Realistic NN and NNN interactions and the nuclear single-particle basis

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Basic Elements of the Ab-Initio No Core Shell Model

- Review of NN interactions - emphasis on Chiral N3LO
- Motivate need for NNN interactions - emphasis on Chiral N2LO
- Choice of single particle basis spaces - Harmonic Oscillator, Saxon-Woods
- Hands-on example - visit “Nuclear Physics Calculator” website

Can we “derive” the NN interaction from QCD?

- What is the role of confinement?
- If derivation is successful, is this the full story?
- What about probing nuclei at ever higher energies & densities?

=> Need a perspective on derivations of interactions

All interactions are "effective" until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD, is an effective theory valid below the Planck scale

$\Lambda < 10^{19}$ GeV/c

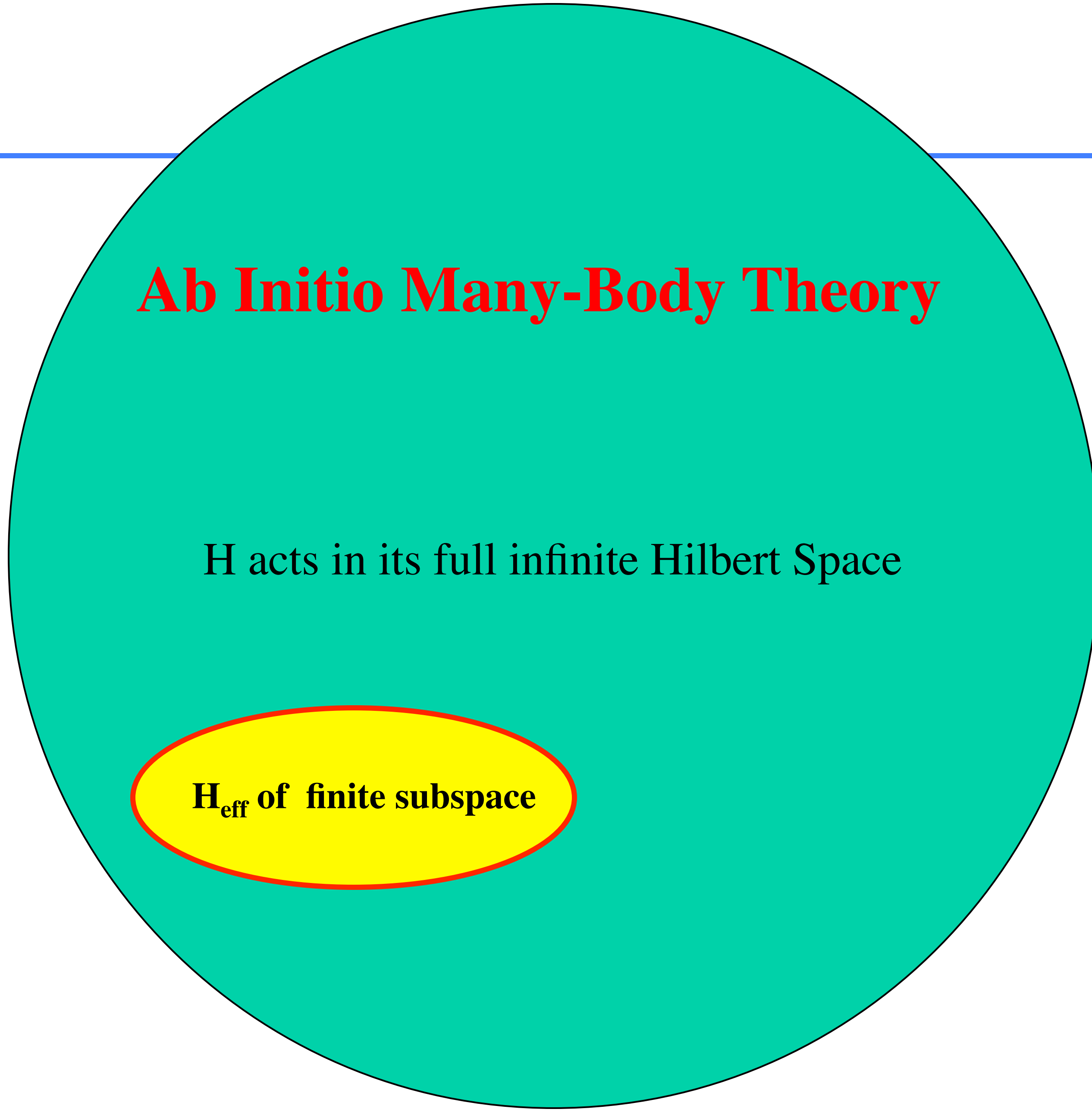
The "bare" NN interaction, usually with derived quantities, is thus an effective interaction valid up to some scale, typically the scale of the known NN phase shifts and Deuteron gs properties

$\Lambda \sim 600$ MeV/c (3.0 fm^{-1})

Effective NN interactions can be further renormalized to lower scales and this can enhance convergence of the many-body applications

$\Lambda \sim 300$ MeV/c (1.5 fm^{-1})

"Consistent" NNN and higher-body forces are those valid to the same scale as their corresponding NN partner, and obtained in the same renormalization scheme.


Ab Initio Many-Body Theory
H acts in its full infinite Hilbert Space
H_{eff} of finite subspace

Recently developed realistic NN interactions
Fit to available phase shifts and deuteron properties

- ❖ Traditional meson-exchange theory (Nijmegen X, CD Bonn X, AVX, etc.,)
- ❖ Effective field theory with roots in QCD (Chiral EFT, Idaho X, NXLO, etc.,)
- ❖ Off-shell variations of bare NN interactions (INOY-X, etc.,)
- ❖ Inverse scattering theory (ISTP, JISPX, etc.,)

"X" represents label specifying versions of that interaction

Take these as valid at least to the scale

$\Lambda \sim 600$ MeV/c (3.0 fm^{-1})

