COMPUTATIONAL MATHEMATICS FOR QUANTUM TECHNOLOGIES

1-5 AUGUST 2022
BATH, UK

MONDAY

Sergio Blanes

University of Valencia, Spain

Splitting methods with complex coefficients to the numerical integration of quantum systems

Mon Aug 1, 9:00

The evolution of most quantum systems is modeled by differential equation in the complex space. However, in general, the equations are numerically solved using integrators with real coefficients. To consider complex coefficients usually does not make the schemes computationally more costly and can provide more accurate results. In this talk, we explore the applicability of splitting methods involving complex coefficients to solve numerically the time-dependent Schrödinger equation. There are pros (high accuracy and not to increase the cost) and cons (instability and loose of qualitative properties) when using complex coefficients. However, there is a class of methods with complex coefficients with a particular symmetry that keep most pros while avoid most cons. This class of integrators are stable and behave as conjugate to unitary methods for sufficiently small step sizes. These are promising methods that we will explore: we build new methods and we analyse their performance on several examples.

Graham Worth

University College London, UK

Solving the Time-Dependent Schrodinger Equation for Molecules using Grids or Gaussians

Mon Aug 1, 10:15

In this talk, a family of methods used to solve the Time-dependent Schrodinger Equation (TDSE) for molecular systems will be presented. This is of particular importance when quantum effects such as tunneling or non-adiabatic crossing is involved. The most straightforward and accurate method is to expand the wavefunction and Hamiltonian in an appropriate basis that effectively discretises the problem onto a grid. Unfortunately, as in all quantum mechanical problems, the scaling of this approach rises exponentially with system size preventing the treatment of typical molecules. The Multi-configuration time-dependent Hartree (MCTDH) method provides the way forward as a contraction of the primitive grid into sets of time-dependent basis functions [1]. In the ultimate multi-layer form (ML-MCTDH), this allows Hamiltonians of many hundreds of degrees of freedom to be solved [2]. The drawback of this approach, however, is that it is not able to treat realistic molecular Hamiltonians as the potential energy function needs to be known a priori. To try and circumvent this problem, we have extended the MCTDH method to use Gaussian basis functions rather than grids, which allows potentials to be calculated on-the-fly [3].

[1] M. Beck, A. Jäckle, G.A. Worth, and H.-D. Meyer. Phys. Rep., 324:1–106, 2000.
[2] H. Wang and M. Thoss, J. Chem. Phys., 119: 1289. 2003.

[3] G. W. Richings et al. Int. Rev. Phys. Chem., 34:269, 2015.

Paul Bergold

University of Surrey, UK

Tensor-Train Chebyshev Method for Multidimensional Quantum Dynamics Simulations

Mon Aug 1, 11:00

Methods for the efficient simulation of multidimensional quantum dynamics are essential for the theoretical studies of chemical systems. In this talk we will explore the tensor-train Chebyshev (TTC) method for rigorous nuclear quantum dynamics simulations. TTC is essentially the Chebyshev propagation scheme applied to the initial state represented in a tensor-train format, which is a special variant of low-rank tensor decompositions that can overcome the curse of dimensionality and is currently at the forefront of research in many different fields. Numerical experiments to simulate high-dimensional quantum dynamics will demonstrate the capabilities of the TTC method.

Nick Blunt

Riverlane, UK

Quantum computation in chemistry: statistical phase estimation and error mitigation

Mon Aug 1, 12:00

We present an application of quantum computing to quantum chemistry. Quantum phase estimation (QPE) is perhaps the most promising quantum algorithm for chemistry, however it requires deep circuits that cannot be performed on current quantum processors. Recently, several authors have proposed statistical alternatives to QPE that involve random sampling, and which have potential advantages, particularly on near-term quantum processors. Here we investigate the quantum eigenvalue estimation algorithm (QEEA) proposed recently by Somma[1] and apply it to small chemical active spaces. This method allows both ground and excited-state energies to be estimated in a single analysis, and its potential in chemistry is yet to be properly explored. We perform this method on Rigetti's current quantum processors and present results. We then discuss our current work on zero noise extrapolation (ZNE)[2,3], which we are implementing together with the QEEA.

