Talks

Calculation Of Generalized Pauli Constraints

Murat Altunbulak
Dokuz Eylül University Izmir

In the talk I am planning to explain two different solutions of N-representability problem and then give the algorithm to calculate GPCs. After that, as examples I will show my calculations for 3 fermions systems of rank 6 and 7 for which the algorithm works smoothly. For higher rank systems we need an additional tool which I will try to explain also.

Quasipinning and Extended Hartree-Fock Method based on Generalized Pauli Constraints

Carlos Benavides-Riveros
University of Halle

It is now known that fermionic natural occupation numbers (NON) do not only obey Pauli's exclusion principle but are even stronger restricted by the so-called generalized Pauli constraints (GPC). So far, the nature of these constraints has been explored in some systems: a model of few spinless fermions confined to a one-dimensional harmonic potential, the lithium isoelectronic series and ground and excited states of some three-, four- and five-electron atomic and molecular systems. Whenever given NON lie on the boundary of the allowed region the corresponding N-fermion quantum state has a significantly simpler structure. By employing this structure a variational optimization method for few fermion ground states is elaborated. We quantitatively confirm its high accuracy for systems with the vector of NON in a small distance to the boundary of the polytope. In particular, we derive an upper bound on the error of the correlation energy given by the ratio of the distance to the boundary of the polytope and the distance of the vector of NON to the Hartree-Fock point. Moreover, these geometric insights shed some light on the concept of active spaces, correlation energy, frozen electrons and virtual orbitals.

This talk is based on
C. L. Benavides-Riveros and C. Schilling, Z. Phys. Chem. (in press).
C. L. Benavides-Riveros and M. Springborg, Phys. Rev. A 92, 012512 (2015).
C. L. Benavides-Riveros, J. M. Gracia-Bonda and M. Springborg, ArXiv:1409.6435 (2014).
C. L. Benavides-Riveros, J. M. Gracia-Bonda and M. Springborg, Phys. Rev. A 88, 022508 (2013).
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Openness of a Many-fermion Quantum System from the Generalized Pauli Principle

Romit Chakraborty
University of Chicago

Information about the interaction of a many-electron quantum system with its environment is encoded within the one-electron density matrix (1-RDM). While the 1-RDM from an ensemble many-electron quantum system must obey the Pauli exclusion principle, the 1-RDM from a pure quantum system must obey additional constraints known as the generalized Pauli conditions [1-4]. By examining the 1-RDM's violation of these generalized Pauli conditions, we obtain a sufficient condition at the level of a single electron for a many-electron quantum system's openness [2]. As the system interacts with the environment, the more stringent generalized Pauli conditions relax to the Pauli principle, the nature and extent of this relaxation serving to quantify the degree openness of a many-electron quantum system [5]. In an application to photosynthetic light harvesting we show that the interaction of the system with the environment (quantum noise) relaxes significant constraints imposed on the exciton dynamics by the generalized Pauli conditions. This relaxation provides a geometric (kinematic) interpretation for the role of noise in enhancing exciton transport in quantum systems [2, 5].

[1] R. Chakraborty and D. A. Mazziotti, Phys. Rev. A 89, 042505 (2014)
[2] R. Chakraborty and D. A. Mazziotti, Phys. Rev. A 91, 010101 (2015)
[3] R. Chakraborty and D. A. Mazziotti, Int. J. Quantum Chem. 115, 1305 (2015)
[4] R. Chakraborty and D. A. Mazziotti, Int. J. Quantum Chem. (2016, in press)
[5] R. Chakraborty and D. A. Mazziotti, (2016, in preparation)

Pinning of Fermionic Occupation Numbers

Matthias Christandl
University of Copenhagen

The Pauli exclusion principle is a constraint on the natural occupation numbers of fermionic states. It has been suspected since at least the 1970's, and only proved very recently, that there is a multitude of further constraints on these numbers, generalizing the Pauli principle. Here, we provide the first analytic analysis of the physical relevance of these constraints. We compute the natural occupation numbers for the ground states of a family of interacting fermions in a harmonic potential. Intriguingly, we find that the occupation numbers are almost, but not exactly, pinned to the boundary of the allowed region (quasi-pinned). The result suggests that the physics behind the phenomenon is richer than previously appreciated. In particular, it shows that for some models, the generalized Pauli constraints play a role for the ground state, even though they do not limit the ground-state energy. Our findings suggest a generalization of the Hartree-Fock approximation.

