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A Study of Nuclear Many Body Problem for Even Nuclei

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ABSTRACT: The nuclear many-body problem is among the most challenging many-body problems in physics. Our group develops and implements many-body methods to advance the understanding of nuclear properties from underlying effective interactions. These properties are important for understanding astrophysical processes, such as nucleosynthesis and supernovas, and for interpreting results expected from new radioactive beam facilities, such as FRIB.

High-performance computing has enabled significant progress in applying various ab initio methods to calculate properties of nuclei, but these methods are mostly limited to light nuclei. One example, density functional theory (DFT), is unique in providing a global theory of nuclei. However, it can miss important correlations beyond the mean field. Another method involves diagonalization of the Hamiltonian within a basis constructed by the configuration-interaction (CI) shell model approach. The CI shell model, a basic model of nuclear structure, provides an attractive framework as it accounts for both shell effects and correlations. However, combinatorial growth of the dimension of the many-particle space hinders its application in mid-mass and heavy nuclei.

KEYWORDS: nuclear, body, problem, even, nuclei, particle, computing, interactions, density

I. INTRODUCTION

We have overcome the difficulty in applying the CI shell-model approach to mid-mass and heavy nuclei by using quantum Monte Carlo methods. In particular, we use the auxiliary-field Monte Carlo (AFMC) method, which is known in the context of the nuclear CI shell model as the shell model Monte Carlo (SMMC). For a recent review of AFMC in nuclei, SMMC enables exact solutions in model spaces that are many orders of magnitude larger than those that can be treated by conventional methods. While fermionic Monte Carlo methods are often limited by the so-called sign problem, the dominant components of nuclear interactions have a good sign in SMMC and often suffice for realistic calculations of statistical and collective properties. The smaller bad-sign components of the interactions can be treated. The SMMC method is particularly useful for the microscopic calculation of statistical and collective properties of nuclei, such as level densities. Level densities are required to estimate transition rates through Fermi's golden rule and are important in the Hauser-Feshbach theory of statistical nuclear reactions, and therefore appear in numerous nuclear physics applications. However, their calculation in the presence of correlations is a difficult many-body problem. We have developed state-of-the-art SMMC methods for the microscopic calculation of level densities, including their dependence on good quantum numbers such as parity, spin and isospin.

We have extended SMMC to heavy nuclei introducing a new proton-neutron formalism and carrying out some of the largest SMMC calculations to date. Heavy nuclei exhibit various types of collectivity that are well described by phenomenological models, but a microscopic description has been lacking. Using SMMC, we have provided the first microscopic description of the crossover from vibrational to rotational collectivity. In a finite-size system such as the nucleus, it is crucial to use the canonical ensemble with a fixed number of particles. However, the projection on an odd number of particles leads to a new sign problem, which has prevented applications of SMMC to odd-even and odd-odd nuclei. We have recently developed a method that circumvents this odd-particle sign problem, enabling accurate

