

Neutron matter with Quantum Monte Carlo: chiral 3N forces and static response

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Abstract. Neutron matter is related to the physics of neutron stars and that of neutron-rich nuclei. Quantum Monte Carlo (QMC) methods offer a unique way of solving the many-body problem non-perturbatively, providing feedback on features of nuclear interactions and addressing scenarios that are inaccessible to other approaches. In this contribution we go over two recent accomplishments in the theory of neutron matter: a) the fusing of QMC with chiral effective field theory interactions, focusing on local chiral 3N forces, and b) the first attempt to find an *ab initio* solution to the problem of static response.

1. Introduction

Neutron matter (NM) is an extended system composed of strongly interacting particles [1, 2]. Not only is it not a toy problem, but it provides crucial information for nuclear astrophysics and nuclear structure. Specifically, the neutron-matter equation of state (EOS) is directly relevant to neutron-star physics: the mass-radius relationship follows from using the EOS and general relativity. Furthermore, neutron matter offers significant input to energy-density functionals (EDFs) tailored to describe nuclei: in addition to fitting properties of known nuclei, the use of “synthetic data” (dependable *ab initio* many-body results) like the EOS of neutron matter extends the physics content of EDFs to the neutron-rich side. Since neutron matter is not self-bound, it provides an intriguing combination of features: it is strongly interacting but also easier to address than isospin-asymmetric systems and symmetric nuclear matter. This has led to the use of NM to probe detailed features of nuclear forces, of both phenomenological [3, 4, 5, 6, 7] and chiral varieties [8, 9, 10, 11, 12, 13, 14]. (See Ref. [15] for a mixed-potential approach).

The state-of-the-art in nuclear physics has advanced to the stage where several challenging problems are attacked using *ab initio* methods, i.e. from first principles: solving the many-nucleon Schrödinger equation. A particularly successful way of doing so is via the use of the non-perturbative many-body methods known as Quantum Monte Carlo (QMC). The two most successful continuum QMC methods used to describe nuclear systems are Green’s Function Monte Carlo (GFMC) [16, 17, 18] and Auxiliary-Field Diffusion Monte Carlo (AFDMC) [19]. Both methods follow the general philosophy of Diffusion Monte Carlo, extracting the ground state by starting out with a trial/variational wave function $|\Psi_T\rangle$ and projecting out excited states in imaginary time τ : $|\Psi_0\rangle = \lim_{\tau \rightarrow \infty} \exp(-\hat{H}\tau)|\Psi_T\rangle$. What makes the nuclear many-body problem especially challenging is that the interactions include central, spin, tensor, spin-



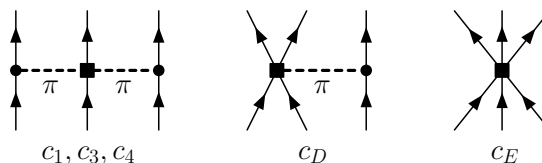


Figure 1. Three-nucleon forces at next-to-next-to-leading order. There are three distinct contributions: a) the two-pion-exchange (containing the couplings c_1, c_3 , and c_4), b) the one-pion-exchange–contact interaction (containing c_D), and c) the contact interaction (containing c_E).

orbit, and more complicated terms. Both GFMC and AFDMC address the coordinate degrees of freedom stochastically. What distinguishes them is how they treat the spin-isospin degrees of freedom: in GFMC they are treated explicitly, while in AFDMC they are also handled stochastically, at the cost of introducing auxiliary fields. Since GFMC is limited to small sizes, AFDMC is more appropriate to describe extended systems like neutron matter, so in what follows we will focus on AFDMC results.

2. Chiral 3N forces

2.1. Formalism

Chiral Effective Field Theory (EFT) forces were developed in order to connect with the symmetries of Quantum Chromodynamics [20, 21, 22]. They contain pion exchanges and shorter-range contact terms. Specifically, they predict consistent three-nucleon (3N) forces, which first appear at next-to-next-to-leading order (N^2LO) [23, 24]. Chiral EFT interactions were adopted as input to many-nucleon calculations by the overwhelming majority of practitioners, with a notable exception: Quantum Monte Carlo methods typically require local potentials as input and were therefore unable to use chiral EFT forces. (For the sake of completeness, note that Monte Carlo methods have been used to study neutron matter based on lattice and other momentum-space techniques [25, 26, 27].) Chiral EFT interactions were usually non-local, due to having been constructed in momentum space (without regard to their locality or non-locality). Starting with Ref. [10], the non-locality of chiral EFT nucleon-nucleon interactions up to N^2LO was fully removed, arriving at local chiral forces that are fully equivalent to the older (momentum-space) potentials. These were then published and used in AFDMC for neutron matter [13], while also being implemented in GFMC for light nuclei [28].