[1] Rolando D Somma (2019) New J. Phys. 21, 123025
[2] Kristan Temme, Sergey Bravyi, and Jay M. Gambetta (2017) Phys. Rev. Lett. 119, 180509
[3] Ying Li and Simon C. Benjamin (2017) Phys. Rev. X 7, 021050

Sam Vinko

University of Oxford, UK

Towards more accurate Exchange-Correlation Functionals using Differentiable Programming

Mon Aug 1, 12:30

Recent advances in combining density functional theory (DFT) calculations of the electronic structure with machine learning are paving a new path towards the construction of chemically-accurate exchange-correlation (xc) functionals [1-7]. These advances promise to have broad application in the predictive modelling of real systems across chemistry, material science, and high energy density physics. In this context, differentiable programming is proving to be a formidable tool to help learn the behaviour of the xc functional, using a combination of higher-level simulations and experimental data, all within the physics-based constraints of the Kohn-Sham framework. Here we provide a brief outline of some recent developments in the field, and present the first fully-differentiable 3D density functional theory simulator (DQC – Differentiable Quantum Chemistry) where the exchange-correlation functional can be efficiently represented by a trainable deep neural network [8]. We demonstrate how this approach helps construct highly accurate exchange-correlation functionals using heterogeneous experimental data even for extremely limited datasets: using only eight experimental values on diatomic molecules, the trained exchange-correlation networks enable improved prediction accuracy of atomization energies across a collection of 104 molecules containing new bonds, new atoms, and new molecules not present in the training dataset [3]. The generalization power of this approach is particularly promising in the context of building accurate functionals for the exploration of extreme states of matter at high densities and temperatures.

[1] Nagai, Akashi, Sugino, Computational Materials 6, 43 (2020).
[2] Li et al., Phys. Rev. Lett. 126, 036401 (2021).
[3] Kasim, Vinko, Phys. Rev. Lett. 127, 126403 (2021).
[4] Dick, Fernandez-Serra, arXiv:2106.04481 (2021).
[5] Chen et al., J. Chem. Theory Comput. 17, 170 (2021).
[6] Kalita et al., arXiv:2110.14846v2 (2021).
[7] Nagai, Akashi, Sugino, arXiv:2111.15593v2 (2021).
[8] Kasim, Lehtola, Vinko, J. Chem. Phys. 156, 084801 (2022).

DQC code available @ https://github.com/diffqc/dqc/

This is joint work with S. Azadi and M. F. Kasim.

Joackim Bernier

Nantes University, France

Exact splitting methods for quadratic evolution equations

Mon Aug 1, 14:15

In this talk I will present some new splitting methods to compute the semigroups generated by quadratic differential operators. These methods consist in factorizing the semigroups as products of semigroups being directly computable by Fast Fourier Transforms. Their specificity is that the factorization is exact: there is no time

discretisation error. Examples of applications to the magnetic linear Schrödinger equations with quadratic potentials and to some Fokker-Planck equations will be given.

Fernando Casas

Jaume I University, Castellón, Spain

A unifying framework for perturbative exponential expansions

Mon Aug 1, 14:45

We propose a unified approach for different exponential perturbation techniques used in the treatment of time-dependent quantum mechanical problems, namely the Magnus, Fer and Wilcox expansions.

The approach is based on carrying out one or several appropriate changes of coordinates (or pictures), and it can be formulated for any time-dependent linear system of ordinary differential equations. In the case of Fer and Wilcox expansions, they result from two particular choices for the initial transformation that seeds the product expansion. In this framework, intermediate expansions can also be envisaged and recurrence formulas are developed. We also provide a new lower bound for the convergence of the Wilcox expansion, as well as some applications of the results. In particular, two examples are worked out up to a high order of approximation to illustrate the behavior of the Wilcox expansion.

This is joint work with Ana Arnal, Cristina Chiralt, and José Ángel Oteo.

