Nuclear physics: a laboratory for many-particle quantum mechanics
or
From model to theory in nuclear structure physics

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1. Models vs. theories
2. The nuclear landscape
3. The unitary fermion gas model
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5. The multiconfiguration shell model
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What are models good for?

Step 1 - Build the Nucleus

The nucleus, the central part of the atom, is made from protons and neutrons. All of your atom's protons and neutrons go in the nucleus. For nitrogen, the nucleus would look something like this:

N. Bohr (1937)

Models:
- capture the essential phenomena
- are simple, at least in formulation
Examples of information nuclear models

The shell model model

\[ H = -\frac{\hbar^2 \nabla^2}{2m} - V_0 f(r) + V_{\ell s} \frac{1}{r} \frac{df}{dr} \ell \cdot s \]

4 parameters
Explains magic numbers,
explains many ground-state spins and parities

The liquid drop model

\[ B(N, Z) = a_v A - a_s A^{1/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N - Z)^2}{A} + \frac{\delta}{A^{1/2}} \]

\[ A = N + Z \]

5 parameters
Reproduces binding energies to 3 MeV r.m.s., out totals
ranging from 100 to 2000 MeV.
Characteristics of good theories

- need only a small set of parameters
- have wide predictive power
- have intrinsic criteria for limits of validity
Starting point: the nuclear interaction

In the two-body sector, the nuclear interaction is just barely able, or not, to produce a bound state.

- nn channel: $r \sim 2$ fm; $a_{nn} \sim 18$ fm
- np channel: $V \sim -100$ MeV; $E_d = -2.2$ MeV

An informative model: the unitary Fermi gas
Interaction is zero-range with a strength that produces a zero-energy bound state
The unitary model in the three-body system--what we learned

1. There are an infinite number of weakly bound 3-body states (Efimov 1971).

2. It is the only nontrivial three-body problem that can be solved exactly.

3. Exact solutions are useful for testing numerical methods (GFMC, hyperspherical harmonics, ...)

Unitary Quantum Three-Body Problem in a Harmonic Trap

Félix Werner and Yvan Castin

Laboratoire Kastler Brossel, École Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France
(Received 18 July 2005; published 10 October 2006)

We consider either 3 spinless bosons or 3 equal mass spin-1/2 fermions, interacting via a short-range potential of infinite scattering length and trapped in an isotropic harmonic potential. For a zero-range model, we obtain analytically the exact spectrum and eigenfunctions: for fermions all the states are universal; for bosons there is a coexistence of decoupled universal and efimovian states. All the universal states, even the bosonic ones, have a tiny 3-body loss rate. For a finite range model, we numerically find for bosons a coupling between zero angular momentum universal and efimovian states; the coupling is so weak that, for realistic values of the interaction range, these bosonic universal states remain long-lived and observable.
The uniform gas of fermions with short-ranged interactions

\[ H = - \sum_i \frac{\nabla_i^2}{2m} + g \sum_{i<j} \delta({\vec{r}}_i - {\vec{r}}_j) \]

Interaction is only defined in a cutoff space; the physical expansion parameter is the scattering length \( a \).

Perturbative limit (1960’s many-body theory):

\[
\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m} \left[ \frac{3}{5} + \frac{2}{3\pi} k_F a + \frac{4}{35\pi^2} (11 - 2 \ln 2)(k_F a)^2 + 0.23(k_F a)^3 + \cdots \right]
\]

(11.71)

Now we look at the limit \( a \to \infty \)

The Hamiltonian has no internal parameters!

\[
\frac{E}{N} = \xi \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{5} \right)
\]
TABLE VI. Historical results for the Bertsch parameter $\xi$ determined experimentally (expt.), by numerical simulation (sim.) and by analytic calculation (anal.), along with publication (pub.) date. Values obtained variationally are upper bounds and are indicated with an asterisk; simulation results without a quoted error bar should be regarded as approximate.

<table>
<thead>
<tr>
<th>Pub. date</th>
<th>$\xi$ (expt.)</th>
<th>Ref.</th>
<th>Pub. date</th>
<th>$\xi$ (sim.)</th>
<th>Ref.</th>
<th>Pub. date</th>
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Getting more realistic

Neutron matter equation of state

Getting more realistic on the nuclear interaction

About 20 parameters are required to describe the nuclear interaction in sufficient detail to reproduce experimental scattering phase shifts and properties of the deuteron.

The Hamiltonian based on that interaction underbinds the 3-nucleon system, overbinds nuclear matter, and produces a spin-orbit field that is too weak.