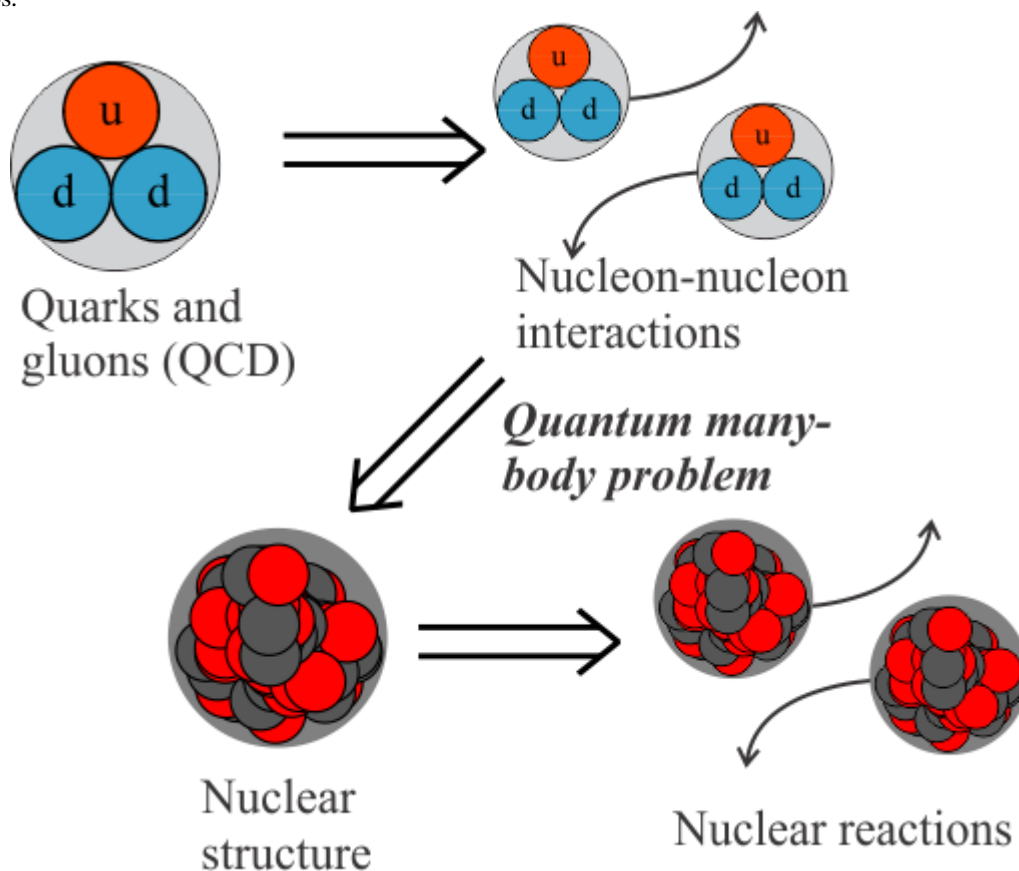
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calculations of the ground-state energy of odd-particle systems .Using this method we have calculated pairing gaps from odd-even mass differences and accurate level densities of odd-mass nuclei .

We have also used a configuration-space Monte Carlo (CSMC) method to solve exactly for the pairing Hamiltonian constructed from a density-dependent contact interaction in the framework of DFT .This improved over the bare DFT+BCS results as measured by the rms deviation between the theoretical and experimental values of ~450 neutron pairing gaps.



Deformation is a key concept in our understanding of heavy nuclei. It arises naturally in the framework of the mean-field approximation, but it breaks the rotational invariance of the underlying nuclear Hamiltonian. We have introduced a novel method to study deformation in the rotationally invariant framework of the CI shell model .We have used SMMC to calculate the axial quadrupole distribution in the laboratory frame, and showed that this distribution carries a model-independent signature of deformation. We have applied the method to isotope chains of lanthanides .Using a Landau-like expansion of the logarithm of the quadrupole distribution in the so-called quadrupole invariants, we have determined its dependence on intrinsic deformation without invoking an intrinsic frame or a mean-field approximation. We can then calculate the dependence of statistical properties of nuclei on intrinsic deformation .This dependence is an important input to models of shape dynamics such as fission.

Most calculations of statistical properties of nuclei are based on mean-field approximations. However, their performance has not been tested against a theory that takes the full correlations into account. Recently, we have benchmarked mean-field results against SMMC results . Finite-temperature mean-field theories are formulated in the grand-canonical ensemble, and it is necessary to project on fixed particle number. We have recently introduced a novel projection formula in mean-field theories in which pairing correlations violate particle-number conservation

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II. DISCUSSION

We begin our discussion of many-nucleon systems by (again) identifying the most important degrees of freedom and writing down the relevant Hamiltonian. Contrary to methods used at a finer level (quarks and gluons) we use here the Hamiltonian picture instead of the Lagrangian density; this is so because most of the analysis can be done in the framework of the standard quantum mechanics, without necessity of applying methods of the quantum field theory. Nevertheless, we shall express our many-body Hamiltonian in the language of the fermion creation and annihilation operators, which is very convenient in any theory that involves many identical particles obeying specific exchange symmetries.