Renormalization schemes preserving all symmetries

- **Lee-Suzuki-Okamoto**

  renormalizes to the shell model basis chosen
- **Vlowk**

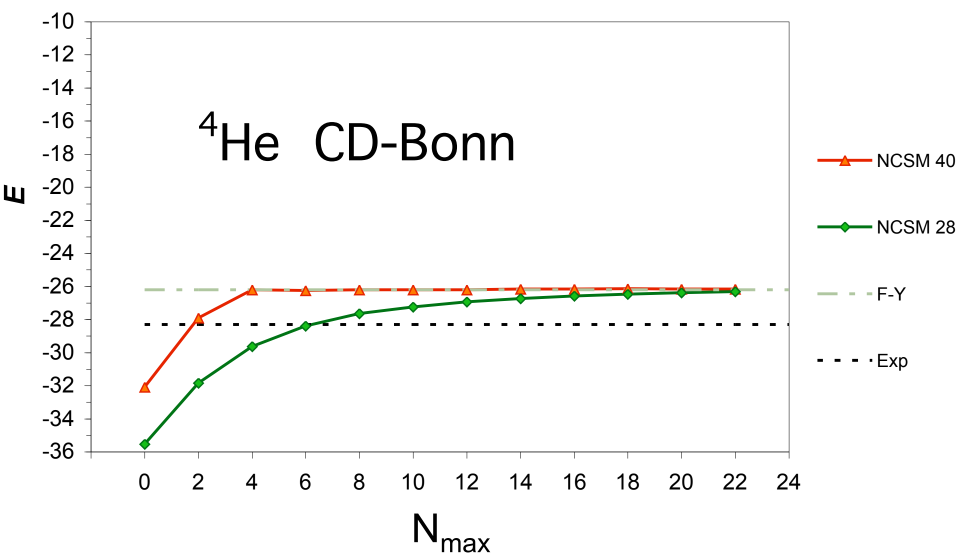
  scales to a lower cutoff momentum
- **Similarity renormalization group (SRG)**

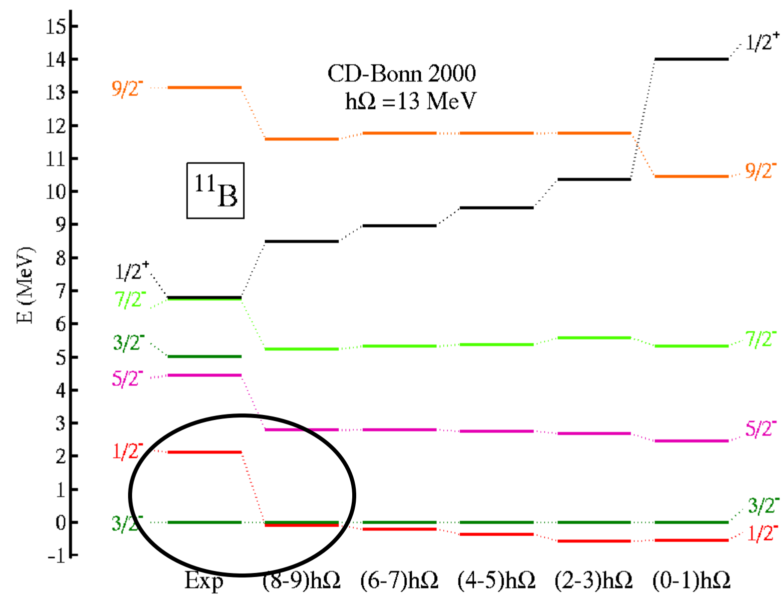
  reduces off-shell couplings
- **Unitary Correlation Operator Method (UCOM)**

  reduces short range repulsion

Comments on need for NNN potentials

- Binding energies of A=3-4 nuclei can be calculated exactly in non-relativistic QM (NRQM). Realistic local NN potentials underbind A=3 by ~500keV and A=4 by 2-4 MeV. Compared to total interaction energy, <GS| V |GS>, these are 2-6% effects.
- Nearly exact results for 5<A<16 nuclei these days indicate spin-sensitive observables (splitting of spin-orbit partners in odd nuclei, ground state spin of ^{10}B, magnetic transitions, neutrino cross sections, etc.) require more than realistic local NN potential.

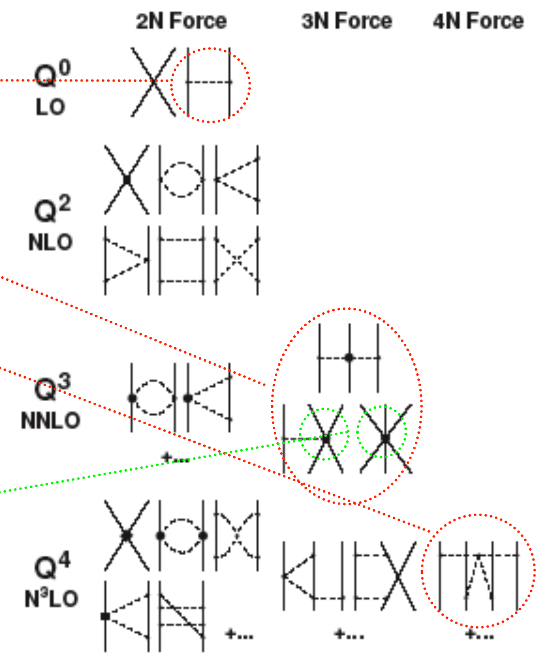




References:
A. Nogga, H. Kamada and W. Gloeckle, Phys. Rev. Lett. 85, 944(2000).
J.L. Friar, et al., Phys. Rev. C 59, 53(1999).
B.S. Pudliner, et al., Phys. Rev. Lett. 74, 4396(1995).
D.R. Entem, et al., Phys. Rev. C 68, 064001 (2002).

