Modern Numerical Methods

for

Quantum Mechanics II

Book
of
Abstracts

University of Gdańsk
&
Polish Academy of Sciences

27–29 June, 2018
Gdańsk, Poland

Wednesday, 27th of June, 2018

Semiclassical computational methods for quantum dynamics with band crossing and uncertainty

9:00 – 9:45

Shi Jin

University of Wisconsin–Madison, USA

Shanghai Jiao Tong University, China

Abstract: Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, chemical reaction etc. In this talk, we will discuss some recent works in developing semiclassical methods for band-crossing in surface hopping. For such systems we will also introduce an "asymptotic-preserving" method that is accurate uniformly for all wave numbers, including the problem with random uncertain band gaps.

Low regularity Fourier integrators for nonlinear Schrödinger equations

9:45 – 10:30

Alexander Ostermann

University of Innsbruck, Austria

Abstract: Nonlinear Schrödinger equations are usually solved by pseudo-spectral methods, where the time integration is performed by splitting schemes or exponential integrators. Notwithstanding the benefits of this approach, its successful application requires additional regularity of the solution. For instance, second-order Strang splitting requires four additional derivatives for the solution of the cubic nonlinear Schrödinger equation. In this talk, we introduce as an alternative low regularity Fourier integrators. For such methods, first-order convergence only requires the boundedness of one additional derivative of the solution, and second-order convergence the boundedness of two derivatives. This allows us to impose lower regularity assumptions on the data. Numerical experiments underline the favourable error behaviour of the newly introduced integrators for low regularity solutions compared to classical splitting and exponential integration schemes.

Joint work with: Marvin Knöller and Katharina Schratz (KIT, Karlsruhe, Germany)

On Quantum Perturbation Theory and Time Averaging

Fernando Casas
Departament de Matemàtiques and IMAC, Universitat Jaume I, Castellón, Spain

11:00 – 11:30

Abstract: The time-dependent quantum perturbation theory developed by Born, Heisenberg and Jordan in 1926 is reformulated in modern language. We show that it not only reproduces the standard theory found in textbooks on quantum mechanics, but also leads to more accurate approximations if time averaging techniques are used. The theory can be rendered unitary even if the expansion is truncated by using a transformation previously suggested by Heisenberg. We illustrate the main features of the procedure on a simple example which clearly shows its advantages in comparison with the standard formalism.

Sharp local error estimation for time-reversible one-step schemes

Winfried Auzinger
Institute of Analysis and Scientific Computing, Technische Universität Wien, Austria

11:30 – 12:00

Abstract: We consider one-step schemes applied to (linear or nonlinear) evolution equations

$$\partial_t u(t) = H(u(t)), \quad u(0) = u_0.$$

Let $\mathcal{E}(t, u_0)$ denote the exact flow and $\mathcal{S}(t, u_0)$ the discrete flow representing a given one-step scheme with stepsize t. For practical estimation of the local error as well as for error analysis, the notion of the defect of the numerical solution,

$$\mathcal{D}(t, u_0) = \partial_t \mathcal{S}(t, u_0) - H(\mathcal{S}(t, u_0)),$$

is a useful quantity, since the local error $\mathcal{S}(t, u_0) - \mathcal{E}(t, u_0)$ can be represented as an integral involving the defect. But there are alternative ways to define the defect. Especially for self-adjoint (time-reversible) schemes, we consider a 'symmetrized' version of the defect which leads to asymptotically sharper a posteriori estimates for the local error and which is also useful for theoretical purposes.

We present the underlying ideas and results and give some numerical examples, including the case of time-dependent vector fields $H = H(u, t)$.

Joint work with: Harald Hofstätter, Othmar Koch, Fakultät für Mathematik, Universität Wien, Austria

Non-relativistic limit of the nonlinear Dirac equation and its numerical methods

12:15 – 12:45

Yongyong Cai

Beijing Computational Science Research Center, China

Abstract: We consider the (nonlinear) Dirac equation in the non-relativistic limit regime, involving a small parameter inversely proportional to the speed of light. The (nonlinear) Dirac equation converges to the (nonlinear) Schrödinger equation in the non-relativistic limit. By a careful analysis, we obtain a semi-relativistic limit of the nonlinear Dirac equation, which enables a design of uniformly accurate multi-scale numerical method. The major difficulty of the problem is that the solution has a rapid oscillation in time depending on the small parameter.

