Effective mass and pairing gap in neutron matter

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Abstract. Microscopic simulations of strongly correlated systems, such as neutron matter (NM), is restricted to a small number of particles due to various complexities. Thus, to understand the physics of infinite systems one has to consider the finite size effects (FSE) arising from these limitations on system size. These conference proceedings are centered around different ways of treating FSE in order to study NM. Specifically, we first present a preliminary study, at the mean field level and beyond, of FSE in the pairing gap of neutron superfluids. We also present a systematic model-independent extraction of the effective mass at various densities in NM using Quantum Monte Carlo (QMC) techniques.

1. Introduction

1.1. Neutron Matter

The properties of Neutron Matter (NM) play an important role in the understanding of various nuclear systems. NM can provide insight into the physics of neutron-rich nuclei while the Equation of State (EoS) is integral in the description of Neutron Stars (NS) [1]. Finally, a resurgence of the interest in the microscopic properties of NM has been observed the past few years following the capture of the first Gravitational Waves signal from a NS merger [2]. Attempts to interpret these observations from a theoretical standpoint have provided constraints on the EoS of dense matter [3–8] which are closely related to the validation of nuclear models.

Often NM is described by a Hamiltonian of the form,

\[
\hat{H} = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_{ij} v_{ij} + \sum_{ijk} v_{ijk},
\]

which corresponds to a kinetic, two-body, and three-body interaction, respectively. The phenomenological approach to constructing these potentials aims to primarily reproduce experimental data. For spin-less calculations, we make use of the Modified Pöschl-Teller (MPT) potential. In order to study systems with spin and isospin degrees of freedom, we turn to the state-of-the-art family of potentials, Argonne, and Urbana, for two- and three-body interactions respectively. The Av8' potential, from the Argonne family includes spin, isospin, spin-orbit and tensor forces [9]. Along with this, we utilize the three-body Urbana-IX (UIX) potential which was fit to light nuclei and allows for more accurate reproductions of nuclear data [10]. We also employ local chiral Effective Field Theory (EFT) interactions [11,12] which attempt to respect the symmetries of Quantum Chromodynamics. These interactions contain contributions which are called leading-order (LO), next-to-leading-order (NLO), next-to-next-to-leading-order (N^2LO), and so on.
Evaluations of observables such as energy via \textit{ab initio} approaches like Quantum Monte Carlo (QMC) are unmanageable for large number of particles. This makes direct evaluations for extended systems, i.e. the thermodynamic limit (TL), impossible. Determining quantities in this limit is of great interest since NM is physically realized as a macroscopic system. In what follows, we detail our investigations of the TL behaviour of two parameters related to NM, the pairing gap, and the effective mass.

1.2. Pairing Gap
The pairing of NM is a well-established phenomenon in the inner crust of neutron stars [13]. In this low-density regime, the neutron-neutron interaction is attractive mainly through the $^1S_0$ channel. Subject to this interaction, the neutrons pair in a spin-singlet state forming a superfluid. An \textit{ab initio} understanding of the microscopic properties of the $^1S_0$ channel superfluidity as well as superfluidity in different channels occurring in deep parts of the star is crucial. This is connected not only to pulse timing irregularities and the dynamical and thermal evolution of the star but also to its magnetic properties and vortex structure [13].

At the mean-field level, one can describe a pure neutron superfluid in the BCS approximation. In this approximation the formalism of the BCS theory of superconductivity is used to describe the pairing correlations and to calculate the pairing gap [14]. Effects beyond the mean-field approach can be introduced by the use of the PBCS theory where finite superfluid systems are described by the component of the BCS ground state that conserves particle number. Ultimately, a fully beyond-mean-field calculation can be done using QMC techniques.

1.3. Effective Mass
The concept of an effective mass has several different definitions in physics. These definitions seek to quantify physical aspects of a system by encapsulating the effects of complicated behaviour involving a particle into a renormalized mass. The ratio of the modified to the original bare mass contains information about the complicated system. We use the effective mass as defined by Landau Fermi Liquid Theory (LFLT), which arises from a quasiparticle treatment of the interactions between a group of particles [18]. This effective mass is extracted from the energy dispersion relation. It has been successful in parametrizing several observables in terms of just a handful of so-called Landau parameters. The effective mass, $m^*$ is related to the leading order spin-symmetric parameter. These Landau parameters show up in other observable quantities like the specific heat [19] effectively making the effective mass an observable. The effective mass is also very important in energy density functional theories, which allow for direct calculations of macroscopic quantities, along with time evolution [20]. We will be describing a systematic extraction of the effective mass in NM.

2. Methods
2.1. Pairing Gap
Calculations of the pairing gap in NM have been done in the past using QMC; these require the extra step of extrapolating to the thermodynamic limit. Calculations at different particle numbers will agree to varying degrees with the TL and those deviations are referred to as the finite size effects.