Federica Agostini

University of Paris-Saclay, France

Theory and simulations of ultrafast processes in molecules with the exact factorization

Mon Aug 1, 15:45

In this talk I will present various applications of the exact factorization [1] to describe ultrafast non-radiative phenomena, such as internal conversion [2, 3] and intersystem crossing [4]. An introduction to the formalism will be given [5], that accounts for kinetic non-adiabatic coupling between electronic states of the same spin multiplicity and for spin-orbit coupling between states of different spin multiplicity. The extension of the formalism to explicitly include the effect of an external time-dependent field will be presented as well [6]. The generalized coupled-trajectory mixed quantum-classical (G-CT-MQC) algorithm [4] will be applied to the study of the photo-isomerization of a retinal chromophore [7] and to the simulation of singlet-to-triplet transitions [4]. Comparisons with vibronic-wavepacket dynamics and various trajectory-based schemes will be employed to evaluate the performance of G-CT-MQC.

[1] Abedi, A.; Maitra, N. T.; Gross, E. K. U., Phys. Rev. Lett. 2010, 105, 123002.
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[5] Agostini, F.; Curchod, B. F. E., WIREs Comput. Mol. Sci. 2019, 9, e1417.

[6] Schirò, M.; Eich, F. G.; Agostini, F., J. Chem. Phys. 2021, 154, 034104.
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Lin Lin

University of California, Berkeley, USA

Quantum algorithms for eigenvalue problems

Mon Aug 1, 16:15

The problem of finding the smallest eigenvalue of a Hermitian matrix (also called the ground state energy) has wide applications in quantum physics, quantum chemistry, materials science etc. I discuss two classes of quantum algorithms for solving such eigenvalue problems with near-optimal query complexities: those suitable for full-scale fault-tolerant quantum computers based on a block encoding input model, and those suitable for early fault-tolerant quantum computers based on a Hamiltonian evolution input model.

[1] L. Lin, Y. Tong, Near-optimal ground state preparation, Quantum, 4, 372, 2020
[2] L. Lin, Y. Tong, Heisenberg-limited ground state energy estimation for early fault-tolerant quantum computers, PRX Quantum. 3, 010318, 2022
[3] Y. Dong, L. Lin, Y. Tong, Ground state preparation and energy estimation on early fault-tolerant quantum computers via quantum eigenvalue transformation of unitary matrices, arXiv:2204.05955

TUESDAY

Weizhu Bao

National University of Singapore, Singapore

Multiscale methods and analysis for highly oscillatory Dirac equation
Tue Aug 2, 9:00

In this talk, I will review our recent works on multiscale methods and analysis for solving the highly oscillatory (nonlinear) Dirac equation including the nonrelativistic regime, involving a small dimensionless parameter which is inversely proportional to the speed of light. In this regime, the solution is highly oscillating in time and the energy becomes unbounded and indefinite, which brings significant difficulty in analysis and heavy burden in numerical computation. Rigorous error bounds are obtained for finite difference time domain (FDTD) methods, time splitting Fourier pseudospectral (TSFP) method and exponential wave integrator Fourier pseudospectral (EWI-FP), which depend explicitly on the mesh size, time step and the small parameter. Then based on a multiscale expansion of the solution, we present a multiscale time integrator Fourier pseudospectral (MTI-FP) method for the Dirac equation and prove its error bound which uniformly accurate in term of the small dimensionless parameter. Finally, by introducing the regularity compensation oscillatory (RCO) technique, we establish improved uniform error bounds on time-splitting methods for the long-time dynamics of the Dirac equation with small electromagnetic potentials and the nonlinear Dirac equation with weak nonlinearity. Numerical results demonstrate that our error estimates are sharp and optimal.

This is joint work with Yongyong Cai, Yue Feng, Xiaowei Jia, Qinglin Tang, and Jia Yin.

Catherine Higham

University of Glasgow, UK

Quantum Annealing in Network Science
Tue Aug 2, 10:15

We propose a new kernel that quantifies success for the task of computing a core-periphery partition for an undirected network. Finding the associated optimal partitioning may be expressed in the form of a quadratic unconstrained binary optimization (QUBO) problem, to which a state-of-the-art quantum annealer may be applied. We therefore make use of the new objective function to (a) judge the performance of a quantum annealer, and (b) compare this approach with existing heuristic core-periphery partitioning methods. The quantum annealing is performed on a commercially available D-Wave machine. The QUBO problem involves a full matrix even when the underlying network is sparse. Hence, we develop and test a sparsified version of the original QUBO which increases the available problem dimension for the quantum annealer. Results are provided on both synthetic and real data sets, and we conclude that the QUBO/quantum annealing approach offers benefits in terms of optimizing this new quantity of interest.

