The hard sphere model of strongly interacting fermion systems

Ph.D. Research Project
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Introduction

The properties of interacting fermion systems, such as liquid $^3$He and nuclear matter, are largely determined by the strongly repulsive nature of the forces acting between the constituent particles at short distance. Figure 1, in which the Lennard-Jones potential [1], describing the interactions between helium atoms, is compared to the Argonne $v_{18}$ potential [2], describing the interaction between two nucleons coupled in a state of total spin and isospin $S = 0, T = 1$, clearly shows that short range repulsion is a prominent and universal feature of fermion dynamics.

![Figure 1: Radial behaviour of the Lennard-Jones potential, describing the interaction between atoms in liquid $^3$He (left panel), and the Argonne $v_{18}$ potential, describing the interaction between two nucleons in the state of total spin and isospin $S = 0, T = 1$ (right panel).](image)

The presence of the strong repulsive core makes “standard” perturbative calculations—carried out using the bare interaction and the basis of eigenstates of the non interacting system—not suitable, and the introduction of a well-behaved effective Hamiltonian essential.

The definition of the effective interactions from the bare Hamiltonian is generally obtained from either of two, conceptually different, approaches. The systematic treatment of short-range repulsion in many-body perturbation theory is based on the replacement of the bare interaction potential, $V$, with the reaction matrix, $G$, originally proposed by Brueckner [3] within the context of nuclear matter theory. This scheme allows one to take into account pair interactions to all orders, through the introduction of a operator describing scattering processes in the medium. The reaction matrix is defined by the integral equation

$$G = V - V \frac{Q}{e} G ,$$

the diagrammatic representation of which is given in Fig. 2. In the above equation, the so-called Pauli operator, $Q$, is a projector that prevents scattering to occupied states, while the denominator $e$ is the energy difference between the initial and final states. The sum of all two-body
Figure 2: Diagrammatic representation of the ladder diagrams, describing two-body multiple scattering processes. The bare interaction and the reaction matrix are represented by dashed and wavy lines, respectively.

multiple scattering processes, usually referred to in diagrammatic language as ladder series, makes the resulting reaction matrix a well-behaved operator, best suited for perturbative calculations in different schemes, such as scattering theory to in free space, time-ordered perturbation theory and the Green’s function method. The main difference between the three cases is the form of the free particle propagators, which determines the explicit form of the integral equation defining for the reaction matrix. Summing up ladder diagrams in free space – the t-matrix method – is equivalent to solving the Lippman-Schwinger equation, while when the presence of the filled Fermi sea is taken into account – the G-matrix method – the same procedure leads to the Bethe-Goldstone equation or to the Bethe-Salpeter equation, respectively, depending on the use of time-ordered (Goldstone) or standard (Feynman) perturbation theory [4].

Variational approaches, originally developed to describe classical and quantum liquids, have been also successfully used to study strongly interacting fermion systems in the high density regime, relevant to the understanding of the properties of astrophysical compact objects.

In this Thesis, we will adopt Correlated Basis Functions (CBF) perturbation theory and the cluster expansion technique [5,6]. This formalism has been recently employed to obtain an effective interaction suitable for use in perturbation theory in the basis of the non interacting Fermi gas [7,8].

Motivated by the universality of the repulsive nature of the interaction at short distance, we will investigate the accuracy of the CBF effective interaction approach studying a variety of properties of the fermion hard sphere system. Within this model, the potentials shown in Fig. 1 are replaced by

\[
v(r) = \begin{cases} 
\infty & r < a \\
0 & r > a 
\end{cases},
\]

where \( r \) denotes the distance between the two interacting particles. Note that neglecting the long-range attractive interaction prevents the possible formation of Cooper pairs, leading to the transition to a superconducting or superfluid phase.