Modeling, analysis and simulation for degenerate dipolar quantum gas

12:45 – 13:15

Weizhu Bao

Department of Mathematics, National University of Singapore

Abstract: In this talk, I will present our recent work on mathematical models, asymptotic analysis and numerical simulation for degenerate dipolar quantum gas. As preparatory steps, I begin with the three-dimensional Gross–Pitaevskii equation with a long-range dipolar interaction potential which is used to model the degenerate dipolar quantum gas and reformulate it as a Gross–Pitaevskii–Poisson type system by decoupling the two-body dipolar interaction potential which is highly singular into short-range (or local) and long-range interactions (or repulsive and attractive interactions). Based on this new mathematical formulation, we prove rigorously existence and uniqueness as well as nonexistence of the ground states, and discuss the existence of global weak solution and finite time blowup of the dynamics in different parameter regimes of dipolar quantum gas. In addition, a backward Euler sine pseudospectral method is presented for computing the ground states and a time-splitting sine pseudospectral method is proposed for computing the dynamics of dipolar BECs. Due to the adoption of new mathematical formulation, our new numerical methods avoid evaluating integrals with high singularity and thus they are more efficient and accurate than those numerical methods currently used in the literatures for solving the problem. In addition, new mathematical formulations in two-dimensions and one dimension for dipolar quantum gas are obtained when the external trapping potential is highly confined in one or two directions. Numerical results are presented to confirm our analytical results and demonstrate the efficiency and accuracy of our numerical methods. Some interesting physical phenomena are discussed too.

Accelerated gradient methods for computing the stationary states of Gross–Pitaevskii Equations

14:30 – 15:00

Xavier Antoine
University of Nancy, France

Abstract: In this talk, I will introduce the application of preconditioned nonlinear conjugate gradient methods for computing the ground states of Gross–Pitaevski equations. After explaining the method, numerical examples will be presented.

Joint work with: Antoine Levitt (Inria, France), Qingling Tang (Sichuan University) and Yong Zhang (Nanjing University)

Computing ground states of spin 2 Bose–Einstein condensates by the normalized gradient flow

15:00 – 15:30

Qinglin Tang
Sichuan University, China

Abstract: In this talk, an efficient and accurate numerical method will be proposed to compute the ground state of spin-2 Bose–Einstein condensates (BECs) by using the normalized gradient flow (NGF) or imaginary time method (ITM). The key idea is twofold. One is to find the five projection or normalization conditions that are used in the projection step of NGF/ITM, while the other one is to find a good initial data for the NGF/ITM. Based on the relations between chemical potentials and the two physical constraints given by the conservation of the total mass and magnetization, these five projection or normalization conditions can be completely and uniquely solved out. This allows one to successfully extend the NGF/ITM to compute the ground state of spin-2 BECs. Additionally, the structures and properties of the ground states in a uniform system are analysed so as to construct efficient initial data for NGF/ITM. Numerical results will be reported to show the efficiency of our method and to demonstrate some interesting physical phenomena.

Elevator Pitch, 16:00–17:00

To be announced

Chunmei Su
University of Innsbruck, Austria

16:00 – 16:05

Abstract: TBA

A computable strict upper bound for Krylov subspace approximations to the exponential of skew-Hermitian matrices

Tobias Jawecki
Vienna University of Technology, Austria

16:05 – 16:10

Abstract: We present a defect-based a posteriori error estimate for Krylov subspace approximations to the exponential of skew-Hermitian matrices. This error estimate constitutes a computable strict upper norm bound on the error and is asymptotically correct. For the proof we use the representation of matrix functions via Hermite interpolation on the spectrum and properties of divided differences. The matrix exponential function itself can be understood as a time propagation with restarts. In practice, we are interested in finding time steps for which the error of the Krylov subspace approximation is smaller than a given tolerance. Finding correct time steps is a simple task with our asymptotic error estimate. Our results obtained in this way are comparable or better than those obtained by existing approaches.

