Tensor Networks: Fundamental theorems and applications

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Abstract

Certain Quantum Many-body states can be efficiently described in terms of tensor networks. Those include Matrix Product States (MPS), Projected Entangled-Pair Etates (PEPS), or the Multi-scale Entanglement Renormalization Ansatz (MERA). Some of them play an important role in quantum computing, error correction, or in the description of topological order in condensed matter physics, and are widely used in computational physics. In this talk I will briefly review one of the basic results in the theory of tensor networks and explain some of its applications in the classification of gapped phases in spin systems, the description of lattice gauge theories, or the characterization of quantum cellular automata. This basic result addresses the following question: If two different tensors generate the same many-body state, how are they related to each other?

*Speaker

Variational and Parquet-diagram theory for strongly correlated normal and superfluid systems

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Abstract

We develop the variational and correlated basis functions/parquet-diagram theory of strongly interacting normal and superfluid systems. The first part of this contribution is devoted to highlight the connections between the Euler equations for the Jastrow-Feenberg wave function on the one hand side, and the ring, ladder, and self-energy diagrams of parquet-diagram theory on the other side. We will show that these subsets of Feynman diagrams are contained, in a local approximation, in the variational wave function, and the approximations to come from one to the other description are the same in all channels.

In the second part of this work, we derive the fully optimized Fermi-Hypernetted Chain (FHNC-EL) equations for a superfluid system. Close examination of the procedure reveals that the naïve application of these equations exhibits spurious unphysical properties for even an infinitesimal superfluid gap. We will conclude that it is essential to go beyond the usual Jastrow-Feenberg approximation and to include the exact particle-hole propagator to guarantee a physically meaningful theory and the correct stability range.

We will then implement the various (variational and local parquet) method and apply it to neutron matter and low density Fermi liquids interacting via a family of Lennard-Jones potentials. We will show that the consistent treatment of the equation of state and the microscpic dynamics is essential for a correct interpretation of the results.

*Speaker

Quantum Phase Diagram of a Frustrated Spin-1/2 Heisenberg Antiferromagnet on a Square-Lattice Bilayer

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Abstract

One of the most powerful *ab initio* formulations of microscopic quantum many-body theory is the coupled cluster method (CCM) [1]. It has been very successfully applied to many strongly correlated systems, spanning areas such as quantum field theory, nuclear and subnuclear physics, condensed matter physics, quantum optoelectronics, and quantum chemistry. The CCM has yielded numerical results among the most accurate available for an incredibly wide range of both finite and extended physical systems. These range from atoms and molecules of interest in quantum chemistry, where the method is now the "gold standard", to atomic nuclei; from the electron gas to dense nuclear and baryonic matter; and from models in quantum optics, quantum electronics, and solid-state optoelectronics to field theories of strongly interacting nucleons and pions [2]. This widespread success for both finite and extended systems defined on a spatial continuum has led more recently to applications to corresponding systems defined on an extended regular spatial lattice. We have shown how the systematic inclusion of multispin correlations for a wide variety of quantum spin-lattice problems can be efficiently and effectively implemented with the CCM [3].
We now apply the CCM to very high orders to study the zero-temperature phase diagram of the spin-half J_1–J_2–$J\_1\hat{}\{\mathrm{perp}\}$ model on an AA-stacked square-lattice bilayer [4]. Both nearest-neighbour (NN) and frustrating next-nearest-neighbour Heisenberg exchange interactions, of strengths $J\_1 > 0$ and $J\_2 = \alpha J\_1 > 0$ respectively, are included in each layer. The two layers are coupled via a NN interlayer Heisenberg exchange interaction with a strength $J\_1\hat{}\{\mathrm{perp}\} = \delta J\_1$. The magnetic order parameter M (viz., the sublattice magnetization) and the spin gap Δ are calculated directly in the thermodynamic (infinite-lattice) limit for the two cases when both layers have antiferromagnetic (AFM) ordering of either the Néel or the striped kind, and with the layers coupled so that NN spins between them are either parallel (when $\delta < 0$) or antiparallel (when $\delta > 0$) to one another. Calculations are performed at nth order in a well-defined (LSUBn) sequence of approximations, which exactly preserve both the Goldstone linked cluster theorem and the Hellmann-Feynman theorem, with $n \leq 10$. The sole approximation made is to extrapolate such sequences of nth-order results for M and Δ to the exact limit, $n \to \infty$. Such extrapolations allow us to calculate the full phase boundaries of the two collinear AFM phases in the α-δ half-plane with $\alpha > 0$ with very high accuracy.