Quantum Marginal Problem and Generalized Pauli Constraints

David Gross
University of Cologne

I will give an introduction to the univariate quantum marginal problem using an elementary mathematical point of view. In particular, I will explain how extremality of the local spectrum carries structural information about the global wave function. The talk will also give some quantum information background, touching e.g. on the computational complexity of general quantum marginal problems and relations to entanglement.

Tba

Duncan Haldane
Princeton

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Physical Meaning of Natural Orbitals and Natural Occupation Numbers

Nicole Helbig
FZ Jülich

By their definition, the natural orbitals and occupation numbers are the eigenfunctions and eigenvalues of the one-body reduced density matrix. This raises the question to which extend one can assign a physical interpretation to them, e.g. if the degeneracies in the occupation numbers reflect the symmetries of the system or if an excitation can be described by simply changing the occupations of the ground-state natural orbitals. We use exactly solvable model systems to investigate the suitability of natural orbitals as a basis for describing many-body excitations. We analyze to which extend the natural orbitals describe both bound as well as ionized excited states and show that depending on the specifics of the excited state the ground-state natural orbitals yield a good approximation or not. We show that the success of reduced density-matrix functional theory in describing molecular dissociation lies in the flexibility provided by fractional occupation numbers while the role of the natural orbitals is minor.

Introduction and Overview of the Reduced Density Matrix Functional Theory

Nektarios N. Lathiotakis
National Hellenic Research Foundation

Reduced density matrix functional theory (RDMFT) is a theoretical framework for approximating the many-electron problem. In RDMFT, the fundamental quantity is the one-body,

reduced, density matrix (1RDM) which plays the same role as the electronic density in density functional theory. Gilberts theorem stands in the foundations of RMDFT, and guarantees that every observable for the ground state is a functional of the 1RDM. This allows for approximating the total energy in terms of the 1RDM and minimizing it under certain conditions for the N-representability of the 1RDM. So far, in almost all practical applications Coleman's ensemble N-representability conditions are employed which are very simple for fermionic systems. They concern the eigenvalues of the 1RDM, known as natural occupations, restricting then in the range between zero and one and their sum which is fixed to be the total number of electrons.

A certain advantage of tackling the many electron problem in this way is that the kinetic energy of the system is a simple expression in terms of the 1RDM, i.e. there is no need for a fictitious non interacting system like the Kohn-Sham system in DFT. Thus, fractional occupations enter the theory in a natural way allowing to construct simple approximations that describe accurately electronic correlations. A central and simple functional in RDMFT is the Mler functional, a relatively simple modification of the expression of the total energy in Hartree-Fock theory. This functional was shown to reproduce the correct physical picture of the dissociation of the Hydrogen molecule, although it is known to overestimate substantially the correlation energy. Several approximations were introduced in the last couple of decades, many of which are corrections to the Mller functional, and were proven to describe accurately such diverse effects and quantities like static correlations and the band gaps of materials. Unfortunately, due to the non-existence of a non-interacting systems, RDMFT calculations are demanding compared to DFT and, at present, are restricted to small molecules or simple periodic systems.

In this presentation, we review the theoretical foundations of RDMFT the most successful approximations and extensions, we assess present-day functionals on applications to molecular and periodic systems and we discuss the challenges and future prospects of the theory.

