Chapter 1

Superfluid Pairing in Neutrons and Cold Atoms

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Ultracold atomic gases and low-density neutron matter are unique in that they exhibit pairing gaps comparable to the Fermi energy which in this sense are the largest in the laboratory and in nature, respectively. This strong pairing regime, or the crossover between BCS and BEC regimes, requires non-perturbative treatments. We describe Quantum Monte Carlo results useful to understand the properties of these systems, including infinite homogeneous matter and trapped inhomogeneous gases.

1. From cold atoms to neutron stars and back

Although the energy and momentum scales of cold atomic gases and atomic nuclei differ by many orders of magnitude, we can gain insight into superfluid pairing in the strongly correlated regime by comparing and contrasting the two systems. Dilute neutron matter and ultracold atomic gases near infinite scattering length (unitarity) are similar in that their equation of state and pairing gaps, when measured in terms of the Fermi energy, are comparable. For this reason these systems can be viewed as “high-temperature superfluids”, even though one occurs at very small and the other at very large temperature. Since the pairing gap $\Delta$ is roughly proportional to the critical temperature $T_c$, both these systems exhibit very strong pairing, the strongest ever observed before in nature or experimented with in the laboratory. In cold fermionic atoms the particle-particle interactions can
be tuned experimentally, thus also mimicking the setting of low-density neutron matter, which is beyond direct experimental reach. More specifically, at low densities $s$-wave scattering can be described using only two parameters: the scattering length $a$ and the effective range $r_e$.

### 1.1. Ultracold Atomic Gases

For ultracold fermionic atoms at low temperature, the superfluid phase arises across the entire spectrum of weak to strong attractive interactions. Experiments with $^6$Li or $^{40}$K have an interparticle spacing that is significantly larger than the characteristic length of the interaction. Over the last decade experimentalists managed to vary the interaction strength (the scattering length $a$) across a resonance, through a regime known as “unitarity”. The cold atom gases are very dilute, so the typical scale of the interaction range (or the effective range $r_e$) is much smaller than the average interparticle spacing. For these broad Feshbach resonances we have $k_Fr_e \ll 1$, where $k_F$ is the Fermi wave vector ($\rho = k_F^2/(3\pi^2)$), so at fixed density the effective-range can be taken to be very small, essentially zero. It may be possible to use narrow and wide resonances in cold atoms to study the case of varying $r_e$ experimentally, and thus directly simulate neutron matter.

A large variety of equilibrium and dynamic properties have been measured in cold Fermi atom experiments. Experiments using $^6$Li at Duke University and at ENS have measured the ground-state energy of the system, essentially finding it to be in good qualitative agreement with Quantum Monte Carlo (QMC) predictions. The ground-state energy per particle is conventionally given in units of the energy of a free Fermi gas at the same density $E_{FG} \equiv 3E_F/5 = 3\hbar^2k_F^2/(10m)$ as $E = \xi E_{FG}$. Recent sign-free auxiliary field QMC calculations and experiments give very precise results $\xi$ at unitary, $\xi = 0.372(5)$ and $0.375(5)$, respectively.

The great advantage of cold atom systems is that they offer quantitative experimental results in the strong-coupling regime with simple interactions. An important example is the pairing gap at unitarity. Experiments at MIT and Rice probed lithium gases with population imbalance (also called “polarized” gases). An MIT experiment established the phase diagram of a polarized gas, revealing spatial discontinuities in the spin polarization. This experiment was then used to extract the pairing gap, which was found to be approximately half of the Fermi energy $E_F$, in good agreement with QMC calculations. The gap is conventionally given in units of $E_F$ as
\( \Delta = \eta E_F \). The MIT group later used RF spectroscopy to independently determine the gap, finding it to be in agreement with the afore-mentioned calculation and extraction.\(^{13}\)

1.2. Neutron matter and neutron drops

As already mentioned, at very low densities, neutron matter is very similar to cold Fermi atoms. The neutron-neutron scattering length is fixed and large \( (a \approx -18 \text{ fm}) \), but by varying the density we can probe different values of \( k_F a \). Neutrons in the inner crust of a neutron star are expected to pair in the \( ^1S_0 \) channel.\(^{15,16} \) at higher densities, also important in neutron stars, the effective range becomes important as do the repulsive parts of the neutron-neutron interaction, and higher partial waves. The inner crust of a neutron star contains a neutron gas embedded in a sea of ions. The properties are largely determined by the EOS and pairing of homogeneous matter. Pairing in neutron matter has been studied for many decades, leading to a large spread of predictions of the \( ^1S_0 \) pairing gap even for this idealized system. The gradient terms in the density functional and the behavior of the pairing gap in an inhomogeneous system are potentially important for the crust of a neutron star and can be studied simulating neutrons in external fields.\(^{17}\)

