Nuclear Structure III: What to Do in Heavy Nuclei

J. Engel

University of North Carolina

June 15, 2005

Outline









Outline









The Situation in Heavy Nuclei

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 $\mathcal{H} \equiv \langle \phi' | H | \phi' \rangle / \langle \phi' | \phi' \rangle$: $\frac{\partial \mathcal{H}}{\partial C_{nj}} = \langle \phi | H a_n^{\dagger} a_j | \phi \rangle = 0 \quad \forall \ n > F, \ j \le F$ (1)

Write H as

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

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

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

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

$$h_{ab} \equiv T_{ab} + \sum_{k \le F} V_{ak,bk} = \delta_{ab} \epsilon_a \quad \forall \ a, b \ . \tag{2}$$

Self Consistency

Note that in equation (2) the potential-energy term depends on **all** the occupied levels. So do the eigenvalues ϵ_a , therefore, and

Solutions are "self-consistent"

To solve equations:

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

Coordinate Space

In coordinate space, equations are

$$\begin{aligned} -\frac{\nabla^2}{2m}\phi_a(\mathbf{r}) &+ \left[\int d\mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) \sum_{j \le F} \phi_j^*(\mathbf{r}') \phi_j(\mathbf{r}') \\ &- \sum_{j \le F} \left[\int d\mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) \phi_j^*(\mathbf{r}') \phi_a(\mathbf{r}') \right] \phi_j(\mathbf{r}) &= \epsilon_a \phi_a(\mathbf{r}) \end{aligned}$$

First potential term involves the "direct" (intuitive) potential

$$U_d(\mathbf{r}) \equiv \int d\mathbf{r}' V(|\mathbf{r}-\mathbf{r}'|)
ho(\mathbf{r}') \; .$$

Second term contains the nonlocal "exchange potential"

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

Self consistency means that these potentials produce wave s.p. wave functions that in turn regenerate the same potentials.

Outline









Brief History of Mean-Field Theory

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



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

$$H = t_0 (1 + x_0 \hat{P}_{\sigma}) \,\delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2} t_1 (1 + x_1 \hat{P}_{\sigma}) \left[(\nabla_1 - \nabla_2)^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + h.c. \right] + t_2 (1 + x_2 \hat{P}_{\sigma}) (\nabla_1 - \nabla_2) \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) (\nabla_1 - \nabla_2) + \frac{1}{6} t_3 (1 + x_3 \hat{P}_{\sigma}) \,\delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^{\alpha} ([\mathbf{r}_1 + \mathbf{r}_2]/2) + i W_0 (\sigma_1 + \sigma_2) \cdot (\nabla_1 - \nabla_2) \times \delta(\mathbf{r}_1 - \mathbf{r}_2) (\nabla_1 - \nabla_2) ,$$

where

$$\hat{P}_{\sigma} = \frac{1 + \sigma_1 \cdot \sigma_2}{2} \; ,$$

and t_i , x_i , W_0 , and α 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

$$\rho_{ab} = \sum_{i \leq F} \langle b | \phi_i \rangle \langle \phi_i | a \rangle, \quad \rho(\mathbf{r}) = \sum_{s} \rho_{\mathbf{r}s,\mathbf{r}'s} = \sum_{i \leq F,s} |\phi_i(\mathbf{r},s)|^2$$
$$\tau(\mathbf{r}) = \sum_{i \leq F,s} |\nabla \phi_i(\mathbf{r},s)|^2, \quad \mathbf{J}(\mathbf{r}) = -i \sum_{i \leq F,s,s'} \phi_i(\mathbf{r},s) [\nabla \phi_i(\mathbf{r},s') \times \sigma_{ss'}]$$

and

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

you find

$$\frac{\partial \left(E - \sum_{i} \epsilon_{i} \rho_{ii}\right)}{\partial \rho_{ab}} = h_{ab} - \epsilon_{a} \delta_{ab} = \mathbf{0}, \ \forall a, b$$

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.

Outline









Modern Results: Shell Structure Near Neutron Drip Line



H. Sagawa, Phys. Rev. C65, 064314 (2002)

Shell Stucture Summary



From J. Dobaczewski et al., Phys. Rev. C 53, 2809 (1996).

Densities Near Drip Lines





Two-Neutron Separation Energies



Experiment

Theory

Deformation



Range of Predictions for Drip Line



http://www.orau.org/ria/RIATG/Blue_Book_6.pdf

Outline









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 $\delta \rho \equiv \rho_{\rm tr}(E)$, is the transition density to $|E\rangle$. Small amplitude approximation is usually called the "random phase approximation" (RPA).

Ground-State Density, Transition Density, etc.

Here, very explicitly, are the various types of densities we've been discussing. The density operator itself in first quantization is

$$ho^{\mathsf{op}}(\mathbf{r}) = \sum_lpha \, \delta(\mathbf{r} - \mathbf{r}^{\mathsf{op}}_lpha)$$

The ground-state and transition densities are then

$$\rho(\mathbf{r}) = \langle 0|\rho^{\mathsf{op}}(\mathbf{r})|0\rangle , \qquad \rho_{\mathsf{tr}}(E,\mathbf{r}) = \langle E|\rho^{\mathsf{op}}(\mathbf{r})|0\rangle .$$

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

$$\langle 0|f(\mathbf{r}^{\mathsf{op}})|0
angle = \int d\mathbf{r} f(\mathbf{r})
ho(\mathbf{r}) \,, \qquad \langle E|f(\mathbf{r}^{\mathsf{op}})|0
angle = \int d\mathbf{r} f(\mathbf{r})
ho_{\mathsf{tr}}(E,\mathbf{r}) \,.$$

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

 $\rho_{ab} \equiv \langle \mathbf{0} | a_b^{\dagger} a_a | \mathbf{0} \rangle \ .$

RPA Collectivization of Transition Strength



This and next 3 slides from N. Paar, http://crunch.ikp.physik.tu-darmstadt.de/~paar/rrpa.html

More Isovector Dipole in RPA



Pygmy Resonances Near the Drip Line?

IV dipole strength



Quadrupole Phonons Near the Drip Line



Smalll Amplitude TDHF: Dipole Resonance in ⁸Be



This slide and next courtesy of T. Nakatsukasa

Surface Octupole Vibration in ¹⁶O



Beyond Mean-Field Theory

Project deformed Slater determinants onto states with good angular momentum and/or mix Slater determinants:

 $|\Psi
angle = \int dq \, g(q) \, |\phi(q)
angle$

The coordinate q can be a deformation parameter like β or an orientation angle θ (for projection).

From M. Bender and P.-H. Heenen, Nuclear Physics **A**713, 390 (2003)

One-dimensional "energy surface", now different for each state in the rotational band.



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