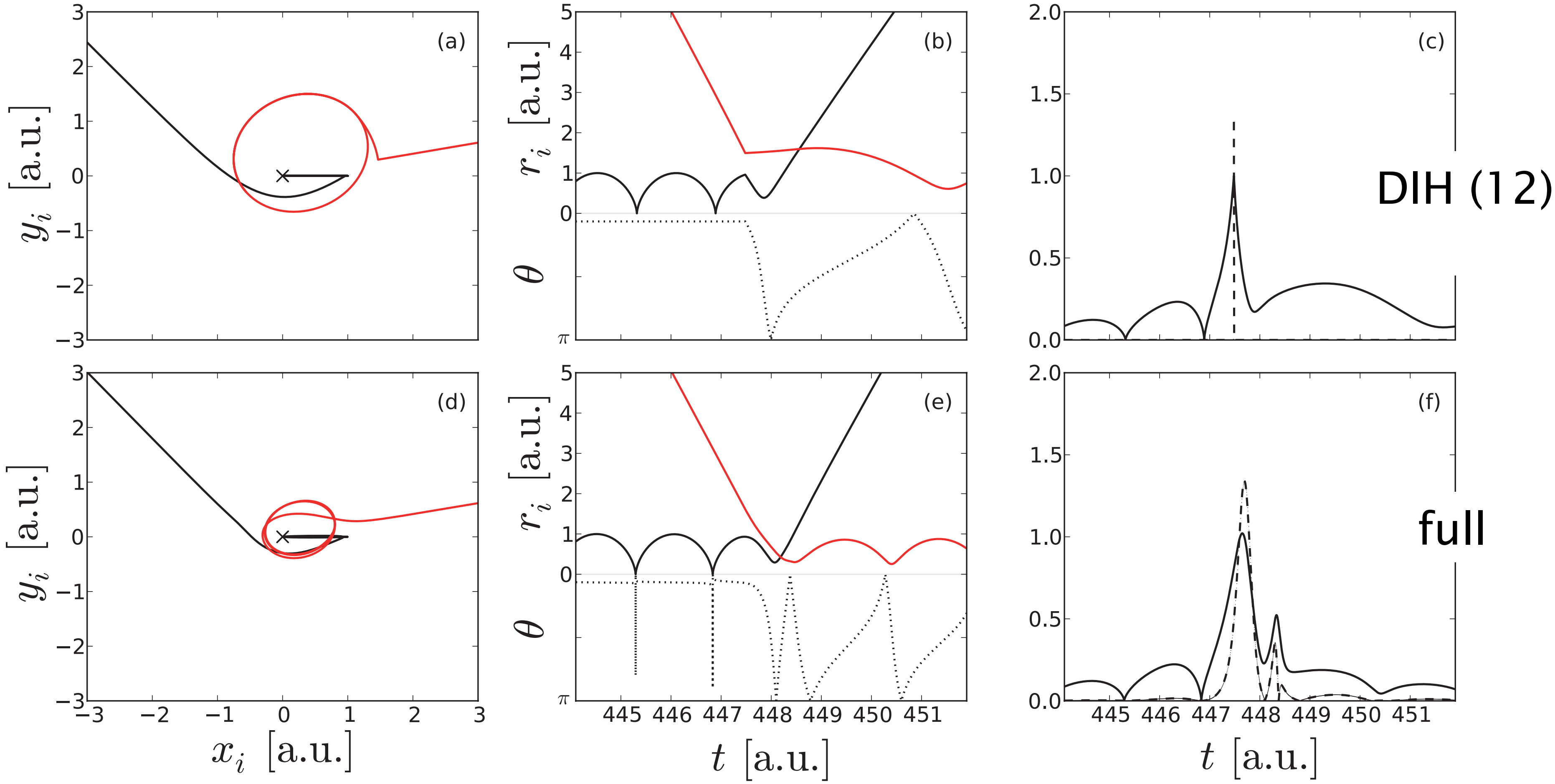


'22': elastic
'12': excitation (classical exchange)



