Thesis title: Quantum-mechanical systems in traps and Similarity Renormalization Group theory

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Aims

The aim of this thesis is to study the structure of fermionic systems using the newly developed Similarity Renormalization Group (SRG) theory. The results will be benchmarked against *ab inito* variational and diffusion function Monte Carlo techniques.

General introduction to possible physical systems

What follows here a general introduction to systems of confined electrons in two or three dimensions. However, although the thesis will focus on such systems, the codes will be written so that other systems of trapped fermions or eventually bosons can be handled. Examples could be neutrons in trap as done in Ref. [1] or ions in various traps [2].

Strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods. Quantum dots in particular, that is, electrons confined in semiconducting heterostructures, exhibit, due to their small size, discrete quantum levels. The ground states of, for example, circular dots show similar shell structures and magic numbers as seen for atoms and nuclei. These structures are particularly evident in measurements of the change in electrochemical potential due to the addition of one extra electron, $\Delta_N = \mu(N+1) - \mu(N)$. Here N is the number of electrons in the quantum dot, and $\mu(N) = E(N) - E(N-1)$ is the electrochemical potential of the system. Theoretical predictions of Δ_N and the excitation energy spectrum require accurate calculations of ground-state and of excited-state energies. Small confined systems, such as quantum dots (QD), have become very popular for experimental study. Beyond their possible relevance for nanotechnology, they are highly tunable in experiments and introduce level quantization and quantum interference in a controlled way. In a finite system, there can not, of course, be a true phase transition, but a cross-over between weakly and strongly correlated regimes is still expected. There are several other fundamental differences between quantum dots and bulk systems: (a) Broken translational symmetry in a QD reduces the ability of the electrons to delocalize. As a result, a Wigner-type cross-over is expected for a smaller value of r_s. (b) Mesoscopic fluctuations, inherent in any confined system, lead to a rich interplay with the correlation effects. These two added features make strong correlation physics particularly interesting in a QD. As clean 2D bulk samples with large r_s are regularly fabricated these days in semiconductor heterostructures, it seems to be just a matter of time before these systems are patterned into a QD, thus providing an excellent probe of correlation effects.

The above-mentioned quantum mechanical levels can, in turn, be tuned by means of, for example, the application of various external fields. The spins of the electrons in quantum dots provide a natural basis for representing so-called qubits [3]. The capability to manipulate and study such states is evidenced by several recent experiments [4, 5]. Coupled quantum dots are particularly interesting since so-called two-qubit quantum gates can be realized by manipulating the exchange coupling which originates from the repulsive Coulomb interaction and the underlying Pauli principle. For such states, the exchange coupling splits singlet and triplet states, and depending on the shape of the confining potential and the applied magnetic field, one can allow for electrical or magnetic control of the exchange coupling. In particular, several recent experiments and theoretical investigations have analyzed the role of effective spin-orbit interactions in quantum dots [6–9] and their influence on the exchange coupling.

A proper theoretical understanding of the exchange coupling, correlation energies, ground state energies of quantum dots, the role of spin-orbit interactions and other properties of quantum dots as well, requires the development of appropriate and reliable theoretical few- and many-body methods. Furthermore, for quantum dots with more than two electrons and/or specific values of the external fields, this implies the development of few- and many-body methods where uncertainty quantifications are provided. For most methods, this means providing an estimate of the error due to the truncation made in the single-particle basis and the truncation made in limiting the number of possible excitations. For systems with more than three or four electrons, *ab initio* methods that have been employed in studies of quantum dots are variational and diffusion Monte Carlo [10, 12, 13], path integral approaches [14], large-scale diagonalization (full configuration interaction) [15–17, 19], and to a very limited extent coupled-cluster theory [20–24]. Exact diagonalization studies are accurate for a very small number of electrons, but the number of basis functions needed to obtain a given accuracy and the computational cost grow very rapidly with electron number. In practice they have been used for up to eight electrons[15, 16, 19], but the accuracy is very limited for all except $N \leq 3$. Monte Carlo methods have been applied up to $N = 24$ electrons [12, 13]. Diffusion Monte Carlo, with statistical and systematic errors, provide, in principle, exact benchmark solutions to various properties of quan-

tum dots. However, the computations start becoming rather time-consuming for larger systems. Hartree[25], restricted Hartree-Fock, spin- and/or space-unrestricted Hartree-Fock[26–28] and local spin-density, and current density functional methods[29–32] give results that are satisfactory for a qualitative understanding of some systematic properties. However, comparisons with exact results show discrepancies in the energies that are substantial on the scale of energy differences.