The deficiencies are corrected by including a 3-body interaction arising from pions.
Calculational method of choice for light nuclei: Green’s function Monte Carlo

S. Pieper et al, Phys. Rev. C70 054325

\[ E = \frac{\langle \Psi_0 | H | \Psi_1 \rangle}{\langle \Psi_0 | \Psi_1 \rangle} \]

\[ \Psi_0 \left( \xi_1, \xi_2, \ldots \right) \text{ is an antisymmetrized function of } \ i = (\xi_i, r_i, \eta_i) \]
with \( r \)-dependence based on shell orbitals.

\[ \Psi_1 = e^{-\beta H} \Psi_0 = \left( e^{-\Delta B \frac{p^2}{2m}} e^{-\Delta B v} \right)^n \Psi_0 \]

\( V \) is a local function of \( r_0 \).

\( e^{-t V^2} \) is the Green’s function for the diffusion equation.

It is applied stochastically by propagating “walkers”

\[ R = (r_1, r_2, \ldots) \Rightarrow R' = (r_1', r_2', \ldots) \]
Excitation energy (MeV)

Argonne \( v_{18} \) with Illinois-7 
GFMC Calculations

Including IL7 gives
- correct s.-o. splitting & \(^{10}\text{B}\) g.s.

S. Pieper et al, Phys. Rev. C70 054325
Argonne $v_{18}$ with Illinois-7 GFMC Calculations
Multi-configuration shell model  


\[ H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{i<j} \sum_{k<l} v_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k \quad i = (n, l, j, m) \]

labels a shell orbital

<table>
<thead>
<tr>
<th>Shell Model Space</th>
<th>Matrix Dimension</th>
<th>Number of Parameters in $H$</th>
<th>Number of Data Fit</th>
<th>Reference</th>
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<td>$\leq 84$</td>
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<td>2s-1d shell</td>
<td>$\leq 9371$</td>
<td>66</td>
<td>$\sim 600$</td>
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<td>2p-1f shell 2p1f+g9_2</td>
<td>$\approx 1.3 \times 10^9$</td>
<td>$10^{15}$</td>
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</table>

[3,4]: Calculations are limited to nuclei not too far from closed shells. Examples:
Domain of configuration-interaction shell model

Matrix size $< 10^8$
Shell-model Monte Carlo method (an early review: Physics Reports 278 2 (1997)).

\[ H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{i<j} \sum_{k<l} v_{ij,kl} a_i^\dagger a_j^\dagger a_k a_l \]

Single-particle energies from the Woods-Saxon potential

\[ v_{ij,kl} \text{ from a self-consistent separable interaction} \]

\[ v(r_1, r_2) = \sum_L v_L f_L(r_1) f_L(r_2) \sum_M Y_{LM}(\hat{r}_1) Y_{LM}(\hat{r}_2) \quad L = 2, 3, 4 \]

plus a pairing interaction (discussed later).
The Monte-Carlo sign problem is avoided by good luck and a good choice of representation. (All $v_L$ are negative and the pairing interaction is expressed as a density-density interaction between like particles.)

The object calculated is the expectation value of an operator in the grand canonical ensemble,

$$<\hat{\mathcal{O}}> = \frac{\text{Tr}(\hat{\mathcal{O}} e^{-\beta \hat{H}_0})}{\text{Tr} e^{-\beta \hat{H}_0}} \quad \hat{H}_0 = H - \mu_n N - \mu_s \hat{\mathcal{N}}$$

The Hubbard-Stratonovich transformation reduces the many-body propagator $e^{-\beta \hat{H}}$ to a sum over single-particle transformations, $\hat{U}_o$. $\text{Tr}(\hat{\mathcal{O}} \hat{U}_o) = \det(1 + \hat{\mathcal{O}} \hat{U}_o)$.

Expectation values are calculated by Metropolis importance sampling.

Refinements:
- projection on particle number
- projection on angular momentum
- A two-time Green's function to calculate odd-$A$
Application to the level density of Dy-162

All the shell orbitals between Z=50-90 and N=82-136 are included.

