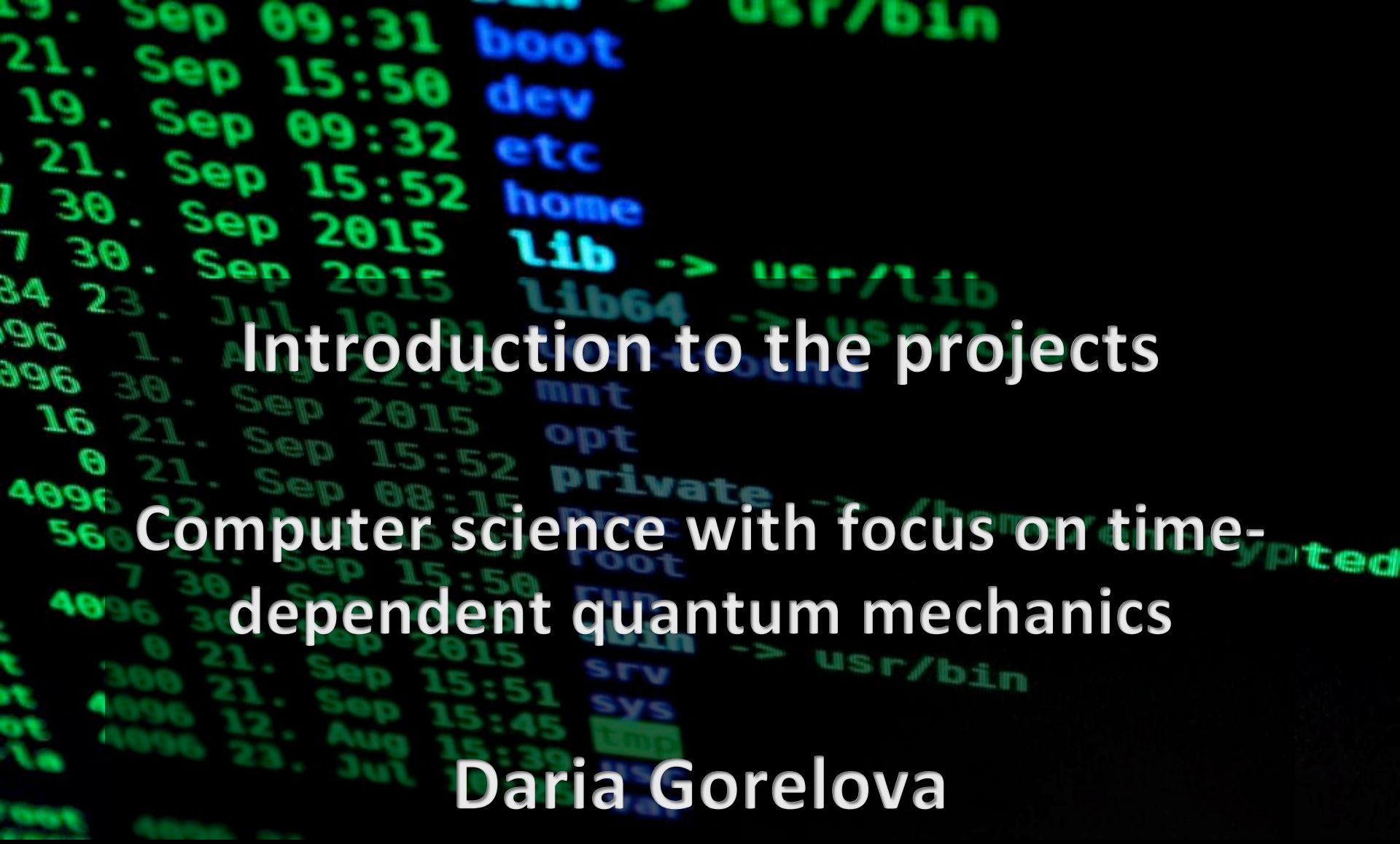


Introduction to the projects

Computer science with focus on time-dependent quantum mechanics

Daria Gorelova

Projects: semester plan

Termine			
	Datum	Von	Bis
1	Di, 24. Okt. 2023	08:30	10:00
2	Di, 7. Nov. 2023	08:30	10:00
3	Di, 14. Nov. 2023	08:30	10:00
4	Di, 21. Nov. 2023	08:30	10:00
5	Di, 28. Nov. 2023	08:30	10:00
6	Di, 5. Dez. 2023	08:30	10:00
7	Di, 12. Dez. 2023	08:30	10:00
8	Di, 19. Dez. 2023	08:30	10:00
9	Di, 9. Jan. 2024	08:30	10:00
10	Di, 16. Jan. 2024	08:30	10:00
11	Di, 23. Jan. 2024	08:30	10:00
12	Di, 30. Jan. 2024	08:30	10:00

Distribution of topics, getting started

Your progress reports

Presentation of projects

Organizational

Projects can be done individually or in a group of two people

The distribution on the 7th of November

Quite late for the reason: fluctuation of participants, but the projects should be given to those, who stay

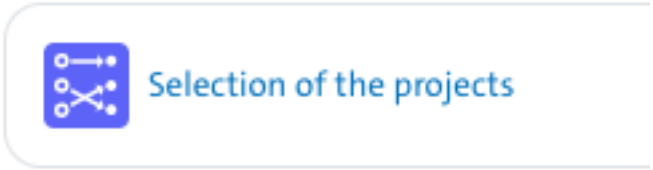
Organizational

Projects can be done individually or in a group of two people

November 7th

Your questions about the projects, voting

Voting in Moodle,
active on: Nov., 7th



If you have a person, with whom you want to do the project: vote together, at the same time

