Programming projects

Lecture: “Computational quantum dynamics”

WS2018/19

Lecturer: Martin Gärttner

Tutor: Ricardo Costa de Almeida

The programming projects are an exercise to apply the numerical tools introduced in the lecture to actual research problems and to reproduce some results of recent publications. This gives the students the opportunity to more deeply access a specific physical system and the corresponding numerical methods used to describe it. You may find the description of the projects vague, even more so than the exercise sheets. This is on purpose. We purposefully leave the exact strategy for solving the problem undefined. The “steps” defined for each project are meant to give you some idea of what we roughly expect. Also the information given in the problem description is incomplete in the sense that you will have to look into the given literature to understand the problem fully.

A written report (pdf) on the results of the project of NO MORE than 10 pages (including plots) should be submitted together with the developed code. The programming language can be chosen freely. The code should be sufficiently documented and styled (such that we can read and understand it).

The projects will be graded with a maximum score of 333 point which adds to the maximal achievable score from the weekly programming exercises 1000 points. In order to pass the course at least 100 points need to be achieved on the programming project. See the “announcements” forum on moodle for a summary of the course requirements.

Students may (and are encouraged to) work in groups of 2.

Please choose a partner and a project until Friday, 18.01.2019 and enter you choice into the database provided on moodle.

The projects should be submitted via email (to martin.gaerttner@kip.uni-heidelberg.de or ricardo.almeida@kip.uni-heidelberg.de) before 10pm on March 10th, 2019.

List of Projects:

1) ***Dissociation dynamics of H_2^+ in XUV and IR laser fields.***

Recent experiments have used pump-probe spectroscopy to study the vibrational and dissociation dynamics of H_2^+. In these experiments H_2 molecules in their electronic and vibrational ground state are ionized forming H_2^+ in its electronic ground state in a superposition of various high-lying vibrational states of the ground state Born Oppenheimer surface of the molecular ion. This transfer happens extremely fast such that the shape of the wave packet is preserved. This vibrational wave packet now oscillates in the Born-Oppenheimer potential of the electronic ground state of the molecular ion. A control pulse with a length of a few fs couples this bound state molecular energy surface to a dissociating one. If this pulse arrives while the wave packet is close to its outer turning point, the molecule dissociates. The resulting fragments (ion and the electron from the initial ionization pulse) are detected with spatial and momentum resolution. This technique of probing the molecules vibrational dynamics has been dubbed "making a molecular movie".

The objective of this project is to simulate the dynamics of the wave packet moving on the two relevant molecular potentials time-dependently coupled by the probe pulse.

Literature: F. Kelkensberg et al., Phys. Rev. Lett. 103, 123005 (2009), A. Fischer et al. PRA 93, 012507 (2016) and references therein.

Methods: Finite difference method, exact diagonalization, split-step Fourier method, Fourier analysis

Steps:

- Find the vibrational eigenstates in the H_2^+ ground state potential
- Simulate the wave packet propagation without the IR laser field
- Simulated the dynamics of the time-dependent system with two coupled energy surfaces, coupled by the time-dependent IR laser field. Visualize the wave packet dynamics.
- Scan the delay time and analyze the momentum distribution of the dissociation products.

The Born Oppenheimer surfaces for the two relevant states, the H_2 ground state wave function (initial state) and the (R-dependent) dipole matrix element between the relevant two electronic states are provided (all in atomic units).

2) ***The Gross-Pitaevskii equation (GPE): Dynamics of solitons and vortices***

The GPE is a mean field equation that has been incredibly successful in describing the dynamics of Bose Einstein condensates (BECs). The equation features a non-linear term and thus allows for stable soliton solutions in 1D and vortices in 2D. The goal of this project is to study these phenomena using the split-step Fourier method.

Literature: Sebastian Erne Diplomarbeit (provided on moodle), M. Karl and T. Gasenzer New. J. Phys. 19: 093014 (2017)

Methods: Mean field approximation, discretization, non-linear partial differential equations, split-step Fourier method

Steps:

- Simulate the evolution of dark solitons in a homogeneous (no trapping potential) 1D Bose gas. Use single and multiple grey solitons and study their propagation.
- Study the dynamics of solitons in a homogeneous 2D Bose gas.
- In 2D other topological defects, called vortices can be present. Use the given routine (to be provided on moodle) to initialize a 2D gas containing vortices and visualize and analyse their dynamics.

3) *The Helium atom*

The Helium is the simplest atom with non-trivial electronic structure and a paradigmatic problem for benchmarking techniques for electronic structure calculations. The goal of this project is to use perturbative, variational, and basis set expansion techniques to calculate the ground state energy of Helium (ignoring relativistic effects and spin-spin coupling and other corrections, i.e. only considering Coulomb interactions). How close can you get to the most precise known experimental value for the ground state energy of −79.005151042(40) eV?

Literature:

The lecture notes of Paolo Giannozzi from the University of Udine (see lecture homepage) contain details of the relevant numerical techniques and briefly review the helium problem and may serve as a starting point.

