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, \textit{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: \textit{Fix} the hamiltonian within an interval of parameters (phase space) and then \textit{jump} to a new fixed H.
Different regions of phase space are dominated by different hamiltonians (DIH)

DIHs are simpler (may be even integrable) than the full $H$

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**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 drosophila of strong field physics)

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

Harmonic Spectrum

\[
\sigma(\omega) = \int e^{i\omega t} a(t) \, dt
\]

with dipole acceleration

- ionisation potential \( I_p \)
- ponderomotive potential \( U_p = \frac{F^2}{4\omega^2} \), \( F = f(t) = \text{const.} \)
High harmonic generation (the drossophila of strong field physics)

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

separable DIH approach:
switch between Coulomb potential only and laser field only (large distances)

spectrum:

\[
\sigma(\omega) = \int e^{i\omega t} a(t) \, dt
\]

with dipole acceleration

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

\[
a(t) = - \langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \rangle
\]
Gaussian wave packet
(initiated at 70 a.u. distance from the nucleus):

laser assisted electron-ion scattering

laser field: $F = 0.1 \text{ au}$, $\omega = 0.038 \text{ au}$, $\gamma = 0.05 \text{ au}$
\[ a(t) = - \langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \rangle \]

\[ \sigma(\omega) = \int e^{i\omega t} a(t) \, dt \]

**QM**

**SC–IVR**

**SC–DIH**

**SC–DIH** (analytical)

**LSC–IVR**

**Volkov**

(free e– in laser field)

- Figure 3.
Switching condition for HHG
(when does an electron, floating with the laser field, get trapped by the ion?)

\[ H_{\text{atom}} = \frac{p^2}{2} + V(x) + xf(t) \cos \omega t \]

V_{\text{ion}}(x) < V_{\text{laser}}(x)

\[ \Rightarrow \text{maximal } x = x_c \]

trapping should occur when the electron is slow:
\[ \Rightarrow p_c = 0 \]

\[ p(t) = p_0 - \frac{\varepsilon}{\omega} \sin(\omega t), \]

\[ q(t) = q_0 + p_0 t + \frac{\varepsilon}{\omega^2} \left[ \cos(\omega t) - 1 \right]. \]

Setting \( p(t_c) = 0 \) leads to switching times
\[ \omega t_c = n\pi + \arcsin \left( \frac{\omega p_0}{\varepsilon} \right), \]
\[ p_0^{(n)}(q_0) = -\frac{\omega}{n\pi} \left( q_0 - \frac{1 - (-1)^n}{2} \frac{2\mathcal{E}}{\omega^2} \right) \]
analytical wave function for HH

\[ |\Psi(t)\rangle = N(t)(|\Psi_V\rangle + c(t)|\Psi_0\rangle) \]

\[ c(t) = \sum_{n=1}^{2N} \Theta(t - nT/2)c_n. \]

\[ c_n \approx \frac{x_c}{\sqrt{\gamma \pi}} \frac{1}{nT} \left( 1 - \frac{(q_\alpha + x_c/2)^2}{\gamma n^2 T^2} \right) \]
1.5 degrees of freedom example: e- - ion scattering under laser pulse (HHG)

5 degrees of freedom example: planar e- He$^+$ scattering
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: $H_{FF} = (\frac{p_1^2 + p_2^2}{2} - \frac{1}{r_1} - \frac{2}{r_2})$ (for $r_1 > r_2$)
  - $H_{FF} = (\frac{p_1^2 + p_2^2}{2} - \frac{2}{r_1} - \frac{1}{r_2})$ (for $r_1 < r_2$)

Temkin – Poet model

*A. Temkin, Phys Rev 126, 130 (1962)*;
*R. Poet, J Phys B 11, 3081 (1978)*
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:
  - $H_{FF} = \frac{(p_1^2 + p_2^2)}{2} - \frac{1}{r_1} - \frac{2}{r_2}$ \hspace{0.5cm} (r_1 > r_2)
  - $H_{FF} = \frac{(p_1^2 + p_2^2)}{2} - \frac{2}{r_1} - \frac{1}{r_2}$ \hspace{0.5cm} (r_1 < r_2)

- interaction event ‘2’: $r_1 = r_2$, then $r_1 \leftrightarrow r_2$ \hspace{0.5cm} ($r'_1 = r_2$, $r'_2 = r_1$)

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How to identify DIH and criteria for switching between them?

