Lecture IV: Nuclear Structure Overview

I. Introduction

J. Engel

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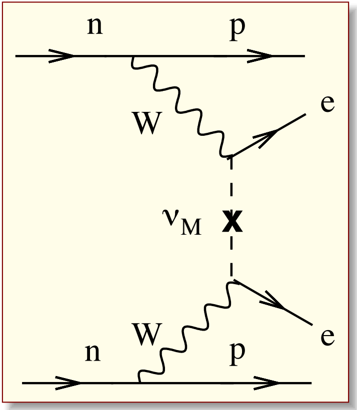
AMHERST CENTER FOR FUNDAMENTAL INTERACTIONS
Physics at the interface: Energy, Intensity, and Cosmic frontiers
University of Massachusetts Amherst

A Little on the Standard Mechanism



Here $m_{\nu_M} \ll m_e$.

How Effective Mass Gets into Rate

$$[T^{0\nu}_{1/2}]^{-1} = \sum_{\text{spins}} \int |Z_{0\nu}|^2 \delta(E_{e1} + E_{e2} - Q) \frac{d^3p_1}{2\pi^3} \frac{d^3p_2}{2\pi^3}$$

$Z_{0\nu}$ contains lepton part

$$\sum_k \bar{e}(x)\gamma_\mu(1-\gamma_5)U_{ek}\nu_k(x)\,\overline{\nu^c_k}(y)\gamma_\nu(1+\gamma_5)U_{ek}e^c(y)\ ,$$

where ν's are Majorana mass eigenstates.
Contraction gives neutrino propagator:

$$\sum_k \bar{e}(x)\gamma_\mu(1-\gamma_5)\frac{q^\rho\gamma_\rho + m_k}{q^2 - m_k^2}\gamma_\nu(1+\gamma_5)e^c(y)\ U^2_{ek}\ ,$$

The $q^\rho\gamma_\rho$ part vanishes in trace, leaving a factor

$$\boxed{m_{\text{eff}} \equiv \sum_k m_k U^2_{ek}.}$$

What About Hadronic Part?

Integral over times produces a factor

$$\sum_n \frac{\langle f|J_L^{\mu}(\vec{x})|n\rangle\langle n|J_L^{\gamma}(\vec{y})|i\rangle}{q^0(E_n+q^0+E_{e2}-E_i)} + (\vec{x},\mu\leftrightarrow\vec{y},\nu)\,,$$

with q^0 the virtual-neutrino energy and the J the weak current.

In impulse approximation:

May not be adequate.

$$\langle p|J^{\mu}(x)|p'\rangle = e^{iqx}\overline{u}(p)\Big(g_V(q^2)\gamma^{\mu} - g_A(q^2)\gamma_5\gamma^{\mu} - ig_M(q^2)\frac{\sigma^{\mu\nu}}{2m_p}q_{\nu} + g_P(q^2)\gamma_5 q^{\mu}\Big)u(p')\,.$$

q^0 typically of order inverse inter-nucleon distance, 100 MeV, so denominator can be taken constant and sum done in closure.

Final Form of Nuclear Part

$$M_{0\nu} = M_{0\nu}^{GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F} + \dots$$

with

$$M_{0\nu}^{GT} = \langle F | \, | \sum_{i,j} H(r_{ij}) \, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \; \tau_i^+ \tau_j^+ \; | I \rangle + \dots$$

$$M_{0\nu}^{F} = \langle F \, | \sum_{i,j} H(r_{ij}) \; \tau_i^+ \tau_j^+ \; | I \rangle + \dots$$

$$H(r) \approx \frac{2R}{\pi r} \int_0^\infty dq \frac{\sin qr}{q + \overline{E} - (E_i + E_f)/2} \quad \text{roughly} \propto 1/r$$

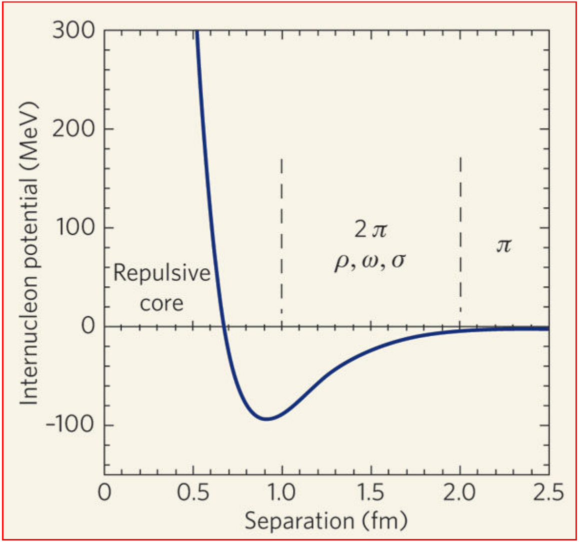
Contribution to integral peaks at $q \approx 100$ MeV inside nucleus.

