Nuclear Structure III: What to Do in Heavy Nuclei

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Outline

1. Hartree-Fock
2. History
3. Results
4. Collective Excitations
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1 Hartree-Fock
2 History
3 Results
4 Collective Excitations
Above $A \approx 100$, shell model is usually unworkable; need too large a valence space. Main alternative is mean-field theory and extensions. Let's begin with Hartree-Fock theory.

Call the Hamiltonian $H$ (it won’t be the NN interaction itself). The Hartree-Fock ground state is the Slater determinant with the lowest expectation value $\langle H \rangle$. Employ:

**Theorem (Thouless)**

Suppose $|\phi\rangle \equiv a_1^\dagger \cdots a_F^\dagger |0\rangle$ is a Slater determinant. The most general Slater determinant not orthogonal to $|\phi\rangle$ can be written

$$
|\phi'\rangle = \exp( \sum_{m>F,i<F} C_{mi} a_m^\dagger a_i )|\phi\rangle = [1 + \sum_{m,i} C_{mi} a_m^\dagger a_i + O(C^2)]|\phi\rangle
$$
Variational Procedure

Find best Slater det. $|\phi\rangle$ by minimizing $\mathcal{H} \equiv \langle \phi'|H|\phi'\rangle/\langle \phi'|\phi'\rangle$:

$$\frac{\partial \mathcal{H}}{\partial C_{nj}} = \langle \phi|Ha_n^†a_j|\phi\rangle = 0 \ \forall \ n > F, \ j \leq F \quad (1)$$

Write $H$ as

$$H = \sum_{\alpha} \frac{p_{\alpha}^2}{2m} + \sum_{\alpha<\beta} V_{\alpha\beta} \implies \sum_a T_{ab}a^{|}_{a}a_b - \sum_{a,b,c,d} \frac{1}{4} V_{ab,cd}a^{|}_{a}a^{|}_{b}a_c a_d ,$$

where $T_{ab} = \langle a|\frac{p^2}{2m}|b\rangle$ and $V_{ab,cd} = \langle ab|V_{12}|cd\rangle - \langle ab|V_{12}|dc\rangle$.

Then equation (1) gives

$$h_{nj} \equiv T_{nj} + \sum_{k<F} V_{jk,nk} = 0 \ \forall \ n > F, \ j \leq F$$

This will certainly be true if we can find a single particle basis in which $h$ is diagonal, i.e. solve the Hartree-Fock equations

$$h_{ab} \equiv T_{ab} + \sum_{k\leq F} V_{ak,bk} = \delta_{ab}\epsilon_a \ \forall \ a, b . \quad (2)$$
Note that in equation (2) the potential-energy term depends on all the occupied levels. So do the eigenvalues $\epsilon_a$, therefore, and

Solutions are “self-consistent”

To solve equations:

1. Start with a set of basis states $a, b, c \ldots$ and calculate the matrix elements of $h$ according to equation (2).
2. Diagonalize $h$ to obtain a new set of basis states $a', b' \ldots$.
3. Repeat steps 1 and 2 until you get essentially the same basis out of step 2 as you put into step 1.
In coordinate space, equations are

\[-\frac{\nabla^2}{2m} \phi_a(r) + \left[ \int dr' V(|r - r'|) \sum_{j \leq F} \phi_j^*(r') \phi_j(r') \right] \phi_a(r) \]

\[-\sum_{j \leq F} \left[ \int dr' V(|r - r'|) \phi_j^*(r') \phi_a(r') \right] \phi_j(r) = \epsilon_a \phi_a(r) \]

First potential term involves the “direct” (intuitive) potential

\[U_d(r) \equiv \int dr' V(|r - r'|) \rho(r') .\]

Second term contains the nonlocal “exchange potential”

\[U_e(r, r') \equiv \sum_{j \leq F} V(|r - r'|) \phi_j^*(r') \phi_j(r) .\]

Self consistency means that these potentials produce wave s.p. wave functions that in turn regenerate the same potentials.
Brief History of Mean-Field Theory

1. Big problem early: HF doesn’t work with realistic NN potentials because of hard core, which isn’t reflected in Slater determinants.

2. Included hard core implicitly through effective interaction: Brueckner G matrix, the solution to Bloch-Horowitz equations for a nucleon pair in the presence of other nucleons. Still didn’t work perfectly.