This joint work with Desmond Higham and Francesco Tudisco is to appear in the proceedings of ACM SIGKDD 2022.

Peter Mosley

University of Bath, UK

Quantum photonics in microstructured optical fibre
Tue Aug 2, 11:00

Here in Bath we design and fabricate optical fibre in which light is guided by a microstructure of tiny holes parallel to the fibre axis. I will discuss the unique properties of this type of fibre and outline how it can be used within photonic quantum technologies. Specific challenges that are being addressed by our research include the development of nonclassical light sources for quantum computation and quantum sensing; building high-efficiency interconnects for disparate nodes in quantum networks; and the creation of gates and memory elements for photonic quantum computers.

Michael Lubasch

Quantinuum, UK

Variational quantum algorithms for nonlinear problems
Tue Aug 2, 12:00

We show that nonlinear problems including nonlinear partial differential equations can be efficiently solved by variational quantum computing. We achieve this by utilizing multiple copies of variational quantum states to treat nonlinearities efficiently and by introducing tensor networks as a programming paradigm. The key concepts of the algorithm are demonstrated for the nonlinear Schroedinger equation as a canonical example. We numerically show that the variational quantum ansatz can be exponentially more efficient than matrix product states (also known as tensor train decompositions) and present experimental proof-of-principle results obtained on an IBM Q device.

Changpeng Shao

University of Bristol, UK

Eigenvalue decomposition on a quantum computer
Tue Aug 2, 12:30

Quantum computers can solve some problems much faster than classical computers. A typical example is quantum algorithms for eigenvalue problems. Quantum phase estimation is a useful technique to solve Hermitian eigenvalue problems. It is the foundation of many useful quantum techniques, such as quantum singular value decomposition. In this talk, I will introduce some recent development of this method on solving generalised eigenvalue problems. The main reference is arXiv:2010.15027.

Stefan Guettel

University of Manchester, UK

Calculation elements of extremely large matrix functions
Tue Aug 2, 14:15

I discuss a simple method for computing elements of matrix functions based on divided differences. The method is applicable to problems where the matrix dimension is so large that not even a single dense vector can be held in memory, hence ruling out Krylov methods and more generally all vector-based approximation methods. We showcase our approach by calculating the matrix elements of the exponential of a transverse-field Ising model and evaluating quantum transition amplitudes for large many-body Hamiltonians of sizes up to 1e19 on a single workstation.

This is joint work with Lev Barash and Itay Hen.

Tobias Jawecki

Vienna University of Technology, Spain

A practical approach on rational approximations to the action of unitary matrix exponentials
Tue Aug 2, 14:45

Approximations to the action of unitary matrix exponentials provide numerical methods for time propagation of spatially discretized linear Schrödinger-type equations. The discretized problem, besides resolving frequencies which are relevant for the given initial state, often includes perturbations in relatively high frequency ranges. Such perturbations can critically affect the convergence of (polynomial) approximations to the action of the matrix exponential. Our approach is to generate unitary rational approximants in barycentric rational form which are accurate in relevant frequency ranges. Due to unitarity, the effect of perturbations is negligible - a property which yields strong advantages in this setting. Relevant frequency ranges (relevant parts of the matrix spectrum) are detected on the run using estimates on the spectral distribution of the initial state. These estimates are based on the Lanczos method and bounds on quadrature weights of Gaussian quadrature formulae.

Di Fang

University of California, Berkeley, USA

Time-dependent Hamiltonian simulation of highly oscillatory dynamics and superconvergence for Schrödinger equation
Tue Aug 2, 15:45

Recent years have witnessed tremendous progress in developing and analyzing quantum algorithms for quantum dynamics simulation of bounded operators (Hamiltonian simulation). However, many scientific and engineering problems require the efficient treatment of unbounded operators, which frequently arise due to the discretization of differential operators. Such applications include molecular dynamics, electronic structure theory, quantum control and quantum differential equations

solver. We will introduce some recent advances in quantum algorithms for efficient unbounded Hamiltonian simulation, including Trotter type splitting and the quantum highly oscillatory protocol (qHOP) in the interaction picture.