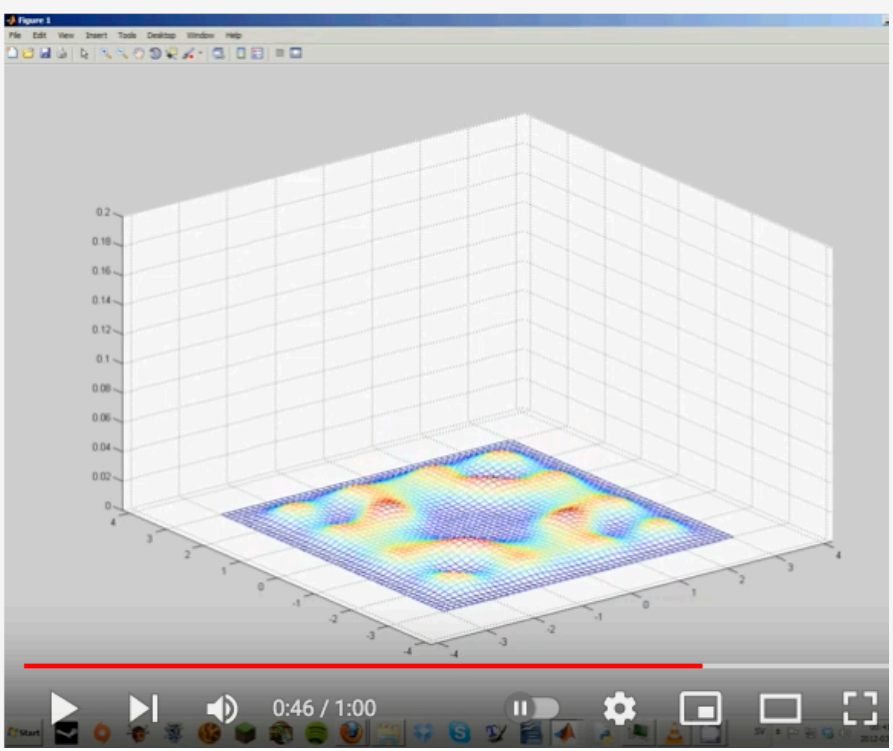
2D Gaussian wave packet

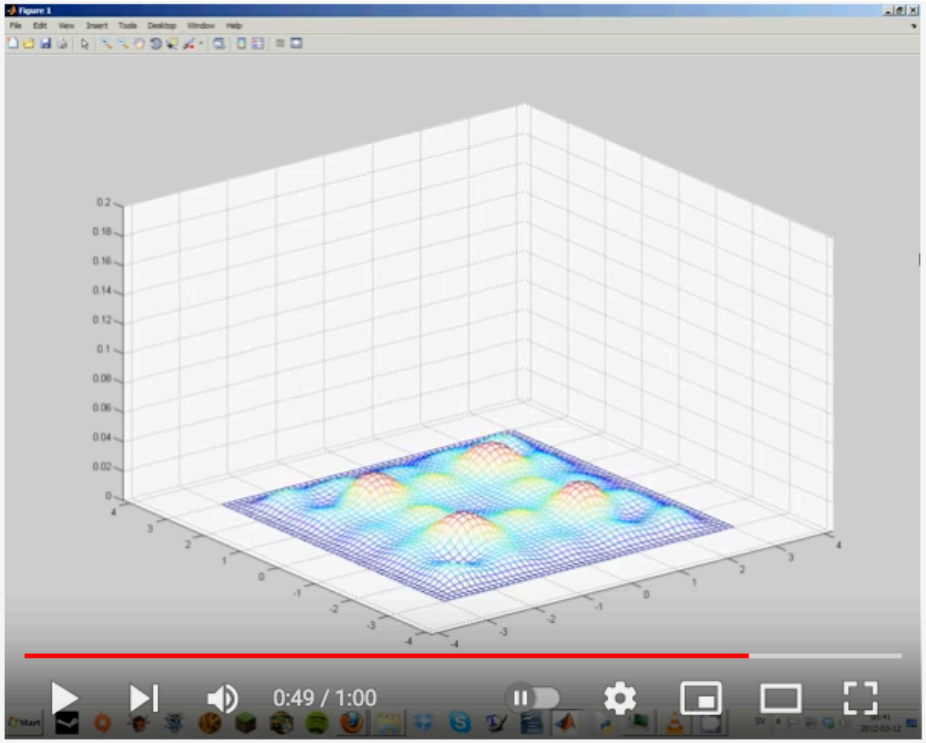
2D Gaussian wave packet

Video 2D box:

https://www.youtube.com/watch?v=tyH7_fhVGLM

2D Gaussian wave packet





https://www.youtube.com/watch?v=EfY3Qbgx3p4

2D Gaussian wave packet

- Think of a potential –
  a 2-D harmonic oscillator
  potential/infinite box, other
  potentials

- Barriers

Calculate probability

Initial condition: Gaussian wave packet

Algorithms for 2d Schrödinger equation

Time-propagation must be beyond Euler method

2D Gaussian wave packet

Literature

Literature

Philipp O.J. Scherer. *Computational Physics. Simulation of Classical and Quantum Systems.*

Rubin H. Landau, Manuel Jose Paez, Cristian C. Bordeianu. *Computational Physics. Problem Solving with Computers.*

Jos Thijssen. *Computational Physics.*

Joshua Izaac and Jingbo Wang. *Computational Quantum Mechanics.*

Tannor, David J. *Introduction to Quantum Mechanics: A Time-Dependent Perspective.*

F. Grossmann. *Theoretical Femtosecond Physics. Atoms and Molecules in Strong Laser Fields.*

Variational calculation

Variational calculation

Widely-used method in Quantum Mechanics

Actively employed in electronic-structure calculations

The possible solutions are restricted to a subspace of the Hilbert space, and in this subspace we seek the best possible solution

Minimization of a functional

Variational calculation

Use the variational calculation to find eigenstates of a particle in the two-dimensional Pöschl–Teller potential