In order to simplify the discussion we disregard the three-body NNN piece of the interaction between the nucleons, and thus the most general Hamiltonian of a many-nucleon system can be written as,

$$\hat{H} = T_{xy} a_x^+ a_y + \frac{1}{4} V_{xyx'y'} a_x^+ a_y^+ a_{y'} a_{x'},$$

where $x \equiv (\mathbf{x}, \sigma, \tau)$, $x' \equiv (\mathbf{x}', \sigma', \tau')$, etc., are the space-spin-isospin variables, and the summation-integration $\int d^3r \sum_{\sigma\tau}$ is implied for every pair of repeated indices. Following the standard notation, we put the

space-spin-isospin arguments as indices of the kinetic energy, T_{xy} , potential energy, $V_{xyx'y'}$, and the creation a_x^+ and annihilation a_y operators. We assume that the two-body potential energy operator is antisymmetrized, $V_{xyx'y'} = -V_{xyy'x'}$.

We can now estimate the order of complication involved in a many-nucleon system. Let us assume that fields a_x^+ (i.e., the s.p. wave functions) have to be known at about $M \simeq 10^4$ space-spin-isospin points. The estimate involves, say, about 20 points of a 1fm lattice in each of the three spatial direction, and four spin-isospin components.

The 1fm lattice may seem to be grossly insufficient to describe a system where a typical s.p. kinetic energy E_k is of the order of 50MeV, and thus involves typical s.p. momenta of nucleons $k = \sqrt{2m_N E_k} \simeq 300\text{MeV} \simeq 1.3\text{fm}^{-1} \simeq (0.7\text{fm})^{-1}$. However, typical scale at which total densities of nucleons vary in a nucleus, are of the order of 2-3fm, so the 1fm lattice is a barely sufficient, but fair compromise to describe a system having the total size (including the asymptotic peripheral region) of at least 20fm.

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The fermion Fock space, i.e., the complete Hilbert space that is relevant to describe a system of many identical

fermions, has the dimensionality of $D = \binom{M}{A}$, which is equal to the number of ways A fermions can be distributed on M sites. For the $A=10$ systems, which at present can still be treated within the GFMC method, we thus obtain $D \simeq 10^{33}$. On the one hand, this number illustrates the power of the existing theoretical descriptions; on the other hand, it explains why it is so difficult to go any further. For example, for a heavy $A=200$ nucleus, the dimensionality reaches 10^{425} . Therefore, it is neither conceivable nor sensible to envisage any exact methods for heavy nuclei.

One has to bear, however, in mind that the physics of a heavy nucleus does not really require such a detailed knowledge of any of its states. To see this, let us consider the energy of an arbitrary state $|\Psi\rangle$ as given by the average value of the Hamiltonian,

$$E = \langle \Psi | \hat{H} | \Psi \rangle = T_{xy} \rho_{yx} + \frac{1}{4} V_{xyx'y'} \rho_{x'y'xy},$$

where the one- and two-body density matrices are defined as

$$\begin{aligned} \rho_{yx} &= \langle \Psi | a_x^+ a_y | \Psi \rangle, \\ \rho_{x'y'xy} &= \langle \Psi | a_x^+ a_y^+ a_{y'} a_{x'} | \Psi \rangle. \end{aligned}$$