It may be possible to access superfluidity in neutron star matter observationally: superfluidity in a neutron star is often used to explain its dynamical and thermal evolution, impacting the specific heat, bremsstrahlung, and pair breaking/formation.\(^ {18,19} \) Additionally, a cooling mechanism that makes use of superfluid phonons has been proposed. Whether this mechanism is competitive to the heat conduction by electrons in magnetized neutron stars or not is a question that is directly correlated to the size of the gap.

Neutron matter and neutron drop computations also hold significance in the context of traditional nuclear physics: equation of state results at densities close to the nuclear saturation density have been used for some time to constrain Skyrme and other density functional approaches to heavy nuclei, while the density-dependence of the \( ^1S_0 \) gap in low-density neutron matter has recently also been used to constrain Skyrme-Hartree-Fock-Bogoliubov treatments in their description of neutron-rich nuclei.\(^ {22} \) Recent \textit{ab initio} results for neutron drops point to a need for more repulsive gradient terms in inhomogeneous neutron matter, and a reduced isovector spin-orbit and pairing strength compared to standard functionals.\(^ {17} \)
2. BCS and Quantum Monte Carlo methods

BCS theory has been critical to understanding many of the pairing properties of nuclei. Quantum Monte Carlo many-body simulations, on the other hand, have been used for some time to calculate the equation of state of strongly-correlated systems, e.g. liquid helium. In such systems, however, QMC methods were unable to reliably calculate pairing gaps because of the vast difference in scale between the energy of the entire system (of the order of eV’s per particle) and the pairing gap (of the order of meV). Thus, the same feature of strongly paired fermionic systems (namely the large pairing gap) that precludes the application of mean-field theories is precisely the reason that allows many-body simulation techniques to be used.

2.1. Weak coupling

We first briefly review the weak-coupling regime where exact results are available. At extremely low densities (|\(k_Fa| < < 1\)) the effective coupling between two fermions is weak and matter properties can be calculated analytically. The ground-state energy of normal (i.e. non-superfluid) matter in this regime was calculated by Lee and Yang in 1957:

\[
\frac{E}{E_{FG}} = 1 + \frac{10}{9\pi} k_F a + \frac{4}{21\pi^2} (11 - 2 \ln 2) (k_F a)^2 ,
\]

where \(E_{FG}\) is the energy of a free Fermi gas at the same density as the interacting gas. While this expression ignores the contributions of superfluidity, these are exponentially small in (1/\(k_Fa\)). In the next section we compare these results to QMC calculations for |\(k_Fa| \geq 1\).

The mean-field BCS approach celebrated in the present volume reduces in the weak-coupling limit to:

\[
\Delta_{BCS}(k_F) = \frac{8}{\pi} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2ak_F} \right) .
\]

As was shown in 1961 by Gorkov and Melik-Barkhudarov the BCS result acquires a finite polarization correction even at weak coupling, yielding a reduced pairing gap:

\[
\Delta^0(k_F) = \frac{1}{(4e)^{1/3}} \frac{8}{\pi} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2ak_F} \right) .
\]

Thus, the polarization corrections reduce the mean-field BCS result by a factor of 1/(4e)^{1/3} ≈ 0.45. Interestingly, if one treats the polarization
effects at the level of sophistication used in the work of Gorkov and Melik-Barkhudarov, this factor changes with $k_Fa$ \cite{25} though there is no a priori reason to expect such an approach to be valid at stronger coupling ($k_Fa$ of order 1 or more). Calculating the pairing gap in this region has been a difficult task, as can be seen from the multitude of publications devoted to this subject over the past twenty years. \cite{15, 16, 26, 36}

