Novel finite range interactions and linear response theory

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Abstract

The tool of choice to describe properties of nuclei from light to heavy and from drip-line to drip-line is the nuclear energy density functional theory. The most popular versions of this theory use functional derived from phenomenological nuclear interactions as Skyrme or Gogny. Despite their success, both families of interactions present clear limits in reproducing nuclear observables.
In a recent article of the Lyon-York-Valencia collaboration, we have explored extensions of these interactions either adding new gradient terms (for the Skyrme case) or adding new Gaussians (for the Gogny case). In both cases, the objective is to introduce extra parameters and, thus, flexibility during the optimisation procedure.

In my talk, I will present a new Gogny-type interaction obtained using three Gaussians and physically motivated ranges. I will also illustrate the new fitting protocol we have developed to overcome the problem of finite-size instabilities. Thanks to the linear response theory, we are now able to identify region of unphysical parameters by studying the behaviour of excited states in the infinite nuclear medium.

*Speaker

Pairing in dilute neutron matter

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Abstract

Superfluidity of dilute neutron matter has important consequences for astrophysical observables such as neutron-star cooling curves and glitches (sudden increase of the rotation frequency of a pulsar). Although it has been a subject of extensive studies for decades, there is still no consensus in the literature on the density dependence of the pairing gap and of the critical temperature. A major uncertainty comes from the induced interactions, also called screening corrections in analogy to the Debye screening of the Coulomb interaction. While at extremely low densities these effects should reduce the critical temperature by a factor of 0.45 (Gor'kov-Melik-Barkhudarov), quantum Monte-Carlo calculations indicate a weaker suppression at the lowest densities relevant for neutron stars. I will discuss that the net effect of the induced interaction is the result of a strong cancellation between the repulsive exchange of spin waves (screening) and the attractive exchange of density waves (anti-screening). While previous studies relied on the (lowest-order) Landau approximation, it turns out to be very important to describe the exchanged excitations within the full RPA, especially at higher densities [1]. At lower densities, neutron matter is close to the so-called BEC-BCS crossover regime. As is well known, e.g. from ultracold atoms, this requires to take into account that there are already non-condensed pairs above the critical temperature (Nozières-Schmitt-Rink). Including simultaneously the effects of non-condensed pairs and induced interactions, it turns out that in neutron matter, the effects from the BCS-BEC crossover physics are much weaker than those of the induced interactions [2]. [1] S. Ramanan and M. Urban, in preparation; [2] S. Ramanan and M. Urban, PRC 98, 024314 (2018).

*Speaker

Lepton-nucleus interactions from quantum Monte Carlo

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Abstract

The development of the world-wide accelerator-based neutrino-oscillation program has been a springboard for the advancement of the theoretical description of lepton interactions with nuclei. I will present first-principle Green's function Monte Carlo calculations of electron- and neutrino-nucleus scattering in the quasielastic region. Particular emphasis will be devoted to the role played by realistic nuclear interactions and on the transverse enhancement brought about by two-body currents. I will also discuss possible approaches suitable to describe lepton-nucleus interactions at higher energies retaining an accurate description of the initial target state.

*Speaker

Self-consistent multiparticle-multihole configuration mixing description of atomic nuclei

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[4]École normale supérieure - Cachan – École normale supérieure de Cachan - ENS Cachan – France

Abstract

The self-consistent multiparticle-multihole configuration mixing approach is an adaptation to nuclei of the method known as 'Multi-Configuration Hartree-Fock or 'Multi-Configuration Self-Consistent Field" which have been used for decades in the fields of atomic physics and quantum chemistry. This method considers the nuclear wave function as a general superposition of Slater determinants. Both the expansion coefficients of the many-body state and the single-particle orbitals are determined simultaneously via a variational principle which ensures full self-consistency between correlations and underlying mean-field picture.
A few years ago, we have applied for the first time the full formalism of this approach to the description of a few light and mid-mass nuclei [1,2]. While these first applications led to an encouraging description of ground- and excited-state properties, they have been obtained using an effective phenomenological interaction (the Gogny force). In order to go towards an 'ab-initio' description of nuclei, we have started implementing an interaction derived from chiral effective field theory. We will show preliminary calculations of light nuclei and make comparisons to results obtained in the framework of quantum Monte-Carlo with the same interaction.
C. Robin, N. Pillet, D. Peña Arteaga and J.F. Berger, PRC 93, 024302 (2016). [2] C. Robin, N. Pillet, M. Dupuis, J. Le Bloas, D. Peña Arteaga and J.F. Berger, PRC 95 044315 (2017).

