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Phys. Rev. Lett. **126**, 132701 — Published 2 April 2021

DOI: [10.1103/PhysRevLett.126.132701](https://doi.org/10.1103/PhysRevLett.126.132701)

Structure Factors of Neutron Matter at Finite Temperature

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(Dated: July 31, 2020)

We compute continuum and infinite volume limit extrapolations of the structure factors of neutron matter at finite temperature and density. Using a lattice formulation of leading-order pionless effective field theory, we compute the momentum dependence of the structure factors at finite temperature and at densities beyond the reach of the virial expansion. The Tan contact parameter is computed and the result agrees with the high momentum tail of the vector structure factor. All errors, statistical and systematic, are controlled for. This calculation is a first step towards a model-independent understanding of the linear response of neutron matter at finite temperature.

INTRODUCTION

As much as 99% of the gravitational binding energy released in core-collapse supernovae escapes the star in the form of neutrinos. This enormous flux, when it interacts with the nuclear matter on its way out of the star, is believed to be an essential ingredient in the explosion of the star [1]. Though neutral-current neutrino-neutron scattering is well-described in vacuum by tree-level Z^0 exchange, neutrino scattering in supernova material is complicated by many-body dynamics induced by the strong force. Due to its non-perturbative nature, however, these effects are hard to calculate (for a review see Ref. [2]). We compute here the exact structure factors of a spin-balanced neutron gas at leading order in the pionless effective field theory [3] using Monte Carlo methods at fugacities of $z \equiv \exp(\beta\mu) = 1.0$ and 1.5 .

The main accomplishments presented here are successful continuum and infinite volume limit extrapolations at such high fugacities. Consequently, all sources of error, both statistical and systematic, are accounted for and add up to a few percent. This was made possible by the import of several methods from lattice QCD for the simulation of fermions including: the conjugate-gradient iterative method [4], pseudofermions [5], and chronological inverters [6]. Since lattice artifacts typically decrease with density, we expect the methods presented here to provide complete control over this system for any fugacity $z \leq 1.5$. Such exact calculations, computed over a range of densities and temperatures, may place the nuclear physics inputs to supernovae simulations on firmer theoretical footing.

The differential cross section of low energy neutrinos off a gas of non-relativistic neutrons is approximately determined by the *static* vector and axial

structure factors ¹

$$\begin{aligned} S_V(q) &= \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \delta n(0, \mathbf{r}) \delta n(0, \mathbf{0}) \rangle \\ S_A(q) &= \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \delta S_z(0, \mathbf{r}) \delta S_z(0, \mathbf{0}) \rangle, \end{aligned} \quad (1)$$

where $\delta n = n - \langle n \rangle$ and $\delta S_z = S_z - \langle S_z \rangle$ are the fluctuations of the density and spin [2, 9]. These quantities are the main object of our calculations. We will also compute the Tan contact C , which determines the asymptotic behavior of the particle distribution function. The result for C provides a non-trivial check for structure factors.

Currently, the only other model-independent approach to finite-temperature neutron matter is the fugacity, or virial, expansion, expected to describe neutron matter well for $z < 1/2$. Within this approach, the equation of state and $S_V(q=0)$ and $S_A(q=0)$ have been computed at second order [10, 11]. Now included in some state of the art simulations [12], these virial results suppress neutrino-neutron scattering rates relative to the free theory [13], which appear to assist the explosion of the star [12, 14]. Our calculation extends these results by providing the full momentum dependence of $S_{V/A}(q)$ and are exact for all fugacity.

We find a clear difference between the structure factors of neutron gas and of the unitary gas [16, 31],

¹ The cross section is determined by the *dynamic* structure factor, but, due to the difficulty in computing it, an approximation involving only the static structure factors is typically used. For S_V , this approximation is reasonable at low neutrino energies ($p_\nu \ll (MT)^{1/2} \sim m_\pi$), but the precise criterion depends on the strength of the interaction. For a fuller discussion, see for instance Ref. [7]. The same holds for S_A until densities where non-central forces become appreciable [8]. We restrict attention here to densities and temperatures low enough that these assumptions hold.

an approximation to the former commonly used. In particular both structure factors are suppressed in neutrons relative to the unitary gas. Qualitative agreement between cold-atom experiments and our calculation give confidence in our results [17].