Planar electron – He^{+} collisions

$$F \equiv \left| \frac{2V_{12}}{V_1 + V_2} \right|$$



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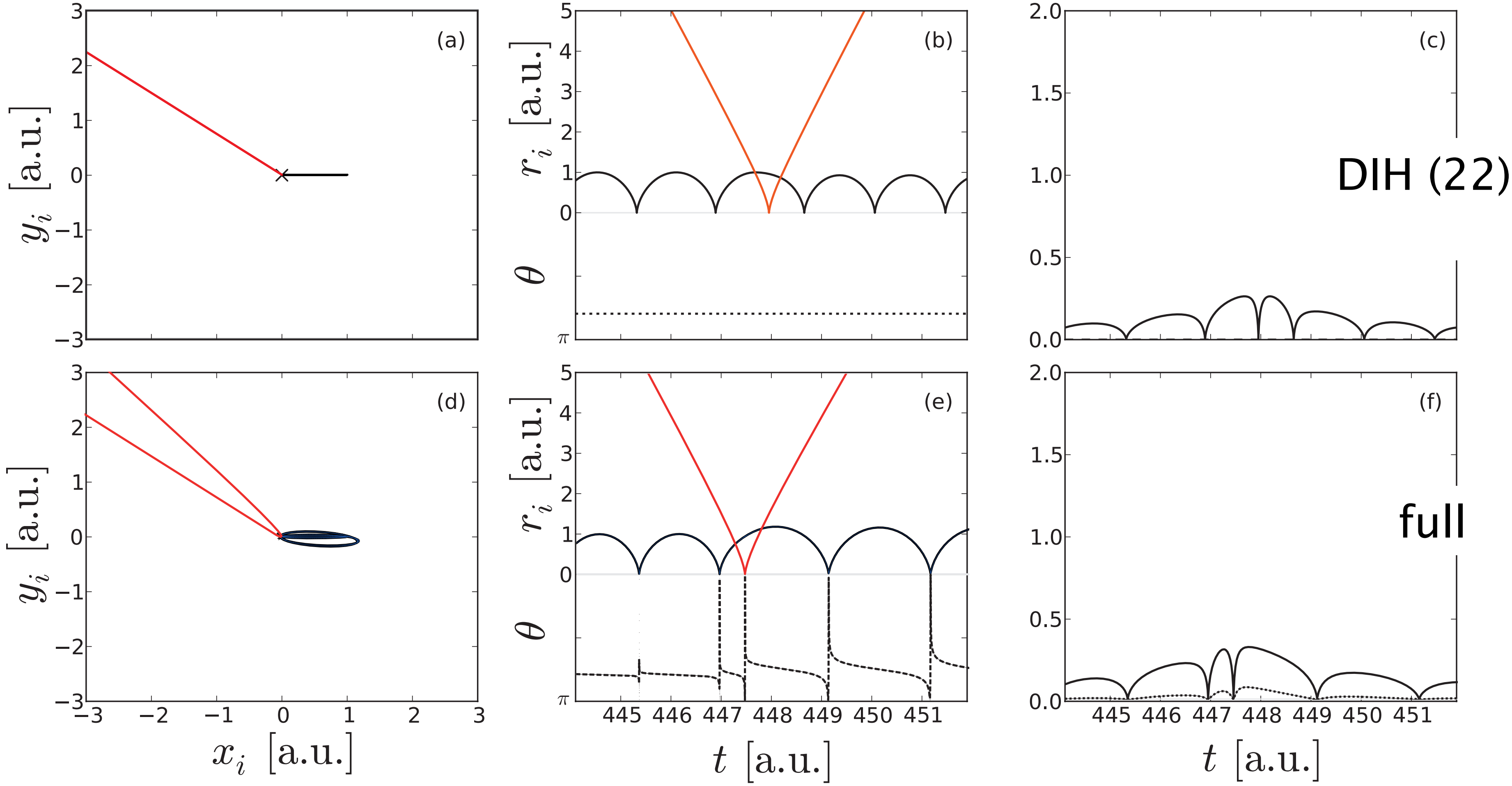
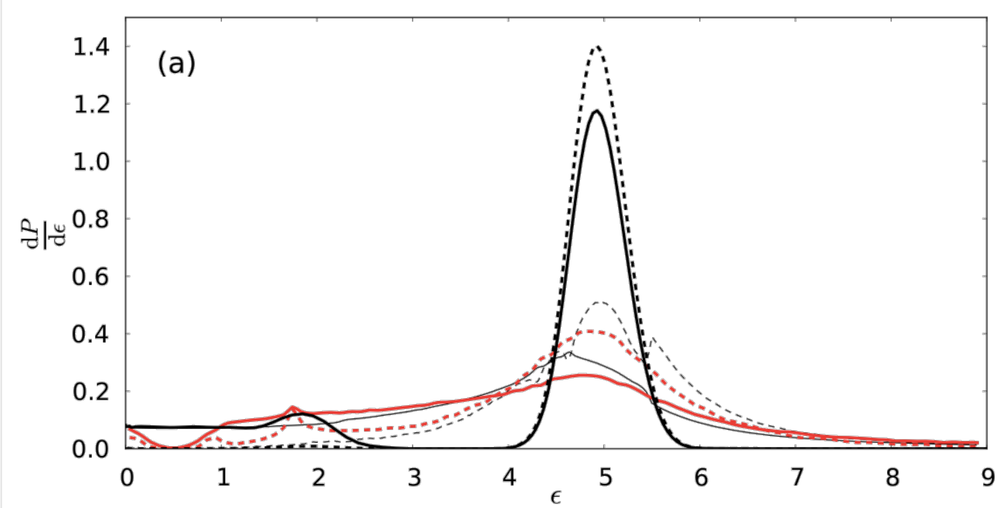
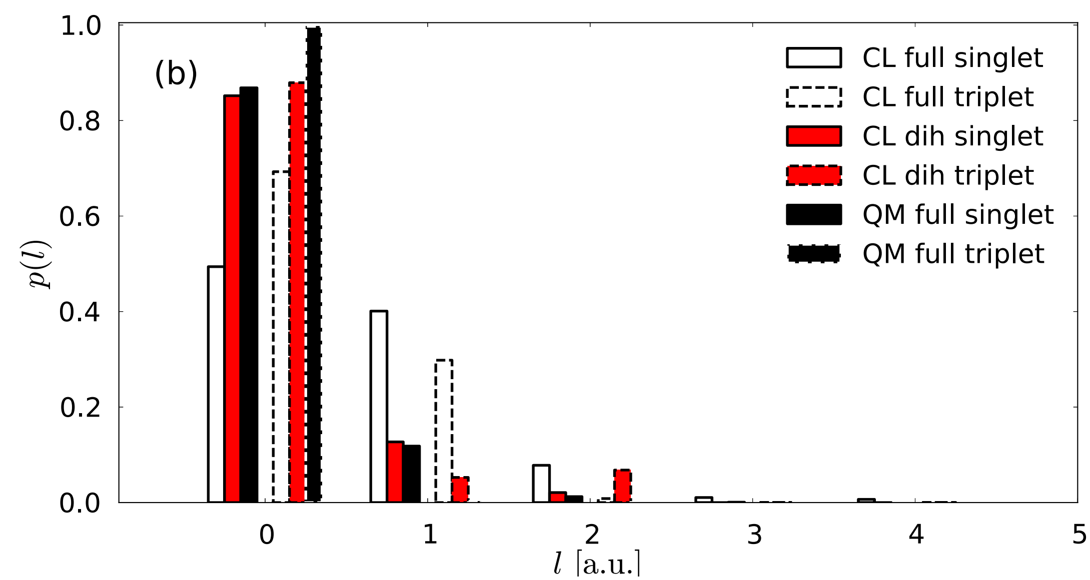


Quantum – Classical – DIH: spectra for energy & angular momentum



Compared to quantum:
DIH better than full classical !?

M Gerlach, S Wüster, and JM Rost,
J Phys B 45, 235204 (2012)
- highlight 2012 -



Summary: Dominant interaction Hamiltonians (DIH)

- *Classical phase space partitioning through dominant interaction*
  - Continuous (chaotic) dynamics split into regular-continuous and chaotic-discrete dynamics
- ***done***
  - classical planar scattering (5 dof)
  - semi-classical laser assisted electron-ion scattering (1.5 dof)
- ***Perspectives***
  - Classification through DIH sequences
  - better qualitative understanding of dynamics
  - better numerical handling of large systems
  - study chaotic map induced by DIH switching

Thanks !

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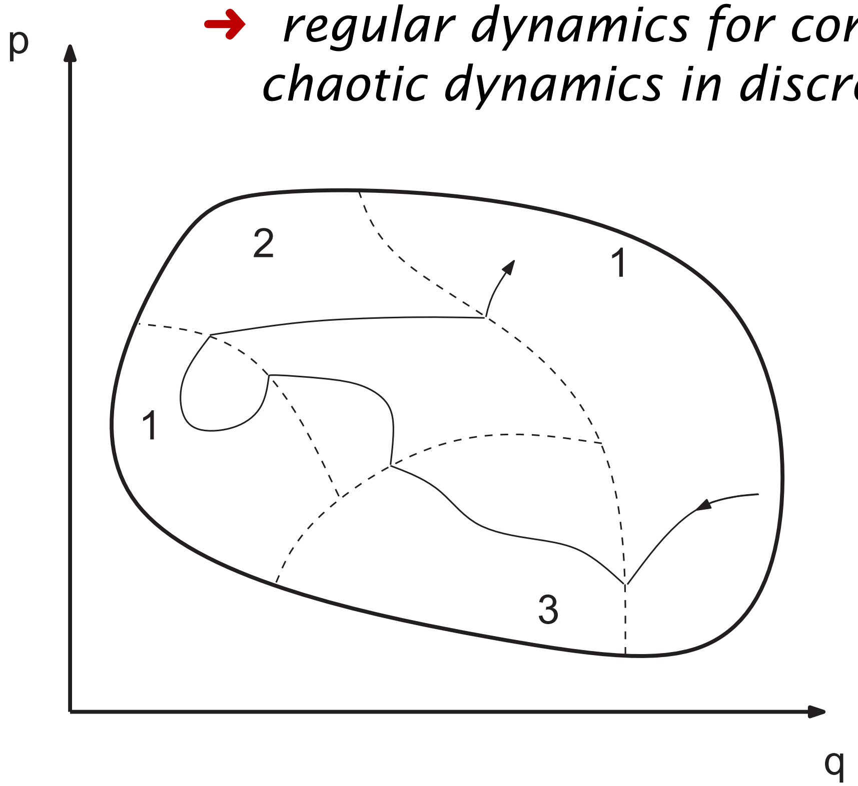
DIH: separating regular and chaotic dynamics