Dimension of space: \( D(M=0) = 6 \times 10^{21} \)

Pairing in nuclei: the phenomenon

Definition of pairing gap:

\[ \Delta_{o,Z}^{(3)}(N) = \frac{1}{2} (E_b(Z, N + 1) - 2E_b(Z, N) + E_b(Z, N - 1)) \]
The seniority model

Define an SU(2) algebra of operators in the Fock space of a j-shell.

\[ P_+ = \sum_{m>0} a_m \dagger a_{-m} \dagger \quad P_- = P_+^\dagger \quad P_0 = \sum_m a_m \dagger a_m \]

The Hamiltonian \[ H = -G P_+ P_- \]

\[ E_v(N) = -\frac{1}{4} G(N-v)(2\Omega - N - v + 2) \]

Ca isotopes in the f\_7/2 shell

\[
H = \sum_i \varepsilon_i a_i^+ a_i - G P_+ P_-
\]

\[
E(\nu) = \sum_i \varepsilon_i \nu_i + \sum_{\alpha} E_{\alpha} \quad \nu_i = 0 \left\{ \begin{array}{ll}
\text{paired} \\
1 \text{single occ.}
\end{array} \right.
\]

\[
N = 2M + \sum_i \nu_i
\]

\[M \text{ equations:} \quad 1 - G \sum \frac{1-\nu_i}{2\varepsilon_i - E_{\alpha}} - 2G \sum \frac{1}{E_{\alpha} - E_{\beta}} = 0\]

Can be generalized to more operators

(Gaudin)

The model has been widely used to assess the accuracy of BCS theory in various contexts.
Pairing gaps calculated by self-consistent mean-field theory

Nuclear deformation

H.B.G. Casimir (1937): “One is led to the conclusion that the quadrupole moment cannot possibly be due to one proton... It might even been that the nucleus as a whole has a prolate shape and that the nucleus as a whole is rotating about its major axis.

Energy gap in the excitation spectrum of even-even nuclei, scaled to 2 Delta(3).
The Nilsson model

\[ H = \frac{P^2}{2M} + \frac{1}{2} M \left( \omega_z^2 z^2 + \omega_\perp^2 (x^2 + y^2) \right) + c (\ell^2 - \langle \ell^2 \rangle) + d \ell \cdot \vec{s} \]

The nucleus is most stable where there are gaps in the single-particle spectrum.
Self-consistent mean field and density-functional theory

\[ H = \sum_{ij} \left( \frac{-\nabla^2}{2m} \right)_{ij} a_i^{\dagger} a_j + \sum_{i<j,k<l} v_{ij,kl} a_i^{\dagger} a_j^{\dagger} a_l a_k + 3\text{body} \]

Minimize \( \langle H \rangle \) in the space of Slater determinants

\[ \langle a_i^{\dagger} a_j \rangle = \rho_{ij} \quad \langle a_i^{\dagger} a_j^{\dagger} a_\ell a_k \rangle = \rho_{i\ell} \rho_{j\ell} - \rho_{i\ell} \rho_{jk} \]

or in the space of Bogoliubov vacua

\[ \langle a_i a_j \rangle = \kappa_{ij} \quad \langle a_i^{\dagger} a_j^{\dagger} a_\ell a_k \rangle = \rho_{i\ell} \rho_{j\ell} - \rho_{i\ell} \rho_{jk} + \kappa_{ji}^* \kappa_{\ell k} \]

Basis of states can be coordinate space mesh, momentum space mesh, or 3-d harmonic oscillator states.

There are two popular families of interactions, the Skyrme family based on contact interactions and derivatives and the Gogny family based on short-ranged Gaussian functions. Both have a density-dependent contact interaction for the 3-body term.

See Bender, Heenen and Reihard, Rev. Mod. Phys. 75 121 (2003).
Performance of SCMF on nuclear binding energies

For comparison, the 5 parameter liquid drop model reproduces binding energies with a 3 MeV RMS error.

- SCMF improvement is a factor 2
- SCMF with phenomenology terms for correlation effects improvement is a factor of 5
- same or better improvement can be obtained with the liquid drop model plus shell corrections plus phenomenological correlation terms
Correlations and the restoration of broken symmetries

SCMF of nuclei breaks translational invariance. Depending on the nucleus, it may also breaks rotational symmetry. In the Bogoliubov theory, it further breaks particle number conservation.

The paradox of self-consistent mean-field theory: the physical states of course respect the symmetries of the Hamiltonian, but one often does better by breaking them.
Extensions of self-consistent mean-field theory for spectroscopy

- RPA, quasiparticle RPA, time-dependent HF, HFB, DFT

Generator Coordinate Methods

- Collective Hamiltonian

- Discrete-basis Hill-Wheeler
Progress on a global theory for even-even nuclei

HFB mapped to the 5-dimensional Bohr Hamiltonian
Delaroche et al., PRC 81 (2010)

13 parameters in the energy functional
The present global study. The experimental spectrum, on the left, is from Ref. [28] as well as from data repository for the $\gamma$ band [24]. Calculated values are those from Ref. [23].
Global assessment of accuracy: first excited J=2 state

