Abstract  We report calculations of equation of state of a model system, representative for a cold Fermi gas, of particles interacting via the Pöschl-Teller interaction. In successively more sophisticated calculations, we determine the importance of correlations and non-localities. We show that the gas displays, at relatively low density, an instability indicated by a divergence of the in-medium scattering length which occurs well before the divergence of the vacuum scattering length and the spinodal density. We also calculate the pairing gap and show that non-local correlations can change the pairing gap by almost an order of magnitude.

Keywords  Superfluidity, Quantum Fluids, Cold Gases

1 Motivation

In the analysis of experiments with cold quantum (Bose- and Fermi-)gases, one is normally interested in a density regime where the short-ranged details of the interaction are irrelevant, and the structure and dynamics of the system can be characterized by low-energy 2-body scattering processes. Much of the physics – with rare exceptions like the “unitary limit” – in this regime can be described by textbook methods, and one of the tasks of microscopic many-body theory is to explore the regime of validity of such approaches. To that end, we examine in this work the equation of state, the stability, and the pairing properties of a low-density Fermi gas interacting via a purely attractive, short-ranged interaction.
2 Generic Many-Body Theory

Our method of choice is the Jastrow-Feenberg\(^1\) variational approach; pedagogical and review material may be found in Refs.\(^1\)–\(^3\); technical details are in Ref.\(^4\).

We assume for a strongly interacting and translationally invariant normal system a non-relativistic many-body Hamiltonian of identical particles interacting via a pair-potential \(v(r_i - r_j)\). The method starts with an ansatz for the wave function

\[
\Psi_0(r_1, \ldots, r_N) = \frac{1}{\sqrt{I_{o,o}}} F(r_1, \ldots, r_N) \Phi_0(1, \ldots, N),
\]

\[
F(r_1, \ldots, r_N) = \exp \left[ \frac{1}{2} \left( \sum_{i < j} u_2(r_i, r_j) + \cdots + \sum_{i_1 < \cdots < i_n} u_n(r_{i_1}, \ldots, r_{i_n}) + \cdots \right) \right],
\]

where \(I_{o,o} = \langle \Phi_0 | F^\dagger F | \Phi_0 \rangle\) is the normalization constant. \(\Phi_0(1, \ldots, N)\) is a model state, which is for normal Fermi systems a Slater-determinant, and \(F\) is a local correlation operator written in the general form (2). In quantum Monte Carlo studies, the wave function (1) is referred to as “fixed-node approximation.” Diagrammatic methods, specifically the optimized Euler-Lagrange Fermi-hypernetted chain (FHNC-EL) method, determine the correlations \(u_n(r_1, \ldots, r_n)\) by functionally minimizing the energy. Truncated at the two-body term \(u_2\), it is the standard Jastrow approximation. These are computationally far less demanding and, more importantly, provide direct information on physical processes; for example phase transitions are reflected in divergences of the theory. The resulting equations are equivalent to the summation of localized parquet–diagrams\(^5\) and can also be derived from Coupled Cluster theory\(^6\) without ever mentioning a Jastrow function. For that reason, we refer to our method as “generic”.

For our specific application, we assume here the “Pöschl-Teller” interaction\(^7\)

\[
V(r) = -\frac{\hbar^2}{m\sigma^2} \frac{V_0(V_0 - 1)}{\cosh^2(r/\sigma)}
\]

characterized by the strength \(V_0\) and the range \(\sigma\). For this interaction, the scattering length can be calculated analytically\(^8\). In the above parametrization, bound states appear at even integer values of \(V_0\); the regime of interest is therefore the range \(1 < V_0 < 2\). The interaction (3) is similar to the attractive square–well potential used by Astrakharchik \textit{et al.}\(^9\) and us\(^10\), it has been used by Gezerlis and Carlson\(^11\) for a Monte Carlo study of strong pairing in cold gases.

We spell out the simplest versions of the equations that are consistent with the variational problem (“FHNC//0-EL”). These equations provide the minimal version of the FHNC-EL theory. In particular, they contain the indispensable physics, namely the correct description of both short- and long-ranged correlations.

The minimization condition for the pair correlations can be written in the form

\[
S(k) = S_F(k) \left[ 1 + 2 \frac{S_F^2(k)}{t(k)} V_{p-h}(k) \right]^{-\frac{1}{2}},
\]
where \( S(k) \) is the static structure factor of the interacting system, \( S_F(k) \) is the static structure factor of the non-interacting Fermi system, and \( t(k) = \hbar^2 k^2 / 2m \). In the FHNC/0 approximation, we have

\[
V_{p-h}(r) = |1 + \Gamma_{dd}(r)| \sqrt{1 + \Gamma_{dd}(r)} + \Gamma_{dd}(r) v_1(r),
\]

(5)

\[
\tilde{w}_1(k) = -t(k) \left[ \frac{1}{S_F(k)} - \frac{1}{S(k)} \right] \left[ \frac{S(k)}{S_F(k)} + \frac{1}{2} \right]
\]

(6)

with the “direct correlation function”

\[
\Gamma_{dd}(k) = (S(k) - S_F(k)) S_F^{-2}(k).
\]

(7)

We define the Fourier transform with a density factor, i.e.,

\[
\tilde{f}(k) \equiv \rho \int d^3 r e^{ik \cdot r} f(r).
\]

More complicated versions of the FHNC-EL method add additional equations for the so-called “ee”, “de,” and “cc” diagrams.