- *Assume chaotic hamiltonian and a set of integrable DIH*
- *Is the chaos lost ?*
- *NO, chaotic dynamics is shifted to the sequence "space"*

➜ *regular dynamics for continuous motion in phase space, chaotic dynamics in discrete sequence space*



Semiclassical Initial Value Representation (IVR)

Heller's Thawed Gaussian Wavepacket Dynamics (TGWD)

$$\boxed{\Psi(x,t) = \left(\frac{\gamma_0}{\pi}\right)^{1/4} \exp\left\{-\frac{\gamma_t}{2}(x-q_t)^2 + \frac{i}{\hbar}p_t(x-q_t) + \frac{i}{\hbar}\delta_t\right\}}$$

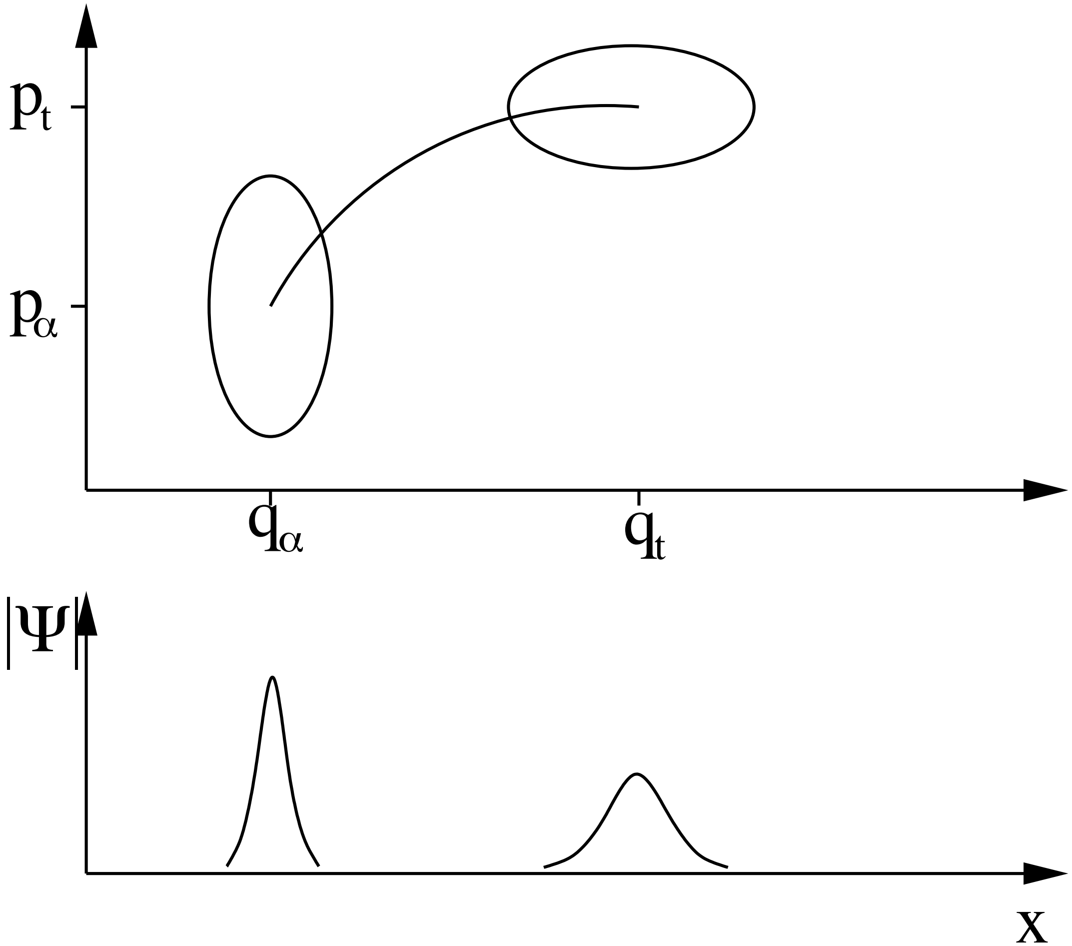
$$\gamma_0, p_t, q_t \in \mathbf{R}, \qquad \gamma_\mathbf{t}, \delta_\mathbf{t} \in \mathbf{C}$$

Ansatz for the solution of the time-dependent Schrödinger equation

$$i\hbar\dot{\Psi}(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t)$$

E. J. Heller, J. Chem. Phys. **62**, *1544 (1975)*

Thawed GWD: Phase- and position space



single trajectory initial value method

Multiple trajectory method for N DOF: FGWD

$$\Psi(\mathbf{x}, t) = \int d\mathbf{x}' K(\mathbf{x}, t; \mathbf{x}', 0)\Psi(\mathbf{x}', 0)$$

Initial value Herman-Kluk propagator

$$\boxed{K(\mathbf{x}, t; \mathbf{x}', 0) \approx \int \frac{d\mathbf{p}' d\mathbf{q}'}{(2\pi\hbar)^N} \langle \mathbf{x} | g_\gamma(\mathbf{p}_t, \mathbf{q}_t) \rangle R e^{iS(\mathbf{p}', \mathbf{q}', t)/\hbar} \langle g_\gamma(\mathbf{p}', \mathbf{q}') | \mathbf{x}' \rangle}$$

$$R = \sqrt{\det \tfrac{1}{2} \left(\mathbf{m}_{pp} + \mathbf{m}_{qq} - \gamma i\hbar \mathbf{m}_{qp} - \tfrac{1}{\gamma i\hbar} \mathbf{m}_{pq} \right)}$$

- $|g_\gamma\rangle$ are Gaussians with fixed width ("frozen")
- Hamilton's principal function $S(\mathbf{p}', \mathbf{q}', t) = \int_0^t L dt'$
- initial value solutions $\mathbf{p}_t(\mathbf{p}', \mathbf{q}'), \mathbf{q}_t(\mathbf{p}', \mathbf{q}')$

Heller ('81), Herman and Kluk ('84), Kay ('94), F.G. and Xavier ('98)