Joint work with: Winfried Auzinger (Vienna University of Technology, Austria)

On the zero-dispersion limit for three coupled long wave-short wave interaction equations

Gulcin M. Muslu
Istanbul Technical University, Turkey

16:10 – 16:15

Abstract: In this talk, we are interested in the mathematical and numerical analysis of zero-dispersion limit for the three coupled long wave-short wave interaction (LSI) equations. We consider the zero- dispersion limit of the LSI equations by using WKB analysis for initial data with Sobolev regularity, before the shocks appear in the limit system. For the smooth solution, the limit system is given by the

two fluids equations. The split-step Fourier method is also employed to justify the numerical simulation of the zero-dispersion limit. The author has been supported by Research Fund of the Istanbul Technical University. Project Number:TGA-2017-40655

Joint work with: Chi-Kun Lin (Xian Jiaotong Liverpool University, Jiangsu, China)

Splitting methods for the time-dependent Klein–Gordon equation

Nikita Kopylov

Polytechnic University of Valencia, Spain

16:15 – 16:20

Abstract: We consider the numerical integration of the non-stationary Klein–Gordon equation with position- and time-dependent mass. The structure of this equation allows us to use unconventional commutators that circumvent this order barrier and at reduced number of stages we build methods up to order six with positive coefficients and small errors leading to efficient symplectic integrators.

Some Remarks on Stability of Differential Equations on Time Scales

Agata Gołaszewska

Gdańsk University of Technology, Poland

16:20 – 16:25

Abstract: We consider the stability and asymptotic stability of the problem

$$x^{\Delta}(t) = f(t, x(t)), \quad x(0) = 0,$$

satisfying the condition

$$2x^{\top} f(t,x) + \mu(t) f(t,x)^{\top} f(t,x) \leq 0,$$

where μ is gridness of the time scale T.

Our main aim is to investigate if conditions for stability of solutions are the same for differential equations on time scales as in a classical case.

Additionally in our considerations the case of one linear equation

$$x^{\Delta}(t) = -g(t)x(t)$$

is discussed more precisely.

Joint work with: Antoni Augustynowicz (Department of Nonlinear Analysis and Statistics, Gdańsk University of Technology, Poland)

How to create "true" potentials needed for dynamics of diatomic molecules

16:25 – 16:30

Patryk Jasik
Gdańsk University of Technology, Poland

Abstract: The new and modern laser techniques allow investigating molecular systems with spectacular precision. The spectra analysis, which is essential in building up the potential energy curves or surfaces, is often very tedious and sometimes impossible due to its complexity. In such tough situations, very high accuracy calculations are needed. Combining experimental results and computational methods one is able to create "true" potentials, which are necessary to perform "real" dynamics of molecular systems. As an example, the deperturbation analysis of the $b(1)^1\pi - c(2)^3\sigma^+$ complex in the KCs molecule is presented. This molecule is an ideal candidate for obtaining a dense gas of ultracold polar particles suitable for the observation of strong anisotropy of their mutual interaction. Thus, it will be possible to investigate the ultracold dipolar many-body physics and novel quantum phases resulting from their anisotropic interactions when they are exposed to an appropriate external electric field.

Ab–initio model potential embeddings in electronic structure calculations of lanthanide doped ionic crystals

16:30 – 16:35

Marek Krośnicki
University of Gdańsk, Poland

Abstract: See abstract in talk below

Ab–initio model potential embeddings in electronic structure calculations of lanthanide doped ionic crystals

16:35 – 16:40

Emilia Przybysz
University of Gdańsk, Poland

Abstract: Photoluminescent properties of activated ionic crystal depend usually on the electronic structure of local defects. This means that an active center formed of dopant ion and its nearest neighbours atoms can be modelled as a cluster under influence of the host lattice [1]. Therefore electronic correlation in the cluster can be calculated using multi reference methods of quantum chemistry whereas the rest of the chunk of solid state crystal can be described on lower level of the theory.