Chiral Effective Field Theory

- Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
- Systematic low-momentum expansion in $(Q/\Lambda_X)^n$; $\Lambda_X \approx$ 1 GeV, Q≈100 MeV
  - Power-counting
  - Chiral perturbation theory (χPT)
- Describe pion-pion, pion-nucleon and inter-nucleon interactions at low energies
  - Nucleon-nucleon sector - S. Weinberg (1991)
    - Worked out by Van Kolck, Kaiser, Meissner, Epelbaum, Machleidt…
- Leading order (LO)
  - One-pion exchange
- NNN interaction appears at next-to-next-to-leading order (N^2LO)
- NNNN interaction appears at N^3LO order
- Consistency between NN, NNN and NNNN terms
  - NN parameters enter in the NNN terms etc.
- Low-energy constants (LECs) need to be fitted to experiment
- N^3LO is the lowest order where a high-precision fit to NN data can be made
  - Entem and Machleidt (2002) N^3LO NN potential
- Only two NNN and no NNNN low-energy constants up to N^3LO



JISP16 NN interaction:
J-matrix Inverse Scattering Potential tuned with phase-shift-equivalent unitary transformations to the binding energy of ^{16}O

- High quality fit to np scattering data (chisq/dof = 1.05)
- High quality fit to Deuteron gs properties
- Finite rank separable in each NN channel in oscillator basis
- Highly non-local, soft and rapidly convergent in nuclear apps
- High quality description of nuclei through the p-shell
- Subroutines and documentation: nuclear.physics.iastate.edu

A.M. Shirokov, J.P. Vary, A.I. Mazur and T.A. Weber,
"Realistic Nuclear Hamiltonian: Ab exitu approach,"
Phys. Letts. B 644, 33(2007), ArXiv nucl-th/0512105

Ab Initio No-Core Shell Model (NCSM)

- Presently the only method capable to apply chiral two- and three-nucleon interactions to all p-shell nuclei
- Many-body Hamiltonian solved by matrix diagonalization

$$H|\Psi\rangle = E|\Psi\rangle$$

- Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) \quad \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

  - Realistic high-precision NN potentials
    - Coordinate space – Argonne …
    - Momentum space - CD-Bonn, chiral …
    - Inverse scattering theory - JISP16
    - Renormalized versions - Lee-Suzuki-Okamoto, Vlowk, Vsrg,…
  - NNN interactions
    - Tucson-Melbourne TM’, χPT N^2LO
    - Renormalized versions - Lee-Suzuki-Okamoto
- Modification by center-of-mass harmonic oscillator (HO) potential (Lipkin 1958)

$$\frac{1}{2} A m \Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$

  - No influence on the internal motion (in infinite space)
  - Introduces mean field for sub-clusters

$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \quad \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

What is our choice of basis states in which to solve this problem?

- Harmonic oscillator - the “standard” choice due to simplicity and ability to retain all the symmetries
- Realistic mean-field basis, such as the Woods-Saxon, offers opportunity for more rapid convergence but may sacrifice exact treatment of the center of mass (CM) motion by introducing spurious CM excitations
- Review similarities and differences by visiting the “Nuclear Physics Calculator” web site - calculate nuclei with the “Extreme Single Particle Shell Model (ESPSM)”

nuclear.physics.iastate.edu/npc.php

The Extreme Single Particle Shell Model "ESPSM" Illustrated with the 197 Au Example

Since the Nobel Prize awarded to Mayer, Haxel, Jenssen and Suess for the phenomenological single-particle shell model, ever improving parameterizations of the single-particle model have emerged.

Basic starting point is to assume nucleons move independently in their average or "mean" field - generated by averaging over all the pairwise and triplet, etc., interactions.

Big ? = How to derive this mean field picture from realistic NN+NNN's

Much of the body of low-energy nuclear structure and nuclear reaction data are interpreted, to first approximation, with this 1-particle quantum mechanical picture of independent Fermions in a 3-D potential well. We can freely adopt this for our choice of basis states.

Hands-on activity - web-based tool for calculating properties of nuclei in this Extreme Single-Particle Shell Model (ESPSM). Potentials are those of C.M. Perey and F.G. Perey, Nuclear Data Tables 10, 540 (1972)

http://nuclear.physics.iastate.edu/npc.php

$$h\psi_\alpha = e_\alpha \psi_\alpha \quad \leftarrow \text{1 - particle problem in QM}$$

$$h = t + u + u_C$$

$$t = \frac{p^2}{2m}$$

$$u(r) = \frac{U_0}{1 + e^{\frac{(r-R)}{a}}} + u_{SO} \leftarrow \text{ Saxon - Woods form}$$

$$U_0 \approx -50\,MeV$$

$$R = r_0 A^{1/3};\ r_0 \approx 1.2\,fm$$

$$a = \text{diffuseness parameter} \approx 0.5\,fm$$

$$u_C(r) = \text{ Coulomb potential of uniformly charged sphere}$$

for the case of protons

$$= \frac{Ze^2}{2R}\left(3 - \frac{r^2}{R^2}\right);\ \ r \leq R$$

$$= \frac{Ze^2}{r};\ \ r \geq R$$

Definition of the Spin-Orbit Potential

$$u_{SO}(r) = \left(\frac{\hbar}{m_\pi c^2}\right)^2 U_{SO}\,\vec{S}\bullet\vec{L}\,\frac{1}{r}\frac{d}{dr}\left[\frac{1}{1+e^{\frac{r-R}{a_{SO}}}}\right]$$

$$\left(\frac{\hbar}{m_\pi c^2}\right)^2 = 2.0\,fm^2$$

$$\langle lj|S\bullet L|lj\rangle = \frac{1}{2}\left(j(j+1) - l(l+1) - \frac{3}{4}\right)$$

Total Nuclear Wavefunctions = Slater Determinants = Antisymmetrized products of these single-particle solutions
Total Nuclear Energies = simple sum of single-particle energies of the occupied orbits

