MASTER THESIS PROJECT FOR CHRISTIAN FLEISCHER: QUANTUM-MECHANICAL STUDIES OF INFINITE MATTER, WITH AN EMPHASIS ON THE INFINITE ELECTRON GAS IN TWO AND THREE DIMENSIONS

INTRODUCTION TO THE THE PHYSICS OF THE ELECTRON GAS

The electron gas is perhaps the only realistic model of a system of many interacting particles that allows for a solution of the Hartree-Fock equations on a closed form. Furthermore, to first order in the interaction, one can also compute on a closed form the total energy and several other properties of a many-particle systems. The model gives a very good approximation to the properties of valence electrons in metals.

The homogeneous electron gas is one of the few examples of a system of many interacting particles that allows for a solution of the mean-field Hartree-Fock equations on a closed form. To first order in the electron-electron interaction, this applies to ground state properties like the energy and its pertinent equation of state as well. The homogeneus electron gas is a system of electrons that is not influenced by external forces except by an attraction provided by a uniform background of ions. These ions give rise to a uniform background charge. The ions are stationary and the system as a whole is neutral. Irrespective of this simplicity, this system, in both two and three-dimensions, has eluded a proper description of correlations in terms of various first principle methods, except perhaps for quantum Monte Carlo methods. In particular, the diffusion Monte Carlo calculations of "Ceperley":"http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.45.566" and "Ceperley and Tanatar":"http://journals.aps.org/prb/abstract/10.1103/PhysRevB.39.5005" are presently still considered as the best possible benchmarks for the two- and three-dimensional electron gas.

The electron gas, in two or three dimensions is thus interesting as a test-bed for electron-electron correlations. The three-dimensional electron gas is particularly important as a cornerstone of the local-density approximation in density-functional theory. In the physical world, systems similar to the three-dimensional electron gas can be found in, for example, alkali metals and doped semiconductors. Two-dimensional electron fluids are observed on metal and liquid-helium surfaces, as well as at metal-oxide-semiconductor interfaces. However, the Coulomb interaction has an infinite range, and therefore long-range correlations play an essential role in the electron gas.

At low densities, the electrons become localized and form a lattice. This so-called Wigner crystallization is a direct consequence of the long-ranged repulsive interaction. At higher densities, the electron gas is better described as a liquid. When using, for example, Monte Carlo methods the electron gas must be approximated by a finite system. The long-range Coulomb interaction in the electron gas causes additional finite-size effects that are not present in other infinite systems like nuclear matter or neutron star matter. This poses additional challenges to many-body methods when applied to the electron gas.

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[1]

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

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 interactions. In second quantization, we can write our Hamiltonian as

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

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

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

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

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

[1] 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.

The curly brackets in Eq. (**??**) 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

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

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 (with the addition of a Yukawa term) as the first benchmark. 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. In addition to the above studies of the electron gas, it is important to study properly the boundary conditions as well. Here we will study so-called periodic boundary conditions following the work of Refs. [**? ? ?**]. See also the recent work of Hagen *et al.* and Baardsen, see Refs. [**? ?**]. One aim of this thesis is to implement so-called twisted boundary conditions, first for the simple electron gas at the Hartree-Fock level. The next step is to perform diffusion Monte Carlo calculations for electron gas in two and three dimensions using the so-called full configuration interaction quantum Monte Carlo approach developed by Ali Alavi *et al* and studied in detail by a former master of science student of the computational physics group, Karl Leikanger, now PhD student at CTCC. The studies can, if time allows, also be extended to studies of finite fermionic systems like electrons in oscillator traps, so-called quantum dots systems or atoms.

The results will be published in scientific journals, if possible.

PROGRESS PLAN AND MILESTONES

The aims and progress plan of this thesis are as follows

- Spring 2016 and partly fall 2016: The first step is to set up a program that uses cartesian coordinates in order to compute the Hartree-Fock energy of the electron gas with a Coulomb interaction with and without a screening term (Yukawa like potential).
- Fall 2016: The next step is to include a proper treatment of periodic boundary conditions using the twisted boudary condition approach described in Refs. [**? ? ?**].
- Fall 2016: Thereafter, correlations at the electron gas level will be studied using a simpler Variational Monte Carlo approach.
- Spring 2017: The final step is to write a code which employs the Full Configuration Interaction Quantum Monte Carlo method of Alavi *et al* for the electron gas in two and three dimensions and compare these results with other many-body methods like density functional theory, coupled cluster theory and many-body perturbation theory.
- Spring 2017: The final step is to perform systematic studies of the infinite electron gas at various densities, both in two and three dimensions.
- Spring 2017: The last part deals with a proper write-up of the thesis.

The thesis is expected to be handed in May/June 2017.

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