The partitioning of the crystal into weakly interacting systems is based on the Group–Function Theory (GFT) proposed by McWeeny [2]. Weak interaction means that electron correlation between groups should be negligible and the number of electrons in each group is constant. Finally, cluster is embedded into crystal lattice by *Ab–Initio* Model Potentials (AIMP) [1], which are obtained within Self Consistent Embedded Ions calculations (SCEI).

We present results of the electronics structure calculations of Y_2O_2S:Ce^{3+} and comparison of the simulated absorption and emission spectra with the experimental data [3]. This work is a part of larger project in which we investigate luminescent properties of lanthanide activated oxysulfides (M_2O_2S, where M stands for Y, La, Lu and Gd respectively).

[1] *The ab-initio model potential method: a common strategy for effective core potential and embedded cluster calculations*, L. Seijo, Z. Barandiaran, in Computational Chemistry: Reviews of Current Trends, vol. 4, ed. by J. Leszczynski (World Scientific, Singapur, 1999), p.55-152

[2] *Methods of Molecular Quantum Mechanics*, R. McWeeny, Academic Press, 1992

[3] *Red luminescence of Ce^{3+} due to the large stokes shifts in Y_2O_2S and Lu_2O_2S*, S. Yokono, T. Abe, T. Hoshina, Journal of Luminescence 24/25 (1981) 309-312.

Joint work with: Andrzej Kedziorski (Institute of Physics, Nicolaus Copernicus University, Toruń, Poland) and Marek Krośnicki (Institute of Theoretical Physics and Astrophysics, University of Gdańsk)

Using sparse grid and tensor methods to compute vibrational spectra of molecules

16:40 – 16:45

Tucker Carrington

Chemistry Department, Queen's University, Kingston, Canada

Abstract: I shall present a new collocation method for solving the Schroedinger equation. Collocation has several important advan- tages over the Galerkin method. Most importantly, it obviates the need for quadrature. The kinetic energy matrix-vector product is evaluated by transforming a vector labelled with (nondirect product) grid indices to a vector labelled by (nondi- rect product) basis indices. Both the transformation and application of the kinetic energy operator scale favourably. Some ideas of general interest: 1) a general scheme for pruning bases and grids when using sparse-grid methods; 2) nested func- tions and grids in which the difference between the number of points in level i+1 and level i is very small

(e.g. one); 3) collocation without a mass matrix; 4) collocation with spectral Lagrange-type functions; 5) hierarchical functions built from non-polynomial general bases. I shall present a rank-reduction tensor method for solving the vibrational Schroedinger equation. The memory cost scales linearly with the number of atoms in the molecule. This method makes possible calculations for molecules with a dozen atoms on a desktop computer, but only if the potential is a sum of products. It uses a direct product basis but: 1) it is not necessary to store a direct-product-basis matrix representation of the Hamiltonian matrix; 2) it is not necessary to store vectors whose length is equal to the size of the direct-product basis. This is accomplished by using sum-of-product (SOP) basis functions stored in a canonical polyadic tensor format and generated by evaluating matrix-vector products. The number of terms in the SOP basis functions is minimized by optimising the factors in the terms of the SOP.t

Thursday, 28th of June, 2018

Using sparse grid and tensor methods to compute vibrational spectra of molecules

9:00 – 9:45

Tucker Carrington

Chemistry Department, Queen's University, Kingston, Canada

Abstract: I shall present a new collocation method for solving the Schroedinger equation. Collocation has several important advan- tages over the Galerkin method. Most importantly, it obviates the need for quadrature. The kinetic energy matrix-vector product is evaluated by transforming a vector labelled with (nondirect product) grid indices to a vector labelled by (nondi- rect product) basis indices. Both the transformation and application of the kinetic energy operator scale favourably. Some ideas of general interest: 1) a general scheme for pruning bases and grids when using sparse-grid methods; 2) nested func- tions and grids in which the difference between the number of points in level i+1 and level i is very small (e.g. one); 3) collocation without a mass matrix; 4) collocation with spectral Lagrange-type functions; 5) hierarchical functions built from non-polynomial general bases. I shall present a rank-reduction tensor method for solving the vibrational Schroedinger equation. The memory cost scales linearly with the number of atoms in the molecule. This method makes possible calculations for molecules with a dozen atoms on a desktop computer, but only if the potential is a sum of products. It uses a direct product basis but: 1) it is not necessary to store a direct-product-basis matrix representation of the Hamiltonian matrix; 2) it is not necessary to store vectors whose length is equal to the size of the direct-product basis. This is accomplished by using sum-of-product (SOP) basis functions stored in a canonical polyadic tensor format and generated by evaluating matrix-vector products. The number of terms in the SOP basis functions is minimized by optimising the factors in the terms of the SOP.t

Numerical methods that conserve or dissipate energy on Riemannian manifolds.