Both density matrices are Hermitian, $\rho_{yx} = \rho_{xy}^*$ and $\rho_{x'y'xy} = \rho_{x'y'x'y}^*$, and the (fermion) two-body density matrix is antisymmetric with respect to exchanging its first two, or last two arguments, $\rho_{x'y'xy} = -\rho_{y'x'xy}$ and $\rho_{x'y'xy} = -\rho_{x'y'yx}$. Hence the total energy of an arbitrary many-fermion state, described by two-body interactions, is

determined by $M^2 + \frac{(M(M-1)/2)^2}{2} \simeq 10^{16}$ real parameters for $M \simeq 10^4$ (independently of A). Even when the three-body interactions are taken into account, this number grows "only" to 10^{24} . This shows explicitly, that the information contained in a many-fermion nuclear state is, in fact, much smaller than the total dimensionality of the Hilbert space, or in other words, only very specific states from this Hilbert space are relevant.

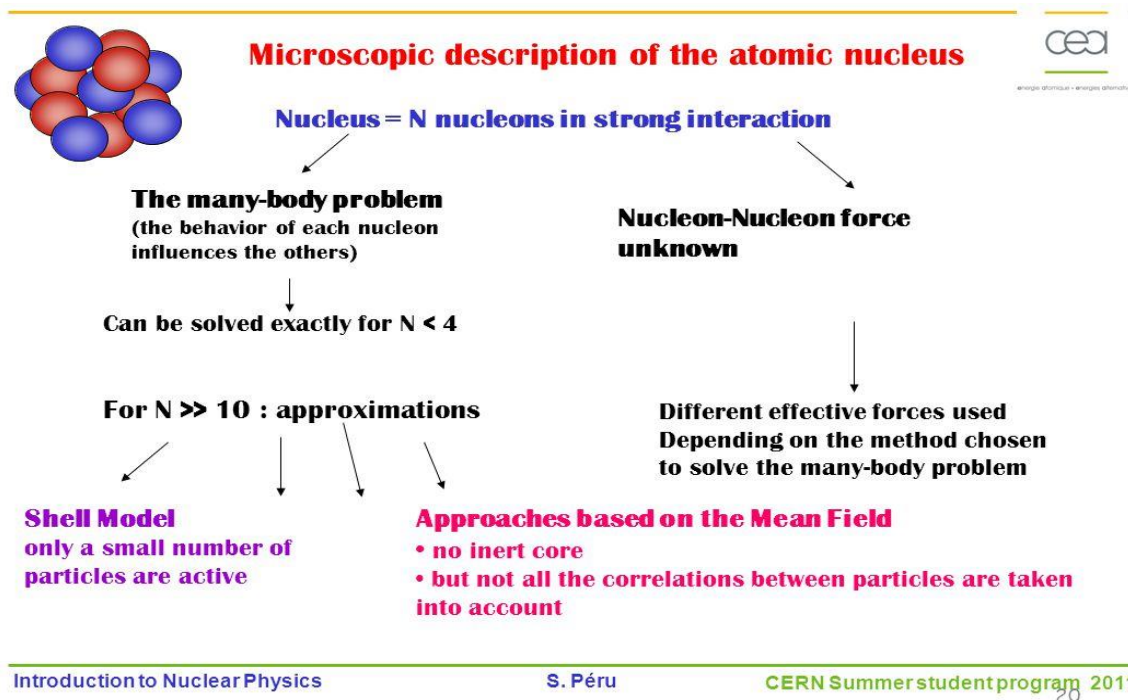
Unfortunately, the presented counting rules, based on the analysis of density matrices, do not help in obtaining practical solutions for many-body problems. The reason for that is the never-solved N -representability problem Col63, Col00, namely, the question: which of the four-index matrices are two-body density matrices of many-fermion states, and which are not. Indiscriminate variation over the density matrices (to look for the ground state) is, therefore,

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inappropriate. Hence, we are back to square one, i.e., we have to anyhow consider the full Hilbert space to look for correct many-fermion states, even if we know that this constitutes an enormous waste of effort. New bright ideas to solve the N -representability problem in nuclear-physics context are very much needed. Before this is achieved, we are bound to look for methods judiciously reducing the dimensionality of the many-body problems.