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Certified Quantum Measurements: Detection of Majorana Fermions

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In the quantum information literature, self-testing refers to the action of uniquely determining a quantum state based solely on the statistics of measurement outcomes and minimal assumptions. These quantum self-testing protocols are more stringent than well-known Bell tests. While violation of a Bell inequality for a bipartite system establishes that its quantum state is entangled, it cannot certify, for instance, that its quantum state is maximally entangled. We extend the self-testing technique used in Quantum Key Distribution to certification of quantum measurements in various physical scenarios. In particular, and because of its importance for realizing the topological qubit, we present a quantum self-testing protocol to certify measurements of fermion parity involving Majorana modes. We derive rigidity conditions for ideal statistics that imply anticommutativity of Majorana fermion and parity operators, a necessary prerequisite for Majorana detection. To assess robustness of our results to experimental errors, rigorous lower bounds to state and observable fidelities, linear in the error, are obtained. For convenience, we propose to analyze experimental outcomes in terms of an entanglement witness W satisfying a contextuality inequality. Its violation contradicts local realism and the departure from the maximum ideal value $\langle W\rangle = 5$ indicates the degree of confidence in the detection of Majorana fermions.

Excitations of correlated nucleons within a higher-order random-phase approximation

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Abstract

The second random-phase approximation (SRPA) is an extension of the standard random-phase approximation (RPA) where two particle-two hole (2p2h) configurations are included together with the RPA one particle-one hole (1p1h) configurations. This beyond mean-field model allows for reliable quantitative predictions to describe the widths and the fragmentation of excited states, due to the coupling between 1p1h and 2p2h elementary configurations.

I will present the formal developments and the practical applications that we have realized in the last years. One important recent achievement was the development of a substantial implementation of the SRPA model, based on a subtraction procedure. This subtraction method was tailored to cure double-counting problems encountered when effective interactions are used in beyond mean-field models, within energy-density functional theories. At the same time, this procedure cures all the instabilities and divergences present in the standard SRPA and produces renormalized single-particle excitation energies. The subtracted SRPA (SSRPA) provides a well-defined theoretical framework for quantitative predictions on nuclear excitation spectra.

Several applications to low- and high-lying states will be shown: for instance, the analysis of dipole excitations in ^{48}Ca and a systematic study on giant quadrupole resonances in medium-mass and heavy nuclei (centroids and widths). A related topic will be discussed, namely the modification (enhancement) of the effective masses induced by the beyond-mean-field SSRPA effects. Finally, low-lying monopole excitations will also be described and a link with the incompressibility modulus of asymmetric nuclear matter will be illustrated.

*Speaker

Mixing time dependent mean-field trajectories to describe the dynamics of collisions between two superfluid nuclei

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Abstract

The highly accurate measurements [1] of the two nucleons transfer in low energy collision between atomic nuclei recently led to a surge of interest on the role of pairing correlations during this many body reaction. In nuclear physics, it is common to treat these correlations with the Hartree-Fock-Bogoliubov (HFB) theory, also known as Bogoliubov-de-Gennes theory, which accurately grasps superfluidity by explicitly breaking the particle number symmetry. However, a precise description of phenomena like the particle transfer during nuclear collisions can only be achieved by considering quantum states with good particle number. The theoretical challenge is then to develop approaches capable of determining the real time evolution of such complex states without a prohibitive numerical cost. We recently took a first step toward this objective by proposing a semi-classical approach to recombine an ensemble of time dependent HFB states [2]. Going further, we are now investigating a fully quantum mixing of the same ensemble of mean-field trajectories that takes properly into account the interferences arising in the dynamics [3].
In this talk, I will first review some recent results on the topic of the transfer of particles in sub-barrier collisions between open shell nuclei. I will insist on the role of the pairing residual interaction on the enhancement factor between the one and two particle exchange channel, and highlight the shortcoming of the time dependent HFB approach when describing these reactions. I will then emphasize our recent attempts to treat the collisions between superfluid nuclei within a semi-classical and fully quantal evolution of an ensemble of time dependent HFB trajectories. Finally, the possibility to apply such methods to describe a realistic nuclear collision will be discussed. [1] D. Montanari, L. Corradi, S. Szilner, *et al.*, Phys. Rev. C **93**, 054623 (2016).