Specific tasks

In addition to the above methods, a very promising first principle method for dealing with quantum mechanical systems with many degrees of freedom has been developed recently, mainly within the nuclear theory community. This method aims at an efficient scheme for decoupling of the high-momentum degrees of freedom, allowing thereby for more tractable dimensionalities for many-particle systems. This is the similarity renormalization group (SRG) method, which was introduced independently by Glazek and Wilson [34] and Wegner [35]. The SRG consists of a continuous sequence of unitary transformations that suppress off-diagonal matrix elements, driving the Hamiltonian towards a band- or block-diagonal form. Writing the unitarily transformed Hamiltonian as

$$H(s) = U(s)HU^\dagger(s) \equiv H^{\rm d}(s) + H^{\rm od}(s)\,,$$

where $H^{\rm d}(s)$ and $H^{\rm od}(s)$ are the appropriately defined "diagonal" and "off-diagonal" parts of the Hamiltonian, the evolution with the flow parameter s is given by

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]\,.$$

Here $\eta(s) \equiv [dU(s)/ds]\,U^\dagger(s)$ is the anti-Hermitian generator of the transformation. The choice of the generator first suggested by Wegner,

$$\eta(s) = [H^{\rm d}(s), H(s)] = [H^{\rm d}(s), H^{\rm od}(s)]\,,$$

guarantees that the off-diagonal coupling of $H^{\rm od}$ is driven exponentially to zero with increasing s [35]. Through different choices for $H^{\rm d}$ and $H^{\rm od}$, one can tailor the SRG evolution to transform the initial Hamiltonian to a form that is most convenient for a particular problem [36, 37]. It is this flexibility, together with the fact that one never explicitly constructs and applies the unitary transformation $U(s)$ [rather it is implemented implicitly through integration] that makes the SRG a powerful alternative to conventional effective interaction methods.

An interesting alternative is to perform the SRG evolution directly in the A-body system of interest [35–37]. Unlike the free-space evolution, the in-medium SRG (IM-SRG) has the appealing feature that one can approximately evolve $3, ..., A$-body operators using only two-body machinery. The key to this simplification is the use of normal-ordering with respect to a finite-density reference state. Starting from a general second-quantized Hamiltonian with two- and three-body interactions, all operators can be normal ordered with respect to a finite-density Fermi vacuum $|\Phi\rangle$ (e.g., the Hartree-Fock ground state), as opposed to the zero-particle vacuum. The details are described in Ref. [38]. In this thesis, the aim is to study the ground state of closed-shell systems of quantum dots in two dimensions and using the same methodology discussed in Ref. [38].

The results and their quality with be compared with the diffusion Monte Carlo results, and eventually also with density functional results developed by fellow students.

Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Fall 2012: In order to become familiar with the SRG method, the first step is to solve the two-electron problem in an oscillator basis, using the approach described in Ref. [39]. These results will be compared with the exact ones from either the diffusion Monte Carlo code, or existing exact results from Coupled-cluster theory or exact diagonalization [24]. To achieve this, the first step is to set up the Coulomb interaction in an oscillator basis. This has been done in for example Ref. [24]. The code and its details can be looked up from the slides for FYS4411 from 2011.

- Fall 2012: In order to perform SRG calculations following the recipe outlined in Ref. [38], one will need to set up a Hartree-Fock basis. Such codes are also available from previous Master of Science theses, see for example Christoffer Hirth's thesis.

- Fall 2012 and begin Spring 2013: The Hartree-Fock interaction is then used as input to the SRG code, a code which needs to be developed. A code for nucleons in three dimensions is available. The results will be compared with available results from large scale diagonalization, variational and diffusion Monte Carlo and coupled-cluster techniques for closed-shell systems up to $\sim 50-70$ interacting electrons.

This method has never before been applied to systems of strongly confined electrons and it will be very interesting to test its pros and cons against other popularly used many-body methods. The thesis is expected to be handed in June 1 2013. Prof. Scott Bogner from Michigan State University will act as a co-advisor. Parts of the thesis work may be conducted at Michigan State University.

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