Exchange statistics - Basic concepts

Jon Magne Leinaas
University of Oslo

In my talk I will review some of the basic ideas and questions related to the exchange symmetry of identical particles. It begins with discussing the braid description of particle exchange and some of the interesting question this raises with respect to geometry and topology. A particularly interesting question is whether the geometric understanding of particle exchange means that the spin-statistics theorem can be given a purely geometric formulation. Even if that so far has not been done, the correct relation between spin and statistics seems in some ways natural from the geometric point of view, as I will discuss. In the last part I will focus on the dynamics of systems of anyons in condensed matter systems, where the physical space has the character of a phase space rather than a configuration space. A semi-classical description is discussed, where the anyon parameter is coupled to an exclusion effect, which in the quantum description is known as exclusion statistics.

Two-electron Reduced Density Matrices in Quantum Chemistry and Physics

David A. Mazziotti
University of Chicago,

Strongly correlated quantum systems are not easily described with conventional quantum chemistry formalism because the number of non-negligible configurations grows exponentially with the number of orbitals actively participating in the correlation. In this lecture we will introduce the concept of reduced density matrices for systems of identical fermions and comment on their relevance to problems in quantum chemistry and physics [1,2], especially the description of strongly correlated quantum systems. We will discuss Coulsons challenge in which Coulson highlighted the potential advantages of a direct calculation of the two-electron reduced density matrix without the many-electron wave function and cautioned against the difficulty of ensuring that the two-electron reduced density matrix represents an N-electron quantum system, known as the N-representability problem [1,2]. We will present recent advances for the direct calculation of the two-electron reduced density matrix including the implementation of N-representability conditions [3] by semidefinite programming [4]. Two-electron reduced density matrix (2-RDM) methods can accurately approximate strong electron correlation in molecules and materials at a computational cost that grows non-exponentially with system size [5]. In an application we will treat a quantum chemical system with sextillion (1021) quantum degrees of freedom to reveal the important role of quantum entanglement in its oxidation and reduction [6].

[1] Reduced-Density-Matrix Mechanics: With Application to Many-Electron Atoms and Molecules (Advances in Chemical Physics) D. A. Mazziotti, Ed.; Wiley: New York, 2007
[2] D. A. Mazziotti, Chem. Rev. 112, 244 (2012)
[3] D. A. Mazziotti, Phys. Rev. Lett. 108, 263002 (2012)
[4] D. A. Mazziotti, Phys. Rev. Lett. 106, 083001 (2011)
[5] D. A. Mazziotti, Phys. Rev. Lett. 93, 213001 (2004)
[6] A. W. Schlimgen, C. W. Heaps III, D. A. Mazziotti, J. Phys. Chem. Lett. 7, 627 (2016)

Exchange symmetry and anyon virial coefficients.

Jan Myrheim
Norwegian University of Science and Technology

I will mention some aspects of the theory of identical particles, for example treating neutrons and protons as identical particles distinguished by a quantum number called isotopic spin. I will also review studies of systems of three or more anyons. In particular, the virial expansion shows that the free anyon gas approximates exclusion statistics, with a correspondence between the anyon parameter and the exclusion parameter which is different from the case of anyons in a magnetic field, discussed in the talk by Jon Magne Leinaas.

Why should anyone care about computing with anyons?

Jiannis Pachos
University of Leeds

Combining physics, mathematics and computer science, topological quantum computation is a rapidly expanding field of research focused on the exploration of quantum evolutions that are resilient to errors. In this talk I will presentation a variety of different topics starting from characterizing knot invariants, their quantum simulation with exotic particles called anyons and finally the possible realization of anyons in the laboratory.

Derivation of the time-dependent Hartree(-Fock)-equation

Peter Pickl
Ludwig-Maximilians-Universität München

Solving the time dependent Schrödinger equation for a system of many interacting Fermions is in many cases impossible, both analytically and numerically. Instead of the microscopic description one uses an effective description which describes the behaviour of the fermions in good approximation and can be treated with a computer. In many cases one uses the fermionic Hartree or Hartree-Fock equation as effective description. In the talk I will present recent progress in proving closeness of the microscopic and effective description for systems of many fermions.