Sheehan Olver

Imperial College London, UK

Infinite Linear Algebra and Spectral Problems

Tue Aug 2, 16:15

We discuss the ∞-dimensional QL algorithm and its use in computing discrete eigenvalues for both discrete Schrödinger operators as well as perturbations of (non-normal) Toeplitz operators. This includes the case where the eigenvalues are embedded in the continuous spectrum.

This is joint work with Marcus Webb.

WEDNESDAY

Yvain Bruned

University of Edinburgh, UK

Approximations of dispersive PDEs in the presence of low-regularity randomness

Wed Aug 3, 9:00

We introduce a new class of numerical schemes that allow for low regularity approximations to the second moment of the solution of a dispersive PDEs with random initial data. This quantity plays an important role in physics, in particular in the study of wave turbulence where one needs to adopt a statistical approach in order to obtain deep insight into the generic long-time behaviour of solutions to dispersive equations. Our schemes used the resonance-based discretisation after applying Wick's theorem that produces Feynman diagrams. To deal with these diagrams, we introduce paired decorated forests which are two decorated trees whose decorations on the leaves come in pairs. The character of the scheme draws its inspiration from the treatment of singular stochastic partial differential equations via Regularity Structures.

This is joint work with Yvonne Alama Bronsard and Katharina Schratz.

Ilya Kuprov

University of Southampton, UK

Spin dynamics simulation algorithms with polynomial complexity scaling

Wed Aug 3, 10:15

A common problem in magnetic resonance simulation is long-range time evolution of dissipative quantum systems that involve irregular three-dimensional networks of anisotropic spin interactions. This regime is exceedingly difficult because tensor network approximations (e.g. DMRG and its variants) fail. To obtain polynomial complexity scaling, a very different set of approximations is necessary, based on reachability under dissipative evolution generators.

This presentation summarises twenty years of research and programming by over 50 people; the result is Spinach – a simulation library that covers the entirety of magnetic resonance, from molecular magnets to metabolic MRI. At the time of writing, complicated pulse sequences on protein spin systems with over 500 interacting nuclear spins can be simulated in the time domain, with accurate account of both coherent and dissipative quantum dynamics. The central approximation is that, in room-temperature spin systems, a vast majority of quantum states is unreachable.

Elizaveta Suturina

University of Bath, UK

Challenges in paramagnetic NMR analysis

Wed Aug 3, 11:00

Nuclear magnetic resonance (NMR) of paramagnetic metal complexes remains a challenging but highly informative analytical technique. In my talk, I will present how improved models for pNMR analysis help to extract more information from standard NMR measurements. These includes:

(i) Ab initio assisted assignment of pNMR spectra of lanthanide complexes relevant for magnetic resonance imaging (MRI) contrast agents; [1]
(ii) Extracting tag mobility information from proteins paramagnetic shift data using analytical and numerical approaches; [2]
(iii) Evaluating electron relaxation parameters from nuclear relaxation enhancement. [3]

References:

[1] Beyond Bleaney's Theory: Experimental and Theoretical Analysis of Periodic Trends in Lanthanide Induced Chemical Shift, EA Suturina, K Mason, CFGC Geraldes, I Kuprov, D Parker, Angew. Chem. Int. Ed., 2017, 56, 12215
[2] Pseudocontact shifts from mobile spin labels, EA Suturina, I Kuprov, Phys. Chem. Chem. Phys., 2016, 18, 26412
[3] Lanthanide-induced relaxation anisotropy, E Suturina, K Mason, CFGC Geraldes, NF Chilton, D Parker, I Kuprov, Phys. Chem. Chem. Phys., 2018, 20, 17676
Observability of paramagnetic NMR signals at over 10 000 ppm chemical shifts, L Gade, JC Ott, EA Suturina, I Kuprov, J Nehrkorn, A Schnegg, M Enders, Angew. Chemie Int. Ed., 2021, https://doi.org/10.1002/anie.202107944

This is joint work with Ilya Kuprov.