Techniques employed - Results generated

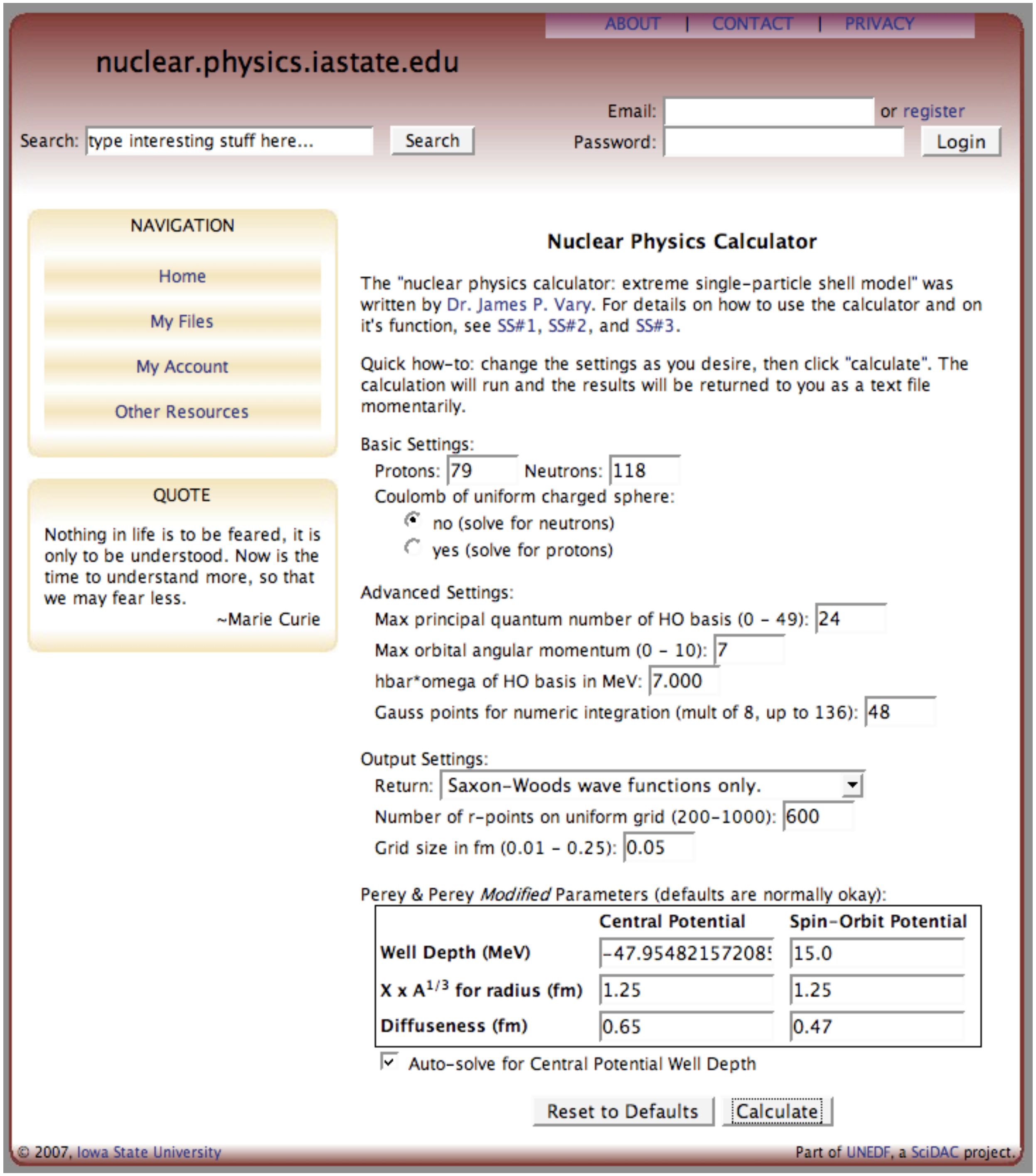
- Numerical evaluation of <H> in oscillator basis - matrix elements by Gauss quadrature, one (l,j) channel at a time

$$h_{ij} = \langle \phi_i | h | \phi_j \rangle; \text{ where } \phi_i \text{ are harmonic oscillator states}$$

- Matrix diagonalization of H by Jacobi method to obtain eigenvalues and eigenfunctions
- Numerical evaluation of eigenfunctions from their expansion in the oscillator basis:

$$\psi_\alpha = \sum_i a_{\alpha i} \phi_i$$

- Sorting of all eigenvalues to occupy states starting from the most deeply bound until all nucleons used (ESPSM ground state)
- Evaluation of density distributions by summation over squares of wavefunctions of occupied orbits (ESPSM ground state)
- Evaluation of rms radius (ESPSM ground state)



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Nothing in life is to be feared, it is only to be understood. Now is the time to understand more, so that we may fear less.

~Marie Curie

Nuclear Physics Calculator

The "nuclear physics calculator: extreme single-particle shell model" was written by Dr. James P. Vary. For details on how to use the calculator and on it's function, see SS#1, SS#2, and SS#3.

Quick how-to: change the settings as you desire, then click "calculate". The calculation will run and the results will be returned to you as a text file momentarily.

Basic Settings:

Protons: 79 Neutrons: 118

Coulomb of uniform charged sphere:

- (•) no (solve for neutrons)
- ( ) yes (solve for protons)

Advanced Settings:

Max principal quantum number of HO basis (0 - 49): 24

Max orbital angular momentum (0 - 10): 7

hbar*omega of HO basis in MeV: 7.000

Gauss points for numeric integration (mult of 8, up to 136): 48

Output Settings:

Return: Saxon-Woods wave functions only.

Number of r-points on uniform grid (200-1000): 600

Grid size in fm (0.01 - 0.25): 0.05

Perey & Perey *Modified* Parameters (defaults are normally okay):

	Central Potential	**Spin-Orbit Potential**
Well Depth (MeV)	-47.95482157208!	15.0
X x $A^{1/3}$ for radius (fm)	1.25	1.25
Diffuseness (fm)	0.65	0.47

[✓] Auto-solve for Central Potential Well Depth

Reset to Defaults Calculate

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Part of UNEDF, a SciDAC project.

It is not necessary to register

Key Parameters for Neutrons in 197Au
The "Default" case at the web site

```
-47.95482  U0 - strength of Saxon-Woods in MeV
  1.25000  r0 - range parameter in fm (multiplies A**(1/3))
  0.65000  a  - diffuseness parameter in fm
 15.00000  USO - strength of spin-orbit in MeV
  0.47000  aSO - diffuseness of spin-orbit in fm
  0.00000  STRC=(0,1) => Coulomb of uniform charged sphere (off,on)
            Controls whether one is calculating the neutrons or protons
118.00000  Neutron number
 79.00000  Proton number
       48  Number of gauss points
       12  Maximum principal Q# of HO basis
  7.50000  hbar*omega of HO basis in MeV
           NB: current default value=7.0 MeV => enter 7.5 to reproduce
           the tables used to generate the HO functions shown here)
      600  Number of r-points on uniform grid
  0.05000  Grid size in fm
```