It is long known that the hard sphere model provides an accurate description of several properties of dilute Fermi systems. Algebraic expressions of the ground state energy, the single-particle energy and the momentum distribution can be written as power series in the parameter \((k_F a)\), where \( k_F \) is the Fermi momentum [9]. We will use the results obtained from these expansions in low density limit as benchmarks to assess the accuracy of the effective interaction approach, thus providing the basis for its generalisation to neutron matter.
Figure 3: Typical shape of the correlation function (green line) obtained solving the Euler-Langrange equation discussed in the text with the hard sphere potential (blu line).

Formalism

Correlated Basis Functions

The formalism based on correlated basis functions is a natural extension of the variational approach employed to describe quantum liquids. Within this scheme, short range correlations induced by the hard core potential are included in the total wave function through a many body correlation operator \( \hat{F} \). With a suitable choice of the correlation operator it is possible to handle both central potentials, such as the interaction between \(^3\)He atoms, and state-dependent potentials, such as those required to describe nuclear interaction.

In general, correlated states are obtained from the non interacting Fermi Gas (FG) states through the transformation

\[
| n \rangle = \frac{\hat{F}|n_{FG}\rangle}{\langle n_{FG}|\hat{F}^\dagger \hat{F}|n_{FG}\rangle^{1/2}}.
\]

The Fermi Gas states, \( |n_{FG}\rangle \), are specified by the occupation numbers of the single particle states, labeled by the momentum \( k \), spin \( \sigma \) and isospin \( \tau \) quantum numbers. For example, the occupation numbers of the ground state, \( |0_{FG}\rangle \), are described by the Heaviside function \( \theta(k_F - |k|) \).

The operator \( \hat{F} \) is defined as the product of pair correlation operators \( \hat{F}_{ij} \),

\[
\hat{F} = S \prod_{j>i} \hat{F}_{ij}.
\]

Note that, for spin-isospin dependent interactions \([ \hat{F}_{ij}, \hat{F}_{ik} ] \neq 0 \), and the right hand side of the above equation needs to be properly symmetrized through the action of the operator \( S \).

In the case of spherically symmetric and spin-isospin-independent interactions, the two-particle correlation function depends on the interparticle distance only, i.e. \( \hat{F}_{ij} = f(r_{ij}) \). Its shape, determined through functional minimization of the ground state energy and shown in Fig. 3 for the hard sphere model, reflects the correlation structure induced by the interaction, implying

\[
f(r < a) = 0 \quad , \quad \lim_{r \to \infty} f(r) = 1.
\]

The CBF effective interaction,

\[
V_{\text{eff}} = \sum_{j>i} v_{\text{eff}}(r_{ij}),
\]  

(2)
is defined in terms of the expectation value of the bare hamiltonian in the correlated ground state through

\[ \langle H \rangle = \langle 0 | H | 0 \rangle = \langle 0_{FG} | T + V_{\text{eff}} | 0_{FG} \rangle , \]

where

\[ H = T + V = \sum_i \frac{p_i^2}{2m} + \sum_{j>i} v(r_{ij}) , \]

with \( v(r_{ij}) \) given by Eq. (1).

The evaluation of the expectation value of bare hamiltonian – or any many-body operator – in a CBF state, involves manyfold integrations, whose dimensionality quickly increases with the number of particles. However, the short range nature of the interaction allows one to exploit the cluster property, and expand the expectation values as sum of terms (clusters) involving an increasing number of particles. Particular classes of these contributions can be summed to all orders solving the Fermi Hyper-Netted Chain (FHNC) integral equations [10,11].

The FHNC summation technique has been extensively used to obtain accurate upper bounds to the ground energy of a variety of interacting many-body systems. Within this approach, the shape of the correlation function is determined from functional minimisation of the ground state expectation value of the hamiltonian, i.e. requiring that

\[ \frac{\delta \langle H \rangle}{\delta f} = 0 . \]

At any given order of the cluster expansion, the above relation provides a Euler-Lagrange equation for the correlation function, \( f \), the range of which, denoted \( d \), is varied to minimise the energy obtained from the full FHNC calculation.