*Speaker

The time-dependent two-particle reduced density matrix method: theory and applications

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Abstract

Describing correlated quantum many-body systems belongs to the greatest challenges of current theoretical physics. This is in particular the case for driven time-dependent systems beyond linear response. While there is a plethora of methods to describe ground state properties of many-body quantum systems ranging from wave function based methods to density based methods, their generalization to time-dependent problems is by far not straightforward. Two of the most widely used methods, multi-configurational time-dependent Hartree-Fock (MCTHDF, or related) and time-dependent density functional methods (TDDFT) can be viewed as two extrema in tackling the problem: While MCTDHF allows, in principle, for an exact treatment if enough orbitals are used, the factorial scaling with particle number restricts practical applications to systems with very few electrons. TDDFT allows for the treatment of hundreds of particles due to its favorable scaling with particle number. The drawback lies in the drastic approximations of the correlation Hamiltonian which have no universal validity and do not allow for systematic improvement. We attempt to bridge the gap between TDDFT and MCTDHF by developing a time-dependent quantum many-body theory which uses the two-particle reduced density matrix (2RDM) as the fundamental variable. In doing so we fully incorporate two-particle correlations and truncate at the level of three-particle correlations. Avoiding the wave function leads to a polynomial scaling with particle number, but comes at the price of dealing with the N-representability problem which in the case of the 2RDM is more severe than for the one-particle reduced density matrix or the density. In my talk I will give an overview of our method and explain how the N-representability problem can be overcome in numerical simulations. Finally, I will report on applications of the method to several driven quantum system, i.e. laser-driven multi-electron atoms, and dynamics of ultra-cold fermionic atoms in optical lattices after a quench.

*Speaker

Density Matrix Simulations of Many-Body Effects in Femtosecond X-Ray Absorption

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Abstract

Density matrix theory to simulate the dynamics of core-electron excitation in solids interacting with a femtosecond x-ray laser pulse is formulated with the time-dependent unrestricted Hartree-Fock (UHF) equations [1]. The one-electron reduced density matrix (RDM) is expressed as a sum of a rapidly oscillating part relevant to x-ray transitions and a slowly varying part describing the response of valence electrons to core holes. The equations of motion for the RDM are solved numerically for a single-shot x-ray pulse. Time evolutions of the off-diagonal elements of the RDM yield the induced electric polarization, whose Fourier transform gives the complex susceptibility relevant to x-ray absorption near-edge spectra (XANES). It is shown that the self-energy matrix, accounting for an electron-hole attractive interaction, gives rise to (i) a renormalization of virtual-orbital energy levels and (ii) an excitonic enhancement of XANES; the latter stems from a mixing of different valence components of RDM and is referred to as the Fermi-edge singularity in the theory of metals [2]. A set of matrix elements of electric dipole transitions and electron-hole interactions are evaluated for a model cluster with the quantum-chemical molecular-orbital method adopting the neglect of diatomic differential overlap approximation, where atomic UHF wavefunctions of valence and low-lying virtual orbitals are used as basis sets. Numerical results for K-shell excitation of copper are presented. Nonlinear effects on XANES, expected in high-intensity x-ray free-electron laser experiments, will also be discussed.

H. Kitamura, Int. J. Quant. Chem. **114**, 1518 (2014); **117**, 25442 (2017)

G.D. Mahan, Phys. Rev. **163**, 612 (1967)

*Speaker

Ab initio field-theory computations in many-fermion systems: beyond ground-state properties

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[2]Department of Physics, College of William Mary – United States

Abstract

Development over the past decade in the ground-state auxiliary-field quantum Monte Carlo (AFQMC) approach has allowed accurate computations in a broad array of systems ranging from Hubbard-like models, ultracold Fermi gases, to solids and quantum chemistry. Here I will discuss recent progress in generailizing the approach to non-zero temperatures. Two bottlenecks had to be removed. The first is the sign or phase problem which appears in most cases, similar to ground-state calculations. The second is the unfavorable scaling of finite-temperature, grand-canonical computations as $N\hat{}3$ (N is the size of the lattice or basis set) in contrast with $N*M\hat{}2$ in ground-state computations (M is the number of fermions), which is a major obstacle in any realistic calculations aiming to describe the continuum limit, since N/M is large and needs to be extrapolated to infinity for convergence. We remove the sign or phase problem by constraining the path-integrals in field space with a gauge condition; a self-consistent procedure is formulated to improve the accuracy of the constraint iteratively. We then introduce a systematically controllable low-rank factorization which changes the scaling of the computations to $N*M\hat{}2$. The method is applicable to both models and real materials. Results will be presented on magnetic and stripe orders in the repulsive Hubbard model, as well as pairing and other properties in the strongly interacting two-dimensional Fermi gas as a function of temperature.

*Speaker

Finite-range effects in ultracold Bose-Bose mixtures

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[3]Faculty of Science, University of Split, Ruera Boškovića 33, HR-21000 Split, Croatia – Croatia

Abstract

We have studied dilute Bose-Bose mixtures of atoms with attractive interspecies and repulsive intraspecies interactions using quantum Monte Carlo methods at $T=0$. Using a number of models for interactions, we determine the range of validity of the universal equation of state of the symmetric liquid mixture as a function of two parameters: the s-wave scattering length and the effective range of the interaction potential. It is shown that the Lee-Huang-Yang correction is sufficient only for extremely dilute liquids with the additional restriction that the range of the potential is small enough. Based on the quantum Monte Carlo equation of state we develop a new density functional which goes beyond the Lee-Huang-Yang term and use it together with local density approximation to determine density profiles of realistic self-bound drops.