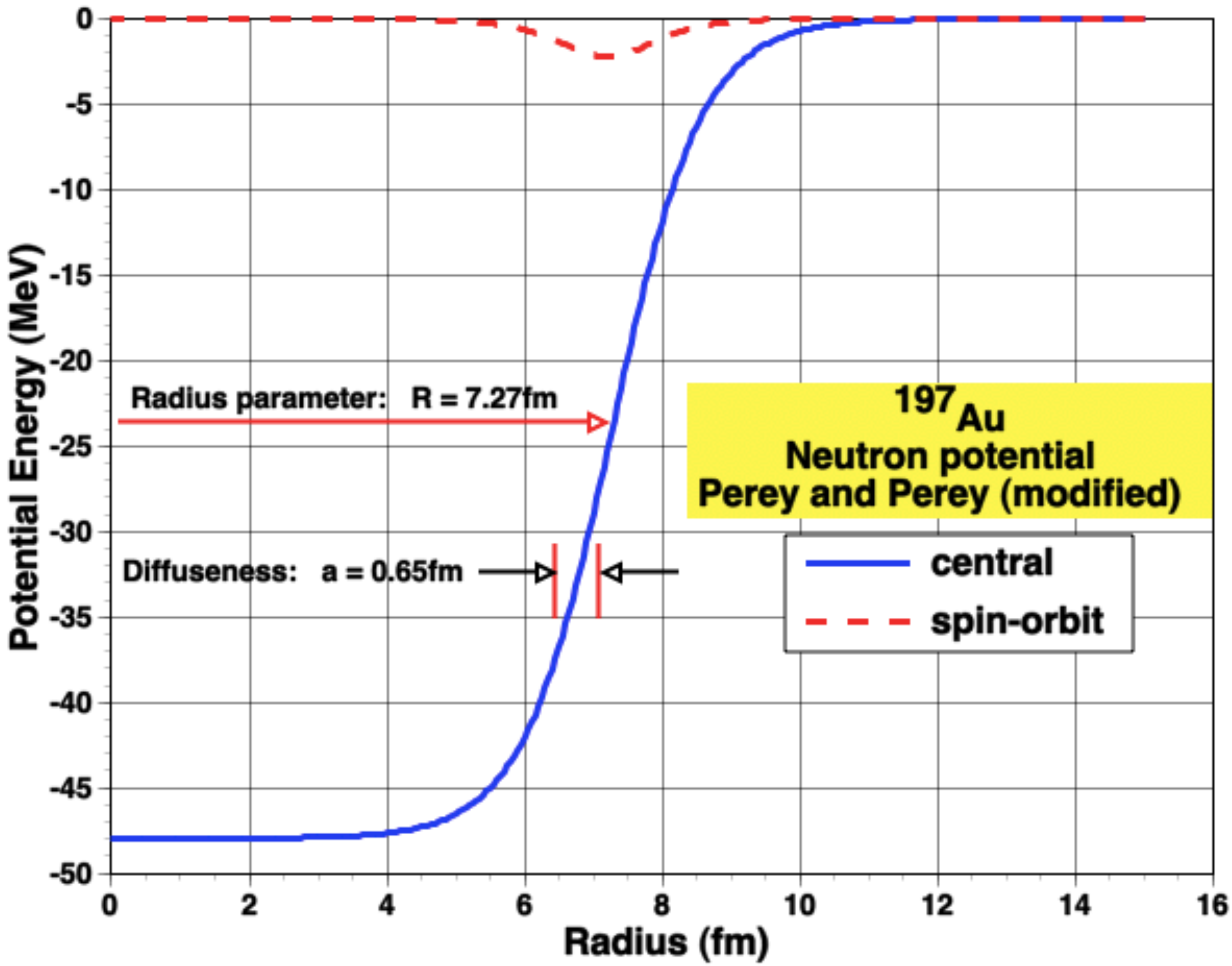
Key Parameters for Protons in 197Au

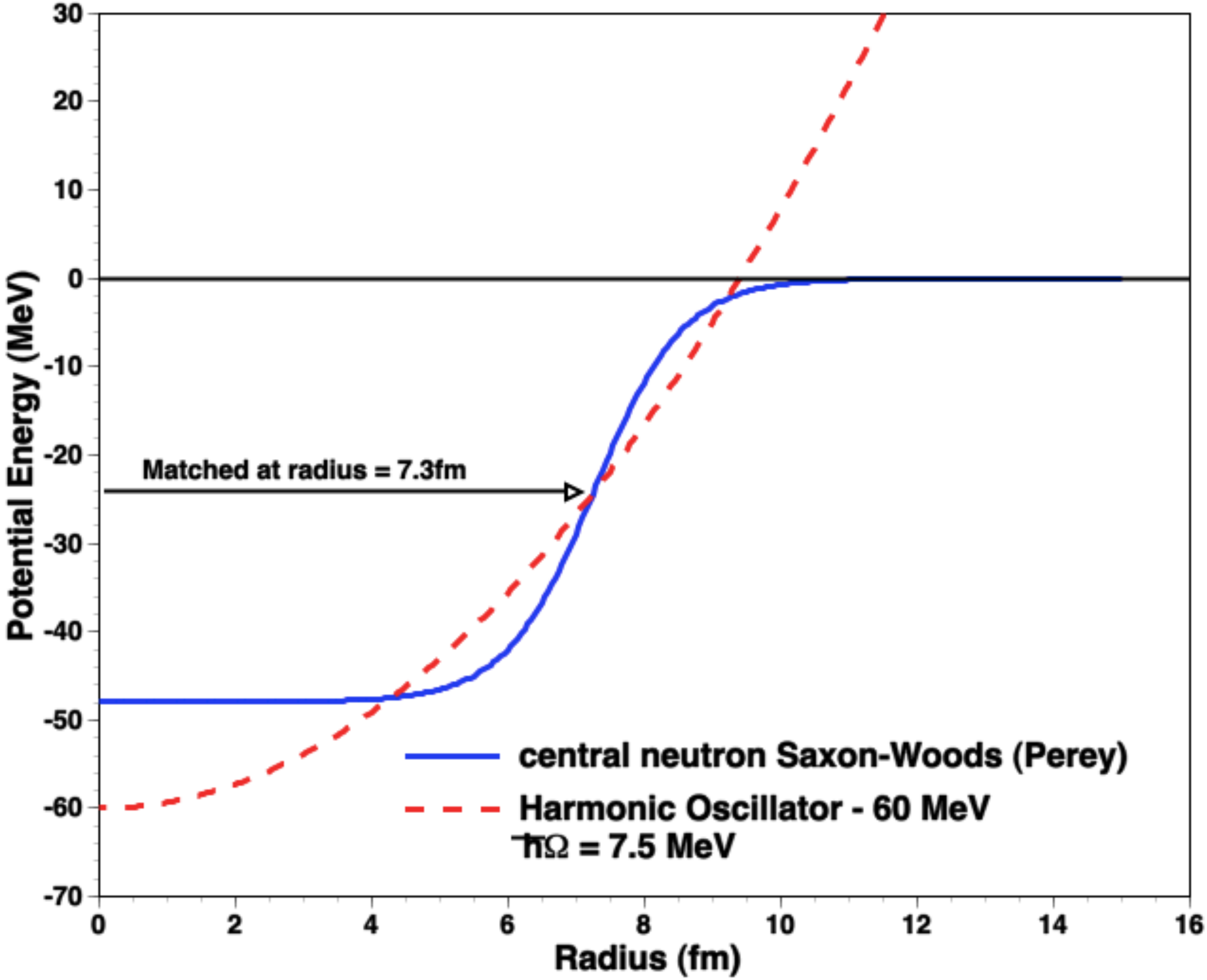
-64.07599	U_0 - strength of Saxon-Woods in MeV
1.25000	r_0 - range parameter in fm (multiplies A**(1/3))
0.65000	a - diffuseness parameter in fm
15.00000	U_{so} - strength of spin-orbit in MeV
0.47000	a_{so} - diffuseness of spin-orbit in fm
1.00000	STRC=(0,1) => Coulomb of uniform charged sphere (off,on) Controls whether one is calculating the neutrons or protons
118.00000	Neutron number
79.00000	Proton number
48	Number of gauss points
12	Maximum principal Q# of HO basis
7.50000	hbar*omega of HO basis in MeV NB: current default value=7.0 MeV => enter 7.5 to reproduce the tables used to generate the HO functions shown here)
600	Number of r-points on uniform grid
0.05000	Grid size in fm