DMRG in Quantum Chemistry: From its relation to traditional methods to n-orbital density matrices and beyond

Markus Reiher
ETH Zürich

In my talk I will attempt to provide an overview on the application of the density matrix renormalization group (DMRG) algorithm in quantum chemistry. I will compare to traditional approaches with respect to limitations and capabilities. I will highlight the matrix product operator structure of our second-generation DMRG program and discuss its features. Emphasis will be put on how orbital-entanglement measures can be exploited to automatically select proper active orbital spaces, a major problem of all multi-configurational approaches.

Entanglement Spectroscopy and its application to the fractional quantum Hall phases

Nicolas Regnault
École normale supérieure, Paris - Princeton

The entanglement spectroscopy, initially introduced by Li and Haldane in the context of the fractional quantum Hall effects, has stimulated an extensive range of studies. The entanglement spectrum is the spectrum of the reduced density matrix, when we partition the system into two. For many quantum systems, it unveils a unique feature: Computed from the bulk ground state wave function, the entanglement spectrum give access to the physics of edge excitations.

In this talk, we will give an overview of the entanglement spectroscopy with a focus on to the fractional quantum Hall phases. We will show how much information is encoded within the ground state and how different partitions probe different types of excitations.

(Almost) 25 Years of DMRG - What Is It About?

Ulrich Schollwöck
Ludwig-Maximilians-Universität München

In this talk, I will introduce DMRG both from the historical (statistical) and modern (matrix product state) perspective, highlighting why it has become the method of choice for one-dimensional quantum systems in and out of equilibrium, as well as why it has made interesting forays into the world of two-dimensional quantum systems. I will also discuss its limitations, as well as the resulting directions of future development.

Fermionic Exchange Symmetry: Quantifying its Influence beyond Pauli's Exclusion Principle

Felix Tennie
University of Oxford

The Pauli exclusion principle has a strong impact on the properties and the behavior of most fermionic quantum systems. Remarkably, even stronger restrictions on fermionic natural occupation numbers follow from the fermionic exchange symmetry. We develop an operationally meaningful measure which allows one to quantify the potential physical relevance of those generalized Pauli constraints beyond the well-established relevance of Pauli's exclusion principle. It is based on a geometric hierarchy induced by Pauli exclusion principle constraints. The significance of that measure is illustrated for a few-fermion model which also confirms such nontrivial relevance of the generalized Pauli constraints.

Generalized Pauli constraints in reduced density matrix functional theory

Iris Theophilou
Max-Planck-Institut Hamburg

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the ground state wavefunction of many electron systems and the first order reduced density matrix (1RDM) and uses the second one as its fundamental valuable. The

ground state of a system is determined within this approach by minimizing the energy functional with respect to the 1RDM while satisfying that the 1RDM corresponds to a fermionic ensemble (Coleman's conditions). As the explicit expression of the energy functional with respect to the 1RDM is not known, different approximate functionals are employed. If we had the exact functional performing the energy minimization using the ensemble representability constraints would be enough to find a 1RDM that corresponds to a pure state (if our ground state is not degenerate so we really have a pure state). However, performing the energy minimization with approximate functionals, as we found for 3 electron systems test cases, results in occupation numbers that do not satisfy the generalized Pauli constraints (GPC). One then could in principle employ the GPC as additional constraints during the energy minimization to ensure that the ground state 1RDM that finds can result from a pure state. However due to the big number of these constraints this is not feasible in practice apart from a few cases of really small systems.

An idea to be explored is constructing energy functionals that satisfy at least some of the GPC. This could serve as a change of paradigm for functional derivation because until now 1RDM functionals were mostly tested on whether they reproduced or not ground state energies correctly. Another idea that we would like to discuss is whether we could apply the GPC in an approximate way to only the electrons that have occupations smaller than one. The electrons with occupation one do not play any role to whether the 1RDM corresponds to a pure state or not. Although it is doubtful whether 1RDMs with occupations that are exactly one can correspond to a ground state of a real fermionic system, in many cases this is a sensible approximation that would significantly reduce the amount of GPC to be considered in a RDMFT minimization.

I. Theophilou et al, J. Chem. Phys. 142, 154108 (2015)