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{1}{\cosh^2(\sqrt{x^2+y^2})}$$

Variational calculation

Construct the 2D finite difference matrix

Basis sets

Convergence

Integration

2D Gaussian wave packet

Literature

Literature

Philipp O.J. Scherer. *Computational Physics. Simulation of Classical and Quantum Systems.*

Rubin H. Landau, Manuel Jose Paez, Cristian C. Bordeianu. *Computational Physics. Problem Solving with Computers.*

Jos Thijssen. *Computational Physics.* **Theory**

Joshua Izaac and Jingbo Wang. *Computational Quantum Mechanics.* **Tips in Chapter 10.3 and exercise P10.8**

Tannor, David J. *Introduction to Quantum Mechanics: A Time-Dependent Perspective.*

F. Grossmann. *Theoretical Femtosecond Physics. Atoms and Molecules in Strong Laser Fields.*

Quantum dots

Quantum dots

Construct artificial systems such that they display certain properties not found naturally

Electrons can be trapped between two layers of semiconductors, effectively confining the electrons to two dimensions

Quantum dots

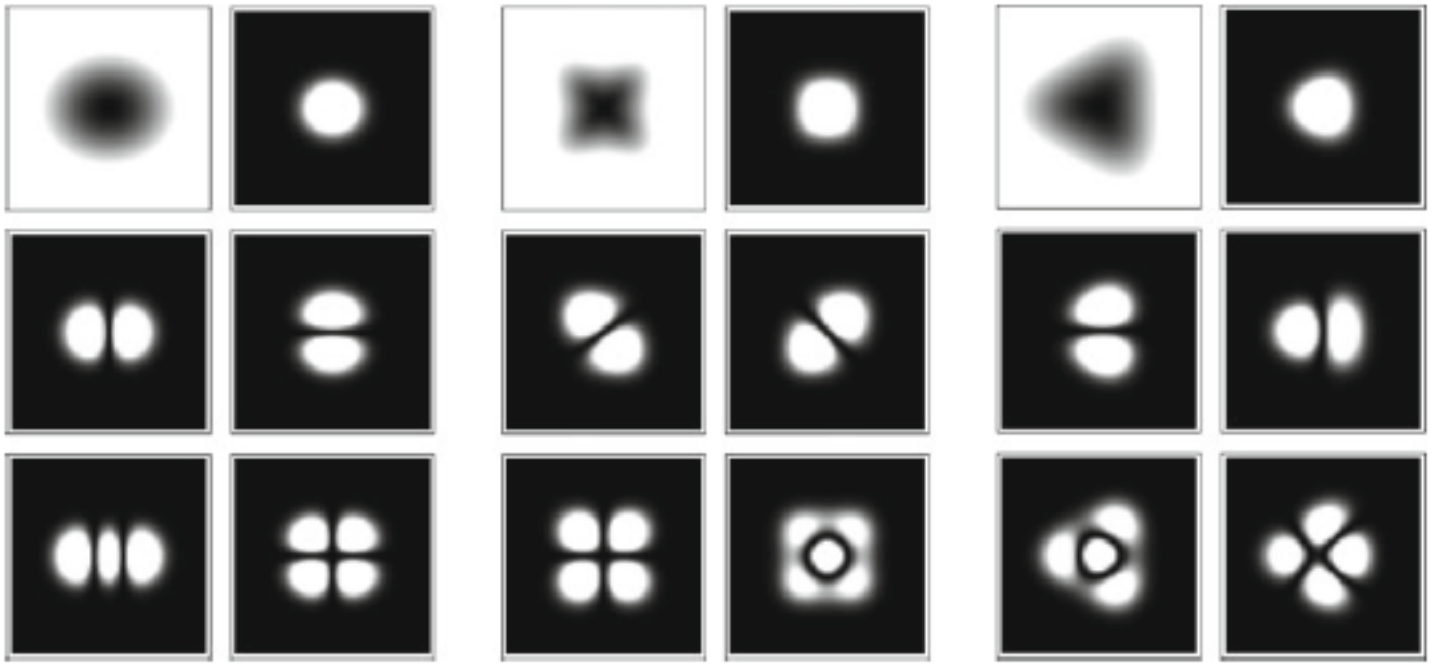
Quantum dots confined to a spherical three-dimensional potential well