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*Speaker

Itinerant magnetism: the importance of many-body correlations

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Abstract

Do electrons magnetise and become ferromagnetic just because of their repulisve Coulomb interaction, as predicted in the most basic model by Stoner?
We have adressed this question performing Variational and Diffusion Monte Carlo calculations for the homogeneous electron gas at low densities where iterative backflow wave functions provide a systematic way to reduce the fixed-node bias.
Our calculations imply that iterinant fermomagnetim of delocalized electrons without lattice or bandstructure is supressed due to many-body correlations as speculated already by Wigner and a possible ferromagnetic transition lowering the densities is preceeded by the formation of the Wigner crystal. Similar bevavior has been observed for different model systems with spin-independent interparticle interactions, e.g. hard-core like interaction as in liquid helium, or repulsive dipolar interaction between fermions in two dimensions, so that many-body correlations generally supress itinerant magnetism in homogeneous systems.

*Speaker

Complex Langevin in Nonrelativistic Rotating Bosonic Systems

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Abstract

Quantum field theories with a complex action suffer from a sign problem in stochastic nonperturbative treatments, making many systems of great interest – such as polarized or mass-imbalanced fermions and QCD at finite baryon density – extremely challenging to treat numerically. Another such system is that of bosons at finite angular momentum; experimentalists have successfully achieved vortex formation in supercooled bosonic atoms, and have measured quantities of interest such as the moment of inertia. However, the rotation results in a complex action, making the usual numerical treatments of the theory unusable. In this work, we use complex stochastic quantization to calculate basic properties of interacting bosons at finite angular momentum.

*Speaker

First principles understanding of nuclear structure in the medium mass region

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Abstract

This talk will mainly review the status of computation of finite atomic nuclei based on self-consistent Green's function theory (SCGF). The SCGF method is one of the few polynomial scaling approaches that allow ab initio computations for nuclear masses in the range A=16-140, and it was the first of such methods to be extended to open-shell nuclei. However, the Gorkov-SCGF formalism (that applies to open shells) was only developed to second order in self-energies until very recently. This talk will present for the first time the so-called Gorkov-ADC(3) formalism, which brings the Gorkov self-energy up to the same level of accuracy of its closed-shell (Dyson) counterpart. Hence, allowing a full all-order resummation of the self-energy that includes particle-vibration couplings and pairing also for open-shells.
Recent ab initio studies based on SCGFs include systematic studies of chiral interactions along complete isotopic chains of oxygen, the calcium region (Ar to Ti), nickel and tin. I will discuss systematics of radii and binding energies, results for optical potential, as well as application of the resulting spectral function to electroweak scattering.