Corrections are from “forbidden” terms, weak nucleon form factors, many-body currents …

II. Basic Ideas of Nuclear Structure

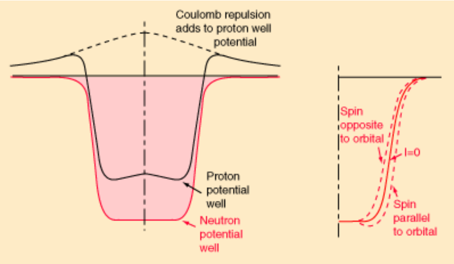
Traditional Nucleon-Nucleon Potential

From E. Ormand, http://www.phy.ornl.gov/npss03/ormand2.ppt

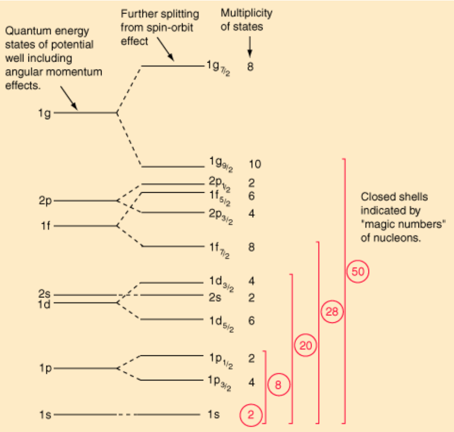


Shell Model of Nucleus

Nucleons occupy orbitals like electrons in atoms. Central force on nucleon comes from averaging forces produced by other nucleons.

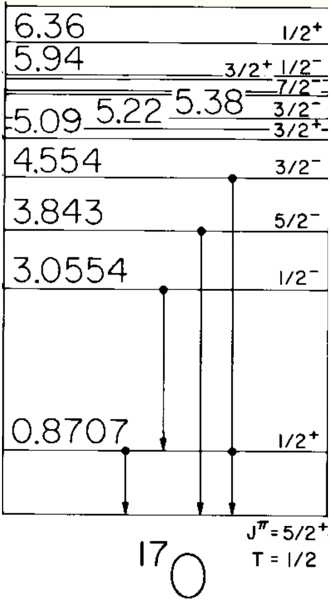


http://hyperphysics.phy-astr.gsu.edu/hbase/nuclear/shell.html



Reasonable potentials give magic numbers at 2, 8, 20, 28, 50, 126

An Example

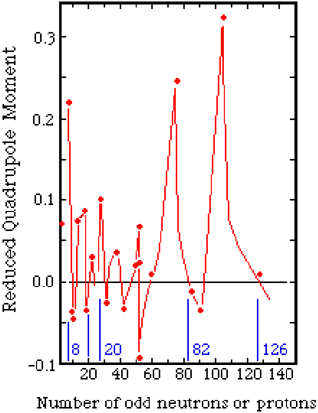


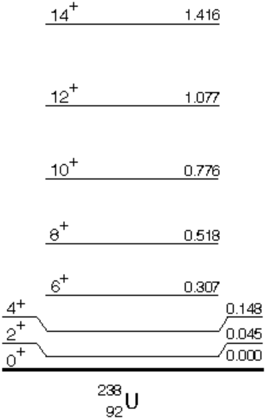
$d_{3/2}$

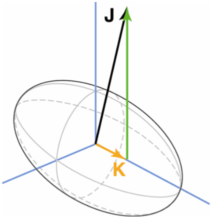
$s_{1/2}$

$d_{5/2}$

Simple Model Can't Explain Collective Rotation…





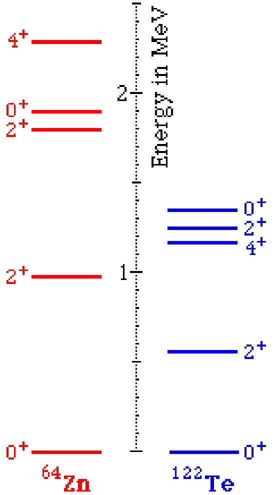


From Booth and Combey, http://www.shef.ac.uk/physics/teaching/phy303/phy303-3.html and

E. Ormand, http://www.phy.ornl.gov/npss03/ormand1.ppt

Collective rotation between magic numbers

Or Collective Vibrations



Two vibrational "phonons" with angular momentum 2 give states with angular momentum 0, 2, 4.

From Booth and Combey, http:///www.shef.ac.uk/physics/teaching/phy303/phy303-3.html and http://www.fen.bilkent.edu.tr/~aydinli/Collective%20Model.ppt

Alternative Early View: "Liquid Drop" Model

Protons and neutrons move together; volume is conserved, surface changes shape.