In this paper the interaction between neutrons will be described with pionless effective field theory [3, 18, 19]. Its applicability is restricted to kinematical regimes where momentum transfers between nucleons is below the pion mass, which is roughly satisfied over the temperature range of interest $T \lesssim 10$ MeV ($1 \text{ MeV} \simeq 1.16 \times 10^{10} \text{ K}$). Over this range the thermal momenta span $p \sim \sqrt{MT} \lesssim 100$ MeV for neutrons of mass $M = 938$ MeV. Pionless effective field theory provides an expansion of observables in powers of typical momentum scales over the pion mass and was shown to converge in a number of few-nucleon processes in the region $q \lesssim 100$ MeV [20–23]. In this work, we will restrict ourselves to leading order in the low energy expansion. At this order, the hamiltonian is given by

$$H = \int d^3x \left[\frac{\nabla\psi^\dagger \cdot \nabla\psi}{2M} - g(\psi_1^\dagger\psi_1)(\psi_2^\dagger\psi_2) \right], \quad (2)$$

where ψ is a spin doublet of quantized fields destroying a neutron, the index $\sigma = 1, 2$ distinguishes two spin components, and the coupling constant g is determined by the s-wave scattering length between neutrons.

FORMALISM

In order to use numerical methods (and to properly define the contact interaction in the hamiltonian in Eq. (2)) we will use a spatial cubic lattice with spacing Δx . The lattice hamiltonian is

$$H = \underbrace{\sum_{xx'} \psi_x^\dagger k_{xx'} \psi_{x'}}_K - \underbrace{\frac{g}{\Delta x^3} \sum_x (\psi_{x1}^\dagger \psi_{x1})(\psi_{x2}^\dagger \psi_{x2})}_V, \quad (3)$$

$$k_{xx'} = \sum_p \frac{p^2}{2M\Delta x^2} e^{-ip \cdot (x-x')},$$

where p are lattice momenta with components $p_i = \frac{2\pi}{N_x} n_i$, and $-\frac{N_x-1}{2} \leq n_i \leq \frac{N_x-1}{2}$ and we use a cubic lattice with N_x^3 sites. The number and spin operators are $N = \sum_x \psi_x^\dagger \psi_x$ and $\mathbf{S} = \sum_x \psi_x^\dagger \boldsymbol{\sigma} \psi_x$, and the chemical potentials coupled to each will be denoted μ and h , respectively. The partition function at inverse temperature β can be written, with the help of the Trotter formula and the Hubbard-Stratanovich

transformation, by using standard steps:

$$Z = \text{tr} e^{-\beta(H-\mu N)} \approx \text{tr} \prod_{t=1}^{N_t} e^{-\Delta t K} e^{-\Delta t(V-\mu N)} \\ = \int \prod_{x,t} D\hat{\psi}_{xt}^\dagger D\hat{\psi}_{xt} D A_{xt} e^{-S(\hat{\psi}^\dagger, \hat{\psi}, A)}, \quad (4)$$

where N_t is the chosen number of time-slices and the error involved in Eq. (4) is of order $\mathcal{O}(\Delta t^2)$ with $\Delta t = \beta/N_t$; the action $S = S_F + S_A$ is given by the fermionic and auxiliary-field contributions

$$S_F = - \sum_{xt} \hat{\psi}_{xt+1}^\dagger e^{A_{xt} + \hat{\mu}} \hat{\psi}_{xt} + \sum_{x,x',t} \hat{\psi}_{xt} B_{xx'} \hat{\psi}_{x't}, \\ S_A = \frac{1}{\hat{g}} \sum_{x,t} (\cosh(A_{xt}) - 1). \quad (5)$$

The matrix $B_{xx'}$ is an $N_x^3 \times N_x^3$ matrix representing spatial hopping:

$$B_{xx'} = \frac{1}{N_x^3} \sum_p e^{-ip \cdot (x-x')} e^{\hat{\gamma} \frac{p^2}{2}} \quad (6)$$

and the parameters of the lattice action are given by

$$\mu \Delta t = \hat{\mu} + \log \frac{f_1(\hat{g})}{f_0(\hat{g})}, \quad \frac{\Delta t}{M \Delta x^2} = \hat{\gamma}, \\ \frac{g \Delta t}{\Delta x^3} = \log \frac{f_2(\hat{g}) f_0(\hat{g})}{f_1(\hat{g})^2}, \quad (7)$$

where $f_\alpha(\hat{g}) \equiv \int_{-\infty}^{\infty} dA e^{-\frac{\cosh(A)-1}{\hat{g}}} e^{\alpha A}$. Eq. (4) and the mappings in Eq. (7) are derived in Ref. [16].