Fundamental constants employed:

Nucleon mass: mc^2 = 938.9185 MeV

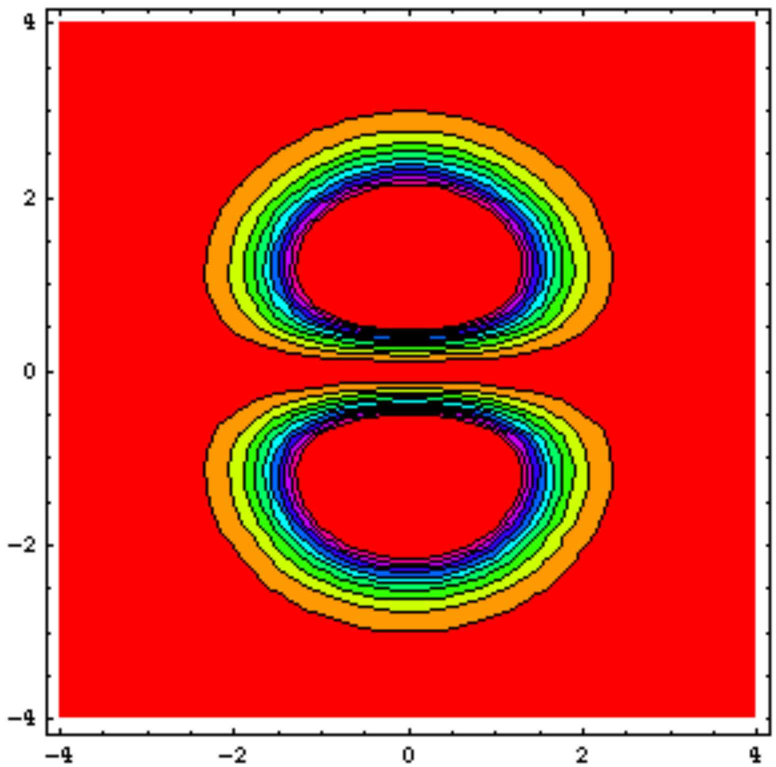
i.e. the average of neutron and proton mass (estimate the importance of this approximation)

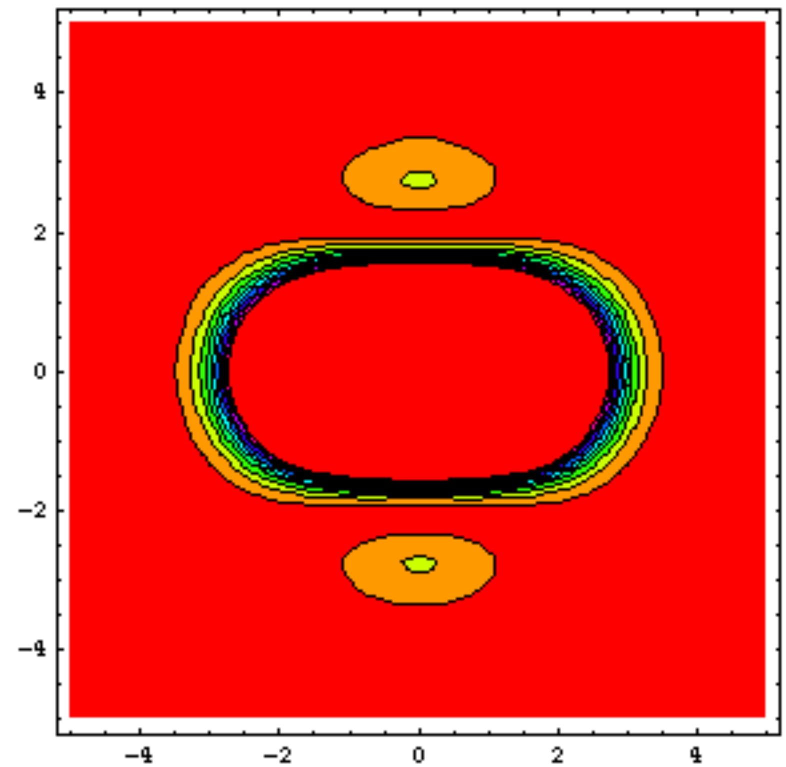

0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
Potential Energy (MeV)
0
2
4
6
8
10
12
14
16
Radius (fm)
Radius parameter: R = 7.27fm
Diffuseness: a = 0.65fm
197Au
Neutron potential
Perey and Perey (modified)
central
spin-orbit