*Speaker

Comparing different t-matrix approaches for a Fermi gas throughout the BCS-BEC crossover

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[2]INFN, Sezione di Perugia, Perugia (PG) – Italy
[3]CNR-INO, Sede di Firenze (FI) – Italy

Abstract

Different many-body diagrammatic theories, all based on the t-matrix self-energy but distinct for the degree of self-consistency, have been proposed in the literature to describe the normal phase of a Fermi gas undergoing the BCS-BEC crossover. In this talk, I will present a comprehensive comparison of the results obtained with the above different t-matrix approaches for both thermodynamic and dynamic quantities [1]. The high accuracy of our implementation of the different schemes throughout the BCS-BEC crossover allows us to analyze also fine details like the residual interaction between the composite bosons in the BEC limit (correcting some statements in the literature), or to point out the inadequacy of certain approximations normally used in the implementation of some of the above schemes. Finally, I will discuss the results of a recent experiment aimed at measuring the number of fermion pairs in the normal phase of an ultra-cold Fermi gas [2] in the light of the above t-matrix approaches.

M. Pini, P. Pieri, G. Calvanese Strinati, Physical Review B **99**, 094502 (2019).

Paintner et al., arXiv:1803.10598 (Physical Review A, in press).

*Speaker

Precision thermodynamics of the homogeneous unitary Fermi gas

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[2]Central Washington University – United States

Abstract

The cold atomic unitary Fermi gas (UFG) is a strongly correlated system which can be realized experimentally and sits in the middle of the BCS-BEC crossover where the s-wave scattering cross section is maximized. This system is known to undergo a phase transition to a superfluid below a certain critical temperature. However, accurate calculation of thermodynamic properties of the UFG across the phase transition has been a major challenge. Specifically, the temperature dependence of the contact, which measures the pair correlations at short distances and appears in a number of exact relations, widely differs among various calculations. Additionally, the extent and nature of a pseudogap regime above the critical temperature for superfluidity is still debated in the literature, both theoretically and experimentally. We present recent results for the homogeneous UFG using finite-temperature auxiliary-field quantum Monte Carlo (AFMC) methods within the canonical ensemble on a spatial lattice. In particular, we determine the temperature dependence of the contact in the continuum limit by performing simulations for multiple filling factors and extrapolating to zero filling factor. We compare our AFMC results with recent precision experiments. We also present results for a model-independent pairing gap of the UFG and discuss possible pseudogap signatures in these results. Our canonical ensemble methods enable a direct calculation of this pairing gap without the need for a numerical analytic continuation that is required in quantum Monte Carlo calculations of the spectral function.

*Speaker

Cluster formation in nuclear systems

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Abstract

Light clusters (mass number A $\leq$ 4) in nuclear matter at subsaturation densities are described
using a quantum statistical approach to calculate the quasiparticle properties and abundances of
light elements. Virial coefficients are derived from continuum contributions
to the partial densities which depend on temperature, densities, and total momentum. The Pauli
blocking is modified taking correlations in the medium into account. Both effects of continuum
correlations lead to an enhancement of cluster abundances in nuclear matter at higher densities.
The properties of light clusters and continuum correlations in dense matter are of interest for nuclear
structure calculations, heavy ion collisions, and for astrophysical applications such as the formation
of neutron stars in core-collapse supernovae.

*Speaker

The Casimir-like effect in a one-dimensional Bose gas

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Abstract

In the most basic formulation, the electromagnetic Casimir effect manifests as the interaction between uncharged conducting objects that are placed in a vacuum. More generally, the Casimir-like effect denotes an induced interaction between external bodies in a fluctuating medium. We study the Casimir-like interaction between two impurities embedded in a weakly interacting one-dimensional Bose gas. We develop a theory based on the Gross-Pitaevskii equation that accounts for the effect of quantum fluctuations [1]. At separations shorter than the healing length of the system, the induced interaction between the impurities decays exponentially with the distance. This is a classical result that can be understood using the mean-field Gross-Pitaevskii equation. At separations r longer than the healing length, the induced interaction crosses over into 1/r^3 dependence due to the quantum fluctuations. Finite temperature destroys the quasi-long-range order of the Bose gas and, accordingly, the induced interaction becomes exponentially suppressed beyond the thermal length. We obtain analytical expressions for the induced interaction at zero and finite temperature that are valid at arbitrary distances [1, 2]. If one of the impurities is infinitely strong, the induced interaction has different dependence and decays as 1/r^2 at zero temperature [3].

Benjamin Reichert, Zoran Ristivojevic, and Aleksandra Petkovic, New J. Phys. **21,** 053024 (2019); https://doi.org/10.1088/1367-2630/ab1b8e

Benjamin Reichert, Aleksandra Petkovic, and Zoran Ristivojevic, Phys. Rev. B **99,** 205414 (2019).

Benjamin Reichert, Zoran Ristivojevic, and Aleksandra Petkovic, in preparation.

*Speaker