Ansatz for surface:

$$R(\theta,\phi) = R_0\left(1 + \sum_m \alpha_m Y_{2,m}(\theta,\phi)\right)$$

The 5 α's are collective variables. For vibrations, Hamiltonian obtained e.g. from classical fluid model:

$$H \approx 1/2B\sum_m |\dot{\alpha}_m|^2 + 1/2C\sum_m |\alpha_m|^2$$

with

$$B \approx \frac{\rho R_0^5}{2} = \frac{3}{8\pi} m A R_0^2\ , \qquad C \approx \frac{a_S A^{2/3}}{\pi} - \frac{3e^2 Z^2}{10\pi R_0}\ , \qquad \omega = \sqrt{C/B}$$

ω is roughly the right size, but real life is more complicated, with frequencies depending on how nearly magic the nucleus is.

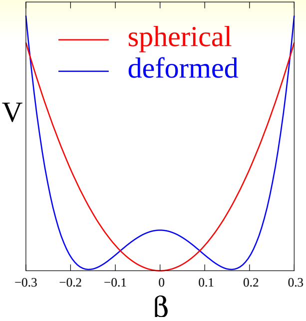
Deformation in Liquid Drop Model

If Coulomb effects overcome surface tension, C is negative and nucleus deforms. 5 "intrinsic-frame" α's replaced by 3 Euler angles, and:

$$\beta \equiv \sqrt{\alpha_0^2 + 2\alpha_2^2}, \qquad \gamma \equiv \tan^{-1}[\sqrt{2}\alpha_2/\alpha_0]$$

so that

$$\Psi(\theta, \varphi, \psi) \approx D^{J*}_{MK}(\theta, \varphi, \psi)\Phi_{\mathrm{int.}}(\beta, \gamma).$$



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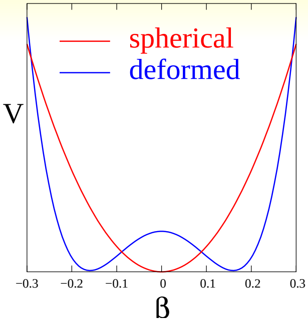
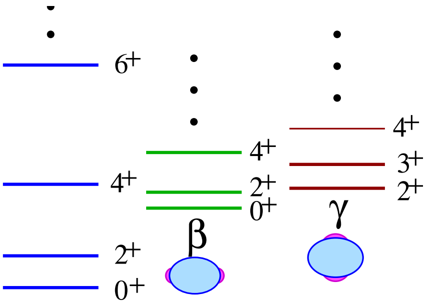


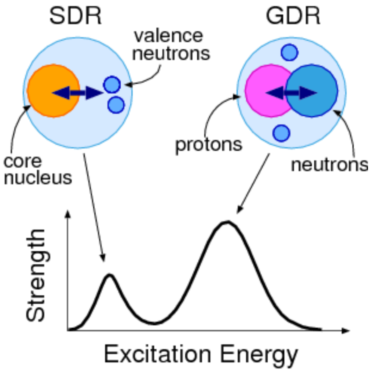


Low-lying states

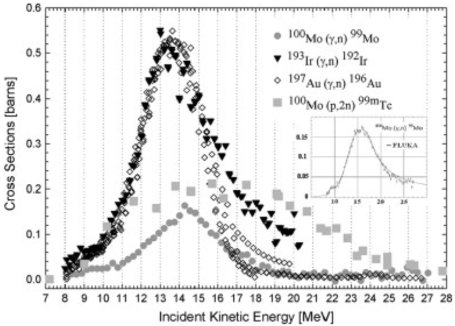
1. Rotations of deformed nucleus
2. Surface vibrations along or against symmetry axis

Density Oscillations

Photoabsorption cross section proportional to “isovector” dipole strength. Resonance lies at higher energy than surface modes.



Ikeda et al., arXiv:1007.2474 [nucl-th]

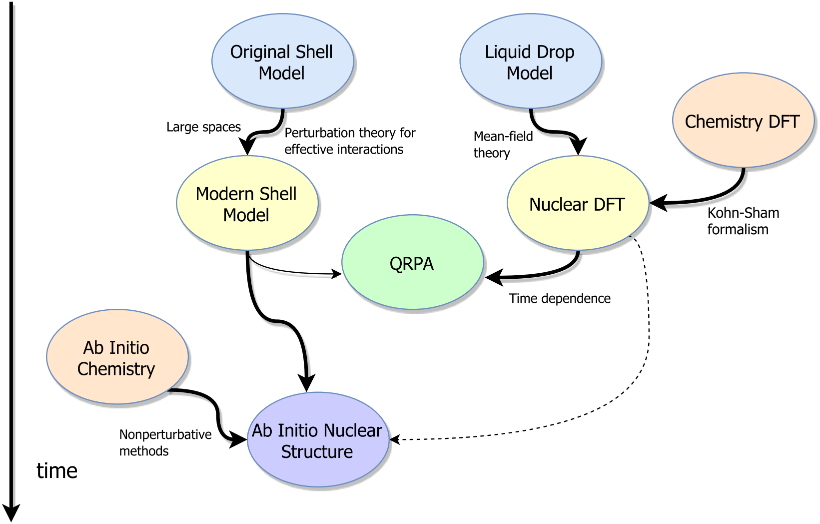


Szpunar et al., Nucl. Inst. Meth. Phys. A 729, 41 (2013)