Chunmei Su

Tsinghua University, China

Scattering and uniform in time error estimates for splitting method in NLS

Wed Aug 3, 12:00

We consider the nonlinear Schrodinger equation with a defocusing nonlinearity which is mass-supercritical and energy-subcritical. We prove uniform in time error estimates for the Lie-Trotter time splitting discretization. This uniformity in time is obtained thanks to a vectorfield which provides time decay estimates for the exact and numerical solutions. This vectorfield is classical in scattering theory, and requires several technical modifications compared to previous error estimates for splitting methods.

Xiantao Li

Pennsylvania State University, USA

Unraveling the dynamics of open quantum systems

Wed Aug 3, 12:30

In most realistic scenarios, the dynamics of a quantum system do not occur in isolation. Rather, it is coupled with an environment that breaks the reversibility and induces decoherence and dissipation. The theory of open quantum systems aims to develop quantum models that do not explicitly involve the degrees of freedom in the environment. We present a class of quantum master equations (QME) that

govern the dynamics of the density matrix. The model can be derived from standard quantum dynamics with both system and bath interactions included. These master equations can be "unpacked" to a system of stochastic Schrodinger equations with multiplicative noise. We explain how the QME can be simulated on classical and quantum computers.

THURSDAY

Simen Kvaal

University of Oslo, Norway

No need for a grid: gaussians for the time-dependent Schrödinger equation

Thu Aug 4, 10:00

Linear combinations of complex gaussian functions, where the nonlinear parameters are allowed to vary, are shown to be an extremely flexible representation for the solution of the time-dependent Schrödinger equation in one spatial dimension. Propagation of such wavefunctions using the Dirac–Frenkel variational principle is notoriously hard, and we present instead a scheme based on the method of vertical lines, or Rothe's method. We apply the method to a simple test system mimicking an atom subject to an extreme laser pulse, producing complicated ionization dynamics. The scheme is shown to perform very well on this model. Since the propagation method can be formulated entirely in terms of gaussian integrals and expectation values, we eliminate the need for large grids using only a handful of gaussian functions but with the same accuracy. This paves the way for accurate and affordable solutions of the time-dependent Schrödinger equation for multi-atom molecules beyond the Born–Oppenheimer approximation.

Alexander Ostermann

University of Innsbruck, Austria

Bourgain techniques for error estimates at low regularity

Thu Aug 4, 10:45

Standard numerical integrators such as splitting methods or exponential integrators suffer from order reduction when applied to semi-linear dispersive problems with non-smooth initial data. In this talk, we focus on the cubic nonlinear Schrödinger equation with periodic boundary conditions. For such problems, we present filtered integrators that exhibit superior convergence rates at low regularity. Furthermore, due to the nonexistence of suitable embedding results, the error analysis at very low regularity cannot be carried out in the usual framework of Sobolev spaces. Instead, completely new techniques are required. They are based on Bourgain's seminal work and will be sketched in the talk. Numerical examples illustrating the analytic results will be given.

Michele Grossi

CERN, Switzerland

Quantum computing's contribution to research projects at CERN: current status and prospects

Thu Aug 4, 12:00

CERN has recently started its Quantum Technology Initiative in order to investigate the use of quantum technologies in High Energy Physics (HEP). A three-year roadmap and research programme has been defined in collaboration with the HEP and quantum-technology research communities. In this context, initial pilot projects have been set up at CERN in collaboration with other HEP institutes worldwide on Quantum Computing and Quantum Machine Learning in particular. These projects, are studying basic prototypes of quantum algorithms, which are being evaluated in the context of LHC experiments for different types of workloads. This talk will provide an overview of recent results obtained by the different studies, including applications in areas ranging from accelerator beams optimisation, nuclear physics, data analysis and classification.