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- interaction event ‘1’: \( F \equiv \left| \frac{2V_{12}}{V_1 + V_2} \right| = 1 \), then \( p'_{12} = K \ p_{12} \)

- approximate Hamiltonian: \( H_{NF} = p_{12}^2 + \frac{1}{r_{12}} \)
  \[ r_{12} = r_1 - r_2 = R, \quad r = \frac{(r_1 + r_2)}{2} \]

- transformation \( K \) uniquely defined by respecting constants of motion and locality:
  \( H, \ p, \ L \) and since the \( r_i \) are fixed for the momentum kick:
  \( p^2, \ l_{12} \)
How to identify DIH and criteria for switching between them?

- Try to concentrate interactions to instants in time
- Approximate Hamiltonian: $H_{FF} = \frac{p_1^2 + p_2^2}{2} - \frac{1}{r_1} - \frac{2}{r_2}$ (for $r_1 > r_2$)

**Interaction event ‘1’:** $F \equiv \left| \frac{2V_{12}}{V_1 + V_2} \right| = 1$, then $p’_{12} = K p_{12}$

- Approximate Hamiltonian: $H_{NF} = p_{12}^2 + \frac{1}{r_{12}}$

- Transformation $K$ uniquely defined by respecting constants of motion and locality:

$H, p, L$ and since the $r_i$ are fixed for the momentum kick: $p^2, L_{12}$
How to identify DIH and criteria for switching between them?

**symmetry arguments, physical intuition, trial & error**

- **interaction event ‘1’**: if \( F = 1 \), then \( \mathbf{p}'_{12} = \mathbf{K} \mathbf{p}_{12} \)

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 \( \mathbf{K} = \ln_x D(-2\alpha) \) with a rotation by \(-2\alpha\) and an inversion in x:

\[
\ln_x = \begin{pmatrix}
-1 & 0 \\
0 & 1
\end{pmatrix}
\]

\[
\mathbf{R} = (0, R)
\]

\( \alpha = \pi/2 \)

\[
F \equiv \frac{2V_{12}}{V_1 + V_2}
\]
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: 
  \[ H_{FF} = p_1^2 + p_2^2 - 1/r_1 - 2/r_2 \quad (r_1 > r_2) \]
  \[ H_{FF} = p_1^2 + p_2^2 - 2/r_1 - 1/r_2 \quad (r_1 < r_2) \]

- interaction event ‘2’: \( r_1 = r_2 \), then \( r_1 \leftrightarrow r_2 \) \( (r'_1 = r_2, r'_2 = r_1) \)
- interaction event ‘1’: \( F \equiv \left| \frac{2V_{12}}{V_1 + V_2} \right| = 1 \), then \( p'_{12} = Kp_{12} \)

<table>
<thead>
<tr>
<th>event</th>
<th>’1’</th>
<th>’2’</th>
</tr>
</thead>
<tbody>
<tr>
<td>condition</td>
<td>( F = 1 )</td>
<td>( r_1 = r_2 )</td>
</tr>
<tr>
<td>action</td>
<td>( p'_2 - p'<em>1 = K</em>{NF}(p_2 - p_1) )</td>
<td>( r_1 \leftrightarrow r_2 )</td>
</tr>
<tr>
<td>effect</td>
<td>( \Delta l_i \neq 0, \Delta E_i \neq 0 )</td>
<td>( \Delta E_i \neq 0 )</td>
</tr>
</tbody>
</table>
DIH qualitative – collision sequences of $2e^-$

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

- ‘22’: elastic
- ‘12’: excitation (classical exchange)

Graphs showing the probability density functions for different sequences.

Legend:
- full
- DIH

Bar graph showing the probability distribution for different sequences.
Planar electron – He\(^+\) collisions

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

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![Diagram of Planar electron – He\(^+\) collisions](image_url)

**Figure 7.**

Same as in Fig. 5, but for a collision sequence, '12'. The specific initial conditions are \(0, 0\) for (a-c) and \(0, 2\) for (d-f).

Classfication of trajectories according to sequences of events '1' and '2' (see table 1).

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[Diagram descriptions and analysis]
Planar electron – He\(^+\) collisions

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

DIH (22)

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

Compared to quantum: DIH better than full classical !?

Figure 9. Energy spectrum from Fig. 4a with contributions shaded according to their event sequences (see table 1), (a) for DIH dynamics (b) for full classical dynamics, for details, see text.