At leading order in the pionless EFT, the s-wave phase shift is given by $k \cot \delta(k) = -1/a$, with scattering length $a = -18.9$ fm. Thus the coupling constant g is adjusted in order for the theory, in the continuum, infinite volume, zero temperature and $\mu = 0$ limits, to reproduce this scattering amplitude.

The way the continuum limit of our lattice theory is approached is subtle. Numerical results indicate that there are terms proportional to powers of $\Delta t/\Delta x^2$ appearing in several quantities. Consequently, we take $\Delta t \rightarrow 0$ first, then $\Delta x \rightarrow 0$. In practice, this is accomplished by keeping $\hat{\gamma} = \Delta t/M\Delta x^2 \ll 1$ as Δx is reduced. In the hamiltonian limit we find that

$$\frac{1}{Mg} = \frac{c_1}{\Delta x} - \frac{1}{4\pi a}, \quad (8)$$

where $c_1^{-1} = 5.14435\dots$. By fixing $M = 938$ MeV, the chemical potential μ , the inverse temperature β , the box size L , and the number of spatial and temporal discretization steps N_x and N_t we can use Eq. (7) and Eq. (8) to compute $\hat{g}$, $\hat{\gamma}$, $\hat{\mu}$ with $\Delta x = L/N_x$ and $\Delta t = \beta/N_t$, and check $\hat{\gamma} \ll 1$.

METHODS

To sample the grand canonical ensemble in Eq. (4) we rewrite the partition function

$$\begin{aligned} Z &= \int D\hat{\psi}_{xt}^\dagger D\hat{\psi}_{xt} DA_{xt} e^{-S_A(A) - \hat{\psi}^\dagger \mathbb{M}(A) \hat{\psi}} \\ &= \int D\phi_{xt}^\dagger D\phi_{xt} DA_{xt} e^{-S_A(A) - \phi^\dagger \mathcal{M}^{-1} \phi}, \end{aligned} \quad (9)$$

using a complex scalar pseudofermion field ϕ_{xt} (no spinor index). The fermion matrix $\mathbb{M}$ is diagonal in spin and in the spin-balanced case it splits into two identical blocks $\mathbb{M}_1 = \mathbb{M}_2$. Furthermore, $\mathcal{M} = \mathbb{M}_1 \mathbb{M}_1^\top$ so $\det \mathbb{M} = \det \mathbb{M}_1 \mathbb{M}_1^\top = \det \mathcal{M}$. The integrand is then positive definite, so we can apply the usual Monte Carlo methods to sample the partition function. We use Hybrid Monte Carlo [24] to sample the field A : we interleave the sampling of ϕ with probability $P(\phi) \propto \exp(-\phi^\dagger \mathcal{M}^{-1} \phi)$, a modified Gaussian distribution, with updates of A generated by a classical mechanics evolution according to a Hamiltonian $H(\pi, A) = \pi^\top \pi / 2 + V(A)$ where $V(A) = S_A(A) + \phi^\dagger \mathcal{M}^{-1} \phi$ and π is canonical momentum conjugate to A sampled randomly according to $P(\pi) \propto \exp(-\pi^\top \pi / 2)$ at the beginning of each classical trajectory.

One ingredient required in the classical evolution of A is the evaluation of the derivative dV/dA (the so-called force term), which involves the calculation of $\mathcal{M}^{-1} \phi$. Since the matrix $\mathcal{M}$ is hermitian and positive definite, we use conjugate gradient [4], an iterative method, to compute $\mathcal{M}^{-1} \phi$. We accelerate the iterative process with the “minimal residue extrapolation” method [6]. This method uses past solutions to construct a trial solution to the present inverse problem (hence its designation as a “chronological inverter”). During the iterative process, the multiplication with $\mathbb{M}_1$ is split into N_t multiplications with diagonal matrix $e^{A+\hat{\mu}}$ and N_t multiplications with the hopping matrix B . The most time consuming piece is the multiplication by B , but this can be done efficiently in the momentum space where B is diagonal. Using the fast Fourier transform [25], the complexity of multiplying by B is reduced to $V_s \log V_s$, with $V_s = N_x^3$ being the number of points in a time slice. The overall complexity of multiplying by $\mathcal{M}$ is then $\mathcal{O}(N_t V_s \log V_s)$, much better than the $\mathcal{O}(N_t V_s^3)$ computational complexity of the Hybrid Monte Carlo algorithm without pseudofermions we used in our previous study [26]. In fact, our simulations indicate that for $N_x \gtrsim 8$ the pseudofermion method wins out. Another advantage is that this method can be parallelized efficiently by dividing the lattice evenly over the temporal direction.

