Master thesis project: Monte Carlo studies of the homogeneous electron gas in two and three dimensions

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Aims

The aim of this thesis is to develop a Full Configuration Interaction Quantum Monte Carlo (FCIQMC) code that can be used to study properties of fermions in infinite systems. The latter can span from the homogenous electron gas in two and three dimensions to infinite nuclear matter present in neutron stars. The formalism to be developed follows the recent work of Alavi and co-workers. The aim is to extend upon the thesis of Karl Leikanger in order to study strongly interacting systems like infinite nuclear matter. If successful, the FCIQMC method has the potential to provide *almost-exact* solutions for ground state properties of strongly interacting many-particle systems.

General introduction to the physical systems

The homogeneous electron gas in two and three dimensions and bulk nucleonic matter are interesting for several reasons. The equation of state (EoS) of neutron matter determines for example properties of supernova explosions and of neutron stars. The determination and our understanding of the EoS for nuclear matter is intimately linked with our capability to solve the nuclear many-body problem. Here, correlations beyond the mean field play an important role. Theoretical studies of nuclear matter and the pertinent EoS span back to the very early days of nuclear many-body physics. Early computations are nicely described in the 1967 review by Day. In these calculations, mainly particle-particle correlations were summed to infinite order. Other correlations were often included in a perturbative way. Coupled cluster calculations of nuclear matter were performed already during the late 1970s and early. In recent years, there has been a considerable algorithmic development of first-principle methods

for solving the nuclear many-body problem. A systematic inclusion of other correlations in a non-perturbative way are nowadays accounted for in Monte Carlo methods, self-consistent Green's function approaches and nuclear density functional theory. The recent Lecture Notes in Physics on Computational Nuclear Physics covers many of the above many-body methods as well as presenting extensive repositories for numerical methods. The homogeneous electron gas has played a central role in solid state physics, not only as a viable model for understanding important aspects of condensed matter systems but also as a benchmark system for various many-body methods. Still, all of the above many-body methods rely on specific approximations (and thereby truncations) to the full set of many-body correlations. The FCIQMC method, as demonstrated by Alavi and co-workers, has the potential to provide almost *exact* results for ground state properties of fermionic and bosonic systems. As such, when applied to both the homogeneous electron gas and infinite nuclear matter, the method has the potential to provide important benchmarks for other many-body methods.

Many-body approaches to infinite matter

For an infinite homogeneous system like nuclear matter or the electron gas, the one-particle wave functions are given by plane wave functions normalized to a volume Ω for a quadratic box with length L. The limit $L \to \infty$ is to be taken after we have computed various expectation values. In our case we will however always deal with a fixed number of particles and finite size effects become important.

$$\psi_{\mathbf{k}m_s}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \exp{(i\mathbf{kr})}\xi_{m_s}$$

where $\mathbf{k}$ is the wave number and ξ_{m_s} is a spin function for either spin up or down

$$\xi_{m_s=+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \xi_{m_s=-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The single-particle energies for the three-dimensional electron gas are

$$\varepsilon_{n_x,n_y,n_z} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2),$$

resulting in the magic numbers 2, 14, 38, 54, etc.

In general terms, our Hamiltonian contains at most a two-body interaction. In second quantization, we can write our Hamiltonian as

$$\hat{H} = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs}\langle pq|v|rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \tag{1}$$

where the operator $\hat{h}_0$ denotes the single-particle Hamiltonian, and the elements $\langle pq|v|rs\rangle$ are the anti-symmetrized Coulomb interaction matrix elements. Normal-ordering with respect to a reference state $|\Phi_0\rangle$ yields

$$\hat{H} = E_0 + \sum_{pq} f_{pq}\{a_p^\dagger a_q\} + \frac{1}{4}\sum_{pqrs}\langle pq|v|rs\rangle\{a_p^\dagger a_q^\dagger a_s a_r\}, \tag{2}$$

where $E_0 = \langle\Phi_0|\hat{H}|\Phi_0\rangle$ is the reference energy and we have introduced the so-called Fock matrix element defined as

$$f_{pq} = \langle p|\hat{h}_0|q\rangle + \sum_i \langle pi|v|qi\rangle. \tag{3}$$

The curly brackets in Eq. (2) indicate that the creation and annihilation operators are normal ordered.