Lihui Chai

Sun Yat-Sen University, China

Frozen Gaussian appoximations for non-strictly hyperbolic systems
Thu Aug 4, 12:30

In this talk, we introduce frozen Gaussian approximation (FGA) to compute high-frequency wave propagation modeled by non-strictly hyperbolic systems, such as the elastic wave equations [J.C. Hateley, L. Chai, P. Tong and X. Yang, Geophys. J. Int., 216, 1394–1412, 2019] and the Dirac system [L. Chai, E. Lorin and X. Yang, SIAM Numer. Anal., 57, 2383–2412, 2019]. We analyze the asymptotic accuracy of FGA for these systems and prove the first order convergence. Unlike the convergence theory of FGA for strictly linear hyperbolic systems, the key estimate lies in the boundness of intraband transitions in diabatic coupling.

This is joint work with J.C. Hateley, E. Lorin, and X. Yang.

Christian Mendl

Technical University of Munich, Germany

Ternary unitary quantum lattice models and circuits in 2 + 1 dimensions
Thu Aug 4, 14:15

We extend the concept of dual unitary quantum gates [Phys. Rev. Lett. 123, 210601 (2019)] to quantum lattice models in $2+1$ dimensions, by introducing and studying *ternary unitary* four-particle gates, which are unitary in time and both spatial dimensions. When used as building blocks of lattice models with periodic boundary conditions in time and space (corresponding to infinite temperature states), dynamical correlation functions exhibit a light-ray structure. We also generalize solvable MPS [Phys. Rev. B 101, 094304 (2020)] to two spatial dimensions with cylindrical boundary conditions, by showing that the analogous *solvable PEPS* can be identified with matrix product unitaries. In the resulting tensor network for evaluating equal-time correlation functions, the bulk ternary unitary gates cancel out. We delineate and implement a numerical algorithm for computing such correlations by contracting the remaining tensors. (Preprint: arXiv:2206.01499)

Stefanos Carlström

Lund University, Sweden

Time-dependent configuration-interaction singles, or the lowest-rank approach to multielectron quantum dynamics

Thu Aug 4, 14:45

We derive the lowest-rank approximation to multielectron dynamics in atoms and small-sized molecules subjected to intense laser radiation and demonstrate its implementation for molecules on a Cartesian grid and for atoms in spherical coordinates. Complications that must be tackled include propagation on a submanifold of the full Hilbert space, as well as the efficient computation of the non-local Coulombic electron–electron repulsion interaction. Finally, we demonstrate the usefulness by comparing with state-of-the-art experimental results.

Yvonne Bronsard Alama

Sorbonne University, France

An approach to low-regularity numerical approximations via decorated trees

Thu Aug 4, 15:45

In this talk I will discuss new time discretization techniques based on decorated tree series for solving a general class of nonlinear evolution equations up to arbitrary order, and in low-regularity spaces. I will illustrate this decorated tree formalism in the context of the Gross-Pitaevskii equation.

In the second part of my talk, I will present an error analysis result for solving the Gross-Pitaevskii equation at low-regularity, and show first and second order convergence in any fractional positive Sobolev space H^r, $r \geq 0$.

These new schemes, together with their optimal local error estimates, allow for convergence under lower regularity assumptions than required by classical methods.

The first part of this talk is joint work with Yvain Bruned (University of Edinburgh), and Katharina Schratz (LJLL, Sorbonne Université).

Jianfeng Lu

Duke University, USA

Taming the dynamical sign problem in diagrammatic algorithms for open quantum systems

Thu Aug 4, 16:15

Numerical simulations for open quantum system dynamics is a profound challenge. In this talk, we will present some recent works on diagrammatic algorithms for open quantum systems. The focus will be an interplay between the dynamical sign problem and error amplification in numerical integration. In particular, our analysis demonstrates that the technique of partial resummation provides a tool to balance these two types of error, and the recently introduced inchworm Monte Carlo method is a successful case to suppress the numerical sign problem.

This is joint work with Zhenning Cai and Siyao Yang.

FRIDAY

Nana Liu

Shanghai Jiao Tong University, China

Quantum computation and pathways for nonlinear partial differential equations

Fri Aug 5, 9:00

Nonlinear partial differential equations have been central to modelling of some of the most significant problems in physics, chemistry, engineering, biology and finance, including climate modelling, aircraft design, molecular dynamics and drug design, deep learning neural networks and financial markets. While quantum computation has shown its advantages for solving linear problems, nonlinear problems have yet remained elusive. This is because quantum mechanics itself is fundamentally linear (as far as we know) and it is not yet known how to model nonlinear problems in a linear way without significant approximations that no longer capture truly nonlinear behaviour. Truly nonlinear behaviour, however, is what makes real physical systems, like the weather and stock markets, interesting, complex and unpredictable.