*Speaker

Some theoretical results for twisted bilayer graphene near magic angle†

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Abstract

When the relative rotation between two sheets of graphene is set to be close to special angles (referred to in the literature as "magic angles"), the low-energy effective theory features Dirac fermions with very flat bands. Interest in understanding the competing mechanisms at play was reignited recently with the experimental observations of superconductivity and strongly correlated insulating phases in such twisted moiré heterostructures. In this talk, I will first discuss the effect of electron-electron interactions on Dirac fermions. Using a combination of nonperturbative numerical and analytical techniques, I will show that the properties of interacting Dirac fermions are governed by two very different fixed points: a Gross-Neveu phase transition to a Mott insulator controlled mostly by the contact interaction, and a semi-metallic state with a diverging Fermi velocity dependent only on the long-range part of the Coulomb interaction [1]. While the various experimental realizations of Dirac fermions span the crossover between these two regimes, changing the twist angle allows one to controllably tune from one regime to another. In the semi-metallic regime, I will show that there is a universal square-root renormalization of the band anisotropy [2], implying that the Dirac fermions in interacting twisted bilayer graphene are more isotropic than predicted from the non-interacting moiré band theory. Using a Boltzmann-RPA theory, I will argue that for small twist angle, gauge phonons dominate the transport properties [3]. For example, at large twist angle, gauge phonons only dominate over charged impurities only for $T > 500$ K, while close to magic angle, this crossover temperature drops to $T_{cr} \sim 5$ K. Finally, close to the Mott insulating regime, starting from a real-space cluster interaction, and using a mean-field analysis, we propose a strong-coupling t-J-D model where fluctuations of the anti-ferromagnetic order mediates superconducting paring. The properties of this model can be solved self-consistently to reveal several proposed experimental signatures including chiral d-wave superconductivity and Majorana edge modes [4].

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Current fluctuations in an out-of-equilibrium Kondo quantum dot

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Abstract

Coulomb interactions play a crucial role in low-dimensionnal systems as they notably affect the I-V characteristic and contribute to time-fluctuations of the electrical current. We have developed a new approach to derive these fluctuations in a Kondo quantum dot without heavy calculations thanks to a careful analysis of all the processes that contribute to the emission noise [1,2]. These processes involve the transfer of an electron-hole pair from one reservoir of electrons to another reservoir of electrons where it emits energy after recombination. We have checked that our results are in agreement with the ones obtained using a more pedestrian approach based on the Keldysh technique where the out-of-equilibrium Green functions need to be calculated. The final analytical expression we obtain for the noise can be seen as the analog of the Meir-Wingreen formula for the current [3] where the inelastic scattering contributions are including via the introduction of an effective transmission coefficient.

To make a qualitative comparison of our theoretical results with experiments, we have treated the Coulomb interactions by solving the self-consistent equations of motion for the Green functions [4,5]. It allows us to describe the Kondo ridge that appears in the Coulomb blockade profile of the differential conductance [6] and the Kondo peak that appears in the derivative of the noise versus voltage at a voltage close to the measurement frequency, in full agreement with recent experiments in a carbon nanotube quantum dot [7]. Moreover, we find that the noise derivative cancels at voltage smaller than the frequency, again in agreement with experiments, and that the cross-correlator in between two distinct reservoirs becomes positive (bosonic statistics) in the presence of interactions, whereas it stays negative (fermionic

*Speaker

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Strong Correlations in Multiorbital System: More is different (and selective)

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Abstract

A huge effort has been devoted to solve the single-band Hubbard model, which is widely believed to be the main building block for the understanding of high-temperature superconductors in doped Mott insulators. The last years have however proposed many examples of multicomponent strongly correlated systems which open completely new scenarios and lead to the emergence of paradigms and concepts such as the 'Hund's metal' or 'Orbital-selective Mott transitions'.
In this talk I will present a comprehensive picture of strong correlations in multiorbital systems focusing on some important aspects which arise in the presence of a moderate Hund's exchange coupling favoring high-spin states, even if similar physics can also be realized for other systems and models, such as multicomponent cold atom fermions [1]

(i) The physical origin of the the Hund's metal, a strongly correlated metal which is however extremely resilient to Mott localization. I will show that, for integer fillings different from global half-filling, the Hund's coupling favors high-spin states which allow for a delocalization of the carriers despite the large value of the interactions [2]

(ii) The link between the Hund's physics and orbital-selective correlations. In this regard I will show that the Hund's coupling leads to an effective decoupling between orbital which allows for a strong differentiation of the electronic properties of different orbitals, even when the differences in the bare Hamiltonian are small [3]

(iii) The relationship between orbital-selective correlations and the phase diagram of iron-based superconductors [4], which will provide a tantalizing new analogy between iron-based superconductors and cuprates

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