2.2. Quantum Monte Carlo

Quantum Monte Carlo simulations typically begin with a local Hamiltonian of the form:

$$\mathcal{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_k^2\right) + \sum_{i<j} v(r_{ij}) + \sum_{i<j<k} v_{ijk}. \quad (4)$$

where $N$ is the total number of particles. In the case of cold atoms the interaction only acts between opposite spin pairs and is effectively a contact interaction (often simulated on the computer using a short-range potential). The neutron-neutron interaction is more complicated, containing one-pion exchange at large distances, intermediate range spin-dependent attraction dominated by two-pion exchange, and a short-range repulsion. One popular NN interaction that fits the experimental phase shifts well is Argonne v18 \cite{37}. At nuclear densities the two-body force is combined to a three-body force that is essential to reproduce the spectrum of light nuclei \cite{38}. At very low densities, though, as found in neutron star crusts or the exterior of neutron-rich nuclei, the scattering length ($a = -18.5 \text{ fm}$) and effective range ($r_e = 2.7 \text{ fm}$) are most crucial to the physical properties of the system. The presence of a short-range repulsive core is important primarily in that it prevents collapse to a higher-density state.

Schematically, Green’s Function Monte Carlo projects out the lowest-energy eigenstate $\Psi_0$ from a trial (variational) wave function $\Psi_V$ by treating the Schrödinger equation as a diffusion equation in imaginary time $\tau$ and evolving the variational wave function up to large $\tau$. The ground state is arrived at using:

$$\Psi_0 = \exp[-(H - E_T)\tau]\Psi_V$$

$$= \prod \exp[-(H - E_T)\Delta\tau]\Psi_V,$$

evaluated as a branching random walk. The short-time propagator is sometimes taken from a Trotter-Suzuki approximation, but the exact two-nucleon propagator can also be employed. The ground-state energy $E_0$ can
be obtained from:

$$E_0 = \frac{\langle \Psi_V | H | \Psi_0 \rangle}{\langle \Psi_V | \Psi_0 \rangle} = \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}.$$  (6)

In the case of more complicated interactions, one can use either the nuclear Green’s Function Monte Carlo method\(^{38}\) or the Auxiliary Field Diffusion Monte Carlo approach\(^{39}\). Schematically, the latter method reduces the spin-isospin dependence of the interaction operators from quadratic to linear by means of the Hubbard-Stratonovich transformation. Given a generic operator \(\hat{O}\) and a parameter \(\lambda\):

$$e^{-\frac{1}{2} \lambda \hat{O}^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + \sqrt{-\lambda} x \hat{O}}.$$  (7)

As a result, the Monte Carlo sampling is no longer limited to the coordinate space positions of the particles, but now extends to sample auxiliary fields. Thus, the AFDMC algorithm limits the exponential growth of the spin-isospin states, and recovers the ground state in polynomial time.

In these Quantum Monte Carlo superfluid simulations the trial wave function was taken to be of the Jastrow-BCS form with fixed particle number:

$$\Psi_V = \prod_{i \neq j} f_P(r_{ij}) \prod_{i' \neq j'} f_P(r_{i'j'}) \prod_{i,j} f(r_{ij}) A[\prod_{i < j'} \phi(r_{ij'})]$$  (8)

and periodic boundary conditions. The primed (unprimed) indices correspond to spin-up (spin-down) neutrons. The pairing function \(\phi(r)\) is a sum over the momenta compatible with the periodic boundary conditions. In the BCS theory the pairing function is:

$$\phi(r) = \sum_n \frac{v_{k_n}}{u_{k_n}} e^{i k_n \cdot r} = \sum_n \alpha_n e^{i k_n \cdot r}.$$  (9)

The Jastrow part is usually taken from a lowest-order-constrained-variational method\(^{40}\) calculation described by a Schrödinger-like equation. The fixed-node approximation guarantees that the result for one set of pairing function parameters will be an upper bound to the true ground-state energy of the system. Variational results with the pairing function alone reproduce BCS calculations with finite particle-number projection. The parameters are optimized in the full QMC calculation, providing the best possible nodal surface, in the sense of lowest fixed-node energy, with the given form of trial function. Comparisons of fixed-node results\(^{9}\) in the cold atom system with recent AFQMC results\(^{10}\) indicate that the fixed node calculations are quite accurate.
In the case of closed-shell neutron drops the antisymmetric part of the trial wave function has the form

$$\psi(R,S) = \left[ \sum \text{Det}\{\phi_\alpha(\vec{r}_i,s_i)\} \right]_{J,M},$$

where \(\alpha = \{n,j,m_j\}\) is the set of quantum numbers of single-particle orbitals, and the summation of more determinants is done in order to have a trial wave function that is an eigenstate of \(J^2\) and \(M\). The single-particle basis is given by

$$\phi_\alpha(\vec{r},s) = \Phi_{n,j}(r) \left[ Y_{l,m}^l(\hat{r}) \xi_{s,m}^s(s) \right]_{j,m_j},$$

The radial components \(\Phi_{n,j}\) are obtained solving the Hartree-Fock problem with a Skyrme force and their width is variationally optimized, \(Y_{l,m}\) are spherical harmonics and \(\xi_{s,m}\) are spinors in the usual up-down base. It is particularly important at low densities (low oscillator frequencies) to incorporate explicit BCS correlations in the trial wave function, essentially using single particle orbitals in the above equation in a form like Eq. (9).