III. RESULTS

We saw that the crucial element of the dimensionality is the number of space-spin-isospin points needed to describe

basic fields a_x^+ . Therefore, we have to use methods that lead to fields as slowly varying in function of position, as it is possible. In this respect, region of the phase space that corresponds to pairs of nucleons getting near one another, is particularly cumbersome, because the wave functions must vary rapidly there, in order to become very small within the radius of the strong repulsion, cf. Fig. 5 above. In the past, very powerful technics have been developed to treat these

hard-core effects. They are based on replacing the real NN interaction $V_{xyx'y'}$ by the effective interaction $G_{xyx'y'}$ that fulfills the following condition

$$\int \int dx' dy' V_{xyx'y'} \Psi_{ij}(x', y') = \int \int dx' dy' G_{xyx'y'} \left[\frac{\phi_i(x')\phi_j(y') - \phi_i(y')\phi_j(x')}{\sqrt{2}} \right],$$

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where the sum-integrals are performed over \mathbf{x}' and \mathbf{y}' .

The two-body wave function in the square brackets on the r.h.s. is the independent-particle, or product wave function,

built as the antisymmetrized product of two s.p. wave functions, $\phi_i(\mathbf{x})$ and $\phi_j(\mathbf{x})$, characterized by quantum numbers i and j . The two-body wave function on the l.h.s., $\Psi_{ij}(\mathbf{x}', \mathbf{y}')$, is a wave function correlated at the short range; it is very small within the region of the hard core. So the real NN interaction, when acting on the correlated wave function, gives a finite result, because the wave function is very small in the region where the repulsion is vary large.

On the other hand, the antisymmetrized product wave function is never small around $\mathbf{x}' = \mathbf{y}'$ (although it vanishes at $\mathbf{x}' = \mathbf{y}'$), and hence the effective interaction fulfilling *has no hard core*. Condition defines, therefore, the effective interaction that can be used in the space of uncorrelated Slater determinants. The whole procedure can be put on firm grounds in the framework of the perturbation expansion, when partial sums of infinite classes of diagrams are performed, but this is beyond the scope of the present lectures. We only mention that within such a formalism, the effective interaction is obtained by solving the Bethe-Goldstone equation

The effective interaction should, in principle, depend on the s.p. states $\phi_i(\mathbf{x})$ and $\phi_j(\mathbf{x})$ for which the Bethe-Goldstone equation is solved. For example, the effective interaction in an infinite nuclear matter, where the s.p. wave functions are plane waves, can be different than that in a finite nucleus. In the past, there were many calculations pertaining to the first case, while the second (and more interesting) situation was successfully addressed only very recently Hax00,Hax02.

On a phenomenological level, one can postulate simple forms of interactions and use them as models of such difficult-to-derive effective interactions. Such a route was adopted by Gogny Gog75b, who postulated the simple local interaction

$$\tilde{G}_{\mathbf{x}\mathbf{y}\mathbf{x}'\mathbf{y}'} = \delta(\mathbf{x} - \mathbf{x}')\delta(\mathbf{y} - \mathbf{y}')G(\mathbf{x}, \mathbf{y}),$$

$$G_{\mathbf{x}\mathbf{y}\mathbf{x}'\mathbf{y}'} = \tilde{G}_{\mathbf{x}\mathbf{y}\mathbf{x}'\mathbf{y}'} - \tilde{G}_{\mathbf{x}\mathbf{y}\mathbf{y}'\mathbf{x}'}$$

where the tilde denotes a non-antisymmetrized matrix element (), in the form of a sum of two Gaussians, plus a zero-range, density dependent part,²

$$G(\mathbf{x}, \mathbf{y}) = \sum_{i=1,2} e^{-(\mathbf{x}-\mathbf{y})^2/\mu_i^2} \times (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) + t_3(1 + P_\sigma)\delta(\mathbf{x} - \mathbf{y})\rho^{1/3} \left[\frac{1}{2}(\mathbf{x} + \mathbf{y}) \right].$$