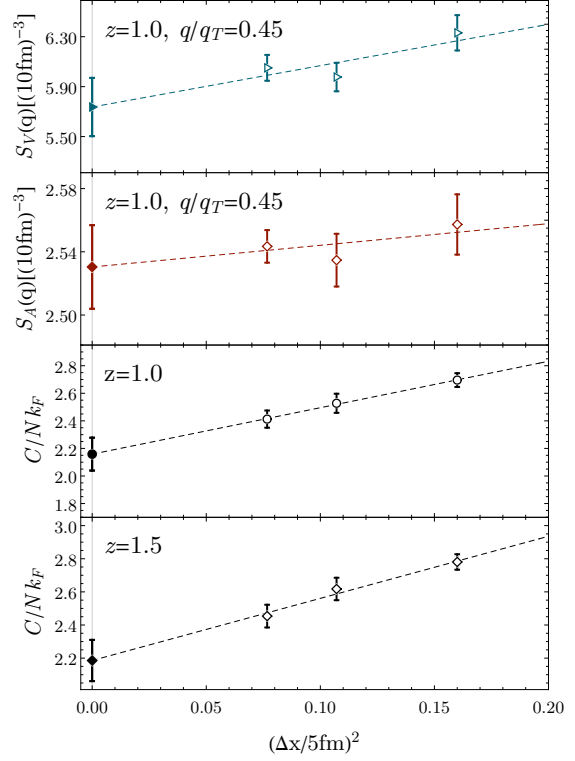


FIG. 1: Continuum limit extrapolation: for S_V and S_A for $z = 1.0$ and $q/q_T = 0.45$ (top) and contact (bottom).

RESULTS

In all calculations the coupling g was determined with from Eq. (8). As an additional check, we ran simulations with $0.05 < z < 0.8$ and compared our results with the virial expansion. The second virial coefficient we extracted, $b_2 = 0.419(3)$, agrees with the Beth-Uhlenbeck prediction $b_2 \simeq 0.415$ [27]. We also found $b_3 = -0.13(5)$.

Physical parameters for our simulations				
T [MeV]	V [fm ³]	z	n/n_0 [%]	ϵ_F [MeV]
4.14	18 ³	1.0	3.2(1)	5.9(2)
—//—	—//—	1.5	5.1(1)	8.0(1)

TABLE I: The temperature, volume, and fugacity are exact inputs to the calculations and have no uncertainty. In contrast, the density n , and Fermi energy ϵ_F are computed quantities and the error bars are obtained by continuum limit extrapolations. Here $n_0 = 0.16 \text{ fm}^{-3}$ is nuclear saturation density.

We used parameters $T = 4.14 \text{ MeV}$, $V = (18 \text{ fm})^3$, $\Delta t = 0.49 \text{ fm}$ and $\Delta x = 1.38 \text{ fm}$ in our “best” calculations. Errors due to finite spatial and temporal lattice spacings, and finite volume, were controlled by performing calculations at different values of V , Δt and Δx . For instance, in order to control for finite volume effects, we performed calculations at three different volumes, $V = (10 \text{ fm})^3$, $(14 \text{ fm})^3$, and $(18 \text{ fm})^3$, while holding $T = 4.14 \text{ MeV}$, $z = 1.0$, $\Delta x = 2.0 \text{ fm}$ fixed. At the largest volumes, errors due to finite volume effects are smaller than 2.0% for S_V and 1.0% for S_A ; these we take as upper bounds on finite volume errors. Similarly, to control for finite Δt errors, we performed calculations at four different temporal lattice spacings, $\Delta t = 0.49 \text{ fm}$, 0.31 fm , 0.245 fm and 0.196 fm , with $T = 4.14 \text{ MeV}$, $V = (6.9 \text{ fm})^3$, $\Delta x = 1.38 \text{ fm}$ held fixed, then extrapolated to the $\Delta t \rightarrow 0$ limit. The typical difference in observables between the $\Delta t \rightarrow 0$ extrapolation and the parameters used in our “best” simulations is 2% for S_V and 0.5% for S_A .