Review about variational bases for He: G.W.F. Drake, (1999). "High precision theory of atomic helium", Phys. Scr. T83, 83–92.

A very nice historic piece (in German): E.A. Hylleraas, Z. Phys. 48, 469 (1928) https://link.springer.com/article/10.1007/BF01340013

Methods: perturbative techniques, variational techniques, basis set expansion

Steps (You don't have to do all of this, but we want you to at least explore one of the advanced methods of Hartree Fock or expansion into variational basis functions):

- Calculate the ground state energy perturbatively, treating the Coulomb interaction between the electrons as a perturbation.
- Use a simple variational Ansatz to get an estimate for the ground state energy.
- Use the self-consistent Hartree (or Hartree Fock) method to estimate the ground state potential
- Use an expansion into products of hydrogen eigenfunctions (or more general variational basis functions) to get an estimate of the ground state energy.

4) *Quantum enhanced sensing and entanglement with collective spins*

The collective Ising model with a transverse field can be used to generate spin-squeezed states useful for sensing, e.g. of small magnetic fields. The goal of this project is to find optimal parameters for a quantum enhanced sensing protocol. To prepare the useful entangled states one can either generate squeezed states under the collective Ising evolution or adiabatically sweep the transverse field though the quantum phase transition, preparing a cat state.

Literature: H. Strobl et al. Science 345, 424-427 (2014), G. Toth and I. Apellaniz, J. Phys. A: Math. Theor. 47, 424006 (2014)

Methods: Exact diagonalization, integration of the Schrödinger equation of a collective spin, evaluating entanglement quantifiers, visualization of collective spins

Steps:

- Simulate the evolution of a collective spin system, initially prepared with all spins along the x-direction under the collective Ising Hamiltonian.
- Simulate and visualize a full interferometric sequence for measuring a magnetic field (implying the evolution under exp[-i*t*dH*Sz] for an interrogation time t).
- Calculate the (optimal) squeezing parameter as a function of time. Evaluate the maximal reachable squeezing and the time at which it is reached. How do these scale with N?
- Calculate the (optimal) quantum Fisher information and the half-chain entanglement entropy of the maximally squeezed state and study their N-dependence.
- Simulate a ramp of the magnetic field form a large value to zero. The initial state is the infinite-field ground state of all spins pointing along x. If the ramp is adiabatic, the system will remain in the ground state, thus reaching the cat state (superposition between all up and all down). Try different ramp profiles and optimize the ramp to reach the maximum quantum Fischer information.

5) *One-dimensional quantum spin models with DMRG*

The density matrix normalization group (DMRG) is the most powerful numerical technique for describing one dimensional quantum many-body systems. It works as an optimization algorithm for matrix product states (MPS) and, as such, can access systems much larger than usually possible with alternative approaches. In this project, you will implement a simple version of this method suited for spin systems and use it to study the Heisenberg model and the Haldane phase.

Literature:

Roman Orus, Annals of Physics 349 (2014) 117-158

U. Schollwöck, Annals of Physics,Volume 326, Issue 1, January 2011, Pages 96-192

T. Kennedy and H. Tasaki, Commun.Math. Phys. (1992) 147: 431

I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, Phys. Rev. Lett. 59, 799

Methods: Variational methods, matrix product states, DMRG

Steps:

- Implement the basic infrastructure for working with MPSs and test it with the exact MPS description of the AKLT model with open boundary conditions.
- Use the DMRG procedure for optimizing and truncating an MPS to find the AKLT ground state and check that it agrees with the analytical result.
- Apply your DMRG to the Heisenberg model to find the ground state for different spins (i.e. local dimension, e.g. spin 1/2,1,3/2…) and study the convergence with the bond dimension.
- It you really want to have fun: Map the phase diagram of model spin 1 Hamiltonians to look for ground states corresponding to the Haldane phase.

6) *Dynamics of a driven dissipative system*

Driven dissipative systems can show bistability, where the state spontaneously changes from a dark, non-emitting state to a strongly emitting one. Such a phenomenon is encountered for an ensemble of atoms driven to a Rydberg excited state. This was studied theoretically by Lee et al.

and later realized experimentally by the group of Charles Adams. The goals of this project is to reproduce some of the results of the theory paper and possibly to extend these simulations to a more realistic scenario with finite range interactions.

Literature: T. Lee et al. PRL 108, 023602 (2012), C. Carr et al. Phys. Rev. Lett. 111, 113901 (2013), N. de Melo et al. Phys. Rev. A 93, 063863 (2016)
Methods: Mean field, quantum jump, unraveling of the master equation
Steps:

- Solve the mean field equations. I.e. solve the Bloch equations including interactions as a mean field shift.
- Solve the Master equation for two interacting two-level atoms. Solve the same problem using the quantum jump approach and compare the results and convergence with respect to the number of trajectories.
- Apply the quantum jump method to arrays of more atoms with all-to-all interactions as in the Lee paper. Try to reproduce the bistable behavior seen in Fig. 4 of the Lee paper.
- Go beyond what was done in the Lee paper by trying different kinds of interactions. Is the bistability robust with respect to changes in the interaction range?