2.1 Correlated Basis Functions

Eq. (4) can be interpreted in terms of linear response theory as follows: Begin with the random phase approximation for the static structure function

\[
S(k) = -\Im m \int_0^\infty d\omega \frac{d\omega}{\pi} \chi_0(k, \omega) \left[ 1 - \tilde{V}_{p-h}(k) \chi_0(k, \omega) \right]^{-1}
\]

(8)

where \( \chi_0(k, \omega) \) is the Lindhard function, and \( \tilde{V}_{p-h}(k) \) is a local quasiparticle interaction or “pseudopotential”. Eq. (4) can be obtained by approximating the Lindhard function \( \chi_0(q, \omega) \) by a “collective” Lindhard function which is constructed by approximating the particle-hole band by an effective single pole such that the \( m_0 \) and \( m_1 \) sum rules of the non-interacting system are satisfied. A way to go beyond local correlation operators of the form (2) is therefore to replace the “collective” expression (4) by Eq. (8), keeping the same particle-hole interaction. With this we go beyond the Jastrow-Feenberg (or fixed-node) approximation. A rigorous proof that this procedure is legitimate can be obtained within correlated basis functions (CBF) theory.

2.2 BCS Theory with correlated wave functions

The natural generalization of the Jastrow-Feenberg approach to a superfluid system is to first project the bare BCS state on a complete set of independent-particle states with fixed particle number. Then apply the correlation operator to that state, normalize the result, and finally, sum over all particle numbers \( N \). Thus, the correlated BCS (CBCS) state becomes

\[
|\text{CBCS}\rangle = \sum_{m,N} |\Psi_{m}^{(N)}\rangle \langle \Phi_{m}^{(N)} | \text{BCS}\rangle, \quad |\text{BCS}\rangle = \prod_k \left[ u_k a^\dagger_k \right] |0\rangle
\]

(9)
where the \( \{ | \phi_m^{(N)} \rangle \} \) is a complete set of normalized, but non-orthogonal \( N \)-particle basis states built with the correlation operator \( F \), and \( u_k, v_k \) are the familiar Bogoliubov amplitudes.

Considering the interaction of only one Cooper pair at a time, we can expand all expectation values in the deviation \( u_k, v_k \) from their normal state values. (In fact, the inclusion of superfluid momentum distributions to all orders has a rather small effect on the pairing gap, even when the gap is comparable to the Fermi energy.) Then, the pairing matrix elements and the single-particle energies entering the gap can be taken from quantities calculated for the normal system.

The calculation of expectation values for correlated states is somewhat tedious; we only give the final result in the approximation used in this work. The energy of the superfluid state becomes

\[
\langle \hat{H} - \mu \hat{N} \rangle_s = H_{oo}^{(N)} - \mu N + 2 \sum_{k, |k| > k_F} v_k^2 (\tau(k) - \mu) - 2 \sum_{k, |k| < k_F} u_k^2 (\tau(k) - \mu) + \sum_{k, k'} u_k v_{k'} \mathcal{R}_{kk'}
\]

in terms of the “pairing interaction” of the form

\[
\mathcal{R}_{kk'} = \langle \uparrow_k, -\downarrow_k | \mathcal{W}(1, 2) | \uparrow_{k'}, -\downarrow_{k'} \rangle + \langle \tau(k) - \mu | + | \tau(k') - \mu | \rangle \langle \uparrow_k, -\downarrow_k | \mathcal{N}(1, 2) | \uparrow_{k'}, -\downarrow_{k'} \rangle.
\]

where \( \mathcal{W}(1, 2) \) and \( \mathcal{N}(1, 2) \) are non-local, energy independent two-body operators. The dominant, local contributions are in momentum space

\[
\mathcal{N}(k) = \tilde{G}_{dd}(k), \quad \mathcal{W}(k) = -\tau(k) \tilde{G}_{dd}(k) S^{-1}(k).
\]

With the result (10), we have arrived at a formulation of the theory which is isomorphic to the BCS theory for weakly interacting systems. Note that, in this formulation, \( \mathcal{W}(1, 2) \) should be identified with a static approximation of the \( T \)-matrix.