Giant dipole resonance

III. Development of Structure Models for for ββ Decay

Development Since the First Models



Modern Shell-Model Basic Wave Functions

Nucleus is usually taken to reside in a confining harmonic oscillator. Eigenstates of oscillator part are localized Slater determinants, the simplest many-body states:

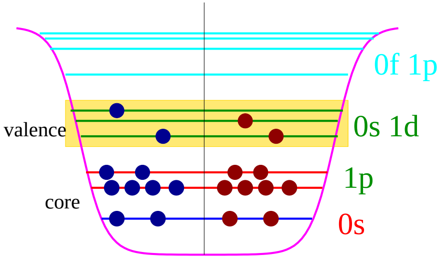
$$\psi(\vec{r}_1 \cdots \vec{r}_n) = \begin{vmatrix} \phi_i(\vec{r}_1) & \phi_j(\vec{r}_1) & \cdots & \phi_l(\vec{r}_1) \\ \phi_i(\vec{r}_2) & \phi_j(\vec{r}_2) & \cdots & \phi_l(\vec{r}_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_i(\vec{r}_n) & \phi_j(\vec{r}_n) & \cdots & \phi_l(\vec{r}_n) \end{vmatrix} \longrightarrow a_i^\dagger a_j^\dagger \cdots a_l^\dagger \left|0\right\rangle$$

They make a convenient basis for diagonalization of the real internucleon Hamiltonian. To get a complete set just put distribute the *A* particles, one in each oscillator state, in all possible ways.

Truncation Scheme of the Modern Shell-Model

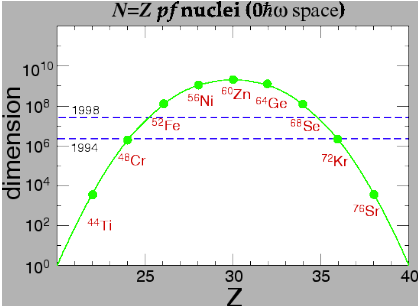
- Core is inert; particles can't move out.
- Particles outside core confined to limited set of valence shells.
- Can't use basic nucleon-nucleon interaction as Hamiltonian because of truncation, which excludes significant configurations. Most Hamiltonians to date are in good part phenomenological, with fitting to many nuclear energy levels and transition rates. All operators need to be "renormalized" as well.

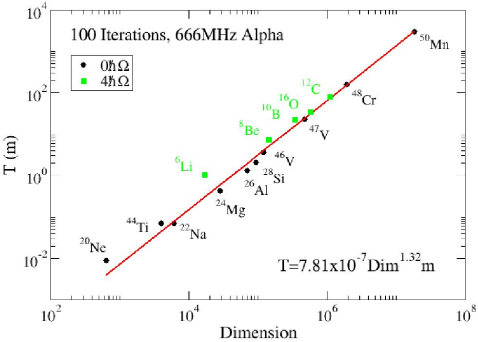
Example: ^{20}Ne



We'll return to this problem later.

What the Shell Model Can Handle



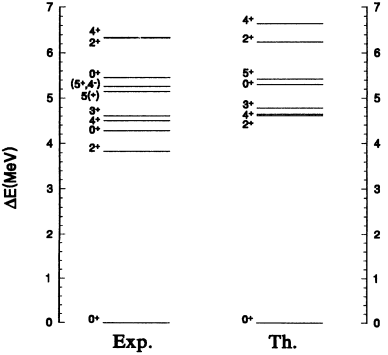


From W. Nazarewicz, http://www-highspin.phys.utk.edu/~witek/

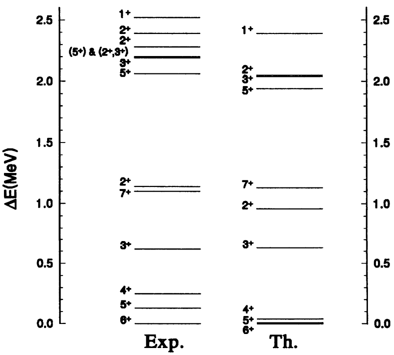
All these are easy now. But more than one oscillator shell still usually impossible.

Level of Accuracy (When Good)

^{48}Ca

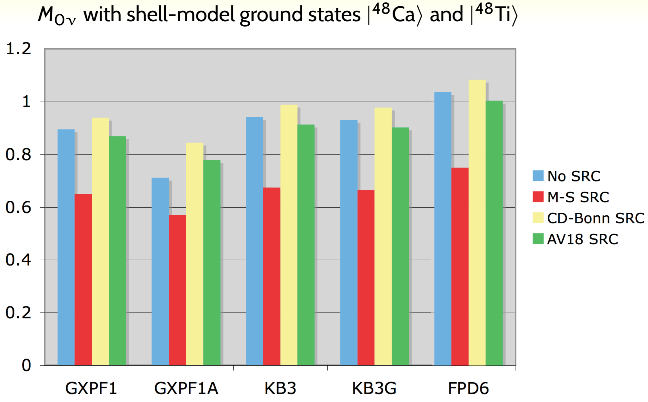


^{48}Sc



From A. Poves, J. Phys. G: Nucl. Part. Phys. 25 (1999) 589 597.