Schrödinger eq -> Solution of the radial eq

$$-\frac{\hbar^2}{2m_e}\frac{d^2\mathcal{P}_{n\ell}}{dr^2}+\left[\frac{\hbar^2\ell(\ell+1)}{2m_e r^2}+V(r)-E_n\right]\mathcal{P}_{n\ell}(r)=0$$

Quantum dots

Solve for single electron quantum dots:
ground + excited states



(a) Circular potential (b) Square potential (c) Triangular potential

Quantum dots

Literature:

Joshua Izaac and Jingbo Wang. Computational Quantum Mechanics.

H_2^+ in a Laser Field

H_2^+ in a Laser Field and fixed nuclei

Coupling an external electric field to the molecular dynamics,

femtosecond spectroscopy,
control of molecular dynamics,
the realization of quantum logic operations …

General aspect of light-matter interaction

H_2^+ in a Laser Field and fixed nuclei

Simplest molecule: two protons and one electron

$$i\dot{\Psi}(\rho,z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + \hat{T}_\rho + V_c(\rho,z) + z\mathcal{E}(t)\right]\Psi(\rho,z,t)$$

The problem has a cylindrical symmetry, if the laser field is polarized along molecular axis

Cylindrical symmetry => expansion in Fourier-Bessel series

Split-operator method

H_2^+ in a Laser Field and fixed nuclei

Literature:

F. Grossmann

Theoretical Femtosecond Physics

Atoms and Molecules in Strong Laser Fields

Chapter 5.2

Magnus expansion

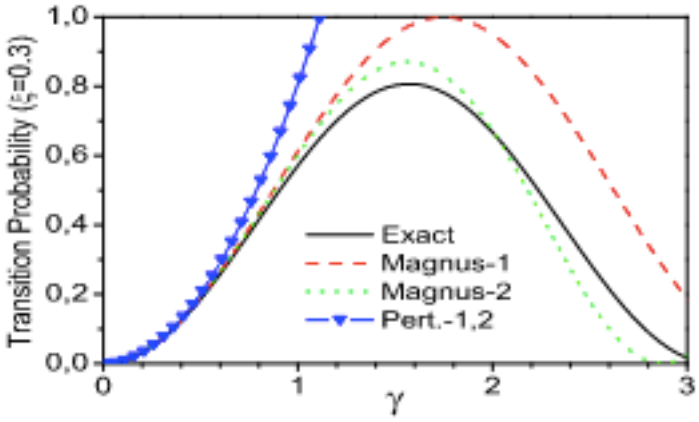
Magnus expansion

Alternative to the time-dependent perturbation theory

Method to solve the time-dependent Schrödinger equation

Magnus expansion is similar to the time-dependent perturbation theory, but there are advantages:

- Unitarity is preserved
- Convergence condition is clear



Magnus expansion

Two-level system and a time-dependent perturbation

$$\hat{H} = \begin{pmatrix} E_1 & f(t) \\ f(t) & E_2 \end{pmatrix}$$

$f(t)$ - some time-dependent function

Magnus expansion

Literature:

(1) F. Grossmann

Theoretical Femtosecond Physics

Atoms and Molecules in Strong Laser Fields

(2) **A pedagogical approach to the Magnus expansion**

S Blanes[1], F Casas[2], J A Oteo[3] and J Ros[4]

Analytical solution to compare to

(3) Magnus expansion applied to a dissipative driven two-level system

Tuguldur Kh. Begzjav[a,*], Hichem Eleuch[a,b]

Dissipation + further analytical solutions

Magnus expansion

Possible studies:

Implement numerically, compare to the analytical solutions

Study different f(t)

Study dissipation

Chebyshev polynomials

(2)

Many different applications in physics. Examples:

Expansions of tight-binding Green's functions
Spin systems
Neutron transport equation
Wave shaping for audio synthesis
… etc

Chebyshev polynomials

Time-dependent quantum harmonic oscillator

$$\hat{H}(t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2(x - \sin t)^2.$$

Example

Chebyshev polynomials

Propagate the initial wave function
under the time-dependent Hamiltonian

$$\psi(x,t) = \left(\prod_{n=1}^{N-1} e^{-i\hat{H}(n\Delta t)\Delta t/\hbar} \right) \psi(x,0)$$

using the Chebyshev polynomials

Play with the initial state, frequency, Hamiltonian

Chebyshev polynomials

Literature:

(1) Joshua Izaac and Jingbo Wang. Computational Quantum Mechanics.

(2) H. Fehske
R. Schneider
A. Weiße (Eds.)

Computational Many-Particle Physics **Chapter 19**

Quantum scattering

Quantum scattering with a spherically symmetric potential

Schrödinger equation involving the (reduced) mass m, the relative coordinate r
and the interaction potential V between the particle and the interaction centre

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Quantum scattering with a spherically symmetric potential

Bombardment of krypton atoms with hydrogen atoms

Lennard–Jones (LJ) potential

$$V_{\mathrm{LJ}}(r) = \varepsilon \left[\left(\frac{\rho}{r} \right)^{12} - 2 \left(\frac{\rho}{r} \right)^{6} \right]$$

Quantum scattering with a spherically symmetric potential

Calculate scattering cross section

Numerov method (studied in the course)

Bessel functions

Explore different potentials

Quantum scattering with a spherically symmetric potential

Literature:

COMPUTATIONAL PHYSICS

Second Edition

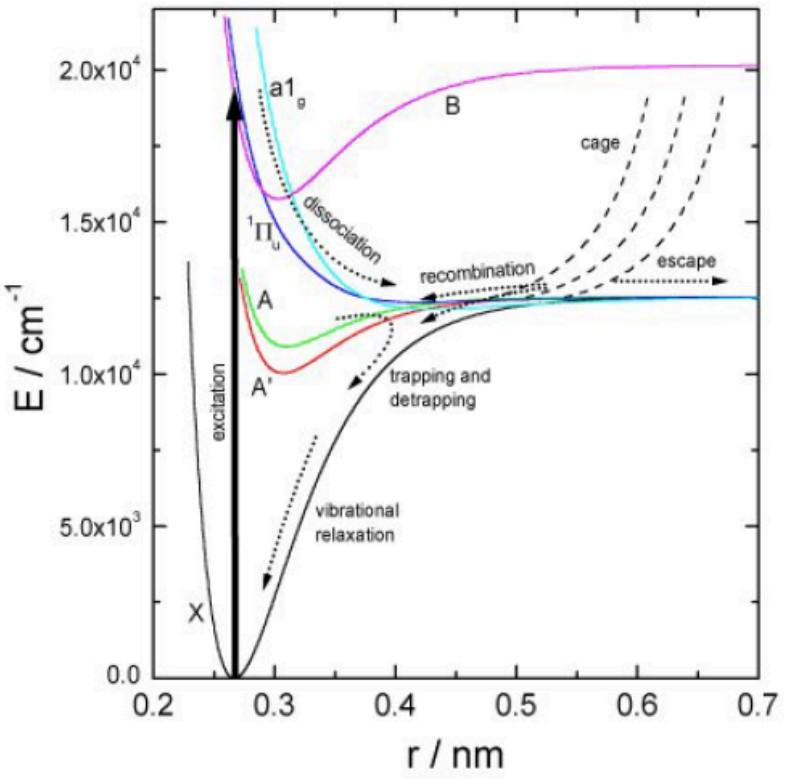
JOS THIJSSEN
Kavli Institute of Nanoscience, Delft University of Technology