9:45 – 10:30

Brynjulf Owren

Norwegian University for Science and Technology (NTNU), Trondheim, Norway

Abstract: Differential equations which conserve one or more first integrals, such as the energy, constitute an important class of dynamical systems. An equally important class consists of problems which dissipate energy at some rate. When we design numerical approximation schemes for problems in either of these classes,

we often which to preserve the conservation or dissipation property in the numerical scheme. A remarkably effective technique for designing such schemes has been the discrete gradients, a construction that mimics the continuous gradient and some of its most important properties. We shall give begin by giving a brief review of discrete gradient methods in linear spaces. Then we shall introduce a framework set on Riemannian manifolds, by deriving energy or dissipation preserving schemes in an intrinsic manner which does not depend on any kind of embedding of the manifold in a larger Euclidean space. We derive convergence estimates for the global error by using a bound for the Levi–Civita connection in its associated operator norm. The methods we obtain exhibit excellent behaviour for certain problems in manifold valued image analysis, such as diffusion tensor imaging. In particular, we shall show some numerical results applied to a case of Total Variation denoising of such images. As an example of an energy preserving integrator, we shall also consider coupled spin systems on two-spheres.

Conservation of energy for various systems of conservation laws. Around Onsager's conjecture.

11:00 – 11:30

Agnieszka Świerczewska-Gwiazda
University of Warsaw, Poland

Abstract: A common feature of systems of conservation laws of continuum physics is that they are endowed with natural companion laws which are in such case most often related to the second law of thermodynamics. This observation easily generalizes to any symmetrizable system of conservation laws. They are endowed with nontrivial companion conservation laws, which are immediately satisfied by classical solutions. Not surprisingly, weak solutions may fail to satisfy companion laws, which are then often relaxed from equality to inequality and overtake a role of a physical admissibility condition for weak solutions. We want to discuss what is a critical regularity of weak solutions to a general system of conservation laws to satisfy an associated companion law as an equality. An archetypal example of such result was derived for the incompressible Euler system by Constantin et al. ([1]) in the context of the seminal Onsager's conjecture. This general result can serve as a simple criterion to numerous systems of mathematical physics to prescribe the regularity of solutions needed for an appropriate companion law to be satisfied. We will also discuss the Euler-Korteweg system. and show that the result applies to the system of Quantum Hydrodynamics.

[1] P. Constantin, W. E, and E. S. Titi. Onsager's conjecture on the energy conservation for solutions of Euler's equation. *Comm. Math. Phys.*, 165(1):207–209, 1994.

[2] Feireisl, Eduard; Gwiazda, Piotr; Świerczewska-Gwiazda, Agnieszka; Wiedemann, Emil; Regularity and Energy Conservation for the Compressible Euler Equations, *Arch. Ration. Mech. Anal.* 223 (2017), no. 3, 1375–1395.

[3] P. Gwiazda, M. Michálek, A. Świerczewska-Gwiazda. A note on weak solutions of conservation laws and energy/entropy conservation, *Arch. Ration. Mech. Anal.*, 229 (2018) 1223?1238.

Energy preserving methods for nonlinear Schrödinger equations

Christophe Besse
University of Tolouse, France

11:30 – 12:00

Abstract: The Schrd̈inger equation is at heart of Bose–Einstein Condensates with the celebrated Gross–Pitaevskii equation. Such dispersive partial differential equations have many preserved quantities such as the mass, the energy or the momentum. It is therefore crucial to build numerical schemes that preserve these invariants. We will present in this talk various way to take this property into account and the pros and cons of the various methods.