Shell Model Calculations of $0\nu\beta\beta$ Decay



Effects of varying the phenomenological Hamiltonian

Problem with shell model: Experimental energy levels tell us, roughly, how to "renormalize" Hamiltonians to account for orbitals omitted from the shell-model space. But what about the $\beta\beta$ operator? How is it changed? Most calculations use "bare" operator.

The Beginning of Nuclear DFT: Mean-Field Theory

For a long time the best that could be done in a large single-particle space.

Call the Hamiltonian H (not the "bare" NN interaction itself). The Hartree-Fock ground state is the Slater determinant with the lowest expectation value $\langle H \rangle$.

Variational Procedure

Find best Slater det. $|\psi\rangle$ by minimizing $\mathcal{H} \equiv \langle\psi| H |\psi\rangle \,/\, \langle\psi|psi\rangle$:
In coordinate space, resulting equations are

$$-\frac{\nabla^2}{2m}\phi_\alpha(\vec{r}) + \left[\int d\vec{r'} V(|\vec{r} - \vec{r'}|) \sum_{j \leqslant F} \underbrace{\phi_j^*(\vec{r'})\phi_j(\vec{r'})}_{\rho(\vec{r'})}\right] \phi_\alpha(\vec{r})$$
$$- \sum_{j \leqslant F} \left[\int d\vec{r'} V(|\vec{r} - \vec{r'}|) \phi_j^*(\vec{r'})\phi_\alpha(\vec{r'})\right] \phi_j(\vec{r}) = \epsilon_\alpha \phi_\alpha(\vec{r}) \, .$$

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

$$U_d(\vec{r}) \equiv \int d\vec{r'} V(|\vec{r} - \vec{r'}|) \rho(\vec{r'}) \, .$$

Second term contains the nonlocal "exchange potential"

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

Self Consistency

Note that in potential-energy terms U_d and U_e depend on all the occupied levels. So do the eigenvalues ϵ_a, therefore, and solutions are "self-consistent." To solve equations:

1. Start with a set of A occupied orbitals $\phi_a, \phi_b, \phi_c \ldots$ and construct U_d and U_e.
2. Solve the HF Schrödinger equation to obtain a new set of occupied orbitals $\phi_{a'}, \phi_{b'} \ldots$
3. Repeat steps 1 and 2 until you get essentially the same orbitals out of step 2 as you put into step 1.

Second-Quantization Version

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 as

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

Minimizing $E = \langle\psi| H |\psi\rangle$:

$$\frac{\partial \mathcal{H}}{\partial C_{nj}} = \langle\phi| H a_n^\dagger a_j |\phi\rangle = 0 \quad \forall\, n > F,\ j \leqslant F$$

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

where $T_{ab} = \langle a| \frac{p^2}{2m} |b\rangle$ and $V_{ab,cd} = \langle ab| V_{12} |cd\rangle - \langle ab| V_{12} |dc\rangle$. This will be true if $\exists$ a single particle basis in which h is diagonal,

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

Another version of the HF equations.

Brief History of Mean-Field Theory

1. Big problem early: Doesn't work with realistic NN potentials because of hard core, which causes strong correlations.

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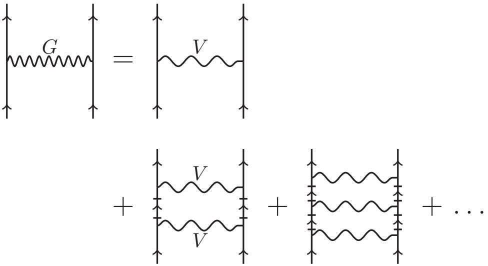

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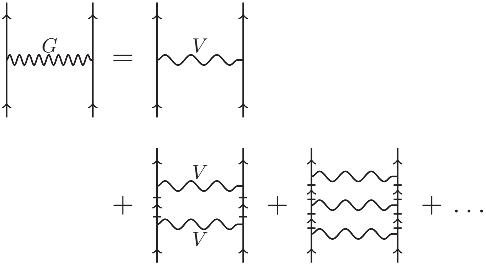


3. Three-body interaction included approximately as orbital-dependent two-body interaction, in the same way as two-body interaction is approximated by orbital-dependent mean field. Results better, and a convenient "zero-range" approximation used.

Brief History (Cont.)