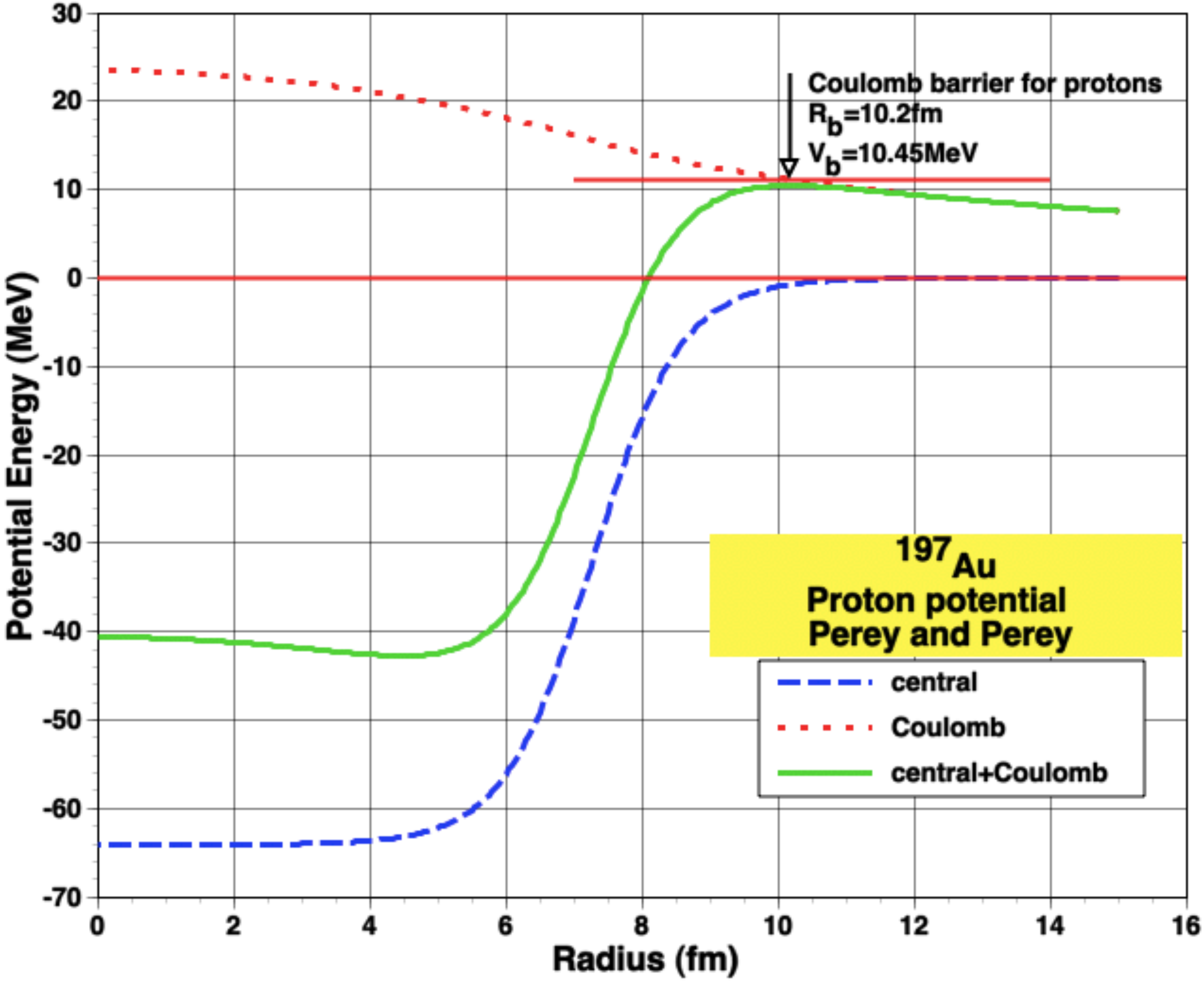


Potential Energy (MeV)
Radius (fm)
Matched at radius = 7.3fm
central neutron Saxon-Woods (Perey)
Harmonic Oscillator - 60 MeV
ħΩ = 7.5 MeV
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
0
2
4
6
8
10
12
14
16