Dynamics of the rotational predissociation of LiH

Józef E. Sienkiewicz
Gdańsk University of Technology, Poland

12:15 – 12:45

Abstract: We have obtained reliable adiabatic Born–Oppenheimer potential energy curves for the LiH dimer. In our computational approach, two valence electrons are taken explicitly into account for building determinants for the multiconguration wave function. The atomic core of Li are described by energy-consistent semilocal pseudopotentials and core polarization potentials. Also, we have described in details dynamics of the rotational predissociation process in LiH and corrected experimentalist's predictions.

Rovibrational predissociation dynamics: spectrum and population decay of selected vibrational levels of the KLi molecule

12:45 – 13:15

Jan Kozicki
Gdańsk University of Technology, Poland

Abstract: A numerical method for solving time dependent Schrödinger equation (TDSE) was implemented into the author's computational framework[1]. The Kosloff method based on Chebyshev polynomials was used, because although computationally intensive, it allows for obtaining results with an unprecedented accuracy. This numerical method was tested against a hydrogen atom with known analytical solutions in one, two and three dimensions. Next, the method was applied for a molecular dynamics problem of photodissociation of the KLi molecule. An initial wavepacket was put into the 2 (second singlet pi) potential of the KLi molecule and its time evolution was calculated. The original part of this work, which hasn't been done before to the author's knowledge, is that the initial wavepacket is chosen as a single eigenfunction obtained by a semiclasical method, which allows for calculation of population decay for the selected rovibrational level.

[1] J. Kozicki and F. Donze, A new open-source software developed for numerical simulations using discrete modeling methods, Computer Methods in Applied Mechanics and Engineering, 26, 7, 2009

Convergence analysis of commutator-free quasi-Magnus exponential integrators for non-autonomous linear Schrödinger equations

14:30 – 15:00

Mechthild Thalhammer
University of Innsbruck, Austria

Abstract: The class of commutator-free quasi-Magnus (CFQM) exponential integrators leads to favourable time integration methods for non-autonomous linear evolution equations. They are formed by products of exponentials involving linear combinations of the defining operator evaluated at certain times. In comparison with other classes of time integration methods such as Magnus integrators, an inherent advantage of CFQM exponential integrators is that structural properties of the operator are well-preserved by the arising linear combinations. A fundamental objective of our work is to provide a rigorous stability and local error analysis of high-order CFQM exponential integrators. In this talk, I will present an appropriate analytical framework for evolution equations of Schrödinger type and main tools for the derivation of local error representations in the presence of unbounded Hamilton operators.

Joint work with: Sergio Blanes, Fernando Casas, Cesáreo González

Exponential propagators for the Schrödinger equation with a time-dependent potential

15:00 – 15:30

Sergio Blanes

Polytechnic University of Valencia, Spain

Abstract: We consider the numerical integration of the Schrödinger equation with a time-dependent Hamiltonian given as the sum of the kinetic energy and a time-dependent potential. Commutator-free (CF) propagators are exponential propagators that have shown to be highly efficient for general time-dependent Hamiltonians. We propose new CF propagators that are tailored for Hamiltonians of said structure, showing a considerably improved performance. We obtain new fourth- and sixth-order CF propagators as well as a novel sixth-order propagator that incorporates a double commutator that only depends on coordinates, so this term can be considered as cost-free. The algorithms require the computation of the action of exponentials on a vector similarly to the well known exponential midpoint propagator, and this is carried out using the Lanczos method. We illustrate the performance of the new methods on several numerical examples.

Joint work with: Philipp Bader and Nikita Kopylov

The Schrödinger method for the Vlasov-Poisson equation in cosmology

16:00 – 16:30

Norbert J. Mauser

Wolfgang Pauli Institute c/o Fak. Math. Univ. Wien, Austria

Abstract: In cosmology, dark matter is modelled by Vlasov–Poisson equations with attractive (gravitation) interaction. In order to reduce the numerical effort from 6-dimensional "phase space" to 3-dimensional "physical space", the "Schrödinger method" was introduced, which is the "inverse semiclassical limit".