E(exp) = E(theory)+/-40% over 2 order of magnitude

Many other observables
The CEA/DAM global survey, on the N=Z line

2+ Excitation energies

Energy (MeV) vs. Z
Evidence for a spin-aligned neutron–proton paired phase from the level structure of $^{92}$Pd

A near-term goal: odd-A nuclei

No collective Hamiltonian to map onto

Restoring angular momentum more difficult

Projection technique

\[ \hat{P}_{MK}^J = \frac{2J + 1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\gamma \, D_{MK}^{*J} \hat{R}, \]

\[ N_J(q) = \sqrt{\int_0^{\pi/2} d\theta \sin(\theta) d_{00}^J(\theta) \langle q | \hat{R}(\theta) | q' \rangle}. \]

Onishi Formula (1966)

\[ \langle \Psi_1 | \Psi_0 \rangle = \sqrt{\det(U_0^\dagger U_1 + V_0^\dagger V_1)} \]

Robledo’s Formula (2009)

\[ \langle \Psi_1 | \Psi_0 \rangle = \text{pf} \left( \begin{array}{cc} (V_1 U_1^{-1})^* & -1 \\ 1 & -(V_0 U_0^{-1}) \end{array} \right) \]
FIG. 3: (Color online) Comparison of the calculated low-lying levels grouped into rotational bands with data taken from Ref. [22].

Let us now illustrate the fourth step of our method for the case shown in Fig. 3. For a given value of $J^\pi$, all the states represented in panels [a] and [b] are being mixed. In the case of the yrast $\frac{3}{2}^+$ and $\frac{5}{2}^+$ levels, this mixing has a limited effect and the energy gain is just a few keV. In contrast, most other levels are significantly shifted, in particular the yrast $\frac{3}{2}^+$ and $\frac{5}{2}^+$ levels, and also the higher $\frac{3}{2}^+$ level in the ground state. This reflects, not surprisingly, that energy surfaces such as those of Fig. 3, obtained from the projection of single $hqp$ configurations and that are drawn as a function of the collective coordinate cannot represent the entire complexity of an odd-$A$ system. The gain in total binding energy from projection strongly depends on the specific configuration. The two $hqp$ HF states that the spectra of panels [a] and [b] of Fig. 3 are projected from differ by keV in energy. This difference is reduced to a few keV by PNP and to a few keV for the lowest levels after combined PNP and xMP. The yrast $\frac{3}{2}^+$ state in panel [a] gains keV from xMP compared to the PNP state, and the yrast $\frac{5}{2}^+$ level in panel [b] even more keV. These values are larger than the typical keV difference that is found for well-deformed even-even systems with the SLy and Gogny EDFs [33]. We attribute this difference to the small effective mass $m^*_0/m$ of SLyMR and indeed large energy gains are also found when calculating adjacent even-even nuclei with SLyMR. The projected states have then been combined for a complete GzM calculation. Sampling the deformations $q_1$ and $q_2$ in steps of keV and considering several $hqp$ states at each combination, we have constructed a basis of $\Omega^+_{\pi,\delta}$ of positive parity and $\Omega^-_{\pi,\delta}$ of negative parity, respectively. After elimination of all redundant states, the Hamiltonian is finally diagonalized in a space of $\Omega^+_{\pi,\delta}$ of $\Omega^-_{\pi,\delta}$ for $J^\pi = \frac{3}{2}^+$ and $\frac{5}{2}^+$ and $\frac{3}{2}^-$ for $J^\pi = \frac{5}{2}^-$. The large number of $hqp$ configurations makes it possible to analyze the calculation's convergence. When adding the states to the GzM in the order of the energy of the $hqp$ state they are projected from, the last few states being considered for each parity just add about a few keV to the energies of the low-lying states, with their energy differences changing even less. This smooth convergence could only be achieved by using a Hamiltonian in the GzM. The GzM gives a quite satisfying description of the low-lying levels, cf. Fig. 3. The overall band structure is reasonably well reproduced, including the excitation energy of the lowest levels with negative parity. yand ic, however, has an incorrect signature splitting and its band head is computed somewhat too low in energy. Within each band, the spectrum is slightly too spread out as is also found for even-even nuclei. This can be corrected for by projecting HF states cranked to finite $B(E2)$ and $B(M1)$ values for transitions between them.

Charge radii-- HFB

Experimental data from Angeli, ADNDT 87 (2004)

(a) Charge radius HFB

Mass Number A

Relative Error
Error assessment

INT09-1: Effective field theories and the many-body problem

Example: intrinsic error from shell truncation in CI fits

Estimated error of 0.2 MeV is close to actual value.