4. Phenomenology successfully evolved toward zero-range density-dependent interactions, with

$$
\begin{aligned}
H = {} & t_0\,(1 + x_0 \widehat{P}_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2) \\
& + \frac{1}{2} t_1\,(1 + x_1 \widehat{P}_\sigma)\,\left[(\vec{\nabla}_1 - \vec{\nabla}_2)^2 \delta(\vec{r}_1 - \vec{r}_2) + h.c.\right] \\
& + t_2\,(1 + x_2 \widehat{P}_\sigma)\,(\vec{\nabla}_1 - \vec{\nabla}_2) \cdot \delta(\vec{r}_1 - \vec{r}_2)(\vec{\nabla}_1 - \vec{\nabla}_2) \\
& + \frac{1}{6} t_3\,(1 + x_3 \widehat{P}_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2)\rho^\alpha([\vec{r}_1 + \vec{r}_2]/2) \\
& + iW_0\,(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot (\vec{\nabla}_1 - \vec{\nabla}_2) \times \delta(\vec{r}_1 - \vec{r}_2)(\vec{\nabla}_1 - \vec{\nabla}_2)\,,
\end{aligned}
$$

where

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

and t_i, x_i, W_0, and α are adjustable parameters.

Abandoning first principles leads to still better accuracy.

Brief History (Cont.)

5. Convenient because exchange potential is local; easy to solve. Also, variational principal can be reformulated in terms of a local energy-density functional. Defining

$$\rho_{ab} = \sum_{i \leqslant F} \langle b|\,\phi_i\rangle\langle\phi_i\,|a\rangle\ , \quad \rho(\vec{r}) = \sum_{i \leqslant F, s} |\phi_i(\vec{r}, s)|^2$$

$$\tau(\vec{r}) = \sum_{i \leqslant F, s} |\nabla\phi_i(\vec{r}, s)|^2\,, \qquad \vec{J}(\vec{r}) = -i \sum_{i \leqslant F, s, s'} \phi_i(\vec{r}, s)[\nabla\phi_i(\vec{r}, s') \times \vec{\sigma}_{ss'}]$$

and

$$E = \langle\phi|\,H\,|\phi\rangle = \int d\vec{r}[\frac{\hbar^2}{2n}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}\rho^3 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau$$
$$+ \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 + \frac{3}{4}W_0\rho\vec{\nabla}\cdot\vec{J} + \frac{1}{32}(t_1 - t_2)\vec{J}^2]$$

and minimizing E gives you back the Hartree-Fock equations.

Brief History (Cont.)

6. "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)

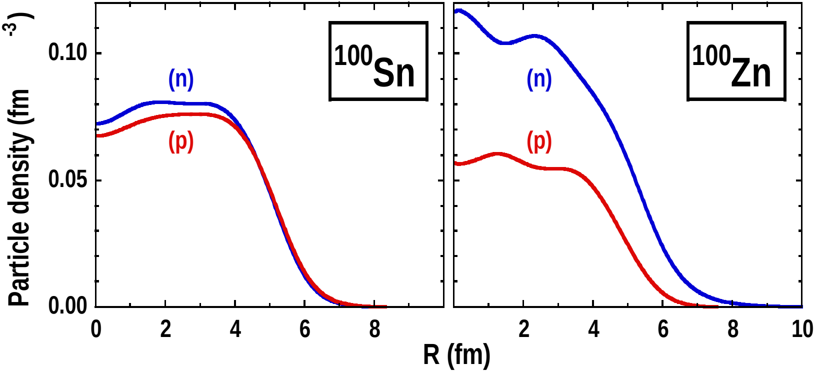
$\exists$ *universal functional of the density that, together with a simple one depending only on external potentials, gives the exact ground-state energy and density when minimized through Hartree-like equations. (Finding the functional is up to you!)*

There is some work to construct functionals form first principles, but they are determined largely by fitting Skyrme parameters.

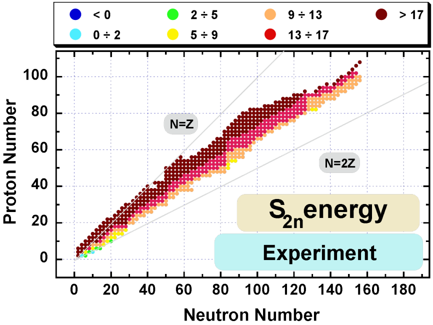
Results are pretty good, but it's hard to quantify systematic error.