The "Quantum Vlasov" or "Wigner equation" is a "phase space" presentation of quantum mechanics that is close to the classical Vlasov equation, but where the "distribution function" $w(x, v, t)$ will in general have also negative values.

We discuss the relation Schrödinger–Wigner–Husimi–Vlasov in the "semiclassical" asymptotics of small Plancks constant. Also, we discuss the numerical task of highly adaptive methods for the solution of Schrödinger–Poisson, including recent progress on Gaussian sum – NUFFT solvers for nonlocal potentials.

Schrödinger equation with time-varying potential: many problems, many approaches.

16:30 – 17:00

Pranav Singh
University of Oxford, U.K.

Abstract: The Schrödinger equation with a time-varying potential arises in a wide range of applications in theoretical chemistry, quantum physics and quantum computing. In this talk I will discuss a variety of Magnus expansion based schemes that have been found to be highly effective for numerically solving these equations.

Recent developments in the field focus on approximation of the exponential of the Magnus expansion via exponential splittings including some asymptotic splittings and commutator-free splittings that are designed specifically for this task.

For the case of laser-matter interaction, in particular, I will present a very recently developed methodology which allows us, with little to no additional cost, to extend any fourth-order scheme for Schrödinger equation with time-indepedent potential to a fourth-order method for Schrdinger equation with laser potential.

Joint work with: Philipp Bader, Arieh Iserles and Karolina Kropielnicka

Friday, 29th of June, 2018

Quantum Dynamics Methods: From Grids to Gaussian Wavepackets.

Graham A. Worth
Dept. of Chemistry, University College London, U.K.

9:00 – 9:45

Abstract: Solving the time-dependent Schrödinger Equation has a natural exponential scaling with system size. This makes it hard to achieve complete (numerical) quantum mechanical results for molecules with more than a few atoms without resorting to approximations. The exponential scaling manifests itself in 2 ways. Firstly, in the computer resources required for the propagation of the nuclear wavepacket. Secondly, in the space to be covered when calculating the potential energy surfaces. These problems are exacerbated for systems involving excited states where couplings between potential surfaces are required and high accuracy is sometimes necessary for even qualitatively correct results.

The multi-configurational time-dependent Hartree (MCTDH) algorithm has gone a long way in solving the first problem [1]. In particular the multi-layer form (ML-MCTDH) is able to propagate multi-dimensional wavepackets with 100s of degrees of freedom. These are effectively efficient contraction schemes for the wavefunction represented in a grid basis-set. MCTDH does, however, require global potential surfaces which can restrict it to using model Hamiltonians rather than general, flexible molecular potentials. [2]. An approach to break both the exponential scaling and allow the use of general potentials is the variational multi-configurational Gaussian (vMCG) method [3]. This uses a set of Gaussian wavepackets (GWP) as a time-dependent basis, but unlike conventional GWP methods, the GWPs follow variational rather than classical trajectories and retains the full quantum description of the system. It is also suited for direct dynamics simulations, calculating the potential on-the-fly using quantum chemistry programs and so opens up the use of flexible potentials [4]. The present state-of-the art of this method will be presented, showing its promise and highlighting the problems still to be solved.

References

[1] M. Beck, A. Jäckle, G. Worth and H.-D. Meyer, Phys. Rep. 324, 1 (2000).

[2] G. A. Worth, H.–D. Meyer, H. Kppel, L. S. Cederbaum and I. Burghardt, Int. Rev. Phys. Chem. 27, 569 (2008).

[3] G. W. Richings, I. Polyak, K. E. Spinlove, G. A. Worth, I. Burghardt and B. Lasorne, Int. Rev. Phys. Chem. 34, 269 (2015).

[4] G. W. Richings and G. A. Worth, Chem. Phys. Lett. 683, 606 (2017).

What happens if the potential is complex-valued?

Caroline Lasser
Technical University of Münich, Germany

9:45 – 10:30

Abstract: Schrödinger equations with complex-valued potentials arise in non-Hermitian quantum mechanics. The non-self-adjoint operators define bounded evolutions operators, but the lack of unitarity results in a couple of surprising new dynamical effects, that will be discussed in the presentation.