We show that an important class of nonlinear partial differential equations - Hamilton-Jacobi and scalar hyperbolic equations - can indeed be fully captured using a quantum algorithm. These equations are important for many applications like optimal control, machine learning, semi-classical limit of Schrodinger equations, mean-field games and many more. Physical quantities like density and energy (and many more) can be computed using a quantum algorithm that can be up to exponentially more efficient compared to a classical device with respect to the dimension of the system and the error of the final answer. In addition, we provide methods for more general classes of nonlinear partial differential equations and show when speedup with respect to the number of initial conditions can be achieved.

Karolina Kropielnicka

Polish Academy of Sciences, Poland

The review of computational approaches for the linear Klein-Gordon equations from low to high frequency regimes

Fri Aug 5, 10:15

In this talk, we consider the Klein–Gordon equation

$$\begin{cases} \frac{\partial^2}{\partial t^2}\psi(x,t) = \Delta\psi(x,t) - m(x,t)\psi(x,t), \quad t > t_0, \quad x \in \mathbb{T}^d \\ \psi(x,t_0) = \psi_0(x), \quad \partial_t\psi(x,t_0) = \varphi_0(x) \end{cases}$$

equipped with periodic initial and boundary conditions and time and space dependant coefficient $m(x,t)$. The latter assumption was proposed only recently and it allows for dealing with the problems of negative probability density and of violation of Lorenz covariance. Moreover application of time and space dependant coefficients extends application of such a problem to the domain of quantum cosmology, where $m(x,t)$ may bring possibly highly oscillatory form

$$m(x,t) = \sum_n a_n(x,t)e^{i\omega_n t}$$

with frequencies $\omega_n \in \mathbb{R}$, $n \in \mathbb{Z}$. Numerical approximation of such a problem requires various approaches when $m(x,t)$ is non-oscillatory, or highly oscillatory. The most challenging form of coefficient $m(x,t)$, however, is when it includes low and high frequencies, for example $m(x,t) = a_0(x,t) + a_1(x,t)\mathrm{e}^{it} + a_2(x,t)\mathrm{e}^{i10^6 t}$.

In this talk we will present various approaches to all the kinds of these problems, will present final error estimates and plenty of numerical examples.

This is joint work with Karolina Lademann (University of Gdansk), Katharina Schratz (Sorbonne Universite),Marissa Condon (Dublin City University), and Rafal Perczynski (University of Gdansk).

Yongyong Cai

Beijing Normal University, China

Numerical methods for computing ground states of spinor Bose-Einstein condensates

Fri Aug 5, 11:00

The remarkable experimental achievement of Bose-Einstein condensation (BEC) in 1995 has drawn significant research interests in understanding the ground states and dynamics of trapped cold atoms. Different from the single component BEC, spinor BEC possesses the spin degree of freedom and exhibits rich phenomenon. In the talk, we will present some recent work for computing ground states of general spin-F BECs.

Yue Feng

National University of Singapore, Singapore

Improved Uniform Error Bounds on Time-splitting Methods for the Long-time Dynamics of the Nonlinear Schrödinger Equation

Fri Aug 5, 12:00

In this talk, we establish improved uniform error bounds for the time-splitting methods for the long-time dynamics of the nonlinear Schrödinger equation (NLSE) with weak nonlinearity. By introducing a new technique of regularity compensation oscillation (RCO) in which high frequency modes are controlled by the regularity of the solution and low frequency modes are analyzed by phase cancellation and energy method, an improved uniform error bound at $O(h^{m-1} + \varepsilon^2\tau^2)$ is carried out in H^1-norm for the long-time dynamics up to the time at $O(1/\varepsilon^2)$ of the cubic NLSE with $O(\varepsilon^2)$-nonlinearity strength. Numerical results are reported to validate our error estimates and to demonstrate that they are sharp.

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TBA

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