3. Tried to include three-body interaction approximately as density-dependent two-body interaction, in the same way as the two-body interaction is approximately a density-dependent mean field. This gave better results and had convenient “zero-range” approximation.
Phenomenology successfully evolved toward zero-range density-dependent (Skyrme) interactions, with

\[
H = t_0 \left( 1 + x_0 \hat{P}_\sigma \right) \delta(r_1 - r_2)
\]
\[
+ \frac{1}{2} t_1 \left( 1 + x_1 \hat{P}_\sigma \right) \left[ (\nabla_1 - \nabla_2)^2 \delta(r_1 - r_2) + h.c. \right]
\]
\[
+ t_2 \left( 1 + x_2 \hat{P}_\sigma \right) (\nabla_1 - \nabla_2) \cdot \delta(r_1 - r_2) (\nabla_1 - \nabla_2)
\]
\[
+ \frac{1}{6} t_3 \left( 1 + x_3 \hat{P}_\sigma \right) \delta(r_1 - r_2) \rho^\alpha([r_1 + r_2]/2)
\]
\[
+ iW_0 (\sigma_1 + \sigma_2) \cdot (\nabla_1 - \nabla_2) \times \delta(r_1 - r_2) (\nabla_1 - \nabla_2)
\]

where

\[
\hat{P}_\sigma = \frac{1 + \sigma_1 \cdot \sigma_2}{2}
\]

and \( t_i, x_i, W_0, \) and \( \alpha \) are adjustable parameters.

Abandoning first principles leads to still better accuracy.
Convenient because exchange potential is local; easy to solve.

Also, variational principal can be reformulated in terms of a local energy-density functional. Defining

\[
\rho_{ab} = \sum_{i \leq F} \langle b | \phi_i \rangle \langle \phi_i | a \rangle, \quad \rho(r) = \sum_s \rho_{rs,r's} = \sum_{i \leq F,s} |\phi_i(r, s)|^2
\]

\[
\tau(r) = \sum_{i \leq F,s} |\nabla \phi_i(r, s)|^2, \quad J(r) = -i \sum_{i \leq F,s,s'} \phi_i(r, s)[\nabla \phi_i(r, s') \times \sigma_{ss'}]
\]

and

\[
E = \int dr \left[ \frac{\hbar^2}{2n} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} \rho^3 + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 + \frac{3}{4} W_0 \rho \nabla \cdot J + \frac{1}{32} (t_1 - t_2) J^2 \right]
\]

you find

\[
\frac{\partial (E - \sum_i \epsilon_i \rho_{ii})}{\partial \rho_{ab}} = h_{ab} - \epsilon_a \delta_{ab} = 0, \quad \forall a, b
\]

i.e. the HF equations. Density dependence makes \( h \) more complicated than what you’d get by just varying \( |\phi\rangle \).
“Shoot, we can include more correlations, get back to first principles, if we mess with the density functional via:”

Theorem (Hohenberg-Kohn and Kohn-Sham, vulgarized)

∃ universal functional of the density that, together with a simple one depending only on external potentials, gives the exact ground-state energy and density when minimized through Hartree-like equations. (Finding the functional is up to you!)

At least two recent EFT-like approaches to constructing functional

- Power counting used to identify important terms; coefficients calculated from first principals (Furnstahl et al).
- Expansion in local-density scheme with coefficients fit to data (Dobaczewski et al).

Both approaches have a way to go. In mean time we have pretty good empirical functionals, with parameters fit in nuclei near closed shells. More sophisticated version of Bethe-Weiszacker.
Modern Results: Shell Structure Near Neutron Drip Line

Shell Structure Summary

Densities Near Drip Lines

This and next 3 slides from J. Dobacewski,
Two-Neutron Separation Energies

Experiment

Theory

SkP volume $\delta$ pairing

$S_{2n}$ energy

Experiment

Theory
Addressing these challenges will require us to exploit advances in the study of microscopic inter-nucleon interactions, in the development of many-body computational techniques, and in raw computer power, as well as to further develop DFT itself as applied to finite, self-bound systems.

The first, most general question to be addressed is just what is the form of the nuclear energy-density functional? Limitations of current functionals in describing isovector and density dependences reflect both insufficient constraints from data (e.g., for time-odd fields) and incomplete physics encoded in the functionals.

To make progress, a concerted effort will be required to study new functionals when applied to finite nuclei and infinite or semi-infinite nuclear matter. For instance, in the particle-hole channel, one would like to enrich the density dependence of the effective mass in order to differentiate between its value in the bulk and at the Fermi surface. Another goal is to understand connections between the symmetry energy and isoscalar and isovector mean fields, and in particular the influence of effective mass and pair correlations on symmetry energy versus isospin. Such an understanding will allow us to better determine isospin corrections to nuclear mean fields and energy density functionals.

In the self-consistent method, the average nucleonic field is obtained from the nucleonic density. Consequently, in the nuclear state with nonzero angular momentum, the self-consistent potential acquires time-odd components. These terms are expected to play a significant role at very high angular momentum when the nucleus is strongly polarized, but they should also influence properties of beta decay and the ground states of odd-mass and odd-odd nuclei.