Joint work with: Roman Schubert and Stephanie Troppmann

Compact splitting methods for Schrdinger equation and their consequences

Karolina Kropielnicka
University of Gdańsk, Poland

11:00 – 11:30

Abstract: In this presentation I am going explain the philosophy behind compact splitting methods for Schrödinger equation, their effectiveness, power, derivation and possible extensions. As will be presented, compact splitting methods together with the Gröbner basis proves that there exists no compact splitting method of order six with only positive real coefficients. Moreover the derivation of order conditions for eight order method, the benefits of such an eight order splitting and the obstacles encountered while working on this problem will be presented.

Measure-valued – strong uniqueness

Piotr Gwiazda
University of Warsaw, Poland

11:30 – 12:00

Abstract: In the last years measure-valued solutions started to be considered as a relevant notion of solutions if they satisfy the so-called measure-valued – strong uniqueness principle. This means that they coincide with a strong solution emanating from the same initial data if this strong solution exists. Following result of Yann Brenier, Camillo De Lellis and Laszlo Szekelyhidi Jr. for incompresible Euler Equation, this property has been examined for many systems of mathematical physics, including incompressible and compressible Euler system, compressible Navier-Stokes system, polyconvex elastodynamics et al. One observes also some

results concerning general hyperbolic systems. Our goal is to provide a unified framework for general systems, that would cover the most interesting cases of systems. Additionaly following result of Eduard Feireisl,Piotr Gwiazda, Agnieszka Swierczewska-Gwiazda and Emil Wiedemann for compresible Euler (and Navier-Stokes) system we introduce a new concept of dissipative measure valued solution to general hyperbolic system.

[1] Brenier, Y., De Lellis, C., Szkelyhidi Jr., L., Weak-strong uniqueness for measure-valued solutions. Comm. Math. Phys., 305(2), 351-361 (2011).

[2] S. Demoulini, D. M. A Stuart, and A. Tzavaras, Weak-strong uniqueness of dissipative measure-valued solutions for polyconvex elastodynamics, Arch. Ration. Mech. Anal., 205 (2012), no. 3, 927-961.

[3] E. Feireisl, P. Gwiazda, A. Świerczewska-Gwiazda and Emil Wiedemann, Dissipative measure-valued solutions to the compressible Navier-Stokes system, Calc. Var. Partial Differential Equations, 55 (2016), no. 6, 55-141.

[4] P. Gwiazda, A. Świerczewska-Gwiazda and E. Wiedemann, Weak-Strong Uniqueness for Measure-Valued Solutions of Some Compressible Fluid Models, Nonlinearity 28 (2015), no. 11, 3873-3890.

[5] T. Debiec, P. Gwiazda, K. Lyczek, A. Swierczewska-Gwiazda, Relative entropy method for measure-valued solutions in natural sciences, to appear in Topol. Methods Nonlinear Anal.

Joint work with: Ondrej Kreml and Agnieszka Swierczewska-Gwiazda

Deep learning as optimal control problems

Elena Celledoni

Norwegian University for Science and Technology (NTNU), Trondheim, Norway

12:15 – 12:45

Abstract: The motivation of this talk comes from recent work of Haber and Ruthotto, where deep learning neural networks have been interpreted as discretisations of an optimal control problem. We review the first order conditions for optimality, and the conditions ensuring optimality after discretization. This leads to a class of algorithms for solving the discrete optimal control problem which guarantee that the corresponding discrete necessary conditions for optimality are

fulfilled. We discuss two different deep learning algorithms and make a preliminary analysis of the ability of the algorithms to generalize.

Geometric Numerical Integration of Differential equations

Reinout Quispel
La Trobe University, Melbourne, Australia

12:45
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13:30

Abstract: This talk will come in three parts: In Part I we start by presenting a number of motivating examples illustrating some of the advantages of using geometric integration methods. We then give a classification of primitive ODEs and their geometric integrators. In Part II we briefly discuss non-primitive ODEs and their integrators, using energy-preserving systems as our examples. Hopefully we will have time to say a few words in Part III about how to find the modified measures and modified integrals of Kahans unconventional method.