The effective interaction employed in our work has been obtained from the the cluster expansion at lowest order, which amounts to including only the contributions arising from two-particle clusters. The resulting potential can be written in the simple form

\[ v_{\text{eff}}(r_{ij}) = v(r_{ij}) f^2(r_{ij}) + \frac{1}{m} (\nabla f(r_{ij}))^2 , \]

where the correlation function is chosen in such a way as to reproduce, at two-body level of the cluster expansion of \( \langle H \rangle \), the variational energies obtained from FHNC minimum of the energy at two body cluster level.

The definition of \( v_{\text{eff}} \) though the equivalence between matrix elements makes the effective interaction finite and well behaved, unlike the bare potential, since it takes into account the effect of the short-range correlations. Moreover, if we assume that correlated states are close to the true eigenstates of the hamiltonian, it follows that non diagonal matrix elements \( \langle m | H | n \rangle \) are small, and the effective interaction \( v_{\text{eff}} \) is adequate for use in perturbative calculations.

The Green’s function

The first objective of our project is the calculation of the Green’s function, defined as [12]

\[ G(\mathbf{k}, \omega) = \langle 0 | a_{\mathbf{k}}^\dagger \frac{1}{H - E_0 + \omega - i\eta} a_{\mathbf{k}} | 0 \rangle - \langle 0 | a_{\mathbf{k}} \frac{1}{H - E_0 - \omega - i\eta} a_{\mathbf{k}}^\dagger | 0 \rangle , \]

\( E_0 \) being the ground state energy, performed using the CBF effective interaction. The Green’s function is fundamental element of the formalism of many-body theory, the knowledge of which is needed for the description of a variety of properties of interacting many-body systems.
The starting point is the relation
\[ G^{-1}(k, \omega) = G_0^{-1}(k, \omega) - \Sigma(k, \omega) , \]
where \( G_0(k, \omega) \) denotes the Green’s function of the non interacting system, allowing to obtain the Green’s function from the perturbative expansion of the self-energy \( \Sigma(k, \omega) \).

We have studied the second order contribution to the Green’s function, arising from the two particle-one hole (2p1h) and two hole-one particle (2h1p) intermediate states. For the self-energy, this analysis requires the calculation of the imaginary parts of the contributions associated with both the polarization and correlation diagrams of Ref. [13]. The resulting imaginary part of \( \Sigma(k, \omega) \) is then used to obtain the real part through dispersion relations.

From the self-energy, it is possible to extract a wealth of information on different properties of the system, ranging from the momentum distribution, yielding the occupation probability of the momentum eigenstates, to the effective mass of the constituent particles.

In perturbation theory, the spectrum of single-particle excitations is determined, order by order, by the poles of the one Green’s function. The on shell imaginary part defines the life-time of the single-particle states, while the real part enters the definition of the corresponding energy
\[ \omega(k) = \frac{k^2}{2m} + \text{Re} \Sigma(k, \omega(k)) , \]
as well as the determination of the effective mass \( m^* \), given by
\[ \frac{m^*}{m} = \left[ \frac{1}{k} \frac{d\omega(k)}{dk} \right]_{k=k_F}^{-1} . \]

The momentum distribution \( \rho(k) \), defined as
\[ \rho(k) = \langle 0 | a_k^\dagger a_k | 0 \rangle , \]
is related to one body Green’s function through an integration in the complex variable \( \omega \), performed on an closed contour in upper half-plane (\( \text{Im} \omega > 0 \))
\[ \rho(k) = \frac{1}{2\pi i} \int_C d\omega G(k, \omega) . \]

The above quantities have been computed using the CBF effective interaction. The corresponding numerical results are shown in Figs. 4, 5, 6 and 7. For all of them perturbative results, obtained using the \( G \)-matrix formalism for dilute Fermi systems, are available in literature. Within this approach, the ground state energy, effective mass and momentum distribution of the hard sphere model are derived as power series in the dimensionless parameter \( k_F a \). Comparison between these results and those obtained from the CBF effective interaction in the low-density limit, provides valuable information to gauge the accuracy of our calculations.