Fundamental questions, such as constraints on the most general form for functionals and the existence of DFT for intrinsic densities, need to be addressed. Effective field theory (EFT) methods, now widely applied for few-nucleon systems, can provide systematic insight into the density dependences along with error estimates.

http://www.orau.org/ria/RIATG/Blue_Book_6.pdf
Collective Excited States

Can do time-dependent Hartree-Fock in an external potential \( f(\mathbf{r}, t) = f(\mathbf{r})e^{-i\omega t} + f^\dagger(\mathbf{r})e^{i\omega t} \). TDHF equation is:

\[
-i\frac{d\rho_{ab}}{dt} = \frac{\partial E[\rho]}{\partial \rho_{ab}} + f_{ab}(t)
\]

Assuming small amplitude oscillations

\[
\rho = \rho_0 + \delta \rho e^{-i\omega t} + \delta \rho^\dagger e^{-i\omega t}
\]

gives

\[
i\omega \delta \rho_{mi} = \sum_{n>F,j\leq F} \frac{\partial h_{mi}}{\partial \rho_{nj}} \delta \rho_{nj} + \frac{\partial h_{mi}}{\partial \rho_{jn}} \delta \rho_{jn} + f_{mi}
\]

Setting \( f = 0 \) gives the condition for a “resonance” — an oscillation that persists in the limit of no forcing — which corresponds to an excited stationary state (a pole in the response function) \(|E = \hbar\omega\rangle\). The resulting \( \delta \rho \equiv \rho_{\text{tr}}(E) \), is the transition density to \(|E\rangle\). Small amplitude approximation is usually called the “random phase approximation” (RPA).
Here, very explicitly, are the various types of densities we’ve been discussing. The density operator itself in first quantization is

\[ \rho^{\text{op}}(\mathbf{r}) = \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}^{\text{op}}_{\alpha}) \]

The ground-state and transition densities are then

\[ \rho(\mathbf{r}) = \langle 0 | \rho^{\text{op}}(\mathbf{r}) | 0 \rangle, \quad \rho_{\text{tr}}(E, \mathbf{r}) = \langle E | \rho^{\text{op}}(\mathbf{r}) | 0 \rangle. \]

To calculate ground-state expectation values or transition matrix elements of an operator:

\[ \langle 0 | f(\rho^{\text{op}}) | 0 \rangle = \int d\mathbf{r} f(\mathbf{r}) \rho(\mathbf{r}), \quad \langle E | f(\rho^{\text{op}}) | 0 \rangle = \int d\mathbf{r} f(\mathbf{r}) \rho_{\text{tr}}(E, \mathbf{r}). \]

Finally, the one-body density matrix we used for the variational principle, which is more general than Slater determinants, is (in second quantization)

\[ \rho_{ab} \equiv \langle 0 | a_{b}^{\dagger} a_{a} | 0 \rangle. \]
RPA Collectivization of Transition Strength

Transition strength $R(E)$ for an operator $f$:

$$R(E) = |\langle E | f | 0 \rangle|^2$$

Figure shows the effects of the “residual” $NN$ interaction — that is, its effects beyond the mean-field approximation — on the isovector dipole strength ($f = e \sum_p z_p$).
More Isovector Dipole in RPA

Strength Distribution

- $^{132}\text{Sn}$
- $E = 14.04$ MeV
- $E = 11.71$ MeV
- $E = 7.60$ MeV

Transition Densities

- $r^2\delta\rho$ for neutrons and protons at various energies.

Graphs showing the distribution and transition densities for different energies.
Pygmy Resonances Near the Drip Line?

IV dipole strength

- $^{22}_{\text{O}}$
- $^{20}_{\text{O}}$
- $^{18}_{\text{O}}$
- $^{16}_{\text{O}}$

E[MeV]

R[e fm$^2$]

self-consistent RQRPA
Quadrupole Phonons Near the Drip Line

- **2^+** 22° quadrupole phonon 2.95 MeV
- **Transition Density**
  - E=2.95 MeV
  - r^2δρ [fm^-2]
- **Plot**
  - 22° quadrupole phonon
  - Red: neutrons
  - Blue: protons
  - E [MeV] vs. r [fm]
Small Amplitude TDHF: Dipole Resonance in $^8$Be
Surface Octupole Vibration in $^{16}$O
Project deformed Slater determinants onto states with good angular momentum and/or mix Slater determinants:

\[ |\Psi\rangle = \int dq \, g(q) \, |\phi(q)\rangle \]

The coordinate \( q \) can be a deformation parameter like \( \beta \) or an orientation angle \( \theta \) (for projection).

Challenges and the Road Ahead

- Better understanding of how much physics can be subsumed into a “Kohn-Sham density functional” (i.e. into mean-field equations)
- Development of methods that include the things mean-field theory cannot
- Better connection with the “bare” NN interaction
- Quantitative predictions in neutron-rich nuclei, before there’s a RIA (important for nucleosynthesis even after RIA)
Double-Beta Decay and Nuclear Structure