Studies of Infinite Matter Systems, from the Homogeneous Electron Gas to Dense Matter

Master of Science thesis project

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Infinite Matter studies

Bulk nucleonic matter is interesting for several reasons. The equation of state (EoS) of neutron matter determines properties of supernova explosions, and of neutron stars and it links the latter to neutron radii in atomic nuclei and the symmetry energy . Similarly, the compressibility of nuclear matter is probed in giant dipole excitations, and the symmetry energy of nuclear matter is related to the difference between proton and neutron radii in atomic nuclei. The saturation point of nuclear matter determines bulk properties of atomic nuclei, and is therefore an important constraint for nuclear energy-density functionals and mass models.

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.

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

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

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

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 (with the addition of a Yukawa term) as the first benchmark in setting up a program for doing Coupled-cluster theories. 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.

The next step is to perform a coupled-cluster calculations at the coupled-cluster with doubles excitations, the so-called CCD approach, for the electron gas. The next step is to include triples correlations and perform full doubles and triples calculations (CCDT) for neutron matter using a simplified model for the nuclear force, the so-called Minnesota potential. This allows for a benchmark of codes to infinite nuclear matter. The next step is to include realistic models for the nuclear forces and study the EoS for pure neutron matter, asymmetric nuclear matter (for different proton fractions) and symmetric nuclear matter. With this one can study β-stable neutron star matter and extract important information about the symmetry energy in infinite matter and the composition of a neutron star. The resulting effective interactions at the two-body level can in turn, if time allows, be included in the study of neutrino emissivities in dense matter. The processes of most interest are the so-called modified URCA prosesses

$$n + n \rightarrow p + n + e + \overline{\nu}_e, \qquad p + n + e \rightarrow n + n + \nu_e. \tag{4}$$

These reactions correspond to the processes for β-decay and electron capture with a bystanding neutron. The calculation of neutrino spectra has important consequences for our basic understanding on how neutron stars cool, the synthesis of the elements and neutrino oscillations in dense matter.