Extrapolation to the spatial continuum limit ($\Delta x \rightarrow 0$) is the largest source of systematic errors for most observables.² To extrapolate, we perform calculations with three different spatial lattice spacings, $\Delta x = 2.00 \text{ fm}$, 1.63 fm and 1.38 fm with $N_x = 9, 11$ and 13 , while $N_t = 96$, $\Delta t = 0.49 \text{ fm}$ and z are held fixed. We then fit observables to the formula $\langle \mathcal{O} \rangle = a + b\Delta x^2$. As an example, we show in Fig. 1 the extrapolations of $S_{V/A}(q)$ for a typical value of $q/q_{\text{th}} = 0.45$, with $q_{\text{th}} \equiv \sqrt{6MT} \approx 153 \text{ MeV}$.

Continuum limits for the structure factors at fugacities $z = 1.0$ and 1.5 are plotted in Fig. 2. All sources of error are included in the error bars. This includes statistical errors, the errors due to the $\Delta x \rightarrow 0$ extrapolation (as shown in Fig. 1), as well as the estimates of the systematic errors due to finite volumes and Δt discussed above. Several features deserve comment. First, we find a $\sim 20\%$ suppression in both structure factors relative to the unitary gas when $a = -18.9 \text{ fm}$ [16]. Thus the finite scattering length produces a detectable effect. Similar reductions in the vector structure factor due to a negative scattering length were found in cold-atom experiments [17]. Second, the suppression of the vector structure factor at low momenta is not captured by second-order virial calculations [7]. On the other hand, fourth-order virial calculations of $S_V(q=0)$ and $S_A(q=0)$

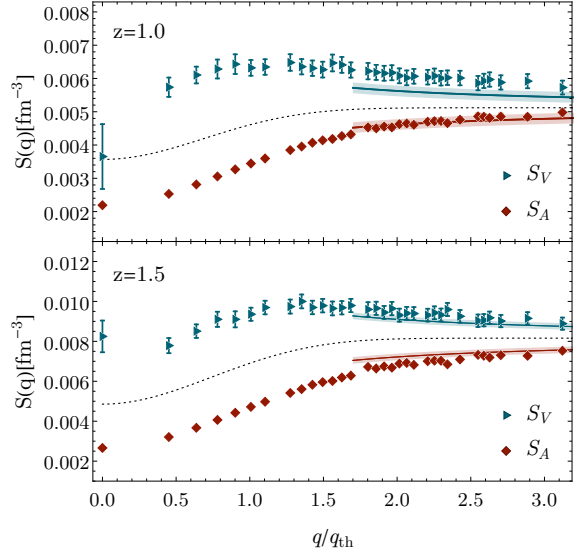


FIG. 2: Continuum limits of the vector and axial structure factors at fixed temperature and $z = 1.0$ and $z = 1.5$. The bands correspond to the OPE asymptotic limits in Eq. (11) and the dotted lines to the free theory result.

for the unitary gas produce qualitatively similar behavior to the $z = 1.0$ results of Fig. 2 [31]. However, naively extrapolating these fourth-order predictions to $z = 1.5$ produces an $S_V(q=0)$ a factor of two smaller than Fig. 2 predicts. Therefore, though it is possible that $z = 1.5$ may lie within the radius of convergence of the virial expansion, the structure factors computed here cannot be captured by currently available virial coefficients.

Since the structure factors are derived directly from a partition function they automatically satisfy the following “sum-rules”

$$S_V(0) = T\partial n/\partial\mu, \quad S_A(0) = T\partial s/\partial h,$$

required for any thermodynamically consistent theory. This consistency ensures that macroscopic conservation laws are obeyed by response functions [32], a feature needed for large-scale supernova simulations [33, 34].

The Tan contact parameter, C [35]:

$$C = \lim_{k \rightarrow \infty} k^4 n(k), \quad (10)$$

characterizes the high momentum behavior of many observables in this system, including both the momentum distribution and structure factors:

$$\begin{aligned} S_V(q) &= \langle n \rangle + \frac{C}{8Vq} + \mathcal{O}(q^{-2}) \\ S_A(q) &= \langle n \rangle - \frac{C}{8Vq} + \mathcal{O}(q^{-2}). \end{aligned} \quad (11)$$

² This can be seen by considering the Symanzik action [28, 29]. The lowest dimension term of this theory not included in Eq. (2) involves *two* extra derivatives and its coefficient is proportional to Δx^2 [30].