The natural next step is to derive (and implement in QMC methods) the consistent three-nucleon interactions up to N^2LO . The relevant terms are shown in Fig. 1. Since QMC is naturally formulated in coordinate space, these contributions need to be Fourier transformed [29]. The 3N contact contribution V_E has the form:

$$V_E^{ijk} = \frac{c_E}{2f_\pi^4 \Lambda_\chi} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}). \quad (1)$$

This contains a two-particle isospin term ($\boldsymbol{\tau} \cdot \boldsymbol{\tau}$) which is 1 in neutron matter; below we similarly find spin terms (e.g. $\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}$). The one-pion-exchange–contact 3N interaction V_D has the following form:

$$V_D^{ijk} = \frac{c_D g_A}{24 f_\pi^4 \Lambda_\chi} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \left[\frac{m_\pi^2}{4\pi} \delta(\mathbf{r}_{ij}) X_{ik}(\mathbf{r}_{kj}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right] \quad (2)$$

which clearly contains not only a one-pion-exchange–contact part ($X\delta$), but also a contact–contact part ($\delta\delta$). Here and above, all the terms that are not delta functions should be taken

to be long-range terms, with the details in Ref. [29]. The two-pion-exchange contribution V_C is most naturally given in three separate expressions:

$$V_{C,c_1}^{ijk} = \frac{c_1 m_\pi^4 g_A^2}{2f_\pi^4 (4\pi)^2} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij} \boldsymbol{\sigma}_k \cdot \hat{\mathbf{r}}_{kj} \times U(r_{ij})Y(r_{ij})U(r_{kj})Y(r_{kj}) \quad (3)$$

and

$$V_{C,c_3}^{ijk} = \frac{c_3 g_A^2}{36f_\pi^4} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \times \left[\frac{m_\pi^4}{(4\pi)^2} X_{ij}(\mathbf{r}_{ij})X_{kj}(\mathbf{r}_{kj}) \right. \\ \left. - \frac{m_\pi^2}{4\pi} X_{ik}(\mathbf{r}_{ij})\delta(\mathbf{r}_{kj}) - \frac{m_\pi^2}{4\pi} X_{ik}(\mathbf{r}_{kj})\delta(\mathbf{r}_{ij}) + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right] \quad (4)$$

and

$$V_{C,c_4}^{ijk} = \frac{c_4 g_A^2}{72f_\pi^4} \sum_{\pi(ijk)} \boldsymbol{\tau}_i \cdot (\boldsymbol{\tau}_k \times \boldsymbol{\tau}_j) \\ \times \left[\frac{m_\pi^4}{2i(4\pi)^2} [X_{ij}(\mathbf{r}_{ij}), X_{kj}(\mathbf{r}_{kj})] - \frac{m_\pi^2}{4\pi} \boldsymbol{\sigma}_i \cdot (\boldsymbol{\sigma}_k \times \boldsymbol{\sigma}_j) (1 - T(r_{ij})) Y(r_{ij}) \delta(\mathbf{r}_{kj}) \right. \\ - \frac{m_\pi^2}{4\pi} \boldsymbol{\sigma}_i \cdot (\boldsymbol{\sigma}_k \times \boldsymbol{\sigma}_j) (1 - T(r_{kj})) Y(r_{kj}) \delta(\mathbf{r}_{ij}) \\ - \frac{3m_\pi^2}{4\pi} \boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij} \hat{\mathbf{r}}_{ij} \cdot (\boldsymbol{\sigma}_k \times \boldsymbol{\sigma}_j) T(r_{ij}) Y(r_{ij}) \delta(\mathbf{r}_{kj}) \\ \left. - \frac{3m_\pi^2}{4\pi} \boldsymbol{\sigma}_k \cdot \hat{\mathbf{r}}_{kj} \hat{\mathbf{r}}_{kj} \cdot (\boldsymbol{\sigma}_j \times \boldsymbol{\sigma}_i) T(r_{kj}) Y(r_{kj}) \delta(\mathbf{r}_{ij}) + \boldsymbol{\sigma}_i \cdot (\boldsymbol{\sigma}_k \times \boldsymbol{\sigma}_j) \delta(\mathbf{r}_{ij}) \delta(\mathbf{r}_{kj}) \right]. \quad (5)$$

