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Some properties and numerical aspects of fractional Schrödinger equations

Xavier Antoine

Université de Lorraine, France

ABSTRACT

The purpose of this talk is to discuss some recent developments concerning the numerical simulation of space fractional Schrödinger and Gross-Pitaevskii equations. In particular, we address some questions related to the discretization of the models (order of accuracy and fast implementation) and clarify some of their dynamical properties. Some numerical simulations illustrate these points.

The Cauchy problem for the quantum hydrodynamics system and the stability of weak solutions

Paolo Antonelli

Gran Sasso Science Institute, Italy

ABSTRACT

The quantum hydrodynamics (QHD) system is a model used to describe macroscopic objects exhibiting quantum features, as for instance in superfluidity, Bose-Einstein condensation or semiconductor devices. They are characterized by a compressible, inviscid flow subject to a stress tensor depending on the particle density and its derivatives, that adds dispersive effects in the system. The Cauchy theory for finite energy weak solutions exploits the analogy between the QHD system and nonlinear Schrödinger (NLS) dynamics, through the Madelung transform. By using a polar factorization approach it is possible to make this analogy rigorous in the space of finite energy weak solutions. Furthermore the hydrodynamic formulation allows to include some dissipative effects which cannot be treated with the NLS dynamics. The polar decomposition can also be exploited to study the problem with non-trivial conditions at infinity. This analysis is motivated by future applications to quantized vortex dynamics. The main drawback of this approach is that the initial data for the hydrodynamical system need to be consistent with a wave function by means of the Madelung transform; at present it is not clear what is the degree of generality of such initial data. We show that in the one-dimensional case we can eliminate this assumption and we prove global existence of finite energy weak solutions to the QHD system with general initial data. Moreover, by introducing a novel functional we are also able to determine a class of solutions for which we can prove stability, namely given a sequence of solutions satisfying some uniform bounds there is a subsequence converging to a weak solution to the QHD system.

This talk is based on a series of works done in collaboration with P. Marcati and our Ph.D. students L. E. Hientzsch and H. Zheng.

Quantized vortex stability and dynamics in superfluidity and superconductivity

Weizhu Bao

National University of Singapore, Singapore

ABSTRACT

Quantized vortices have been experimentally observed in type-II superconductors, superfluids, nonlinear optics, etc. In this talk, I will review different mathematical equations for modeling quantized vortices in superfluidity and superconductivity, including the nonlinear Schrodinger/Gross-Pitaevskii equation, Ginzburg-Landau equation, nonlinear wave equation, etc. Asymptotic approximations on single quantized vortex state and the reduced dynamic laws for quantized vortex interaction are reviewed and solved analytically in several cases. Efficient and accurate numerical methods will be presented for computing quantized vortex lattices and ther dynamics. Direct numerical simulation results from different PDE models are reported for quantized vortex dynamics and they are compared with those from the reduced dynamics laws. Some open problems and emerging applications will be discussed. This is a joint work with Qiang Du, Dieter Jaksch, Alexander Klein, Qinglin Tang and Yanzhi Zhang.

Ground states of spinor Bose-Einstein condensates

Yongyong Cai

Beijing Computational Science Research Center, China

ABSTRACT

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 introduce some mathematical results for ground states of spin-1,2 BECs, and a practical imaginary time propagation method for numerical simulation with several different projection strategies.

On hyperbolicity and convergence of Grad's moment method

Zhenning Cai

National University of Singapore, Singapore

ABSTRACT

Horald Grad was the pioneer of the moment method in the gas kinetic theory. His thirteen-moment model has achieved significant success in engineering. However, Grad's models with many moments seem to be quite fragile, the numerical computation easily breaks down for moderate nonequilibrium. Such an issue has been attributed to the loss of hyperbolicity of the equations. But even if the hyperbolicity problem is fixed, the method still fails for hypersonic flows. To solve the mystery, we reviewed the debate between Holway and Weiss on the existence of the smooth shock structure for Grad's method, and pointed out that the convergence of Grad's series ought to be another reason for the failure of Grad's method. Possible solutions are propos ed to fix the convergence issue.