3. Infinite Matter Results

The \(T = 0\) equations of state for homogeneous cold atoms and neutron matter of Ref. [8] are compared in Fig. 1. The horizontal axis is \(k_F a\), with the equivalent Fermi momentum \(k_F\) for neutron matter shown along the top. The vertical axis is the ratio of the ground-state energy to the free Fermi gas energy \(E_{FG}\) at the same density; as discussed in the previous section (Eq. (1)), it must go to one at very low densities and decrease as the density increases and the interactions become important. The curve at lower densities shows the analytical result by Lee and Yang mentioned previously. The QMC results shown in this figure seem to agree with the trend implied by the Lee-Yang result. The neutron matter and cold atom equations of state are very similar even for densities where the effective range is comparable to the interparticle spacing. Near \(k_F a = -10\) the energy per particle is not too far from QMC calculations and measurements of the ratio \(\xi\) of the unitary gas energy to \(E_{FG}\) shown as an arrow on the right (it corresponds to \(k_F a = \infty\)); previous calculations give \(\xi \approx 0.4\), more recent results in Refs. [9,10] are slightly lower). At larger densities the cold-atom and neutron matter results start to diverge, due to: i) the neutron finite effective range, and ii) the fact that the neutron results also incorporate a simple attempt to include the \(S = 1, M_S = 0\) pairs. When the density is very low, the \(s\)-wave contribution is dominant so cold atoms
and neutron matter agree very well. As the density increases, the effective range, as well as higher order terms in momentum and higher partial waves, become important.

The pairing gap at T=0 is calculated using the odd-even staggering formula:

$$\Delta = \left[ E(N+1) - \frac{1}{2} [E(N) + E(N+2)] \right] (-1)^N,$$

(12)

where $N$ is the number of particles. In Fig. 2 we plot the gap as a function of $k_F a$ for both cold atoms and neutron matter, taken from Ref. 8. BCS calculations are shown as solid lines, and QMC results are shown as points with error bars. QMC pairing gaps are shown from calculations of $N = 66 - 68$ particles. For very weak coupling, $-k_F a < 1$, the pairing gap is expected to be reduced from the BCS value by the polarization corrections calculated by Gorkov and Melik-Barkhudarov, $\Delta/\Delta_{BCS} = (1/4e)^{1/3}$, as mentioned in the previous section (Eq. 3). The QMC calculations at the lowest density, $k_F a = -1$, are roughly consistent with this reduction from the BCS value. At slightly larger yet still small densities, where $-k_F a =
Fig. 2. Superfluid pairing gaps versus $k_F a$ for cold atoms ($r_e \approx 0$) and neutron matter ($|r_e/a| \approx 0.15$). BCS (solid lines) and QMC results (points) are shown.

$O(1)$ but $k_F r_e \ll 1$ for neutron matter, one would expect the pairing gap to be similar for cold atoms and neutron matter. The results at $k_F a = -2.5$, where $k_F r_e \approx 0.35$, support this expectation. Beyond that density the effective range becomes important and both the BCS and the QMC results are significantly reduced in relation to cold atoms where $r_e \approx 0$.

In cold atoms, the suppression from BCS is reduced as the density increases, with a smoothly increasing fraction of the BCS results as we move from the BCS to the BEC regime. At unitarity the measured pairing gaps\cite{12,13} are 0.45(0.05) of the Fermi energy, for a ratio $\Delta/\Delta_{BCS} \approx 0.65$, in agreement with predictions by QMC methods\cite{5,7,8}. In the BEC regime where two fermions are tightly bound, the BCS and QMC values would both give a gap of half the binding energy of the pair. In neutron matter, the finite range of the potential reduces $\Delta/E_F$ as the density increases. We find a ratio $\Delta/\Delta_{BCS}$ that increases slightly from $|k_F a| = 1$ to 2.5, but then remains roughly constant up to $|k_F a| = 10$.