### 3 Results and Discussion

#### 3.1 Energetics

A condition for the existence of solutions of the Euler equation is that the term under the square-root in Eq. (2) is positive, or, in CBF, that the static density-density response function is positive. This is expressed in terms of Landau’s stability criterion \( F_s^0 > -1 \), and we must identify the limit

\[
\tilde{\nu}_{p=0}(0+) = \frac{\hbar^2 k_F^2}{3m} F_s^0 \equiv m(c^2 - c_F^2)
\]

where \( c_F^2 = \frac{\hbar^2 k_F^2}{3m} \) is the speed of sound of the free Fermi gas. The Landau-parameter \( F_s^0 \) can also be obtained from the equation of state

\[
mc^2 = \frac{d}{dp} \rho^2 \frac{dE}{dp} \frac{N}{N}. \tag{14}
\]
Fig. 1 (color online) The left figure shows the Fermi-liquid parameter \( F_s \) of the “Pöschl-Teller” liquid for a sequence of interaction strengths \( V_0 \) as shown in the legend as a function of density, as calculated from Eq. (13). The right figure shows the ratio between the in-medium scattering length \( a \) and the vacuum scattering length \( a_0 \) for the same sequence of interaction strengths.

The values of \( mc^2 \) obtained via Eq. (14) and from a diagrammatic expansion of the particle-hole interaction via (13) agree normally only in an exact theory\(^{16} \), their discrepancy can be used as a convergence test. We have checked this by fitting the energy per particle by the kinetic energy \( \hbar^2 k^2/10m \) plus a polynomial of \( k^3 \) and \( k^5 \) and compared the results obtained from Eqs. (14) and (13). We found that the numerical values are practically identical for weak couplings. They can differ by about 30 percent for strong coupling strengths \( V_0 > 1.7 \) which is consistent with the fact that the convergence of cluster expansions becomes worse with increasing interaction strength.

Let us now go through the calculation of the energetics and stability of the equation of state. The left panel of Fig. 1 shows the Fermi liquid parameter \( F_s \) as obtained from Eq. (13) for a sequence of interaction strengths as a function of the density.

The fact that the equations of state all come to an endpoint has been identified in Ref. 10 as due to a divergence of the in-medium scattering length which is, in the local approximation used here

\[
a \equiv \frac{m}{4\pi\rho h^2} \bar{\mathcal{W}}(0+).
\]

This divergence is the reason that the Landau stability limit \( F_s \rightarrow -1 \) could not be reached. The same situation occurs, expectedly, in the present case, see the right panel in Fig. 1. Due to this instability we have not been able to reach the rather large values of \( -k_F a_0 \) reported in Ref. 11 before the optimization of the correlations diverged.

3.2 BCS pairing

The wave function (1) determines the pairing interaction uniquely. Since the effective interaction (12) contains chain diagrams, the important polarization effects\(^{17,18} \) are included in the density channel in a static manner. We have, however, pointed out in section 2.1 that this approximation can be improved by replacing

\[
\tag{15}
\]
the “collective approximation” by the proper Lindhard function. Again, we take this here as a plausibility argument; the rigorous derivation that such a procedure is legitimate can be obtained by deriving the generalization of the expansion (10) in correlated basis functions.\textsuperscript{19}

\[
\tilde{\mathcal{V}}_{\text{eff}}(k, \omega) = \tilde{\mathcal{V}}_{p-h}(k) \left[ 1 - \chi_0(k, \omega) \tilde{\mathcal{V}}_{p-h}(k) \right]^{-1}
\]

which we take, following Ref.\textsuperscript{18} at $\omega = 0$.

Fig.\textsuperscript{2} shows the calculated energy gap in FHNC/0-EL and CBF approximation. Evidently, inclusion of the energy-dependent effective interaction can change the value of the gap by almost an order of magnitude. This is, of course, not a statement on the specific FHNC approximation, but more generally on the quality of the locally correlated (or “fixed–node”) wave function which must, therefore, be seriously questioned.

\subsection*{3.3 Conclusion}

We have described in this paper new calculations of stability regime and the pairing gap in a model system interacting via the purely attractive Pöschl-Teller interaction. Similar to what we found in previous work\textsuperscript{10}, we have encountered an instability of the system with increasing density and increasing potential strength $V_0$, well before the vacuum scattering length $a_0$ of the interaction potential diverges.

We have also demonstrated that local correlation functions perform poorly for pairing phenomena: The plausible reason for that is that the wave function (2) treats all particles in the same way. This is a reasonable assumption for Fermi–sea averaged quantities like the energy per particle or the static structure function. However, this approximation is particularly poor for observables that are determined by the dynamics close to the Fermi surface. Since this is the case for BCS type pairing, our results are as expected and fully consistent with our earlier work\textsuperscript{20,21}.

In conclusion, we note again that going beyond the “weak coupling” approximation (10) makes very little difference in our results but causes a number of serious formal difficulties.\textsuperscript{15} This is an interesting statement per-se: Note that in a
weakly interacting system, the gap equation can describe the transition between a “BCS” state where the Cooper pairs are weakly coupled, to a “BEC” phase where the pairs are strongly bound. The gap equation is a proper subset of our diagram summation; but we find a divergence of a set of diagrams that are not included in weakly interacting systems described by the gap equation alone. The issue deserves further investigation.

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