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A R T I C L E I N F O A B S T R A C T

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The behavior of QCD at high baryon density and low temperature is crucial to understanding the properties of neutron stars and gravitational waves emitted during their mergers. In this paper we study small systems of baryons in periodic boundary conditions to probe the properties of QCD at high baryon density. By comparing calculations based on nucleon degrees of freedom to simple quark models we show that specific features of the nuclear spectrum, including shell structure and nucleon pairing, emerge if nucleons are the primary degrees of freedom. Very small systems should also be amenable to studies in lattice QCD, unlike larger systems where the fermion sign problem is much more severe. Through comparisons of lattice QCD and nuclear calculations it should be possible to gain, at least at a semiquantitative level, more understanding of the cold dense equation of state as probed in neutron stars.

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1. Introduction

Understanding quantitatively the properties of QCD at low temperature and high baryon density remains one of the most challenging problems in nuclear physics. It is increasingly important as it governs the behavior of neutron stars including their massradius relations (see Refs. [\[1–4\]](#page--1-0) and references therein), cooling, and the emission of gravitational waves in neutron star mergers [\[5\]](#page--1-0). At low to moderate densities (up to about nuclear saturation density) it is natural to model neutron star matter via a system of interacting nucleons, and much progress has been made along these lines [\[6–9\]](#page--1-0). At asymptotically large densities the problem is also tractable: at low temperatures, the ground state will be a color–flavor-locked superfluid phase of quark matter with large superfluid pairing gaps [\[10,11\]](#page--1-0). At intermediate densities (several times nuclear saturation density) the situation is much less clear. One expects the dominant degrees of freedom to transition from nucleons to quarks and gluons, but the density at which this occurs remains very difficult to determine even qualitatively.

Studying the neutron star mass-radius relationship and cooling of neutron stars has been an important goal to constraining the equation of state through astrophysical observations [\[12\]](#page--1-0). The recent observations of two solar mass neutron stars $[13,14]$, for example, have severely constrained possible equations of state at densities higher than nuclear saturation. Nevertheless these provide only some constraints on the equation of state, and less about the relevant degrees of freedom at high density.

In this paper we study the behavior of small numbers of baryons at high density (or equivalently small volumes) in periodic boundary conditions. It may soon be possible to study these systems in lattice QCD, as the sign problem for small baryon number is less severe. The sign problem grows exponentially with imaginary time and is proportional to the number of nucleons times the mass of the nucleon minus three halves the mass of the pion [\[15\]](#page--1-0). We evaluate these systems in both nucleonic models and quark models, and identify specific features that arise in the spectra as the degrees of freedom change from nucleons to quarks. These features rely on the relatively high momenta and short distances that arise in small periodic volumes. The most important of these features are shell closures for small numbers of nucleons and pairing in open-shell systems. The latter is important even for very small systems, in particular for the $N = 4$ systems we study.

The small lattice length *L* needed to simulate high densities with a small number of baryons may be subject to significant cor-

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rections from long-range physics. However, we can expect that some of the longest-distance effects due to pions should be the same in nuclear and QCD simulations as long as nucleon–pion interactions are consistently included in the nuclear Hamiltonians. In any case the smallest box considered in this study (corresponding to *N* = 4 at ρ = 0.48 fm⁻³) has a box size of *L* \approx 2.03 fm.

It may also be possible to perform lattice QCD and nuclear simulations for unphysical heavy up- and down-quarks, resulting in heavy pions. This would reduce the sign problem and the corrections due to finite volume at the cost of unphysical pion masses. Studying the transition even for high pion masses may be instructive as pion degrees of freedom may not play a very important role in the high-density phase transitions. See Ref. [\[16–20\]](#page--1-0) for some studies of *NN* phase shifts at high pion mass.

Small volumes will typically result in large excitation energies, reflecting the wider spacing in the single-particle spectra, as discussed below. This will be less true for comparison of different pairing symmetries that are degenerate in the free-particle limit. However, in general, both the quantum Monte Carlo (QMC) and lattice QCD simulations will converge more quickly with imaginary time for small systems.

Although studies of small systems are ill-suited to capture critical behavior and cannot precisely identify possible phase transitions, this work is well motivated because presently we lack even a qualitative understanding of how quark degrees of freedom might emerge at high density. The signatures we identify below suggest that these small systems could be quite valuable in this regime. Eventually one can add protons and/or hyperons to look at the density dependence of the symmetry energy and/or the presence of hyperons in neutron stars. In these initial studies, we concentrate on pure neutron matter.

