Polarization in low-density neutrons

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Abstract. We examine selected aspects of strongly interacting neutrons. We first go over the basics of Green’s Function Monte Carlo and then provide some specifics on the variational wave functions used. We then turn to results for the ground-state energies of polarized neutron matter, finding that phase separation is energetically favored with respect to a homogeneous polarized superfluid. Polarized neutron matter is of possible relevance to the physics of highly magnetized neutron stars as well as to terrestrial experiments with ultracold fermionic atoms. Furthermore, the simulation results we show can function as microscopic constraints for phenomenological energy-density functional theories of nuclei. We make this connection more explicit by also discussing the “neutron polaron”.

1. Introduction

Neutron matter is a system that has a long history in nuclear physics [1]. While finite nuclei are bound systems composed of neutrons and protons, neutron matter is pure (it contains no protons) and infinite (unbound). These two aspects lead to simplifications, both physically and algorithmically, that make it possible to apply Quantum Monte Carlo (QMC) methods. The lack of protons makes the many-body problem simpler, as now there are only 2 components to deal with and no long-range Coulomb forces. Neutron matter has direct physical relevance to the physics of neutron stars: it impacts their crusts (which contain a sea of dripped neutrons) [2, 3, 4] as well as their cores. Furthermore, the physics of neutron matter is related to properties of neutron-rich nuclei, such as neutron skins, which will be explored at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt and the Facility for Rare Isotope Beams (FRIB) in Michigan. Neutron matter equation of state and pairing gap results can constrain phenomenological treatments of neutron-rich nuclei [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. The general case of imbalanced neutrons (at larger density) has also been studied by many groups [20, 21, 22, 23, 24, 25].

An appealing aspect of low-density neutron matter is that its physics is especially clean: at intermediate densities only the scattering length and the effective range are relevant, and at even lower density only the former is important. Thus, low-density neutron matter is directly related also to the physics of strongly interacting ultracold atomic gases. This field has experienced an explosion of interest in the last decade, attracting both condensed-matter and nuclear physicists [26, 27]. The main reason for this has to do with the experimentalists’ ability to not only cool and trap $^6$Li and $^{40}$K atoms, but also to directly tune the interatomic $S$-wave scattering length by means of Feshbach resonances. As a result of this, cold atomic systems now routinely function as laboratories of strong interaction theory.
2. Methodology

2.1. Green’s Function Monte Carlo

When interested in the ground-state energy of a strongly interacting system, we often start out with a Variational Monte Carlo calculation which is computationally straightforward, but is contaminated with contributions coming from excited states. The results of this variational calculation are then used as input to a Green’s Function Monte Carlo (GFMC) simulation. GFMC works by projecting out the lowest-energy eigenstate $\Psi_0$ from a variational wave function $\Psi_V$. The ground-state energy is usually computed using a combination of the variational wave function as well as the “evolved” one, giving what is known as a “mixed estimate”:

$$
\langle H \rangle_M = \frac{\langle \Psi_V | H | \Psi(\tau) \rangle}{\langle \Psi_V | \Psi(\tau) \rangle} = \frac{\langle \Psi_V | H e^{-\frac{(H-E_\tau)\tau}{2}} | \Psi_V \rangle}{\langle \Psi_V | e^{-\frac{(H-E_\tau)\tau}{2}} | \Psi_V \rangle} e^{-\frac{(H-E_\tau)\tau}{2}}
$$

where $E(\tau/2)$ is the expectation value of $H$ in the state $\Psi(\tau/2)$, a quantity which approaches $E_0$ from above as $\tau \to \infty$. Let us note parenthetically that expectation values of quantities that do not commute with the Hamiltonian can be calculated using a combination of the mixed and variational estimate:

$$
\langle \Phi | \hat{S} | \Phi \rangle \approx 2\langle \Phi | \hat{S} | \Psi_V \rangle - \langle \Psi_V | \hat{S} | \Psi_V \rangle,
$$

where $\hat{S}$ is the operator corresponding to the relevant physical quantity, and the error in this expression is of second order in $\Phi - \Psi_V$. Such a combination of estimates is often called the “extrapolated estimate”.

2.2. Wave function

The choice of the wave function used in these numerical calculations, despite the fact that GFMC is in principle an exact method whose result should not depend on it, is a significant one because this wave function is used in three distinct ways: i) as the initial/trial wave function, ii) in calculating the importance-sampling function, and iii) as the fixed-node constraint.

We have chosen to write the variational wave function in the following form, which is in principle capable of educing pairing in the system under consideration:

$$
\Psi_V(\mathbf{R}) = \prod_{i \neq j} f_P(r_{ij}) \prod_{i' \neq j'} f_P(r_{i'j'}) \prod_{i,j'} f(r_{ij'}) \Phi(\mathbf{R}).
$$

The $f_P$ and $f$ are called “pair correlation functions” (also known as “Jastrow functions”). In principle they correlate both same-spin pairs and opposite-spin ones. The term $\Phi(\mathbf{R})$ describes the entire collection of $N$ particles and in these studies we have taken it to be either of the “Slater” or of the “BCS” form.

