Neutron-rich Nuclei and Matter

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We used advanced large-scale computational techniques to determine the properties of inhomogeneous matter. Recent advances allow us to calculate the properties of up to 50 neutrons bound in external wells. These results place significant new constraints on the density functionals relevant for large neutron-rich nuclei and inhomogeneous neutron matter.

Neutron-rich nuclei and matter in the neutron star crust are the subject of intense interest, and are an important component of the new Facility for Rare-Isotope Beams (FRIB) being constructed by the Department of Energy (DOE) Office of Science [1]. The properties of very neutron-rich matter are typically studied using density-functional theories that are extrapolated from already-measured nuclei to the regime of very large neutron excess [2].

Typical large nuclei have only a 10–20% excess of neutrons, so the extrapolation to neutron star matter, with approximately 90% neutrons, is quite large. As part of the UNEDF–SciDac project (Universal Nuclear Energy Density Functional–Scientific Discovery through Advanced Computing) through the DOE Office of Science, LANL scientists in collaboration with ANL and other members of the UNEDF project, have used ab initio methods with realistic interactions to examine the properties of inhomogeneous matter consisting of neutron matter only.

The equation of state of uniform neutron matter has been studied extensively, and largely determines the masses and radii of neutron stars [3]. The recent observation of a nearly two-solar-mass neutron star [4] has put severe constraints on the equation of state of this homogeneous matter. The properties of inhomogeneous matter have received comparatively little attention, though.

LANL scientists have examined this matter by performing microscopic calculations of from 8–50 neutrons trapped in external potentials. By varying the shape and depth of the potential, several different properties of the neutrons can be examined. Figure 1 shows the ground-state energies of neutrons confined to external wells of frequency 5 and 10 MeV, respectively.

The solid red points in Fig. 1 are the results of Green’s function Monte Carlo (GFMC) calculations, pioneered at LANL. The blue points are the results of a new algorithm, auxiliary field diffusion Monte Carlo (AFDMC), which treats the spin degrees of freedom, as well as the spatial coordinates, with Monte Carlo techniques. The energies are scaled by the harmonic oscillator frequency and the number of particles, so that free particles would be essentially flat at one.

Previous density functional models are indicated by open symbols and by the black line—the latter is the often-used SL Y4 model. These models significantly overbind these neutron drops compared to the microscopic calculations. We find that these density functionals can be improved by including a repulsive gradient correction to the energy, proportional to $|\nabla \rho|^2$. This term is not well constrained by fits to known nuclear masses. This repulsive contribution brings the results much closer to the ab initio results. We also found that a smaller superfluid pairing and spin-orbit splitting improve the agreement. The functional adjusted to neutron matter is indicated by the magenta line in Fig. 1.

The same functional also greatly increases agreements of energies of neutrons bound in a Woods-Saxon well, and the root mean square (rms) radii and density distributions in that well. A plot of the rms radii for the different wells is shown in Fig. 2. The blue points are the GFMC calculations and the black line the original density functional. The
magenta line indicates results with the same improved functional used for the energies.

The UNEDF project will use these results to help produce improved density functionals that are more accurate when extrapolated to neutron-rich systems, such as large neutron-rich nuclei and the neutron star crust.

Fig. 1. Ground state energy of neutrons in harmonic wells.

Fig. 2. Rms radii of neutrons bound in external wells.


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