On a kinetic Elo rating model for players with dynamical strength

Bertram Düring

University of Sussex, UK

ABSTRACT

We propose and study a new kinetic rating model for a large number of players, which is motivated by the well-known Elo rating system. Each player is characterised by an intrinsic strength and a rating, which are both updated after each game. We state and analyse the respective Boltzmann type equation and derive the corresponding nonlinear, nonlocal Fokker-Planck equation. We investigate the existence of solutions to the Fokker-Planck equation and discuss their behaviour in the long time limit. Furthermore, we illustrate the dynamics of the Boltzmann and Fokker-Planck equation with various numerical experiments.

Nonequilibrium dynamical mean-field theory and hidden phases of quantum matter

Martin Eckstein

Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

ABSTRACT

Non-equilibrium dynamical mean-field theory and its generalisations provide a versatile approach to understand the non-equilibrium dynamics in strongly correlated electron systems, and to unravel pathways to reach novel transient or metastable phases: How does the electronic structure of correlated insulators and metals change under strong electric field transients or photo-excitation? How can such fields be used to engineer emergent superconducting or magnetic low energy states? After a review of these questions, we focus on possible electronic pathways to hidden phases, i.e., states which are different from any equilibrium state.

Polynomial and rational approximation for electronic structure theory

Simon Tobias Etter

National University of Singapore, Singapore

ABSTRACT

Computer simulations based on Density Functional Theory (DFT) and related electronic structure models spend a large part of their compute time on evaluating functions of large, sparse matrices. Traditionally, such matrix functions have been computed by means of the eigenvalue decomposition, but the cubic scaling of standard eigensolvers with respect to the matrix size renders this ansatz prohibitively expensive in many applications. Several alternative algorithms have been developed in recent decades, among which the Pole Expansion and Selected Inversion (PEXSI) algorithm by Lin Lin and collaborators stands out for its ease of use and excellent parallel scaling. However, the runtime of the PEXSI scheme grows with $N^{3/2}$ for two-dimensional systems of N atoms and with N^2 for three-dimensional systems, which is an important drawback of this method compared to most of its competitors.

The first part of this talk will present a modification of the PEXSI algorithm which reduces its cost to linear in the system size regardless of the dimension. This modification is based on the observation that the LU factorisation of a sparse, well-conditioned matrix is localised, i.e. the magnitudes of the fill-in entries decay exponentially as we move away from the nonzero entries of the original matrix. The second part of this talk will discuss conductivity calculations, which introduce a new twist to the theory of electronic structure algorithms in that the matrix function to evaluate in this case is a bivariate one. The runtime of such calculations is proportional to the number of significant Chebyshev coefficients of the function $f(x, y) := 1/(x - y + s)$ with small imaginary s, and we will see that this number scales with only $|s|^{3/2}$ rather than $|s|^2$ as one might expect based on tensor-product arguments.

Gibbs equilibrium for Gross-Pitaevskii equation

Reika Fukuizumi

Tohoku University, Japan

ABSTRACT

The stochastic Gross-Pitaevskii equation is used as a model of Bose-Einstein condensation(BEC) at positive temperature. The equation is a complex Ginzburg-Landau equation with a trapping potential and an additive space-time white noise. A positive temperature effect, for example, the spontaneous vortex formation by a sudden quench in BEC (seen as a phase transition) is of great interest in Physics, and to analyze this phase transition from the point of view in statistical physics, the convergence of the physical system to the Gibbs equilibrium in large time is essential.

In this talk we present some recent studies on the Gibbs measure defined for the two-dimensional stochastic Gross-Pitaevskii equation, and the existence of solution.

This talk is based on joint works with Anne de Bouard(Ecole polytechnique), Arnaud Debussche(ENS Rennes).

The Cauchy problem stability for the quantum Boltzmann- BEC condensation system

Irene Gamba

The University of Texas at Austin, USA

ABSTRACT

We discuss a new model for a coupled quantum Boltzmann-Condensation system that describes the evolution of the interaction between a well formed Bose-Einstein Condensate (BEC) and the quasi-particles cloud interacting with the condensed part at very low temperature. The kinetic dynamics of the quasi-particles, derived as weak turbulence kinetic model from a quantum Hamiltonian, is valid for a dilute regime at which the temperature of a bosonic gas is very low compared to the Bose-Einstein condensation critical temperature. In particular, the system couples the density of the condensate from a Gross-Pitaevskii type equation to the kinetic equation through the potential as much as on the dispersion relation in the kinetic model and the corresponding transition probability rate from pre to post collision momentum states.