Note that effective interaction approach is based on the assumption that a suitable choice of the correlation function allows one to truncate the cluster expansion of \( \langle H \rangle \) at lowest order and still obtain a very accurate estimate of the ground state energy. However, in principle it is not obvious that the same correlation function may reproduce other physical properties of the system. Hence, the agreement between our results and the momentum distribution obtained by the authors of Ref. [6] and [14] is very promising, in view of the further applications of the effective interaction approach.
Figure 4: Dependence upon $y = \omega / \omega_F$ of the imaginary part of the self-energy obtained through CBF effective interaction for two momenta $k$, below ($k/k_F=0.5$) and above ($k/k_F=1.5$) Fermi momentum ($k_F = 0.7 \text{ fm}^{-1}$, $\nu=4$, $a=1$).

Figure 5: Dependence on $y = \omega / \omega_F$ of the real part of correlation and polarization diagrams for $\nu = 4$, $a = 1$, $k_F=0.7 \text{ fm}^{-1}$ and $k=0.1k_F$ obtained through CBF effective interaction.
Figure 6: Momentum distributions of a hard sphere Fermi system for degeneracy \( \nu = 4 \), core \( a = 1 \) and Fermi momenta \( k_F = 0.4 \) and 0.7 fm\(^{-1}\) obtained though CBF effective interaction (full lines), \( G \)-matrix for \( k_F = 0.7 \) fm\(^{-1}\) of Ref. [9] (short dashed line) and FHNC for \( k_F = 0.4 \) fm\(^{-1}\) of Ref. [14] (long dashed line).

Figure 7: Dependence upon \( k/k_F \) of the quantity \( m^*(k)/m \) for Fermi momentum \( k_F = 0.4 \) (preliminary results). The enhancement, due to second order contributions, has a peak at momentum \( k = k_F \).
Summary and prospects

We plan to use the self-energy to obtain the spectral functions $P_h(k, E)$ and $P_p(k, E)$, appearing in the Källén-Lehmann representation of the Green’s function. The knowledge of these quantities, yielding the probability of removing or adding a particle of momentum $k$ to the system in its ground state, leaving the resulting $(N \pm 1)$-particle system with excitation energy $E$, allows one to obtain the linear response to a probe delivering momentum $q$ and energy $\omega$

$$S(q, \omega) = \sum_n \langle 0 | \rho_q^\dagger | n \rangle \langle n | \rho_q | 0 \rangle \delta (\omega + E_0 - E_n),$$

where the operator $\rho_q = \sum_k a_k^\dagger a_k + q$ describes the fluctuations of the density of the system induced by the interaction with the probe. In the impulse approximation regime, i.e. when the spatial resolution of the probe is larger than interparticle distance, the linear response is directly related to spectral function the above definition is in fact expected to reduce to [15,16]

$$S(q, \omega) = \int dE d\mathbf{k} P_h(k, E) P_p(k + q, \omega - E).$$

Finally, we will exploit the flexibility of the effective interaction approach, allowing for a consistent calculation of the effective mass and the in-medium scattering cross section, to calculate the transport coefficients, e.g. the shear viscosity and thermal conductivity, within the framework of the Landau-Abrikosov-Khalatnikov formalism [8,17]. The understanding of the transport properties of dense matter is of paramount importance for astrophysical applications, as they determine the stability of rapidly rotating neutron stars [18], as well as the scattering rates of low energy neutrinos [19], which in turn drive the evolution of supernovae and protoneutron stars. The results of our study of the hard sphere system, besides being interesting in their own right, will be of great value for the assessment of the applicability of the effective interaction approach to neutron star matter.

References