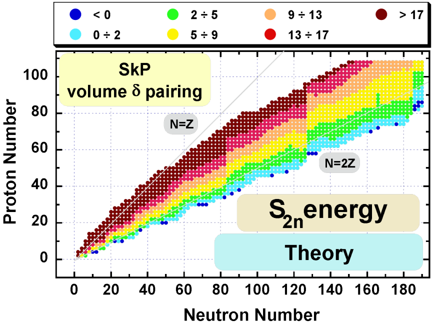
Densities Near Drip Lines

This and next 2 slides from J. Dobacewski



Two-Neutron Separation Energies

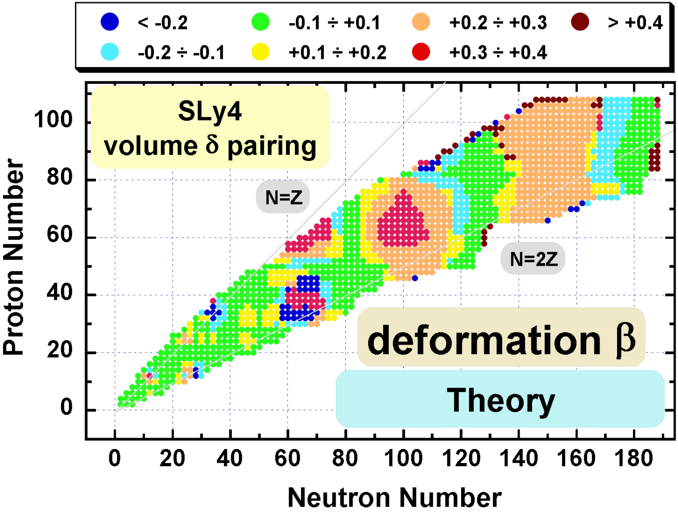




Experiment

Theory

Deformation



Collective Excited States

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

$$-i\frac{d\rho}{dt} = \frac{\partial E[\rho]}{\partial\rho} + f(t)$$

Assuming small amplitude oscillations

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

gives equation for $\delta\rho_\omega$, the transition density to the state with with energy $E = \hbar\omega$. Square of matrix element connecting ground state of operator f to that state is (schematically)

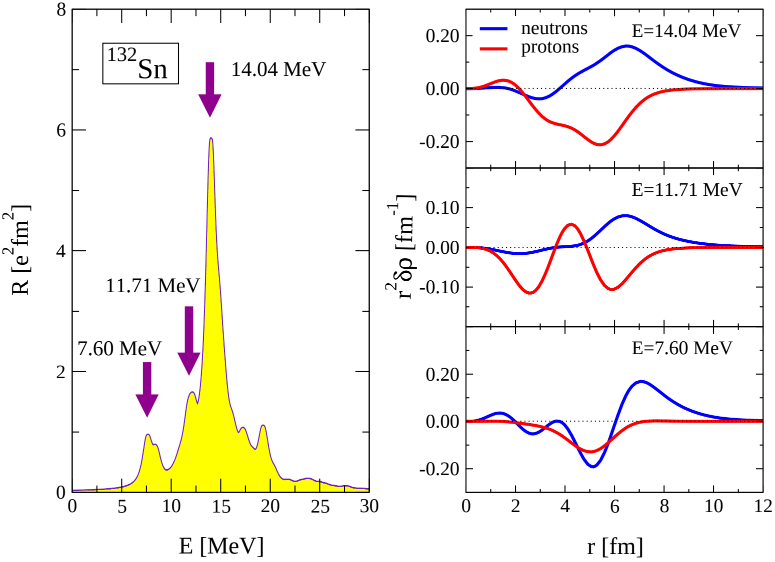
$$Im\left(\int d\vec{r} f(\vec{r})\delta\rho_\omega(\vec{r})\right) .$$

This is the "random phase approximation" (RPA).

Isovector Dipole in RPA

Strength Distribution

Transition Densities



Generalization to Include Pairing

HFB (Hartree-Fock-Bogoliubov) is the most general "mean-field" theory in these kinds of operators:

$$\alpha_a = \sum_c \left(U^*_{ac} a_c + V^*_{ac} a^\dagger_c \right) , \qquad \alpha^\dagger_a = \sum_c \left(U_{ac} a^\dagger_c + V_{ac} a_c \right) ,$$

Ground state is the "vacuum" for these operators.

In addition to having ordinary density matrix $\rho(\vec{r})$, one also has "pairing density:"

$$\kappa(\vec{r}) \equiv \langle 0 | \, a(\vec{r}) a(\vec{r}) \, | 0 \rangle \ .$$

Quasiparticle vacuum violates particle-number conservation, but includes physics of correlated pairs.

Energy functional $E[\rho]$ replaced by $E[\rho, \kappa]$. Minimizing leads to HFB equations for U and V.

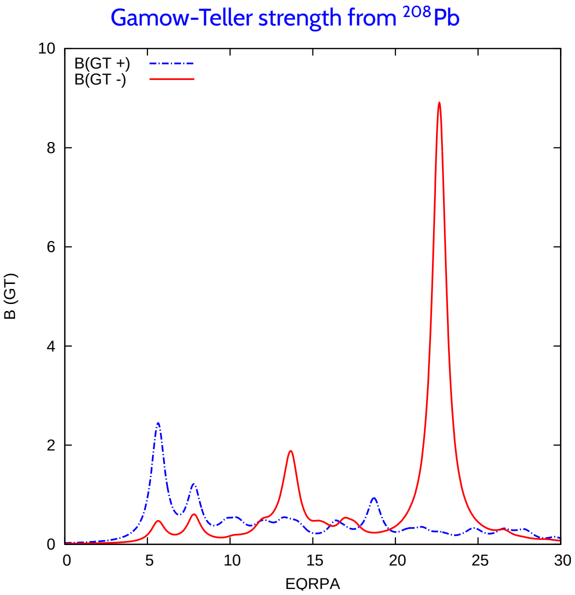
Generalization to linear response is called the quasiparticle random phase approximation (QRPA).