We show the well-posedness of the Cauchy problem to the system for bounded solutions with a sufficiently large number of statistical moments and prove stability leading to a global in time existence and uniqueness of bounded, finite energy solutions to an initial value problem for the quantum Boltzmann-Condensation system. The proof entices finding qualitative properties of the solution such as instantaneous creation of polynomial and exponential moments (L^1-weighted norms), and finding estimates that related to the initial mass and boundness relation between condensed particles and quasi-particles.

This is work in collaboration with Ricardo J. Alonso and Minh Binh Tran.

On-demand topological matter by periodic driving

Jiangbin Gong

National University of Singapore, Singapore

ABSTRACT

Periodically driven quantum systems can be used to explore many novel aspects of topological matter. In this talk, I shall first introduce some basic notions on the so-called Floquet topological matter and then discuss recent progresses made by my research group at NUS. Emphasis is placed on possible applications of novel topological matter, without going into the technical details. These include, for example, topological insulators with arbitrarily large number of chiral edge states, topological semimetals with exotic topological linkages between nodal loops, measurement-based quantum computing based on topological corner states, and long-distance entangled-state transfer, etc.

Correlated topological states with interfaces and disorder

Walter Hofstetter

Goethe-Universität, Germany

ABSTRACT

The last years have witnessed dramatic progress in experimental control and theoretical modeling of quantum simulations with ultracold atoms. Major developments include synthetic gauge fields for neutral atoms, induced by time-periodic driving, which allow the simulation of topologically nontrivial phases of matter with strong interactions and disorder. I will discuss two recent theoretical results:

Two-dimensional topological insulators possess conducting edge states at their boundary while being insulating in the bulk. We investigate the edge state emergent at a smooth topological phase boundary of interacting fermions within the time-reversal invariant Hofstadter-Hubbard model. We characterize the localization of the edge state and the topological phase boundary by means of the local compressibility, the spectral density, a generalized local spin Chern marker as well as the Hall response and find good agreement between all these quantities. Computing the edge state spectra at the interface we observe robustness of the edge state against fermionic two-body interactions and conclude that interactions only shift its position. Hence the bulk-boundary correspondence for the interacting system is confirmed. Since experimental probing of edge states remains a challenge in ultracold atom setups, we propose the detection of the local compressibility by using a quantum gas microscope.

We furthermore study transport properties and the topological phase transition in two-dimensional interacting disordered systems. Within real-space dynamical mean-field theory we derive the Hall conductance, which is quantized and serves as a topological invariant for insulators, even when the energy gap is closed by localized states. In the spinful Harper-Hofstadter-Hatsugai model we find that the repulsive on-site interaction can assist weak disorder to induce the integer quantum Hall effect, while in the topologically nontrivial regime, it impedes Anderson localization. Generally, the interaction widens the regime of the topological phase in the disordered system.

Random batch methods for interacting particle systems and its applications in consensus-based high dimensional global optimization in machine learning

Shi Jin

Shanghai Jiao Tong University, China

ABSTRACT

We develop random batch methods for interacting particle systems with large number of particles. These methods use small but random batches for particle interactions, thus the computational cost is reduced from $O(N^2)$ per time step to $O(N)$, for a system with N particles with binary interactions.

For one of the methods, we give a particle number independent error estimate under some special interactions. Then, we apply these methods to some representative problems in mathematics, physics, social and data sciences, including the Dyson Brownian motion from random matrix theory, Thomson's problem, distribution of wealth, opinion dynamics and clustering. Numerical results show that the methods can capture both the transient solutions and the global equilibrium in these problems.

We also apply this method and improve the consensus-based global optimization algorithm for high dimensional machine learning problems. This method does not require taking gradient in finding global minima for non-convex functions in high dimensions.

Emergent behaviors of the Schrödinger-Lohe model for quantum synchronization

Dohyun Kim

National Institute for Mathematical Sciences, Korea

ABSTRACT

We investigate the coupled nonlinear Schrödinger equation, namely Schrödinger-Lohe (S-L) model as a phenomenological model for describing possible quantum synchronization. To reflect real-world situations, we employ several dynamical properties such as general network structures and interaction frustration, and sufficient conditions leading to the complete and practical synchronizations are presented. First, we begin with the all-to-all network in which the complete synchronization occurs generically. Second, general network structure is studied to observe that several asymptotic behaviors including repulsive behavior and period orbits can arise. Finally, we consider interaction frustration which triggers the competition between synchronous and periodic behavior.