The unperturbed part of the Hamiltonian is defined as the sum over all the single-particle operators $\hat{h}_0$, resulting in

$$\hat{H}_0 = \sum_i \langle i|\hat{h}_0|i\rangle = \sum_{\mathbf{k}_i m_{s_i}} \frac{\hbar^2 k_i^2}{2m} a^\dagger_{\mathbf{k}_i m_{s_i}} a_{\mathbf{k}_i m_{s_i}}.$$

We will throughout suppress, unless explicitely needed, all references to the explicit quantum numbers $\mathbf{k}_i m_{s_i}$. The summation index i runs over all single-hole states up to the Fermi level.

The general anti-symmetrized two-body interaction matrix element

$$\langle pq|v|rs\rangle = \langle \mathbf{k}_p m_{s_p} \mathbf{k}_q m_{s_q}|v|\mathbf{k}_r m_{s_r} \mathbf{k}_s m_{s_s}\rangle,$$

is given by the following expression

$$\begin{aligned}
&\langle \mathbf{k}_p m_{s_p} \mathbf{k}_q m_{s_q}|v|\mathbf{k}_r m_{s_r} \mathbf{k}_s m_{s_s}\rangle \\
=&\frac{e^2}{\Omega}\delta_{\mathbf{k}_p+\mathbf{k}_q,\mathbf{k}_r+\mathbf{k}_s}\left\{\delta_{m_{s_p}m_{s_r}}\delta_{m_{s_q}m_{s_s}}(1-\delta_{\mathbf{k}_p\mathbf{k}_r})\frac{4\pi}{\mu^2+(\mathbf{k}_r-\mathbf{k}_p)^2}\right. \\
&\left.-\delta_{m_{s_p}m_{s_s}}\delta_{m_{s_q}m_{s_r}}(1-\delta_{\mathbf{k}_p\mathbf{k}_s})\frac{4\pi}{\mu^2+(\mathbf{k}_s-\mathbf{k}_p)^2}\right\},
\end{aligned}$$

for the three-dimensional electron gas. The energy per electron computed with the reference Slater determinant can then be written as (using hereafter only atomic units, meaning that $\hbar = m = e = 1$)

$$E_0/N = \frac{1}{2}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right],$$

for the three-dimensional electron gas. This will serve as the first benchmark in setting up a program for the FCIQMC method. The electron gas provides a very useful benchmark at the Hartree-Fock level since it provides an analytical solution for the Hartree-Fock energy single-particle energy and the total energy per particle.

Most of the details for setting up a single-particle basis and performing a Hartree-Fock calculation for infinite systems can be found in chapter 8 of the recent Lecture Notes in Physics mentioned above.

Specific tasks

The first task of this thesis is to develop a code which implements the above-mentioned single-particle basis for a two-dimensional and three-dimensional infinite homogeneous gas of electrons using a cartesian basis. With this basis, the next task is to write a code which computes the Hartree-Fock energy. These results will be benchmarked against analytical results for the electron gas as well as existing numerical results for infinite nuclear matter. The next step is, using a Hartree-Fock basis, to develop a Variational Monte Carlo code that uses a simple form for the two-body correlation function based on perturbation theory to second order. The final task is to develop an FCIQMC code for infinite systems using as input the Hartree-Fock and the optimal energy from the Variational Monte Carlo calculations. The results will be benchmarked against other many-body methods and can easily lead to publications in international journals.

Progress plan and milestones

The aims and progress plan of this thesis are as follows

- Fall 2017: Develop a program which sets up a cartesian single-particle basis for infinite systems and perform Hartree-Fock calculations for the infinite electron gas in two and three dimensions.
- Fall 2017: Set up a Variational Monte Carlo code that uses a Jastrow factor based on many-body perturbation theory to first order in the wave operator.
- Fall 2017: Start developing the FCIQMC method and perform the first calculations for simpler two-electron systems in two and three dimensions.
- Spring 2018: Develop and finalize a fully object-oriented and parallelized FCIQMC code which can be used to study the infinite electron gas. The results can in turn be benchmarked with other first principle calculations.
- Spring 2018: The last part deals with a proper write-up of the thesis, final runs and discussion of the results.

The thesis is expected to be handed in May/June 2018.