Figure 10. Spectra of the projectile electron after the collision with parameter as in Fig. 3 in singlet/triplet symmetry (solid/dashed). The different curves provide the quantum result (thick/black), the classical full trajectory result (thin/white) and the classical DIH result (red). Part (a) gives the (continuous) energy spectrum, part (b) the binned distribution of final angular momentum of the projectile electron.

Fact that the quantum triplet dynamics is less reactive than the singlet dynamics due to a symmetry enforced nodal line at \( r_1 = r_2 \). Classically, this effect is resembled to a certain degree by the DIH dynamics compared to the full classical dynamics. In the former "reactivity" is limited to the events '1' and '2', discrete in time.

6. Summary

We have introduced the concept of dominant interaction hamiltonians which approximates dynamics described by a complicated, non-separable classical hamiltonian with different simplified hamiltonians. Each of them is valid in a specific phase space volume where it dominates all other simplified hamiltonians formulated. Applied to planar electron-ion scattering, we have demonstrated that the DIH approach provides a good approximation to the full classical dynamics. More importantly, and somewhat surprisingly, quantum results regarding differential spectra (energy and angular momentum of the projectile) agree better with the DIH result than with the full classical dynamics. Whether this is accidental or systematic will have to be investigated in future studies. A second appealing aspect of the DIH concept is...

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

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

\(\gamma_0, p_t, q_t \in \mathbb{R}, \quad \gamma_t, \delta_t \in \mathbb{C}\)

Ansatz for the solution of the time-dependent Schrödinger equation

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

Thawed GWD: Phase- and position space

\[ \Psi \]

single trajectory initial value method
Multiple trajectory method for N DOF: FGWD

\[
\psi(x, t) = \int dx' K(x, t; x', 0) \psi(x', 0)
\]

Initial value Herman-Kluk propagator

\[
K(x, t; x', 0) \approx \int \frac{dp'dq'}{(2\pi\hbar)^N} \langle x | g_\gamma(p_t, q_t) \rangle R e^{iS(p', q', t)/\hbar} \langle g_\gamma(p', q') | x' \rangle
\]

\[
R = \sqrt{\det \frac{1}{2} \left( m_{pp} + m_{qq} - \gamma i\hbar m_{qp} - \frac{1}{\gamma i\hbar} m_{pq} \right)}
\]

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

Heller (’81), Herman and Kluk (’84), Kay (’94), F.G. and Xavier (’98)
Frozen GWD: Phase- and position space

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

$$M = \begin{pmatrix} m_{pp} & m_{pq} \\ m_{qp} & m_{qq} \end{pmatrix} = \begin{pmatrix} \frac{\partial p_t}{\partial p'} & \frac{\partial p_t}{\partial q'} \\ \frac{\partial q_t}{\partial p'} & \frac{\partial q_t}{\partial q'} \end{pmatrix}$$

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

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

$\Rightarrow$ purely classical input!
multitrajectory initial value method
- Time-dependent initial value method for arbitrary dynamics
- no storage problems due to locality \( \Rightarrow \) DIH
- Initial Gaussian \( \Rightarrow \) Monte Carlo integration over phase space
- SPA \( \Rightarrow \) Van Vleck-Gutzwiller propagator

\[
K(x, t; x', 0) \sim \sum_j \left| \frac{1}{\det m_{qp}} \right|^{1/2} \exp\{iS_j(x, x', t)/\hbar - i\pi\nu_j/2\}
\]

- “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
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

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

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

\((E_1 = -2; E = 0.5; \quad \epsilon^* = E_2^{(f)}/E)\)
DiH quantitativ-spectra: energy & angular momentum
‘1’: kick (near field)
‘2’: switch (far field)

DiH qualitative – collision sequences

(a)

(b)

full
DiH qualitative – collision sequences

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

‘22’: elastic
‘12’: excitation (classical exchange)
DiH two electrons, summary
Stability of periodic orbits & orbiting resonances

trajectories with $1.5 < E_{\text{fin}} < 2.5 \text{ eV}$ and $\alpha < 5^\circ$ ($p_{z,\text{ini}} = 0 \text{ a.u.}$)
Stability of periodic orbits & orbiting resonances

phase = 9.9°

- $p_{x,ini} = 0.035$ a.u. (left)
- $p_{x,ini} = 0.04638$ a.u. (minimum)
- $p_{x,ini} = 0.062$ a.u. (right)
final energy (angle) as a function of initial perpendicular momentum ($p_{z,\text{ini}}=0$) for different ionization times (phases)
Thanks!