The whole Chapter 2

Coupled electron-nuclear dynamics

Coupled electron-nuclear dynamics

One of the main applications of atto- and femtosecond pulses:

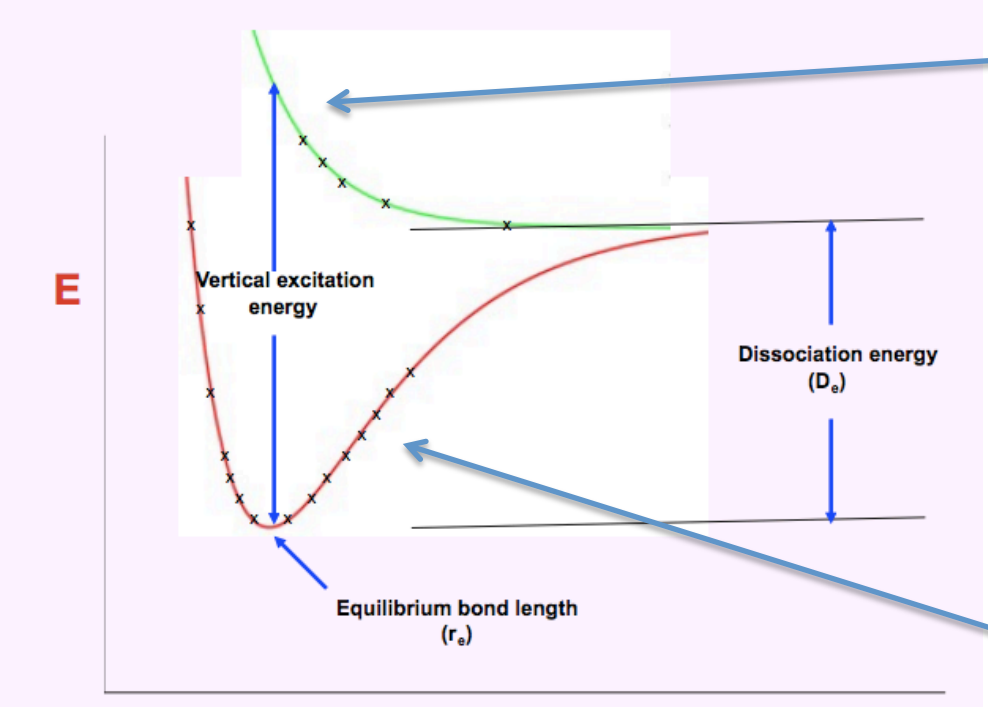


Light speaks to electrons,
electrons speak to nuclei

⇒ light-energy conversion
⇒ chemical reactions
⇒ light harvesting
⇒ …

Coupled electron-nuclear dynamics

In this project



Repulsive potential: $+A/r^{12}$

Lennard-Jones potential

Coupled electron-nuclear dynamics

Wigner distribution of molecular geometries about the equilibrium geometry of the electronic ground state account for the spread of the initial N dimensional vibrational wave function.

Coupled electron-nuclear dynamics

Sample x and p according to the Wigner distribution for the ground state of the harmonic oscillator (advanced option: ground state of the Lennard-Jones potential)

Obtain an ensemble of twenty trajectories and propagate them classically in the dissociation potential