Frozen GWD: Phase- and position space

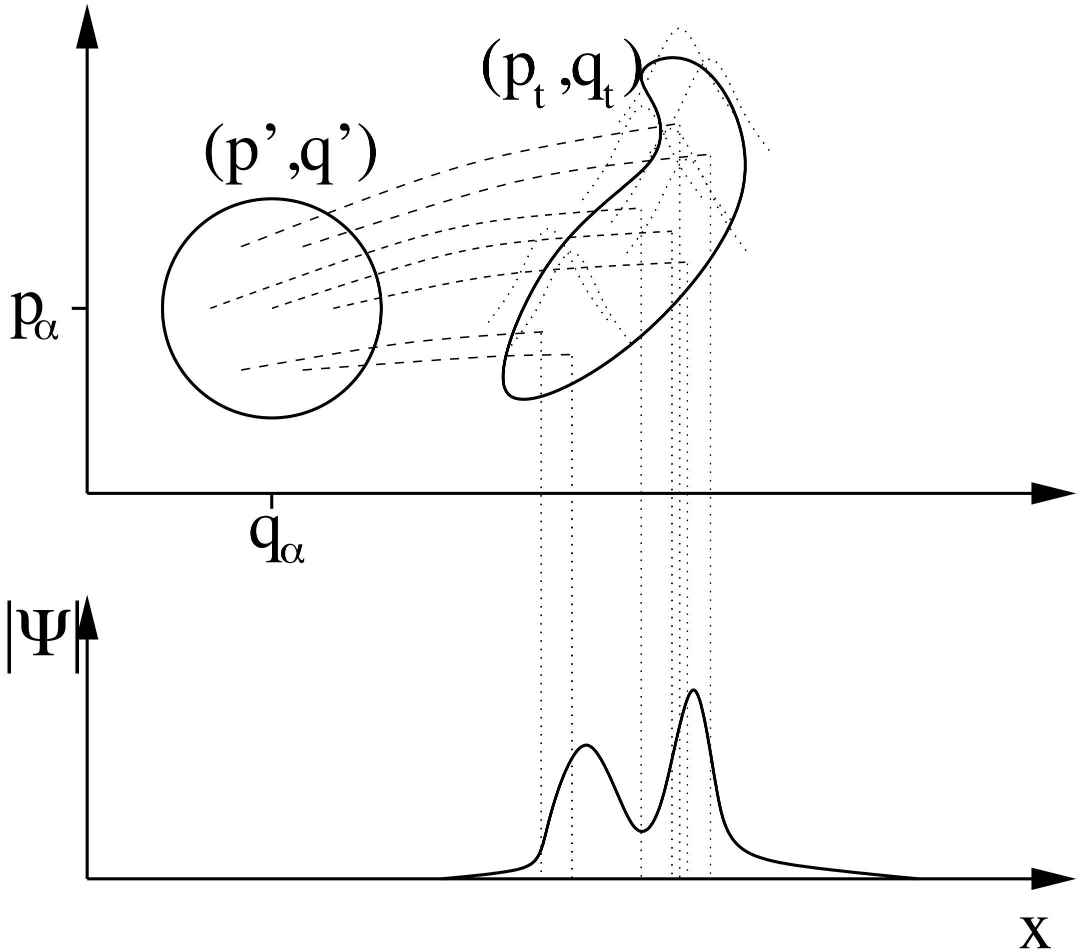
- $\mathbf{m}_{pp}, \mathbf{m}_{qq}, \ldots$ are elements of the stability (monodromy) matrix $\mathbf{M}$

$$\mathbf{M} = \begin{pmatrix} \mathbf{m}_{pp} & \mathbf{m}_{pq} \\ \mathbf{m}_{qp} & \mathbf{m}_{qq} \end{pmatrix} = \begin{pmatrix} \partial\mathbf{p}_t/\partial\mathbf{p}' & \partial\mathbf{p}_t/\partial\mathbf{q}' \\ \partial\mathbf{q}_t/\partial\mathbf{p}' & \partial\mathbf{q}_t/\partial\mathbf{q}' \end{pmatrix}$$

$$\frac{d}{dt}\mathbf{M} = \begin{pmatrix} 0 & -H_{qq} \\ H_{pp} & 0 \end{pmatrix} \mathbf{M}$$

- H_{qq}, H_{pp}: Hessian

$\Rightarrow$**purely classical input!**



*multi*trajectory initial value method

- Time-dependent initial value method for *arbitrary* dynamics
- no storage problems due to laocality $\Rightarrow$DIH
- Initial Gaussian $\Rightarrow$Monte Carlo integration over phase space
- SPA $\Rightarrow$Van Vleck-Gutzwiller propagator

$$\boxed{K(\mathbf{x}, t; \mathbf{x}', 0) \sim \sum_j \left| \frac{1}{\det \mathbf{m}_{qp}} \right|^{1/2} \exp\{iS_j(\mathbf{x}, \mathbf{x}', t)/\hbar - i\pi\nu_j/2\}}$$

- "Maslov-Phase" is already incorporated
- no problems at caustics, FGA is uniform $\Rightarrow$Kay (2006)
- FGA is unitary (in SPA) $\Rightarrow$Herman (1986)
- Approximation to CCS $\Rightarrow$Shalashilin and Child
- iterative improvement is possible $\Rightarrow$Pollak group, Kay group