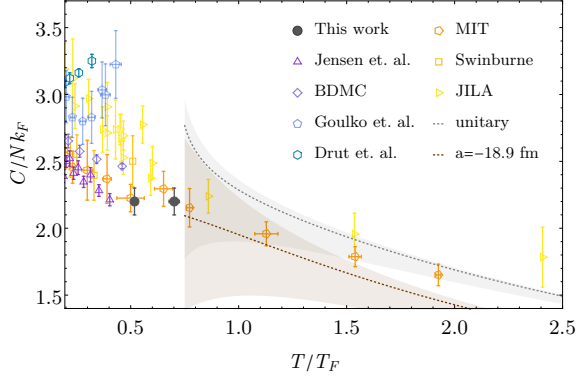


FIG. 3: Experimental data for the value of the contact of the unitary gas is shown in warm colors (Swinburne [37], JILA [38], MIT [39]), while theoretical results are shown in cool colors (Bold diagrammatic Monte Carlo [40], Jensen [41], Drut [42], Wingate [43]). The dashed grey curve is the third-order virial expansion for the unitary gas [44] and the brown dashed line shows the second-order results for $a = -18.9$ fm. The band around the virial curves incorporates an estimate of the next-order contribution.

The contact C may be written as

$$C = g^2 M^2 \int d^3x \langle \psi_1^\dagger \psi_1 \psi_2^\dagger \psi_2(x) \rangle, \quad (12)$$

as was shown in Ref. [36] using the operator product expansion. We compute C using Eq. (12) and its continuum extrapolation, shown in Fig. 1, gives $C/Nk_F = 2.1(1)$ (at $z = 1.5$) and $C/Nk_F = 2.1(1)$ (at $z = 1.0$). The uncertainty is dominated by statistical and continuum extrapolation errors. In Fig. 2 we show, besides the continuum extrapolated results for the structure factors, the asymptotic limits at high q predicted by Eq. (11) and our measured values of $\langle n \rangle$ and C . The agreement between the OPE prediction Eq. (11) and high-momentum tails of $S_{V/A}$ is a further consistency check for our calculation.

There are also a number of theoretical calculations and experimental measurements of the contact for the unitary gas (scattering length $a = -\infty$). A direct comparison with the values we obtained is complicated by the difference in scattering lengths, the different values of the temperature (in units of the Fermi energy) and the tensions between different experiments and numerical calculations. In Fig. 3 we present the available experimental and Monte Carlo data along side our values for the contact and the predictions of the virial expansion. The agreement we find is a further check on our calculations.

CONCLUSIONS

We report a Monte Carlo calculation of the structure factors of neutron matter at temperatures and densities relevant to supernovae and neutron star mergers. All sources of numerical error, statistical and systematic, are accounted for and add up to a few percent. This control was possible in large part due to technologies seldom used in this context. The results show a definite change from both the free theory and the unitary limit as the scattering length is changed, agreeing qualitatively with experiment [17]. We also calculate the contact and verify its consistency with the high-momentum dependence of the structure factors.

After controlling for these errors the dominant source of uncertainty is the hamiltonian. Experience with pionless EFT in few-nucleon systems [3, 20, 21, 45, 46] suggests that pionless EFT converges well in this regime and that inclusion of next-order interactions improves the results significantly. At third-order in the EFT, tensor forces appear that are likely to be particularly important to the axial structure factors. Extensions to larger densities and lower temperatures appear possible. Thus, the calculation presented here opens up a path for a definitive calculation, including a more realistic description of nuclear forces, encompassing most temperatures and densities relevant to supernova physics. Extension to higher temperature, however, is more complex, as typical momenta exceed the range of convergence of the pionless EFT and a substantially more complicated hamiltonian will be required. Even more difficult would be the calculation of *dynamical* structure factors, as those depend on fundamentally new ideas (perhaps those reviewed in [47–51]) to deal with the real time dependence inherent to the problem.

ACKNOWLEDGMENTS

We are grateful to Martin Zwiernien and Biswaroop Mukherjee for providing experimental data and we thank Sanjay Reddy and David Radice for discussions. A.A. is supported by U.S. DOE Grant No. DE-FG02-95ER40907. P.B and E.B are supported in part by the US DoE under contract No. DE-FG02-93ER-40762. N.C.W is supported in part by the U.S. DOE under Grant No. DE-FG02-00ER41132.

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