In Refs. 36-41 new QMC values for neutron matter were compared to selected previous results.\cite{29,24,112,13,15} The results of the QMC calculations are much larger than most diagrammatic approaches. As these approaches
assume a well-defined Fermi surface or calculate polarization corrections based on single-particle excitations it is not clear how well they can describe neutron matter in the strongly paired regime, or the similar pairing found in cold atoms. Finally, the QMC results seem to qualitatively agree (at least for the lowest densities considered) with a determinantal Quantum Monte Carlo lattice calculation.\cite{35}

4. Neutron drops

A neutron drop is an idealized system where neutrons, interacting via realistic nuclear forces, are confined in external potentials. They provide a simple model to study neutron-rich nuclei. In Refs. 42,43 the neutron-rich isotopes of oxygen and calcium have been studied as neutrons confined in external fields, and this model provided good results for both bound and excited states. In addition, these models can be used to constrain density functionals in the large isospin-asymmetry region. Ab initio study of neutrons confined in different geometries showed that some Skyrme forces, typically fitted to nuclei with small isospin-asymmetry, are not accurate when dealing with pure neutron systems.\cite{17} The energies computed using
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Fig. 4. Pairing gap of neutrons confined in a harmonic well with frequencies $\omega = 5$ (left) and 10 (right) MeV. Results were arrived at using different Hamiltonians with only a two-body force, and including different three-body forces are presented.

QMC show that Skyrme forces tend to overbind confined neutrons, the main contribution to the difference being the poorly constrained gradient term. In Fig. 3 we plot the energy of confined neutrons computed using QMC techniques, compared with selected Skyrme forces.

The harmonic oscillator potential introduces another element into the pairing of neutrons, namely the mean field or the spacing of single-particle levels in the neutron drop. By studying the odd-even staggering of neutron drops with different frequencies, it is possible to examine the pairing as it evolves from small finite systems to infinite matter. The drops we have considered to date have harmonic oscillator frequencies of 5 and 10 MeV. In both these cases the pairing is much smaller than the single-particle spacing, so the BCS wave function is largely that occurring in the lowest shell of the drop. The GFMC calculations have included this pairing into the trial wave function, and have been used to examine both trap frequencies. At a frequency of 10 MeV, the pairing is reduced particularly for the larger drops. Early results are shown in Fig. 4 where the gap of confined neutrons...
is calculated using different Hamiltonians. The dominant physics is provided by the NN interaction, with modest changes introduced by the three-nucleon interaction. Further studies of these systems are underway.

5. Summary and Future Work

In summary, this review has examined the application of Quantum Monte Carlo methods to strongly-paired matter, including homogeneous and trapped systems of atoms or neutrons. For infinite matter, the calculated equation of state and pairing gap match smoothly with the known analytic results at low densities, and provide important constraints in the strong-coupling regime at large $k_Fa$. The low-density equation of state can help constrain Skyrme mean-field models of finite nuclei. The pairing gap for low-density neutron matter is relevant to Skyrme-Hartree-Fock-Bogoliubov calculations of neutron-rich nuclei and to neutron-star physics, since it is expected to influence the behavior of the crust. Similarly, results for neutron drops can also be used to constrain Skyrme and other energy-density functional approaches. Furthermore, the newly determined value of the gap implies that a new mechanism that makes use of superfluid phonons is competitive to the heat conduction by electrons in magnetized neutron stars.

Another consequence of the gap magnitude is related both to neutron-star observations and heavy-nuclei phenomenology: polarized neutron matter may be plausible within the context of magnetars, and has recently been attacked using Quantum Monte Carlo.

Microscopic many-body simulations will undoubtedly continue to straddle the divide between atomic and nuclear physics. Such simulations started with two species and equal populations, soon thereafter moving to spin-polarization. Further examination of the evolution of pairing from small to large systems is an intriguing area of study, including both cold atoms and neutron matter. For example, one avenue of future research is related to optical lattice experiments with cold atoms: to first approximation these are equivalent to periodic external potentials. In the nuclear case, an external potential would allow us to study the static response of neutron matter and would also facilitate the understanding of the impact on neutron pairing of the ion lattice that exists in a neutron star crust. Such microscopic results for the static response could provide further constraints on energy-density functionals used to describe the crust of neutron stars.
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