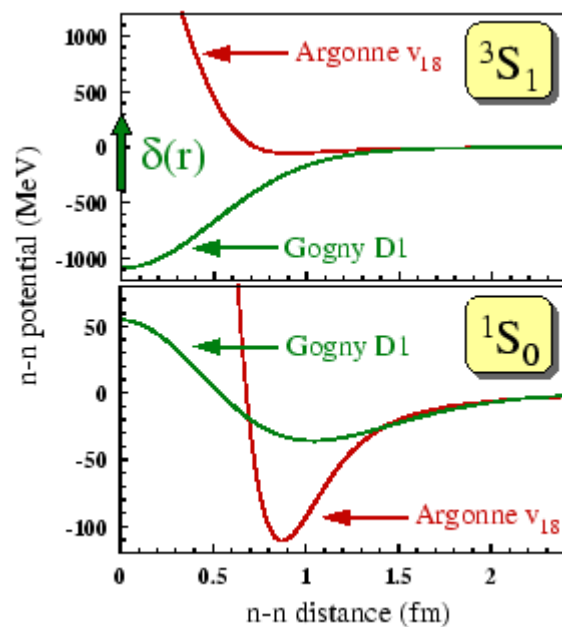
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$$P_\sigma = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2) \quad P_\tau = \frac{1}{2}(1 + \vec{\tau}_1 \cdot \vec{\tau}_2)$$

In this Equation, P_σ and P_τ are, respectively, the spin and isospin exchange operators of particles 1 and 2, $\rho(\mathbf{r})$ is the total density of the system at point \mathbf{r} , and $\mu_i, W_i, B_i, H_i, M_i, t_3$ are parameters.



Comparison of the Gogny and Argonne v_{18} $n-n$ potentials in the 3S_1 (top) and 1S_0 (bottom) channels. Note very different scales of the top and bottom panels.

Hence we compare the real $n-n$ interaction (Argonne v_{18}) with the effective Gogny interaction (the D1 parametrization Gog75b,RS80) in the $L=0$ channels, i.e., in the 3S_1 channel ($P_\sigma = 1$ and $P_\tau = -1$) and 1S_0 channel ($P_\sigma = -1$ and $P_\tau = 1$). It is clear that real and effective interactions are very different near $\mathbf{r}=0$. The zero-

range piece of the interaction acts only in the 3S_1 channel; it is represented by the green arrow at $\mathbf{r}=0$. One should keep in mind that the Gogny interaction is meant to represent the effective interaction, and hence it can only act on the product wave functions. In particular, an attempt to solve exactly, e.g., the two-body (deuteron) problem goes beyond the range of applicability of the effective interaction. The Gogny interaction is mostly used within the mean-field approximation.

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IV. CONCLUSIONS

We know that such composite particles (called nuclei or nuclides, as you know) exist in Nature. There exist exactly 253 species of stable nuclei. About 2500 other ones have been synthesized in laboratories - they decay by different processes, like electron, positron, proton, or neutron emission, or by fission, i.e., by splitting into two lighter nuclei (including the case when one of the lighter nuclei is the ^4He nucleus, called the α particle). According to theoretical predictions, there probably exist another 3000 nuclei, not synthesized yet, that are stable with respect to nucleon emission. At present, their synthesis, investigation, and description is at the centre of interest of nuclear structure physicists, and most of the lectures presented during this Summer School were devoted precisely to this subject.

Nuclei are fascinating objects. They are fermionic systems that exhibit single-particle (s.p.) and collective features at the same scale. Apart from very light ones, they contain too many constituents for an application of exact methods, and too few constituents for an application of statistical methods. Their elementary modes of excitation can, nevertheless, be very well defined based on using quasi-constituents and/or effective interactions.

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