Highly-oscillatory evolution equations with time-varying vanishing frequency: asymptotics and numerics

Mohammed Lemou

Université de Rennes 1, France

ABSTRACT

In asymptotic analysis and numerical approximation of highly-oscillatory evolution problems, it is commonly supposed that the oscillation frequency is either constant or, at least, bounded from below by a strictly positive constant uniformly in time. Allowing for the possibility that the frequency actually depends on time and vanishes at some instants introduces additional difficulties from both the asymptotic analysis and numerical simulation points of view. I will present a first step towards the resolution of these difficulties. In particular, we show that it is still possible in this situation to infer the asymptotic behavior of the solution at the price of more intricate computations and we derive a second order uniformly accurate numerical method.

Deriving order parameter from the reduced density matrix

Hai-Qing Lin

Beijing Computational Science Research Center, China

ABSTRACT

By establishing a connection between a frequently used quantum information concept, the mutual information, and the conventional order parameter in condensed matter physics, we are able to derive the order parameters corresponding to some long-range correlations in the ground state of a system, without any knowledge of the existing symmetries. We demonstrate our scheme on the one-dimensional Hubbard model and the spinless Su-Schrieffer-Heeger (SSH) model. All the derived order parameters and their possible corresponding quantum phases are verified by the entanglement entropy and electronic configuration analysis results. In particular, the order parameter appropriate to the topological regions is proposed and further proved by calculating the Berry phase under twisted boundary conditions. We found that the topological nontrivial phase is robust to the introduction of repulsive intersite interactions and can appear in the topological trivial parameter region when appropriate interactions are added.

A bi-fidelity method for multiscale kinetic equations with random parameters: computation and error analysis

Liu Liu

The University of Texas at Austin, USA

ABSTRACT

In this talk, we first study the multiscale Boltzmann equation with multi-dimensional random parameters by a bi-fidelity stochastic collocation (SC) method developed in [A. Narayan, C. Gittelson and D. Xiu, SIAM J. Sci. Comput., 36 (2014); X. Zhu, A. Narayan and D. Xiu, SIAM J. Uncertain. Quantif., 2 (2014)]. By choosing the compressible Euler system as the low-fidelity model, we adapt the bi-fidelity SC method to combine computational efficiency of the low-fidelity model with high accuracy of the high-fidelity (Boltzmann) model. With only a small number of asymptotic-preserving solver runs for the Boltzmann equation, the bi-fidelity approximation can capture well the macroscopic quantities of the solution to the Boltzmann equation in the random space.

Then we will develop a framework on obtaining an error estimate between the high-fidelity and bi-fidelity solutions in solving a more general class of multi-scale kinetic equations with uncertainty. Extensive numerical experiments will be presented to verify the efficiency and accuracy of our proposed method.

Analysis of convergence of Schwarz waveform relaxation methods for the Schroedinger equation

Emmanuel Lorin

Carleton University, Canada

ABSTRACT

This talk is dedicated to the analysis of convergence of Schwarz Waveform Relaxation (SWR) methods for the stationary and evolution Schroedinger equations. We are more specifically interested in the rate of convergence of SWR methods, depending on the type of transmission conditions, namely Dirichlet (Classical SWR), transparent/absorbing (quasi-Optimal SWR) conditions and optimized Robin-type (Optimized SWR) transmission conditions. Some numerical experiments illustrating the analytical results will be proposed, and application to the N-body Schroedinger equation will also be discussed.

This is a joint work with X. Antoine (IECL).