mpipks

Finite
Systems

Dominant interaction hamiltonians
DIH

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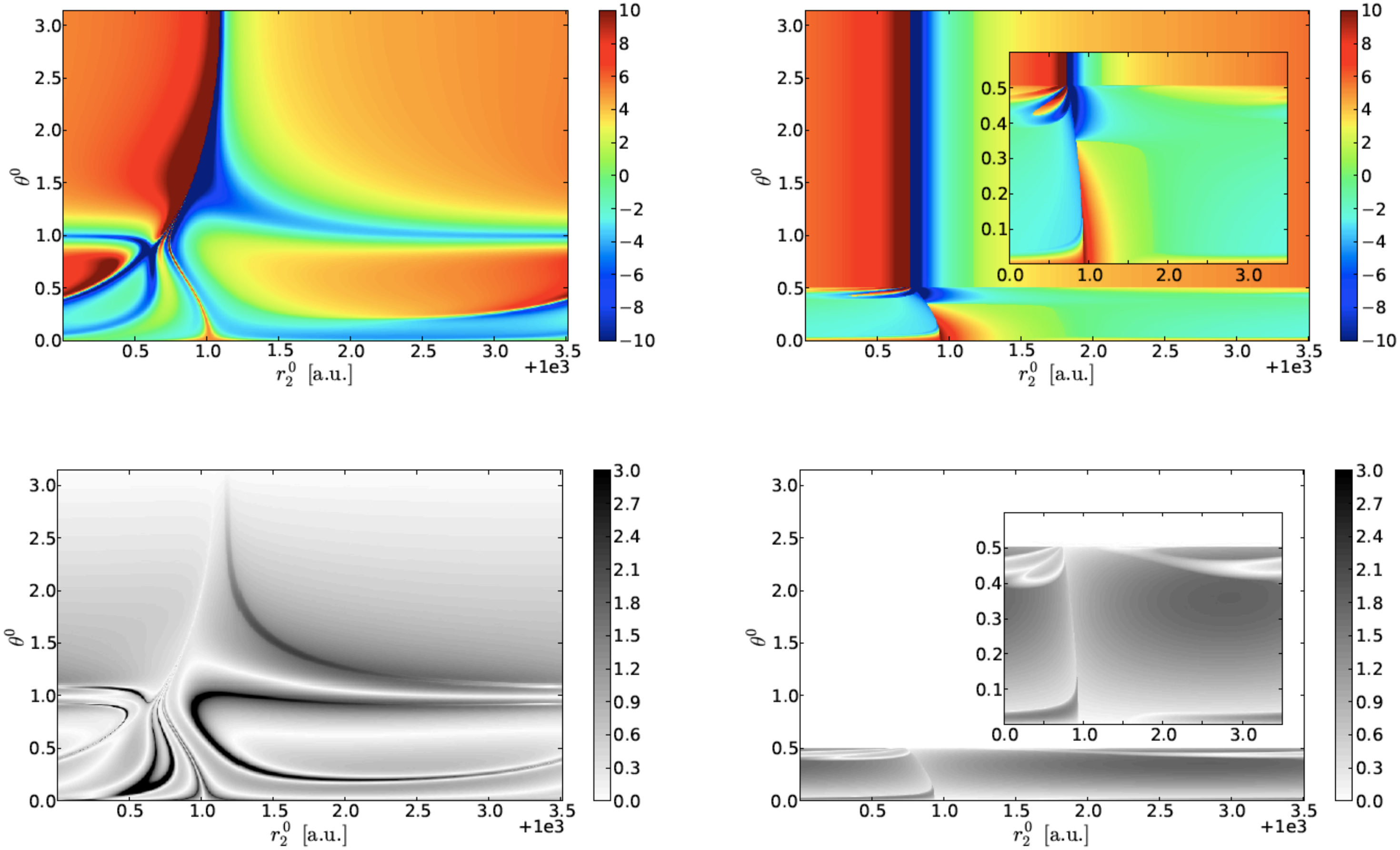
Overview

- 5 dof example: planar e- He^+ scattering
- 1.5 dof example: e- - ion scattering under laser pulse (HHG)

Deflection functions: energy & angular momentum

full | DIH



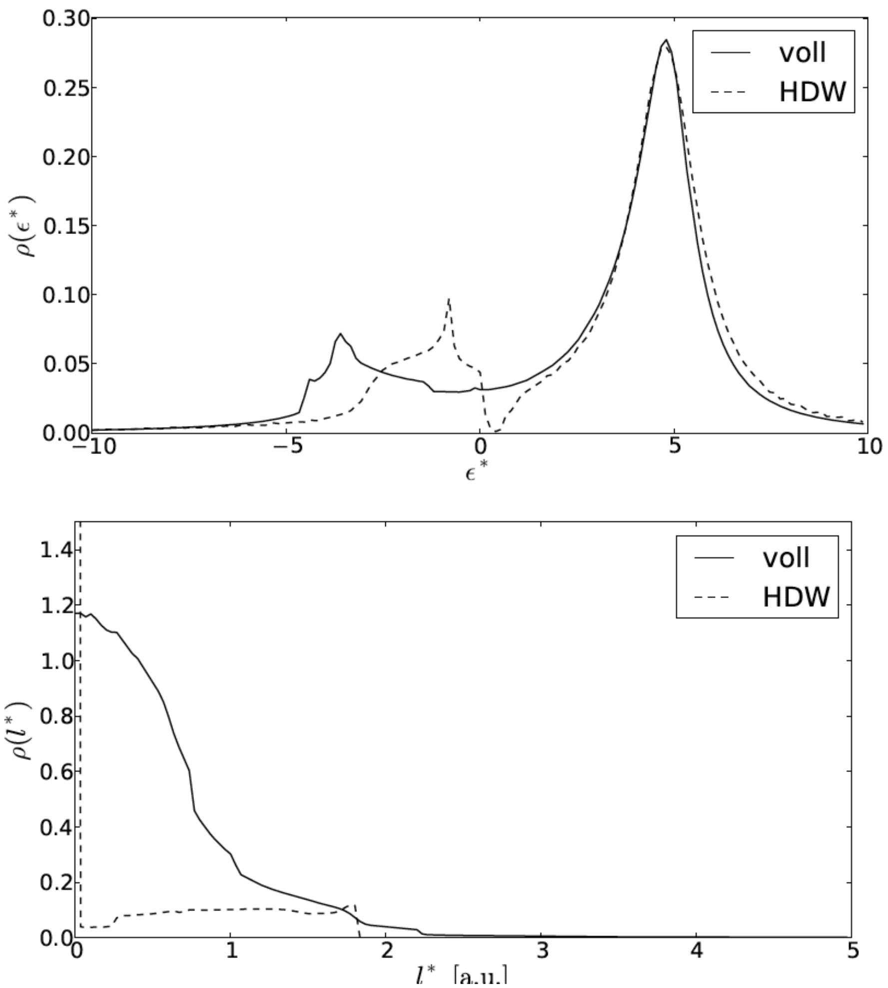
$\epsilon^*(r_2^0, \theta^0)$

(projectile)

$l^*(r_2^0, \theta^0)$

(E_1= -2; E = 0.5; $\varepsilon^* = E_2^{(f)}/E$)

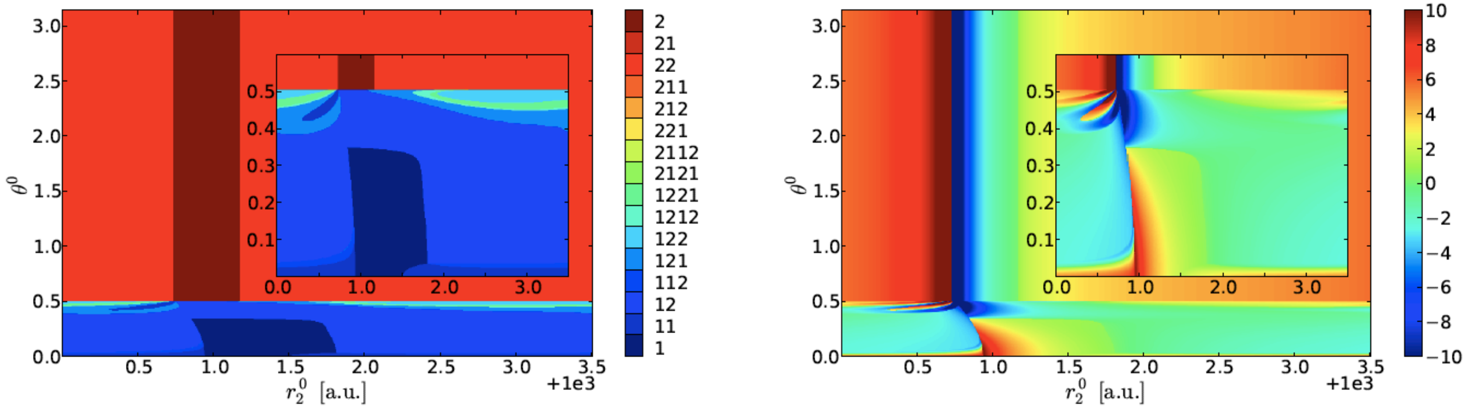
DiH quantitativ-
spectra: energy & angular momentum