The simplest approximation that can be used to calculate $\Phi(\mathbf{R})$ in Eq. (3) is to describe the particles as being in a free Fermi gas (i.e., let all the correlations lie within the Jastrow functions). Solving this elementary exercise gives the following form for $\Phi(\mathbf{R})$:

$$
\Phi_S(\mathbf{R}) = \mathcal{A}[\phi_n(r_1)\phi_n(r_2) \ldots \phi_n(r_{\frac{N}{2}})] \mathcal{A}[\phi_n(r_1')\phi_n(r_2') \ldots \phi_n(r_{\frac{N}{2}}')],
$$

where $\mathcal{A}$ is the antisymmetrizer, and $\phi_n(r_k) = e^{i\mathbf{k}_n \cdot \mathbf{r}_k}/L^{3/2}$. Each of the two terms in Eq. (4) can be written as a Slater determinant (one for spin-up particles and one for spin-down ones).
A choice for $\Phi(R)$ that can also describe pairing is the well-known BCS wave function $\Phi_{BCS}(R)$. In the canonical ensemble, it can also be written as an antisymmetrized product of the pairing functions $\phi(r)$:

$$\Phi_{BCS}(R) = \mathcal{A}[\phi(r_{11'})\phi(r_{12'}) \ldots \phi(r_{n2n'})],$$

or, equivalently, in the form of a determinant. It is possible to generalize such a determinant so as to describe systems that contain $n$ pairs of particles, $u$ unpaired spin-up particles and $d$ unpaired spin-down particles. In this formulation the unpaired particles are in $\psi_{i\uparrow}$ and $\psi_{j\uparrow}$ single-particle states. This leads to an $(n + u + d) \times (n + u + d)$ determinant. For example, when $u = 2$ and $d = 3$, one obtains the following determinant:

$$ \begin{vmatrix}
\phi(r_{11'}) & \phi(r_{12'}) & \ldots & \phi(r_{1(n+d)'}) & \psi_{1\uparrow}(r_1) & \psi_{2\uparrow}(r_1) \\
\phi(r_{21'}) & \phi(r_{22'}) & \ldots & \phi(r_{2(n+d)'}) & \psi_{1\uparrow}(r_2) & \psi_{2\uparrow}(r_2) \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\phi(r_{(n+u)1'}) & \phi(r_{(n+u)2'}) & \ldots & \phi(r_{(n+u)(n+d)'}) & \psi_{1\uparrow}(r_{n+u}) & \psi_{2\uparrow}(r_{n+u}) \\
\psi_{1\downarrow}(r_{1'}) & \psi_{1\downarrow}(r_{1'}) & \ldots & \psi_{1\downarrow}(r_{(n+d)'})) & 0 & 0 \\
\psi_{2\downarrow}(r_{1'}) & \psi_{2\downarrow}(r_{2'}) & \ldots & \psi_{2\downarrow}(r_{(n+d)'})) & 0 & 0 \\
\psi_{3\downarrow}(r_{1'}) & \psi_{3\downarrow}(r_{2'}) & \ldots & \psi_{3\downarrow}(r_{(n+d)'})) & 0 & 0 
\end{vmatrix}. \quad (6)$$

To summarize the situation with the wave functions: for an unpolarized superfluid we use a determinant containing only pair-wave functions; for a normal gas (whether polarized or unpolarized) a product of two single-particle state-determinants (one for spin-up particles, one for spin-down); for a homogeneous superfluid the form of Eq. (6) where $d = 0$ and $u$ varies.

**Figure 1.** We show the energy of a normal neutron gas (the black solid line shows a simple fit to the Quantum Monte Carlo results), along with homogeneous superfluid results (red square points), and a tangent construction showing the phase coexistence curve (green dashed line). For large values of the relative fraction, the phase separated state is favored with respect to a homogeneous polarized superfluid.
3. Results

We begin by showing ground-state energy results for a fixed low total density of neutrons, in Fig. 1. The polarized normal neutron gas results are the black solid line from Ref. [28]. We also show as red square points the unpolarized superfluid result from Ref. [29] (at $x = 1$) and the homogeneous polarized superfluid results of Ref. [30] (at smaller $x$). In addition, we show a coexistence curve which is arrived at by a tangent construction from the unpolarized superfluid to the normal polarized curve. This coexistence line meets the normal curve at $x_c = 0.74$. As is obvious, the coexistence line lies below the homogeneous polarized superfluid Quantum Monte Carlo results, implying that these are not energetically favored. This is similar to the behavior of ultracold fermionic gases at unitarity, where $x_c = 0.44$ [31, 32, 27].

We have also focused our attention on the Fermi polaron in nuclear physics. The polaron is a single spin-down impurity embedded in a Fermi sea of spin-up particles, which has been studied by Quantum Monte Carlo methods for ultracold atomic gases [31, 32]. We show the binding energy of the neutron polaron [33] in Fig. 2. Diffusion Monte Carlo calculations for a system of the order of 100 particles provide a tight upper bound, which we use to constrain phenomenological theories (like the Skyrme functionals shown in the figure) that describe neutron-rich nuclei. Such approaches are fit to a number of empirical properties, e.g., the energy of nuclear matter. Skyrme functionals in their present form provide very different predictions for the binding energy of the polaron, none of which obey the expected behavior at weak coupling. Our results thus provide direct input for nuclear density functionals at the extreme physics of the neutron polaron.

![Figure 2](image-url)

**Figure 2.** Binding energy of neutron polaron in GFMC and AFDMC compared with Skyrme energy-density functionals. The GFMC results shown include only $s$-wave interactions, while AFDMC also uses higher partial waves, as well as tensor, and spin-orbit interactions. The microscopic results serve to exclude the behavior exhibited by a large class of phenomenological functionals.
4. Summary

Using insights and experimental guidance from the field of ultracold atomic gases, we have studied polarized low-density neutron matter in the general case and in the extreme case of the polaron. Quantum Monte Carlo provides microscopic benchmarks that can be of use to phenomenological theories of nuclear physics. This line of reasoning can be readily extended, to the case of external potentials, 3 or 4 species, lower-dimensional systems and more. These are all relatively clean systems that have a lot to teach us on the physics of neutron-rich nuclei.

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