It's worth mentioning that the two-pion exchange V_C , which could be expected to be long-range from the Feynman diagram in Fig. 1, clearly also contains terms that are short-range and intermediate-range.

As in all nuclear-force formulations, the local 3N forces need to be regulated. Similarly to what is done in the NN sector, we regularize the 3N forces by smearing out the δ functions:

$$\delta(\mathbf{r}) \rightarrow \delta_{R_{3N}}(\mathbf{r}) = \frac{1}{\pi\Gamma(3/4)R_{3N}^3} e^{-(r/R_{3N})^4}, \quad (6)$$

where R_{3N} is the 3N cutoff. Also, the long-range contributions are multiplied with a long-range regulator:

$$Y(r) \rightarrow Y(r) \left(1 - e^{-(r/R_{3N})^4}\right). \quad (7)$$

The NN and 3N cutoffs can be and have been varied: this reflects the fundamental fact that there is not one true nuclear potential: cutoffs are arbitrary, so it is worth probing what effect, if any, this technical feature has on the physics. The NN cutoff was varied between $R_0 = 1.0 - 1.2$ fm [10, 13]. Smaller cutoffs lead to the appearance of spurious bound states, while larger cutoffs cut off the (physically significant) pion exchanges.

2.2. Results

Neutron matter was chosen as the first system to study using the new local chiral 3N forces because in it the structure of the 3N interaction is considerably simplified. Specifically, for $R_{3N} \rightarrow 0$ the short-range and intermediate-range parts of V_C (as well as the V_E and V_D

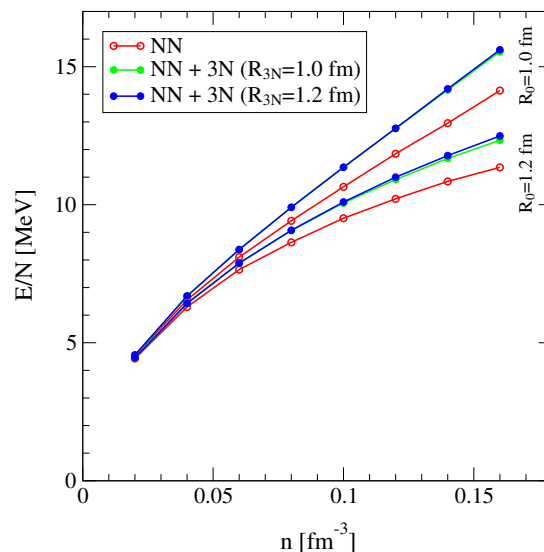


Figure 2. Energy per particle vs density for neutron matter at N^2LO , including NN forces and the 3N interaction V_C . The NN and 3N cutoffs are varied in the range 1.0 – 1.2 fm.

contributions) vanish in neutron matter. Thus, their contribution in neutron matter for finite cutoffs is only a regulator effect. Consistently with what was done for the NN cutoff $R_0 = 1.0 - 1.2$ fm, we have varied the 3N cutoff in the range $R_{3N} = 1.0 - 1.2$ fm.

In Fig. 2 we show AFDMC results from Ref. [29] for the equation of state of neutron matter using chiral NN and 3N forces at N^2LO . Specifically, the energy per particle is shown as a function of density including NN forces and the 3N V_C interaction. The NN and 3N cutoffs have been varied in the same range, 1.0 – 1.2 fm. For the softer NN potential ($R_0 = 1.2$ fm, lower lines) the energy per particle is 12.3 – 12.5 MeV at saturation density for the different 3N cutoffs. The corresponding NN-only energy is 11.4 MeV, so the 3N V_C has an impact of ≈ 1 MeV. For the harder NN potential ($R_0 = 1.0$ fm, upper lines) the energy per particle is 15.5 – 15.6 MeV (cf. 14.1 MeV for an NN-only calculation), so the effect the 3N V_C is ≈ 1.5 MeV. The variation of the total energy with the 3N cutoff is ≈ 0.2 MeV, much smaller than the variation due to the NN cutoff.

