- **MS13: Modeling and numerics of (relativistic) Schrödinger equations**

    - Timon Gutleb, Oxford, UK
    - Norbert Mauser, MMM c/o Univ. Wien, Austria
    - Hans Peter Stimming, MMM c/o Univ. Wien, Austria

3+3+2 speakers

Monday morning 11h-12h30 : Block A (3 speakers) :
Chair : Hans Peter Stimming

A1) Jakob **Möller** (Univ. Vienna), jakob.moeller@univie.ac.at

Title: The semiclassical limit of the Pauli - Poiswell system

Abstract:
The self-consistent Pauli equation or Pauli-Poiswell equation for 2-spinors is a semi-relativistic approximation of the Dirac-Maxwell equation for 4-spinors.
It consists of a vector valued magnetic Schrödinger equation with an extra term coupling spin and magnetic field via the Pauli matrices and of 1+3 Poisson type equations as the "magnetostatic approximation" of the Maxwell equations. The Pauli-Poiswell equation is a consistent O(1/c) model, with c being the speed of light, that keeps the relativistic effects magnetism and spin, which are both absent in the non-relativistic Schrödinger-Poisson equation. The semiclassical limit of the Schrödinger-Poisson equation has been established by Markowich-Mauser and Lions-Paul using Wigner methods. We extend this result to the Pauli-Poiswell equation in a density matrix formulation under an additional assumption on the statistical weights of the density matrix.

A2) Timon Salar **Gutleb** (Oxford) timon.gutleb@gmail.com

Title: Splitting methods for the Pauli equation and the Pauli-Poiswell system

Abstract:
The Pauli equation is obtained as the semi-relativistic approximation of the Dirac equation or as an extension of the scalar magnetic Schrödinger equation to a 2 spinor NLS. In this talk we discuss numerical splitting methods to the linear Pauli equation and sketch proofs of stability and convergence. We also discuss recent advances and challenges which appear when trying to extend these methods to the self-consistent Pauli-Poiswell system which couples the Pauli equation to a semi-classical variation of Maxwell's equations.

A3) Peter Allmer (Univ. Vienna) peter.allmer.94@gmail.com

Title: A time splitting spectral method for the Klein-Gordon Maxwell system

Abstract:
In this talk we consider numerics for the time dependent Klein-Gordon Maxwell system, which describes a charged spin-0 particle in flat Minkowski space-time with a self consistent coupling to the electromagnetic force. We introduce an operator splitting scheme in time using spectral methods in space coupled to a spectral Crank-Nicolsen scheme to solve the Klein-Gordon and Maxwell equations respectively in each time step.
The goal of this talk is to present of our method and the numerical analysis of it. Thereby the method achieves a second order convergence rate in time and also conserves the total electric charge of the system.

Monday 16h30-18h00 : Block B (3 speakers) :

Chair : Norbert Mauser

B1) Stéphane **Descombes** (Univ. Nice) Stephane.DESCOMBES@univ-cotedazur.fr

Title : Building energy preserving methods for nonlinear Schrödinger equations

Abstract:

The numerical integration in time of nonlinear Schrödinger equations using different methods preserving the energy or a discrete analog of it is an old problem. The Crank-Nicolson method is a well known method of order 2 but is fully implicit and one may prefer a linearly implicit method like a relaxation method for the cubic nonlinear Schrödinger equation. In this talk we focus on difficulties to construct such methods and to give a rigorous proof of convergence with optimal order. Numerical simulations for different physical models will illustrate the efficiency of these methods.

B1) Pranav **Singh** (University of Bath), ps2106@bath.ac.uk

Title: Convergence of Magnus based methods for Schrödinger equations

Abstract:
Magnus expansion based methods are an efficient class of integrators for solving Schrödinger equations that feature time dependent potentials such as lasers. These methods have been found to be highly effective in computational quantum chemistry since the pioneering work of Tal Ezer, Kosloff and Cerjan in the early 90s. The convergence of the Magnus expansion, however, is understood only for ODEs and traditional analysis suggests a much poorer performance of these methods than observed experimentally. It was not till the work of Hochbruck and Lubich in 2003 that a rigorous analysis justifying the application to PDEs with unbounded operators, such as the Schrödinger equation, was presented.
In this talk I will present the extension of this analysis to the semiclassical regime, where the highly oscillatory solution conventionally suggests large errors and a requirement for very small time steps.

B2) Mark **Tennyson** (University of Bath), mt767@bath.ac.uk

Title: Rational Krylov Methods for Schrödinger Equations

Abstract:
Discretised linear differential equations require a matrix exponential solution. In general the equation matrix is large, making direct computation unfeasible. However, the matrix is often sparse or structured, so Polynomial and Rational Krylov methods are effective. When the norm is large, Polynomial Krylov requires small steps. Rational Krylov aims to remove the small step restriction. In this talk I describe how pole selection affects the performance of these methods, and techniques for identifying optimal poles.

<u>Tuesday morning 11h00 - 12h30 : Block C (2 speakers) :</u>

<u>Chair : Timon Gutleb</u>

C1) Norbert J **Mauser** (MMM Univ. Wien) mauser@courant.nyu.edu

Title: Absorbing boundary conditions for nonlinear Schrödinger equations

Abstract:

In this talk we discuss several options to impose boundary conditions for time dependent Schrödinger equations on finite space domains. Periodic boundary conditions (p.b.c.) allow for very efficient numerical methods based on FFT. We present Absorbing Boundary Layer techniques where p.b.c. are combined with absorbing boundary conditions realized by adding a complex ("optical") potential in a layer next to the limit of the domain, thus avoiding the numerical pollution appearing after some time from the p.b.c.

C2) Speaker: Hans Peter **Stimming** (MMM c/o Univ. Wien) hans.peter.stimming@univie.ac.at

Title: Numerical models for Quasi-1 d Bose Condensates: Generalized Hydrodynamics

Abstract:

Generalized Hydrodynamics is a recent mathematical model for quantum many body problems related to cold quantum gases. Hydrodynamic theory yields in a kinetic equation with "rapidities" as kinetic variable. This model is an alternative to Gross Pitaevskii and Sine-Gordon equations. The model is extended by a component representing transverse excited states that occur in a quasi-1D setting accounted for by a Boltzmann type collision term. We discuss the theory and compare to results in a Quantum Newton's cradle experiment.