1.1. Nucleonic models

M

To study nucleonic matter we consider nonrelativistic nucleons interacting via two-nucleon (NN) interactions:

$$
H = -\sum_{i} \frac{\hbar^2 \nabla_i^2}{2m} + \sum_{i < j} V_{ij},\tag{1}
$$

where the *NN* interaction is taken as either the Argonne AV18 [\[21\]](#page--1-0), the AV8' $[22]$, or the local next-to-next-to-leading order (N^2LO) chiral interactions of Ref. [\[23\]](#page--1-0). At low densities such interactions should be able to faithfully reproduce the properties of QCD. Of course the three- (and eventually four- and many-) nucleon forces will be present, and eventually play a significant role. The simple spectral features we identify below will remain, though, even in a more sophisticated picture. These features depend primarily upon the single-particle states available to a nucleon in periodic boundary conditions, indeed some are present even for noninteracting neutrons.

In this paper we consider only cubic simulation volumes with periodic boundary conditions. Other geometries, such as elongated volumes or different types of boundary conditions, might allow one to identify additional spectral features [\[24\]](#page--1-0), but since present lattice calculations typically use cubic symmetry, we will adopt it in this study. Below we show results for different densities with various numbers of neutrons in cubes of length *L* on each side, and we show results as a function of the density $\rho = N/L^3$.

The nuclear interaction models described above are defined in the continuum. To maintain periodic boundary conditions, we add the contributions from periodic images for each pair:

$$
V_{ij} = \sum_{i_x, i_y, i_z = -M}^{M} V \left[r_{ij} + L(i_x \hat{x} + i_y \hat{y} + i_z \hat{z}) \right],
$$
 (2)

where r_{ij} is the minimum separation in the periodic box and we include the self interaction of particles with their own image in the cases where this is not negligible $(N = 3, 4$ and high-density). We find that $M = 1$ to 2 images in each direction are sufficient to obtain periodic solutions since the *NN* interaction is at most of pion range. We note that the longest-range corrections from pions "wrapping around" the box are also present in lattice QCD simulations [\[25\]](#page--1-0). For heavier pion masses these long-range periodic images will play much less of a role.

For the larger number of neutrons $(N > 4)$, we restrict ourselves to solutions fully symmetric under cubic rotations. For the smallest systems, we also investigate states that would correspond most closely to *p*-wave ($N = 3, 4$) or *d*-wave ($N = 4$) solutions in the continuum. The couplings to nonzero angular momenta prove quite interesting in comparing neutron potential models to quark models.

Calculations are performed using QMC methods: Either the Green's function Monte Carlo or Auxiliary Field Diffusion Monte Carlo methods. More details are described in [\[26\]](#page--1-0). The simulations are fairly simple as there are only a modest number of neutrons and the small volumes raise the energies of the excited states allowing for a more rapid convergence.

1.2. Quark model

For comparison, we also consider very simple quark models of high-density QCD in periodic boundary conditions. These models are not intended to be realistic or predictive of the behavior of QCD in this regime, but they should illustrate possible alternative behaviors when deconfined quarks are the dominant degrees of freedom.

We consider both free and interacting quarks in periodic boundary conditions. In general the models can be written as:

$$
H = \sum_{i} T_i + \sum_{i < j} V_{ij} \,. \tag{3}
$$

In the free case we consider for the kinetic energies T_i of the $\sqrt{p_i^2 + m_i^2}$ and $T_i = m_i + p_i^2/2m_i$, respectively. For the interacting quarks relativistic and nonrelativistic dispersion relations $T_i =$ quark model, we shall assume that chiral symmetry is not fully restored when quark degrees of freedom first manifest in the spectrum and use a relatively large value of $m = 300$ MeV. Under these conditions we treat the quarks as nonrelativistic even for the small volumes that we consider. For the free case we also explore the opposite case with full restoration of chiral symmetry and $m_i = 0$.

The pair potential is chosen in order to reproduce the pairing pattern expected from a Nambu–Jona-Lasinio-like model [\[27\]](#page--1-0) where interactions are antisymmetric with respect to color. Furthermore, for 3 colors and 2 flavors, we look for a color superconducting ground-state called the 2SC phase where two species are paired in a color and flavor anti-symmetric channel while the third does not interact with either and is effectively decoupled [\[28\]](#page--1-0). In the following we will consider the blue quarks to be the decoupled species.

For a given neutron number *N* the occupation numbers in flavor–color–spin space are chosen in order to satisfy the following constraints

baryon number $3N = (N_U + N_D)$ **color neutrality** $N_R = N_B = N_G$ **charge neutrality** $N_D = 2N_U$ **spin neutrality** $N_{\uparrow} = N_{\downarrow}$

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