Workshop on "Generalized Pauli Constraints and Fermion Correlation"

THURSDAY

13:15 - 13:30	Opening Remarks (Gottlieb)
13:30 - 14:15	***Quantum marginal problem and generalized Pauli constraints*** (Schilling)
14:15 - 14:30	Discussion
14:30 - 15:15	***Pinning and quasipinning in quantum chemistry*** (Benavides-Riveros)
15:15 - 16:00	Discussion / Coffee
16:00 - 16:45	***Geometry of the Borland-Dennis setting: the W-type class*** (Gottlieb)
16:45 - 17:00	Discussion

FRIDAY

10:00 - 10:30	***Quasi-separated electron pairs in small molecules*** (Gottlieb)
10:30 - 11:00	Discussion / Coffee
11:00 - 11:45	***Solving time-dependent many-body quantum problems using the two-particle reduced density matrix*** (Brezinova)
11:45 - 12:15	Discussion
12:15 - 14:00	Lunch
14:00 - 14:45	***Fermionic exchange symmetry: quantifying its influence beyond Pauli's Exclusion Principle*** (Schilling)
14:45 - 15:15	Discussion / Coffee
15:15 - 16:00	***Natural extension of Hartree-Fock through extremal 1-fermion information*** (Benavides-Riveros)
16:00 - 16:15	Discussion
16:15 - 17:15	Workshop session

SATURDAY

10:00 - 13:00	Workshop session

Quantum marginal problem and generalized Pauli constraints

Christian Schilling

The question whether given reduced density operators (marginals) for subsystems of a multipartite quantum system are compatible to a common total state is called quantum marginal problem (QMP). We present the solution found by A. Klyachko just a few years ago as well as the main steps for its derivation. Applying those concepts to fermionic systems reveals further constraints on fermionic occupation numbers beyond Pauli's famous exclusion principle. We introduce and discuss these so-called generalized Pauli constraints in great detail and comment on their potential physical relevance.

Pinning and quasipinning in quantum chemistry

Carlos Benavides-Riveros

It is now known that fermionic natural occupation numbers (NONs) do not only obey Pauli's exclusion principle but are even stronger restricted by the so-called generalized Pauli constraints (GPC). Whenever given NONs lie on or close to the boundary of the allowed region the corresponding N-fermion quantum state has a significantly simpler structure. We explore this phenomenon in the context of quantum chemistry.

Geometry of the Borland-Dennis setting: the W-type class

Alex Gottlieb

We call the Hilbert space for three fermions in six orbitals the Borland-Dennis setting. It is isomorphic to the alternating tensor product of three copies of the standard 6-dimensional Hilbert space C^6. Slater determinant states in the Borland-Dennis setting correspond to "decomposable" trivectors, i.e., simple wedge products of three vectors from C^6. Generic wave functions in the Borland-Dennis setting can be written as a sum of just two decomposable trivectors. The wave functions that cannot be written as a sum of fewer than decomposables constitute the "W-type entanglement class." I will discuss the geometry of the W-type class within the ambient Borland-Dennis space.

Quasi-separated electron pairs in small molecules

Alex Gottlieb

Some of the electrons in a molecule are tightly bound to the nuclei. The closely bound "core electrons" can be relatively uncorrelated with the rest of the electrons in the molecule, and may even form what we call a "quasi-separated" pair. [Let F be the electronic wave function of a molecule with N+2 electrons. We say that F features a "quasi-separated pair" if it is approximately equal to the wedge product G ^ H of a geminal G that describes the state of the separated pair and an N-electron wave function H that is strongly orthogonal to G.] We have computational evidence of such quasi-separated electron pairs in the ground states of very small molecules (like LiH or the Be atom) whose correlated electronic structure can be very accurately approximated with full CI calculations.

Solving time-dependent many-body quantum problems using the two-particle reduced density matrix

Iva Brezinova

In this talk we will give an overview over our recent progress in solving time-dependent many-body problems using the two-particle reduced density matrix (2RDM) as the fundamental variable. The wavefunction is completely avoided and with this all problems arising from the exponentially increasing complexity with particle number. Key is the reconstruction of the 3RDM which couples to the dynamics of the 2RDM. At this point the approximation to the full solution of the Schrödinger equation enters: while two-particle correlations are fully incorporated, three-particle correlations are only approximated. We will discuss the reconstruction of the 3RDM, how we overcome the N-representability problem, and demonstrate the accuracy of our theory on two-examples: multi-electron atoms in strong fields, and ultra-cold atoms in optical lattices.

Fermionic exchange symmetry: quantifying its influence beyond Pauli's Exclusion Principle

Christian Schilling

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.

Natural extension of Hartree-Fock through extremal 1-fermion information

Carlos Benavides-Riveros

By employing the simpler structure arising from pinning and quasipinnig a variational optimization method for few fermion ground states is elaborated. We quantitatively confirm its high accuracy for systems whose vector of NON is close 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. These geometric insights shed some light on the concept of active spaces, correlation energy, frozen electrons and virtual orbitals.