Gamow-Teller Strength

i.e. Square of Gamow-Teller Transition Matrix Element

Transition operators are those that generate allowed β decay:

$$\vec{f} = \vec{\sigma}\tau_{\pm} \; .$$



QRPA Calculations of $0\nu\beta\beta$ Decay

These very different in spirit from shell-model calculations, which involve many Slater determinants restricted to a few single-particle shells. QRPA involves small oscillations around a single determinant, but can involve many shells (20 or more).

Recall that the 0ν operator has terms that look like

$$\hat{M} = \sum_{ij} H(r_{ij}) \sigma_i \cdot \sigma_j \, .$$

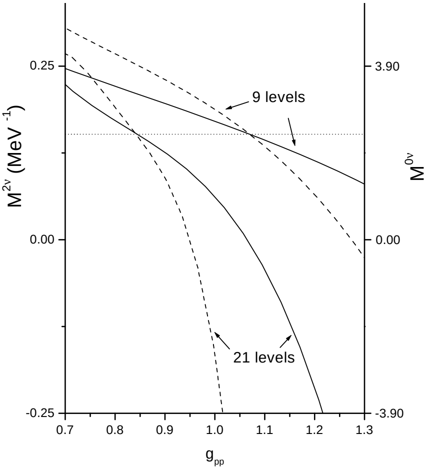
where i and j label the particles. QRPA evaluates this by expanding in multipoles, and inserting set of intermediate-nucleus states:

$$\langle F | \hat{M} | I \rangle = \sum_{ij,JM,N} \langle F | \hat{O}_{i,JM} | N \rangle \langle N | \hat{O}_{j,JM} | I \rangle \ ,$$

and uses calculated transition densities to evaluate the matrix elements.

More on QRPA

Strength of neutron-proton pairing in effective interaction is not well determined by data, often fit to reproduce 2ν lifetime.



Problem: Computation of transition densities for initial and final nuclei are completely separate. No way to match the states *N* computed in initial-nucleus and final-nucleus QRPA." Must cheat.

Beyond Mean-Field Theory: Generator Coordinates

Sometime called "EDF"

Sometimes a single mean field won't do, even with density functionals that includes the effects of many correlations.

Basic idea: Construct set of mean fields by constraining coordinate(s), e.g. quadrupole moment:

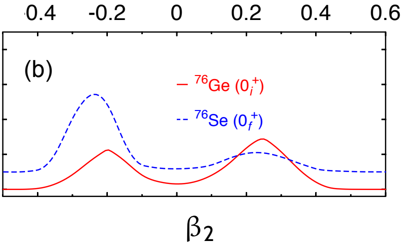
$$\langle Q_0 \rangle \equiv \langle \sum_i r_i^2 Y_i^{2,0} \rangle \ .$$

Minimize

$$\langle H' \rangle = \langle H \rangle - \lambda \langle Q_0 \rangle$$

for a whole range of the coordinate $\langle Q_0 \rangle$. Then diagonalize H in space of quasiparticle vacua (projected onto good particle number and angular momentum) with different $\langle Q_0 \rangle$.

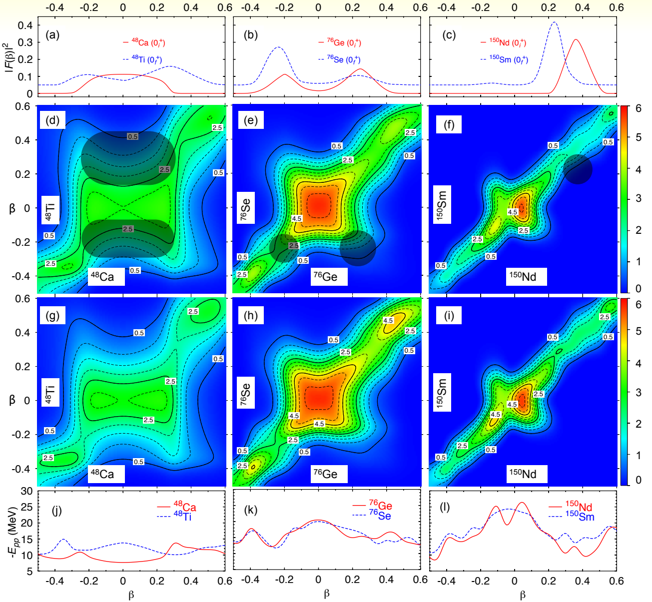
Collective wave functions



Wave functions peaked at $\beta_2 \approx \pm .2$

Calculating $\beta\beta$ Decay with Generator Coordinates

Rodríguez and Martinez-Pinedo



Level of Agreement So Far

Significant spread. And all the models could be missing important physics.

Uncertainty hard to quantify.