In the BCS and PBCS approximations, respectively, the collection of paired neutrons is described by the ground states [21]:
Figure 1. [Left] The \( N \)-dependence of the pairing gap in BCS for a density that corresponds to \( k_F a = -10 \). The inset focuses on the region of \( \langle N \rangle = 66 \) where we observe a minimum in FSE. The green line corresponds to the TL value which was obtained by solving the gap equations at the TL. [Right] The \( N \)-dependence of the energy per particle in BCS and PBCS scaled by their TL values which were obtained by solving the gap equations at the TL. The insets focus on the regions of \( N = 66 \) and \( N = 90 \).

\[
|\psi_{BCS}\rangle = \prod_{k} (u_k + v_k \hat{c}^\dagger_{k \uparrow} \hat{c}^\dagger_{-k \downarrow}) |0\rangle \quad (2)
\]

\[
|\psi_{PBCS}\rangle_N = \int \frac{dz}{2\pi i} z^{M-1} \prod_{k} (u_k + z v_k \hat{c}^\dagger_{k \uparrow} \hat{c}^\dagger_{-k \downarrow}) |0\rangle \quad (3)
\]

where \( M = N/2 \) is the number of pairs. The BCS ground state is defined in a grand canonical ensemble and therefore describes systems with particle number fluctuations. The PBCS ground state, Eq (3), is the particle conserving component of a corresponding BCS ground state. The functions \( v_k^2 \) and \( u_k^2 \) represent the probability to find a pair with momentum \( k \) or not, respectively. The pairing gap is defined as the energy released from the system when a pair is formed on the Fermi surface \( k_F \). This definition, in the context of BCS, corresponds to the minimum of the excitation energy \( E^q_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2} \), where \( \epsilon_k \) is the single particle kinetic energies, \( \mu \) is the chemical potential, and \( \Delta_k \) is the gap distribution. An example of the \( N \)-dependence of the pairing gap calculated using this definition for a density that corresponds to \( k_F a = -10 \), where \( a = -18.5 \) fm is the neutron-neutron scattering length can be found in the left panel of Fig. 1.

2.2. Effective Mass

Our effective mass calculations are carried out using QMC, a non-perturbative method for evaluating both excited energies and ground-state energies [10, 15–17]. The non-interacting problem has plane-wave solutions with the dispersion relation, \( E = \frac{\hbar^2}{2m} k^2 \). Our quasi-particle energy at the Fermi surface can be extracted from the difference in energy between a box containing \( (N+1) \) particles and \( N \) particles, where the additional particle is in some excited momentum state \( k \). After some extrapolations derived in [22] we arrive at a quasi-particle energy of

\[
\Delta E_{TL}^{(k)} = \Delta E^{(k)} - \Delta T^{(k)} + \frac{\hbar^2}{2m} k_{TL}^2,
\]
where the delta terms are interacting and non-interacting (unextrapolated) quasi-particle energies and $k^2_{TL}$ is an extrapolated momentum. This is an approximation to the TL since there is still an $N$-dependence. To perform our effective mass extraction, we attempt to match the energy of an interacting particle to the energy of a non-interacting particle. The only freedom in matching the quasi-particle energy to the non-interacting energy is in the mass. Naturally, this introduces our effective mass, $m^*$ in the form $\Delta E(k) = (\hbar^2/2m^*)k^2$, which again can be extrapolated to give,

$$\Delta E_{TL}^{(kTL)} = \frac{\hbar^2}{2m^*}k^2_{TL}. \quad (5)$$

We can extract effective masses as the slope of a linear fit between the quasi-particle energy and the momentum squared of the excited particle. Figure 2 shows the dependence of $N$ on Eq. (4). To determine the optimal $N$, we choose a multiple of $k^2_{TL}$ that best fits to the overall $N$-dependence of $\Delta E_{TL}^{(kTL)}$. The best agreement occurs at $N = 66$, making it our ideal choice to study for the TL.

3. Results
We calculated the energy of the states in Eq. (2) and Eq. (3) and studied its $N$-dependence. Figure 1 shows the energy per particle in the BCS and PBCS case where one can easily identify the particle numbers that would be of use in a QMC calculation. Both for $k_Fa = -10$ and $k_Fa = -5$, in the context of BCS, we find that the particle number $N = 66$ is a good approximation to the infinite system and it can be used to extrapolate to the TL. Applying PBCS theory which is, by design, a better description of the finite system since it encapsulates some of the beyond-mean-field correlations [23], we observe that the region of $N = 90$, for $k_Fa = -10$, and $N = 100$, for $k_Fa = -5$, can approximate an infinite system very well.
Figure 3. The effective mass ratio, $m^*/m$ for various number densities, $n$ and potentials. The upper panel makes use of only two-body interactions, while the lower panel makes use of both two- and three-body interactions.

The density dependence of the effective mass can be investigated now that FSE are under control, using $N = 66$. In Fig. 3 we show the trend of effective mass as a function of density for various potentials. The effective mass tends to unity at low densities, as the diminishing influence of the interactions makes the system act as a non-interacting system, while as the density increases there is a steady decrease in the effective mass. Both the phenomenological and chiral potentials exhibit the same general behaviour. For the chiral interactions, the notable increase in the effective mass at the highest density prompted additional calculations. These were carried out with a different three-body cut-off, that preserves the QMC EoS, and yielded a less significant increase. Thus, the effective mass is largely independent of the interaction details.

4. Conclusion
For a range of densities relevant to the inner crust of a NS, we applied PBCS theory to improve on the BCS description of finite superfluid systems and we determined a better approximation of the $N$-dependence of the energy per particle. Finally, we identified particle numbers that can act as candidates for minima in the FSE of the pairing gap. Once the existence of those minima is verified by pairing gap calculations within PBCS, these particle numbers will be optimal for use in QMC calculations for the pairing gap in NM with higher accuracy than before.

In addition, our work presents a systematic model-independent extraction of the effective mass in NM. The use of periodic boundary conditions allowed our finite QMC calculations to approximate infinite systems, further improved by our extrapolation prescription in the energy. This allowed us to carefully study the $N$-dependence and reliably extract effective masses.

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