Nonlinear dissipative photonics with spin-orbit coupling

Boris Malomed

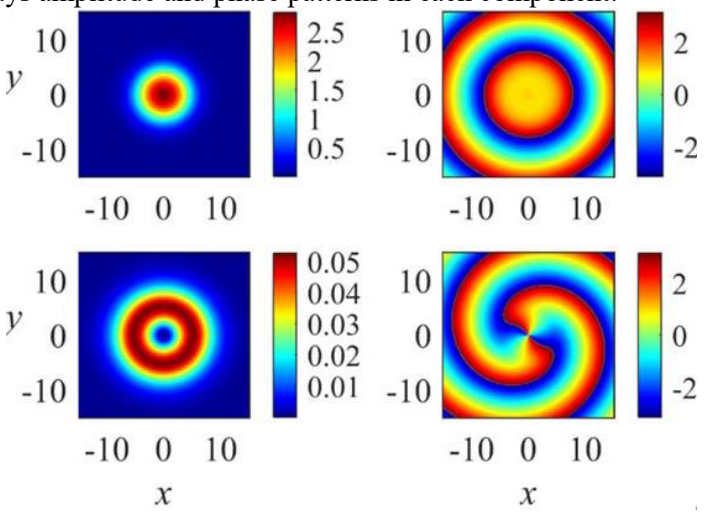
Tel Aviv University, Israel

ABSTRACT

Nonlinear dissipative optics in 2D settings has been a subject of studies for a long time [1]. Currently, a great deal of interest is drawn to 2D patterns in polariton condensates [2]. An important effect in binary polariton condensates, including TE- and TM-polarized photon fields, is spin-orbit coupling (SOC). The present talk aims to summarize recent results predicting robust localized vortex modes (quasi-solitons) supported by the interplay of gain, loss, nonlinearity, and SOC. Dissipative SOC-driven solitons were first obtained in the 2D model including saturable gain ($g > 0$), loss ($a > 0$) and SOC constant β [3]

$$i\partial_t \psi_\pm = \left(-\nabla^2 + if\right)\psi_\pm + \beta\left(\partial_x \mp i\partial_y\right)^2 \psi_\mp, f = -1 + \frac{g}{1+\varepsilon\left(|\psi_+|^2 + |\psi_-|^2\right)} - \frac{a}{1+\left(|\psi_+|^2 + |\psi_-|^2\right)}.$$

SOC couples terms with vorticity difference $\Delta S = 2$ between components $\psi_\pm$. As a result, the model generates two species of stable 2D solitons: vortex-antivortex (VAV) pairs and semi-vortices, the latter ones being a bound state of a zero-vorticity soliton in one component and vortex in the other, as shown in the figure, which displays amplitude and phase patterns in each component:



Further, in a physically relevant setting localization can be provided not by self-trapping but by an external trapping potential $\sim r^2$ [4]:

$$i\partial_t \psi_\pm = \left[-(1-i\eta)\nabla^2 + \left(|\psi_\pm|^2 + \alpha|\psi_\mp|^2\right) + i\left(\varepsilon - \sigma|\psi_\pm|^2\right) + r^2\right]\psi_\pm + \beta\left(\partial_x \mp i\partial_y\right)^2 \psi_\mp.$$

This model generates stable VAVs and mixed modes (MMs) states, which combine terms with vorticities 0 and ± 2 in both components.

In nonlinear optical settings per se, SOC can be realized in a dual-core planar waveguide with *PT* symmetry, represented by the balanced linear gain and loss in the two cores. Stable soliton families of the MM type have been found in this setting [5].

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Recent progress in the derivation of gyrokinetic models for magnetized plasmas

Florian Méhats

Université de Rennes 1, France

ABSTRACT

In this talk, we will present the mathematical derivation of the gyrokinetic model for the approximation of the Vlasov-Poisson system under a strong magnetic field in dimension 3. The proof relies on Littlejohn's derivation.

Computational quantum mechanics in phase space

Sihong Shao

Peking University, China

ABSTRACT

The Wigner function has provided an equivalent and convenient way to render quantum mechanics in phase space. It allows one to express macroscopically measurable quantities, such as currents and heat fluxes, in statistical forms as usually does in classical statistical mechanics, thereby facilitating its applications in nanoelectronics, quantum optics and etc. Distinct from the Schrödinger equation, the most appealing feature of the Wigner equation, which governs the dynamics of the Wigner function, is that it shares many analogies to the classical mechanism and simply reduces to the classical counterpart when the reduced Planck constant vanishes. Despite the theoretical advantages, numerical resolutions for the Wigner equation is notoriously difficult and remains one of the most challenging problems in computational physics, mainly because of the high dimensionality and nonlocal pseudo-differential operator. On one hand, the commonly used finite difference methods fail to capture the highly oscillatory structure accurately. On the other hand, all existing stochastic algorithms, including the affinity-based Wigner Monte Carlo and signed particle Wigner Monte Carlo methods, have been confined to at most 4D phase space. Few results have been reported for higher dimensional simulations. My group has made substantial progress in both aspects.