We note that the magnitude of the local 3N two-pion-exchange V_C contribution (no more than 1.5 MeV at saturation density), is smaller than the momentum-space/nonlocal-regulator contribution, which is typically ~ 4 MeV [8]. This difference between 1.5 and 4 MeV is presumably due to the locality vs non-locality of the regulators in the two approaches. Similar conclusions have been drawn using coupled-cluster theory [12].

3. Static response

3.1. Formalism

Quantum Monte Carlo studies of neutron matter have also recently tackled a situation that probes further aspects of the interaction, namely the static-response problem [30]. The static response of neutron matter is synonymous to the behavior of an extended neutron system in the presence of a periodic external potential. This is equivalent to a neutron-star crust: there, unbound neutrons interact strongly with each other and with a lattice of nuclei. The unbound neutrons experience the nuclei as a periodic modulation, which one can model as a one-body potential. Approaches to this general problem were until now limited only to mean-field approaches [31, 32]. Note also that the static response of neutron matter is closely

analogous to that of the three-dimensional electron gas and to liquid ^4He at vanishing pressure and temperature [33]. Similarly, cold fermionic atomic gases in optical lattices provide another experimental realization of related physics [34, 35].

We start from the following microscopic Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + V_{\text{ext}}. \quad (8)$$

In addition to a non-relativistic kinetic energy, this contains a two-nucleon interaction V_{ij} and a three-nucleon interaction V_{ijk} (Argonne v8' and Urbana IX, respectively). The last term corresponds to the external periodic potential: $V_{\text{ext}} = \sum_i V_i$, where $V_i = 2v_{\mathbf{q}} \cos(\mathbf{q} \cdot \mathbf{r}_i)$. The situation can be viewed as the application of a static (i.e., not dynamic) external potential to an unperturbed Hamiltonian. The periodicity of the potential is contained in q . Continuum QMC simulations for extended systems are carried out inside a simulation volume with periodic boundary conditions. It is important to ensure that the box length is an integer multiple of the period of the external potential.

We now discuss the fundamentals of response theory. One typically starts from an unperturbed system characterized by a Hamiltonian \hat{H}_0 (here, the first three terms in Eq. (8)). The last term in Eq. (8) then represents the coupling of an external potential $V_{\text{ext}}(\mathbf{r})$ to the one-body density operator $\hat{n} = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$. It is easy to see that $\int d^3r \hat{n}(\mathbf{r}) V_{\text{ext}}(\mathbf{r})$ is merely a rewriting of the last term in Eq. (8). One can define the linear density-density static response function using the functional expansion of the perturbed density $n_{\text{tot}}(\mathbf{r})$ in terms of $V_{\text{ext}}(\mathbf{r})$:

$$n_{\text{tot}}(\mathbf{r}) = n_0 + \int d^3r' \chi(\mathbf{r}' - \mathbf{r}) V_{\text{ext}}(\mathbf{r}'). \quad (9)$$

This $\chi(\mathbf{r}' - \mathbf{r})$ is the density-density response function of order 1, so a $\chi^{(2)}$ response function would involve two $V_{\text{ext}}(\mathbf{r})$ terms, and so on. It is possible to write down a corresponding expansion for the perturbed energy E_{tot} . This can then be re-expressed in terms of the Fourier components $v_{\mathbf{q}}$ of the modulating potential, $V_{\text{ext}}(\mathbf{r}) = \sum_{\mathbf{q}} v_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r})$, and the Fourier transform of the response, $\chi(q)$, to give:

$$E_{\text{tot}} = E_0 + \frac{\chi(q)}{n_0} v_{\mathbf{q}}^2 + C_4 v_{\mathbf{q}}^4 + \dots. \quad (10)$$

Note that this expression explicitly includes higher-order response functions (hidden in the higher-order coefficients). The response function $\chi(q)$ is related to an energy integral over the dynamic structure factor, familiar from standard response theory.