Calculate the averaged probability

Coupled electron-nuclear dynamics

Molecular geometries generation. *Wigner sampling.* A central motivation to build a dataset beyond MD17 is that the quantum mechanical distribution of the configurational space is much broader than the one provided by classical AIMD at 500 K[48]. The zero-point energy stored in each degree of freedom is usually much bigger than the classical thermal energy, meaning that the vibrational amplitudes are much more prominent in the quantum than in the classical picture. A straightforward way of sampling the configurational space (or, more generally, the phase space) to match the zero-point energy requirement is through a quantum-harmonic-oscillator Wigner distribution of the nuclei[38]. The optimized molecular geometries and their corresponding harmonic frequencies described in the previous section form the basis for generating an ensemble of non-equilibrium structures sampled from a Wigner probability distribution function[38,49]. This function maps the nuclear wave function—written as a product of ground-state harmonic oscillator wave functions, one for each normal mode—on the classical phase space[50]. Within this approach, each of the $N_F = 3N_{at} - 6$ normal mode coordinates and momenta are randomly sampled according to the probability distribution function

$$P_W(\mathbf{Q}, \mathbf{P}) = \prod_{i=1}^{N_F} \frac{1}{\pi\hbar} \exp\left(-\frac{1}{\hbar\omega_i} (\omega_i^2 Q_i^2 + P_i^2) \right) \quad (1)$$

where $Q_i = \mu_i^{1/2} q_i$ and $P_i = \mu_i^{-1/2} p_i$ are the mass-scaled coordinate and momentum for each normal mode i with coordinate q_i and momentum p_i, reduced mass μ_i, and angular frequency ω_i. After the sampling, the normal-mode coordinates and momenta are converted to Cartesian coordinates and momenta.

(nice explanation from https://doi.org/10.1038/s41597-023-01998-3)

Coupled electron-nuclear dynamics

Literature

Several papers and book chapters in moodle

See “THE JOURNAL OF CHEMICAL PHYSICS 133, 044313 2010” for sampling strategies

The project is recommended for two students

Floquet physics

Floquet formalism

Describe light-matter interaction using Floquet formalism

Floquet formalism − intensively used approach in modern quantum mechanics

Describes periodic driving of a (quantum) system

- Time crystals
- Extreme nonlinear optics

Floquet formalism

Light-matter interaction

According to the perturbation theory, the probability of an effect involving transitions from the initial state to

one state $\propto I$
two states $\propto I^2$ breaks down
three states $\propto I^3$ …

Problem – this is true only for small intensities.
Intensity of light pulses can be made very high nowadays

Floquet formalism

Create Floquet matrix for 4 electronic states driven by a periodic electro-magnetic field

Obtain eigenstates and eigenvalues

Use eigenstates to calculate high-harmonic generation spectrum

(If in a couple) Extend to a simple tight-binding model

Floquet formalism

Literature:

A new topic, less educational literature (speak to me, I have lecture on it)

F. Grossmann. *Theoretical Femtosecond Physics. Atoms and Molecules in Strong Laser Fields.* **Chapter 2.3**

Exploring different time-propagation methods

Different time-propagation methods

Consider these three methods that will be studied in the course:

Split-step
4.-order Runge-Kutta
Crank-Nicolson

Apply to a same time dependent problem
Compare advantages and disadvantages of the methods

Different time-propagation methods

Advantage of the project:

all algorithms have to be written in any case

Challenge:

High responsibility, because serves for educational purposes

This project can be done only by one

Project presentation

Four aspects to be addressed:

- **Algorithm**
- **Results**
- Error analysis
- Physics background

Project presentation

If you do the project in a couple

Prepare different presentations

Presentations should not repeat each other

More creativity is expected

Two presentations must cover all 4 aspects, a single presentation must cover the two important aspects

It should be clear to me, who wrote which parts of the code

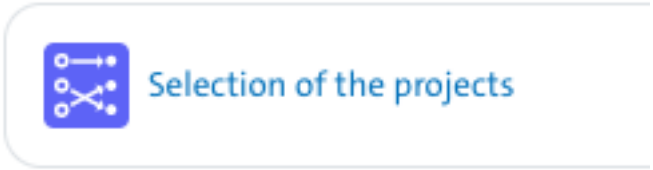
Organizational

Projects can be done individually or in a group of two people

November 7th

Your questions about the projects, voting

Voting in Moodle,
active on: Nov., 7th



If you have a person, with whom you want to do the project: vote together, at the same time