(1) We completed the design and implementation of a highly accurate numerical scheme for the Wigner quantum dynamics in 4-D phase space. Our algorithm combines an efficient conservative semi-Lagrangian scheme in the temporal-spatial space with an accurate spectral element method in the momentum space. This accurate Wigner solver has been successfully applied into the investigation of quantum tunneling in double well and quantum double slit interference. Moreover, the Wigner function for a one-dimensional Helium-like system was clearly shown for the first time.

2) We explored the inherent relation between the Wigner equation and a stochastic branching random walk model. With an auxiliary function, we can cast the Wigner equation into a renewal-type integral equation and prove that its solution is equivalent to the first moment of a stochastic branching random walk. The accuracy of the resulting implementation can be systematically improved and is hardly affected by the choice of time step. In order to further gain a substantial reduction in variances, we propose an asymptotical approach using stationary phase approximation which may ameliorate the sign problem. The performance of 6-D and higher-dimensional simulations demonstrate the accuracy and the efficiency of our asymptotical approach.

It should be noted that all proposed numerical schemes fully exploit the mathematical structure of the Wigner equation. Our target is an efficient simulator for analyzing some fundamental issues in many-body quantum mechanics, such as the nuclear quantum effect and dynamical correlation.

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High friction limits from Euler flows to gradient flows

Athanasios Tzavaras

King Abdullah University of Science and Technology, Saudi Arabia

ABSTRACT

I will review some recent works that address the problem of passing to the high-friction limit (or small mass approximation) from Euler flows to advection-diffusion equations that are gradient flows. This problem is addressed at the level of single component systems and I will discuss analogous issues at the level of multi-component systems.

Angular momentum radiation by a benzene molecule

Jian-Sheng Wang

National University of Singapore, Singapore

ABSTRACT

It is well-known that all bodies emit energy in the form of thermal radiation. It is much less well-known that they can also carry a nonzero angular momentum. In this talk, we present our study of a benzene molecule in a nano-junction geometry under voltage bias and show that there is a total angular momentum transfer. The mechanism is highly non-trivial and we explain it with a picture that involves four distinct angular momentum states of the molecule.

Algorithms for computing eigenvalues of quantum spin chains

Chao Yang

Lawrence Berkeley National Laboratory, USA

ABSTRACT

We present algorithms for computing eigenvalues and eigenvectors of quantum spin chains. In particular, we will examine efficient algorithms for computing interior eigenvalues of a finite size disordered spin chain with local interactions. We will also examine algorithms for computing the ground state of a translational invariant spin chain with infinite number of spins. One way to solve such a problem is to use an infinite translational invariant tensor ring to represent the approximation to the eigenvector to be computed and update the core of such a tensor ring through a flexible power iteration. We discuss approximations made in each step of the power iteration and how these approximations affect the convergence of the method.

Trapped Bose-Einstein condensates with attractive s-wave interaction

Su Yi

Chinese Academy of Sciences, China

ABSTRACT

Within the framework of the Gaussian-state theory, we show that the quantum many-body ground state of a trapped condensate with weakly attractive interaction is a single-mode squeezed vacuum state, as oppose to the coherent state under repulsive interaction. The spatial mode of the squeezed-state condensates satisfies a Gross-Pitaevskii like equation in which the interaction strength is augmented by a factor 3 due to the large particle fluctuation of the squeezed state. We also study the collective excitations of the condensates by the tangential space projection, which leads to new two-particle excitations and confirms the phase transition from coherent-state to squeezed-state condensates. Our investigation clarifies the quantum states of the attractive condensates and will shed new light on research of the droplet phases in dipolar and multicomponent condensates.

arxiv.org/abs/1909.02432

Multiscale methods and analysis for the Dirac/nonlinear Dirac equation

Jia Yin

National University of Singapore, Singapore

ABSTRACT

In this talk, numerical methods for the Dirac/nonlinear Dirac equation in different limit regimes are studied.