3.2. Results

One can carry out AFDMC simulations for a fixed value of q : these would vary the one-body strength $2v_{\mathbf{q}}$. For that specific q , then, Eq. (10) can be used to extract the $\chi(q)$ by fitting in powers of $v_{\mathbf{q}}$. Then, changing q this process can be repeated, leading to a better understanding of the behavior of $\chi(q)$. This is clearly a computationally intensive approach, requiring dozens of simulations of ~ 100 strongly interacting particles. The results from Ref. [30] are shown in Fig. 3. The q_F used is the Fermi wave vector: the values of q/q_F available to us are prescribed by the need to respect translational invariance.

In order to provide a physical interpretation for these QMC results, Fig. 3 also shows the static response function of a non-interacting Fermi gas, known as the Lindhard function:

$$\chi_L = -\frac{mq_F}{2\pi^2\hbar^2} \left[1 + \frac{q_F}{q} \left(1 - \left(\frac{q}{2q_F} \right)^2 \right) \ln \left| \frac{q + 2q_F}{q - 2q_F} \right| \right]. \quad (11)$$

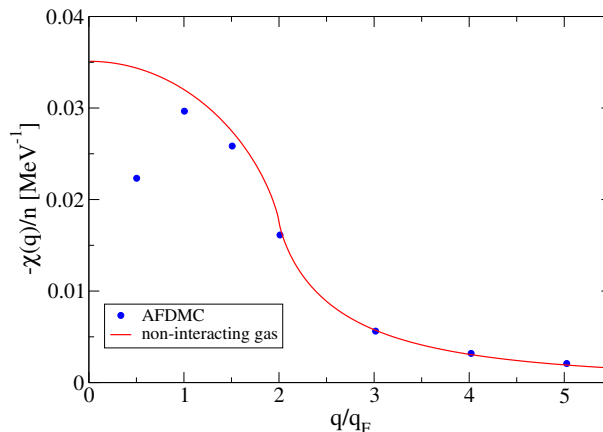


Figure 3. Static density-density linear response function of neutron matter. Points follow from AFDMC simulations using NN and 3N interactions, as well as several one-body strengths and periodicities. The line is the Lindhard function, which corresponds to the response of a non-interacting Fermi gas.

Some general features are immediately obvious. First, at large q (i.e., for the case of several clusters) the AFDMC results match the Lindhard values very well. This reflects the fact that in that scenario the interactions are vastly outweighed by the effect of the confining potential. Second, at low q we see a clear suppression, bringing to mind the case of the three-dimensional electron gas (3DEG). However, it's important to note that in the 3DEG the response function goes to 0 at $q = 0$. It is easy to see, e.g. using the random-phase approximation, that this result is specific to the Coulomb interaction, i.e., a finite-range potential changes this trend. Qualitatively, as can be seen from Eq. (10), a suppression with respect to the non-interacting gas means that the modulated interacting gas highlights the repulsion between the particles (when they are brought closer together by the external potential). It is important to note that the problem being solved here is always strongly coupled: even when $q \rightarrow 0$ the one-body strengths used extend to large fractions of the Fermi energy.

4. Summary & Conclusions

In this contribution we have touched upon two major recent developments in the study of neutron matter using QMC methods: i) local chiral forces, and ii) the static-response problem. Starting with the former, we briefly discussed the motivation behind chiral EFT and its fusing with QMC methods. We then gave the expressions describing local chiral 3N forces. After that, we turned to results for the ground-state energy of pure infinite neutron matter. We varied the 3N cutoff from $R_{3N} = 1.0$ fm to $R_{3N} = 1.2$ fm and found a much smaller dependence on this cutoff than on the NN cutoff, R_0 . This finding, along with similar explorations of regulator effects in neutron matter, has motivated further studies of specific regulator choices. We then turned to the second recent advance, namely the study of periodically modulated strongly interacting neutron matter. After a brief overview of the basics of response theory, we showed the first QMC results on the static density-density linear response function of neutron matter. This required heavy-duty computations at several strengths and periodicities of the external potential. We found a suppression with respect to the response of the non-interacting gas, of a form that is special to the nuclear problem. This has opened up several new possibilities in the study of the interplay between matter and nuclei in neutron-star crusts.

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