DiH qualitative – collision sequences

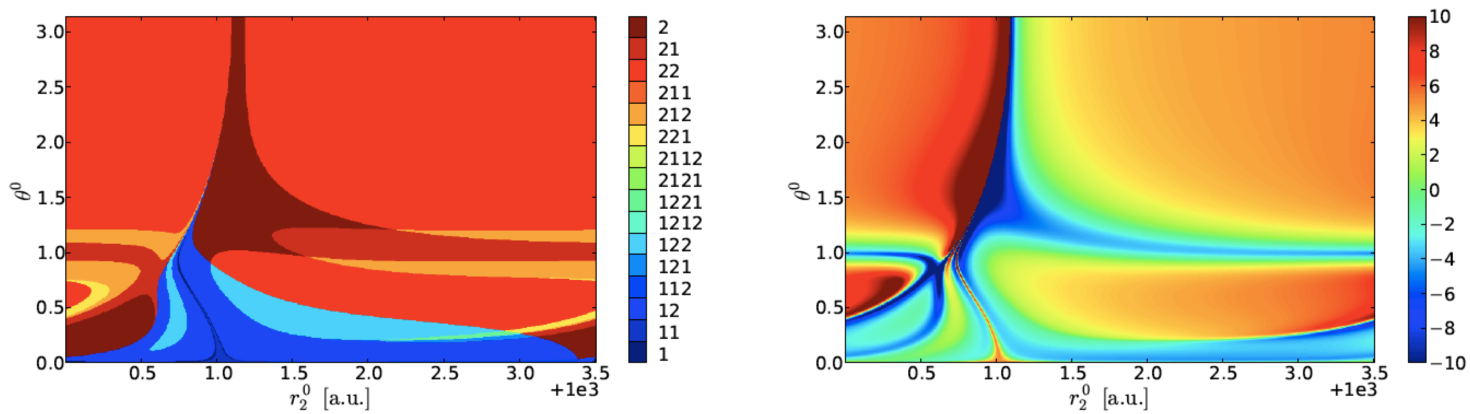
'1': kick (near field)
'2': switch (far field)

DIH



(a) (b)

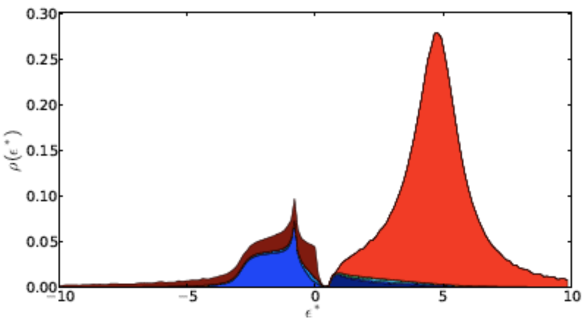
full



‘1’: kick (near field)
‘2’: switch (far field)

DiH qualitative – collision sequences

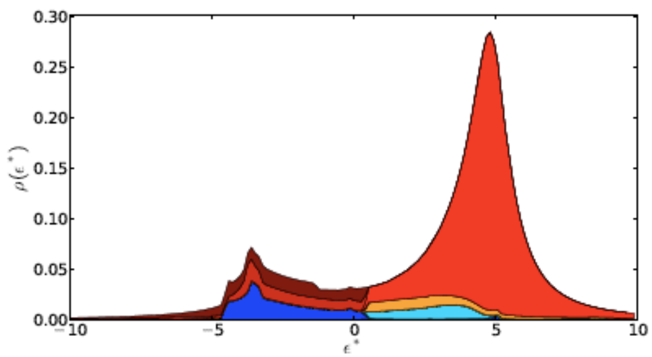
DIH

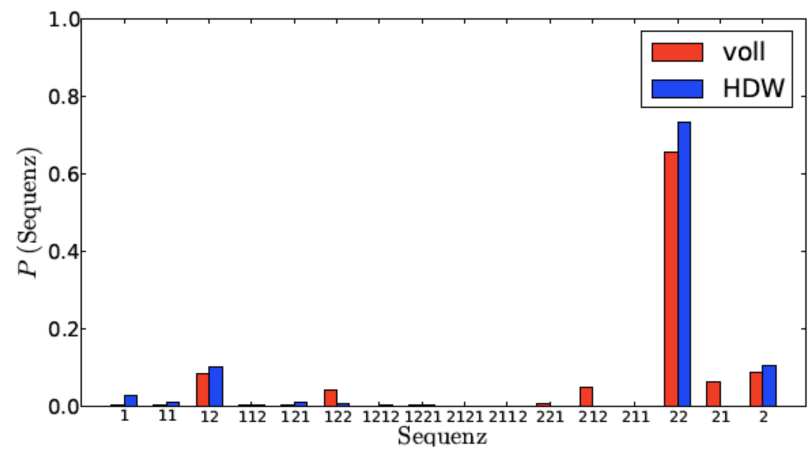


‘22’: elastic

‘12’: excitation (classical exchange)