A new fourth-order compact time-splitting (S_{4c}) Fourier pseudospectral method is put forward for the Dirac equation without magnetic potential by using a double commutator. It is explicit, fourth-order in time and spectral order in space, and it is called compact time-splitting since, at each time step, the number of sub-steps in S_{4c} is much smaller than those in the standard fourth-order splitting and the fourth-order partitioned Runge-Kutta splitting. This method is superior to the above mentioned fourth-order splitting methods in efficiency and accuracy, which is verified by the numerical results.

In the nonrelativistic limit regime, the surprising super-resolution of the time-splitting methods, especially the Lie-Trotter splitting (S_1) and the Strang splitting (S_2), for the Dirac and nonlinear Dirac equation is discovered and analyzed. More specifically, the splitting methods break the resolution In this talk, numerical methods for the Dirac/nonlinear Dirac equation in different limit regimes are studied. A new fourth-order compact time-splitting (S_{4c}) Fourier pseudospectral method is put forward for the Dirac equation without magnetic potential by using a double commutator. It is explicit, fourth-order in time and spectral order in space, and it is called compact time-splitting since, at each time step, the number of sub-steps in S_{4c} is much smaller than those in the standard fourth-order splitting and the fourth-order partitioned Runge-Kutta splitting. This method is superior to the above mentioned fourth-order splitting methods in efficiency and accuracy, which is verified by the numerical results. In the nonrelativistic limit regime, the surprising super-resolution of the time-splitting methods, especially the Lie-Trotter splitting (S_1) and the Strang splitting (S_2), for the Dirac and nonlinear Dirac equation is discovered and analyzed. More specifically, the splitting methods break the resolution constraint under the Shannon's sampling theorem, i.e. the methods can capture the solution accurately even if the time step size τ is much larger than the sampled wavelength at $O(\varepsilon^2)$, where $0 < \varepsilon \leq 1$ is a small parameter inversely proportional to the speed of light.

It is found out that S_1 and S_2 both exhibit uniform $1/2$ order convergence. This order could even be improved under non-resonant time step sizes, to 1 for S_1, and to $3/2$ for S_2. It is also noted that super-resolution is still valid for higher order splitting methods.

Furthermore, the error bounds of four frequently-used finite difference time domain (FDTD) methods for the Dirac equation in the semiclassical regime are rigorously studied. This regime involves a small dimensionless parameter $0 < \delta \leq 1$ representing the scaled Planck constant, and there are highly oscillatory propogating waves with wavelength $O(\delta)$ in both time and space of the solution. It is proved that the FDTD methods share the same error bounds, which are explicitly related to time step size τ, mesh size h, as well as the small parameter δ. Based on the error bounds, in the semiclassical regime, i.e. $0 < \delta \ll 1$, to obtain 'correct' numerical solutions, the δ-scalabilities $\tau = O(\delta^{3/2})$ and $h = O(\delta^{3/2})$ are required. Numerical tests are carried out to support the error estimates.

Fast convolution-type nonlocal potential solvers in nonlinear Schrödinger equation and lightning simulation

Yong Zhang

Tianjin University, China

ABSTRACT

Convolution-type potential are common and important in many science and engineering fields. Efficient and accurate evaluation of such nonlocal potentials are essential in practical simulations. In this talk, I will focus on those arising from quantum physics/chemistry and lightning-shield protection, including Coulomb, dipolar and Yukawa potential that are generated by isotropic and anisotropic smooth and fast-decaying density, as well as convolutions defined on a one-dimensional adaptive finite difference grid. The convolution kernel is usually singular or discontinuous at the origin and/or at the far field, and density might be anisotropic, which together present great challenges for numer-ics in both accuracy and e?ciency. The state-of-art fast algorithms include Wavelet based Method(WavM), kernel truncation method(KTM), NonUniform-FFT based method(NUFFT) and Gaussian-Sum based method(GSM). Gaussian-sum/exponential-sum approximation and kernel truncation technique, combined with finite Fourier series and Taylor expansion, finally lead to a $O(NlogN)$ fast algorithm achieving spectral accuracy. Applications to NLSE, together with a useful recently-developed sum-of-exponential algorithm are reviewed. Tree-algorithm for computing the one-dimensional convolutions in lighting-shield simulation is also covered as the last application.

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