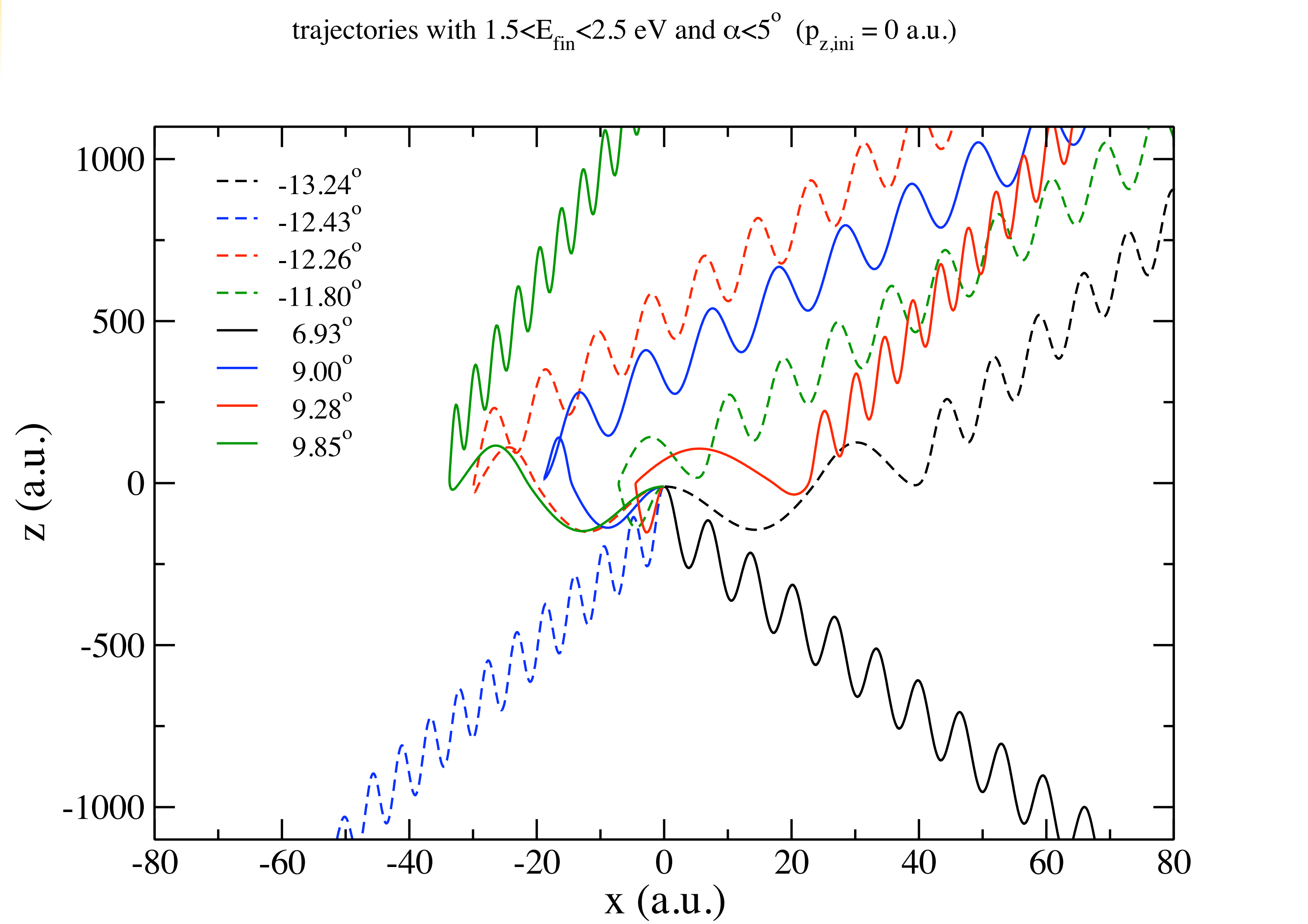
full



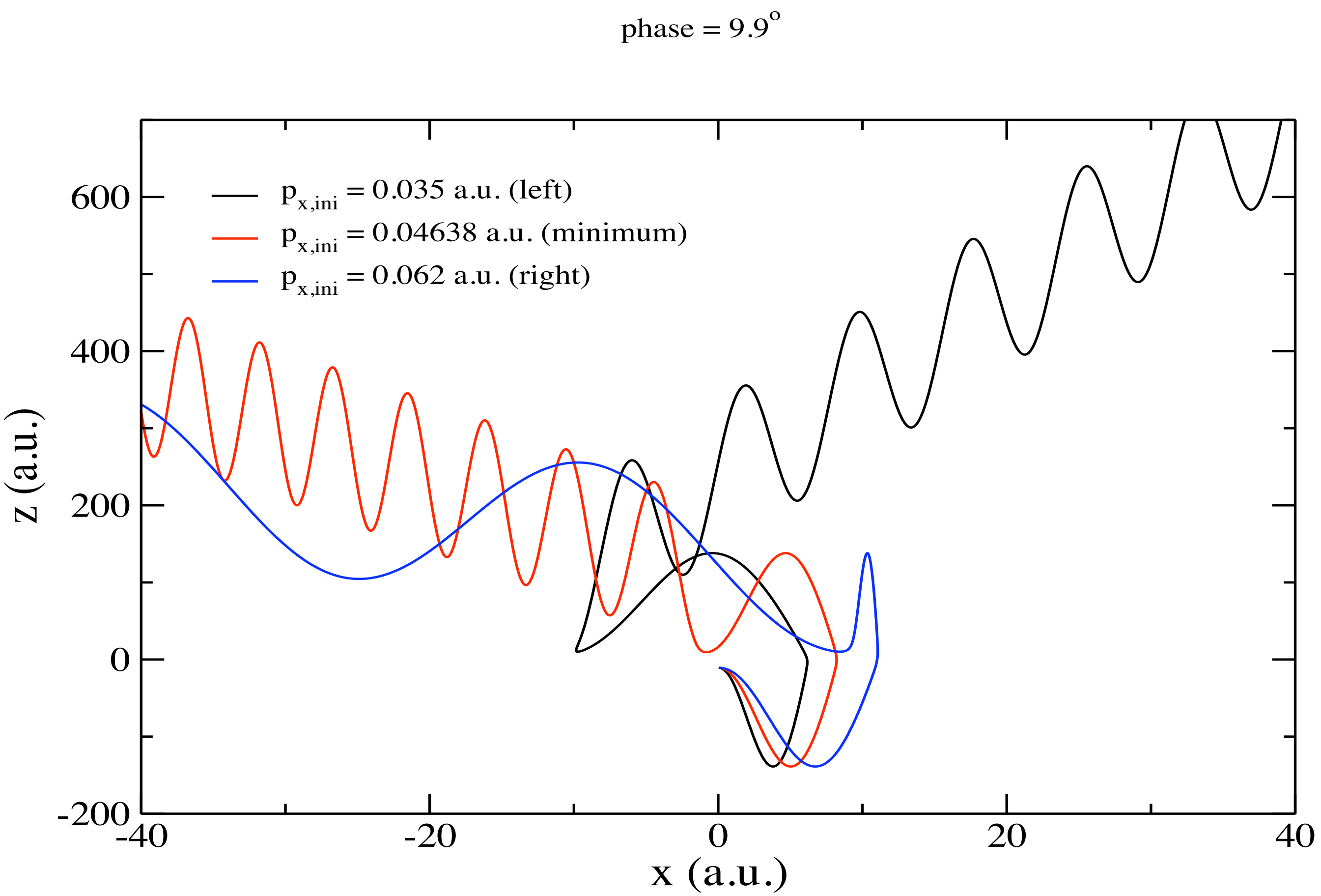


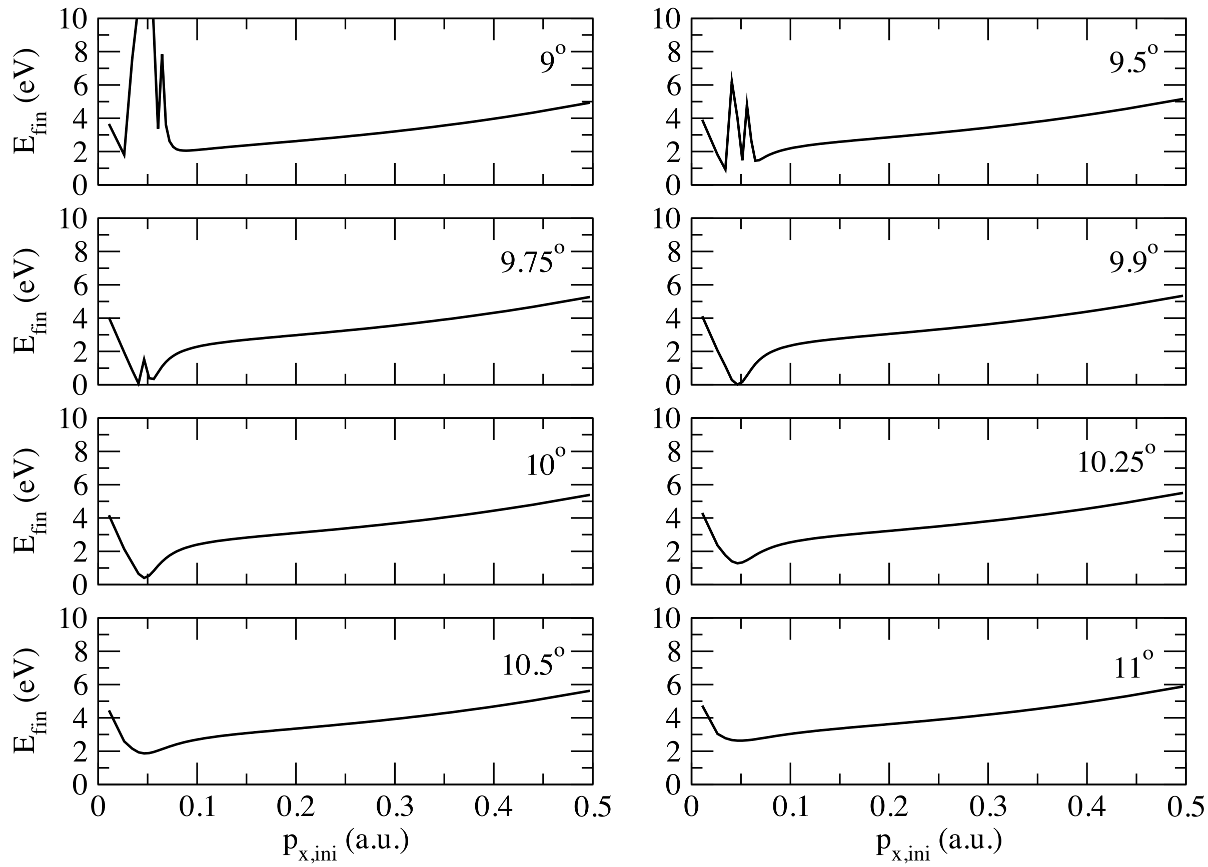
DiH two electrons, summary

Stability of periodic orbits & orbiting resonances

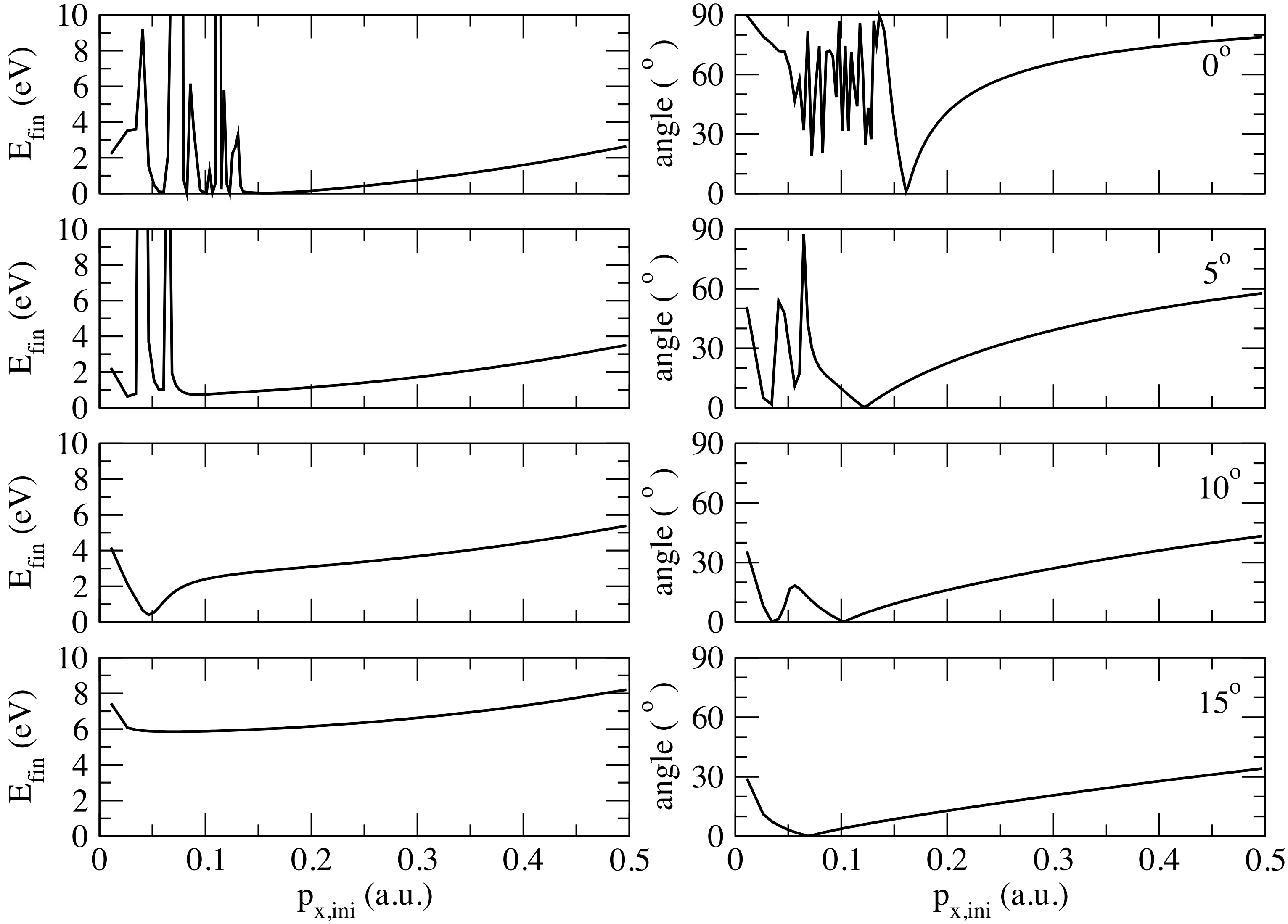


Stability of periodic orbits & orbiting resonances




9°
9.5°
9.75°
9.9°
10°
10.25°
10.5°
11°
E_{fin} (eV)
$p_{x,ini}$ (a.u.)
0
2
4
6
8
10
0.1
0.2
0.3
0.4
0.5

final energy (angle) as a function of initial perpendicular momentum ($p_{z,ini}$=0)
for different ionization times (phases)



Thanks !