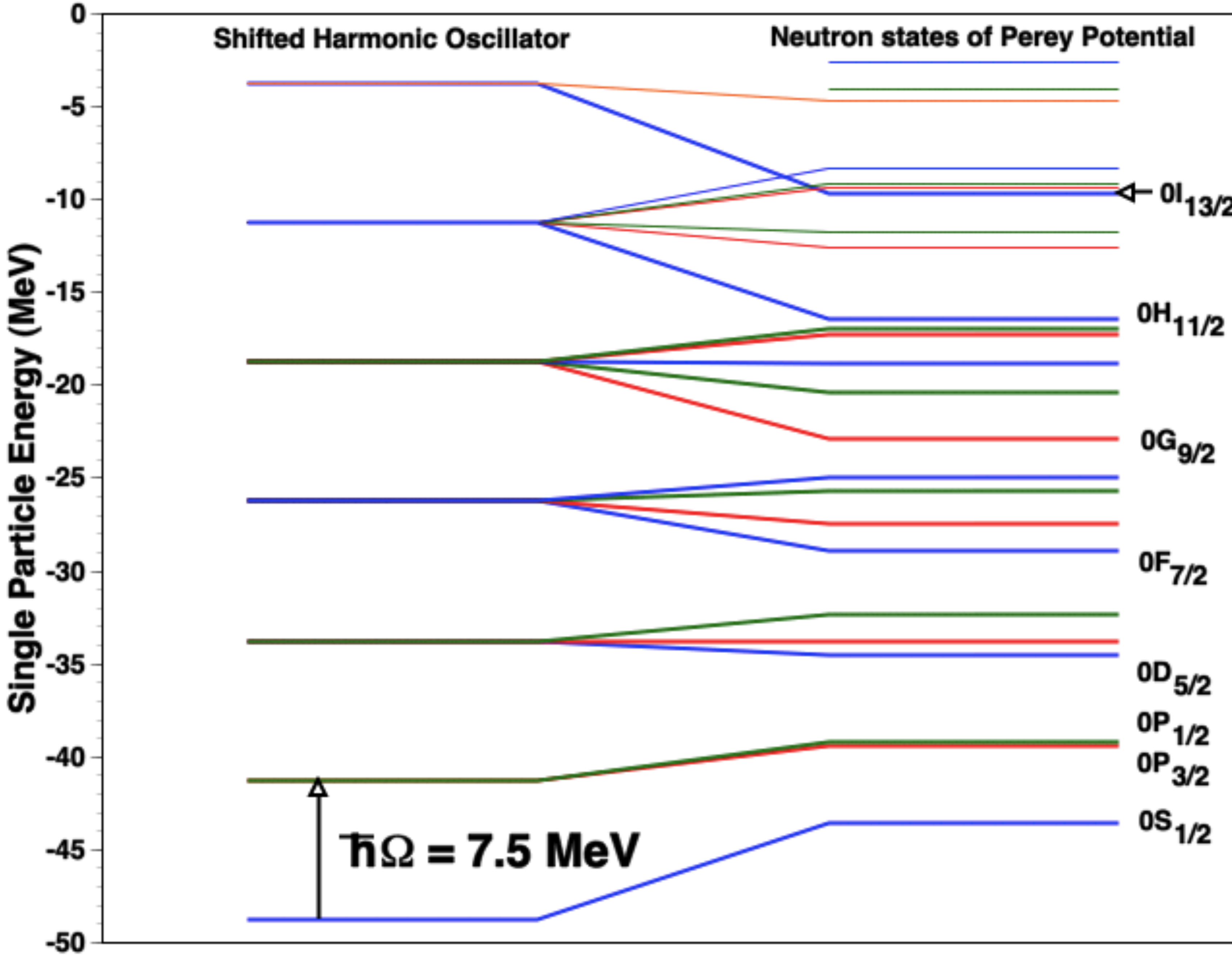
“Walkthrough” of HO wavefunctions
nlm = 221 & superposition: 111+331



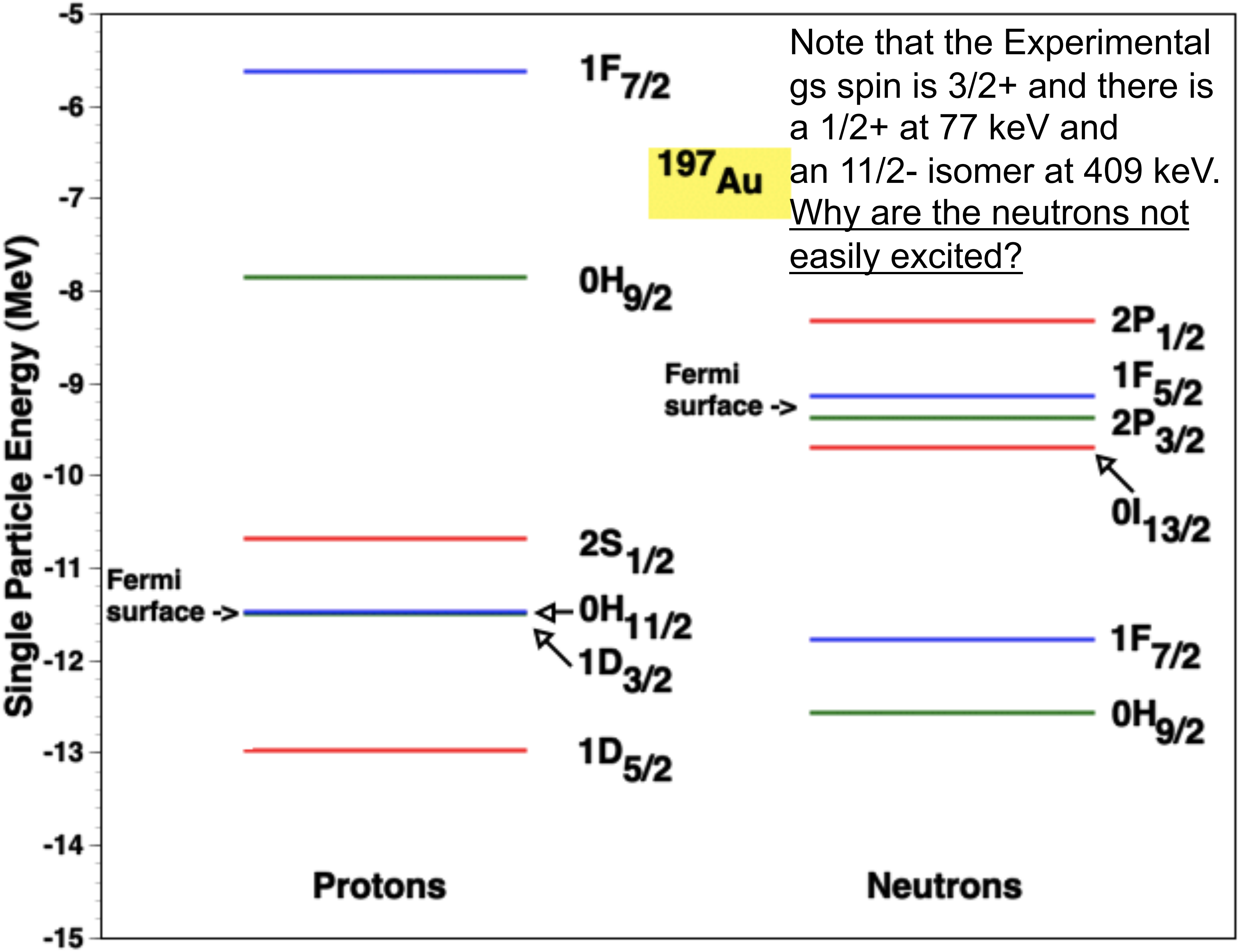




Coulomb barrier for protons
R_b=10.2fm
V_b=10.45MeV
197Au
Proton potential
Perey and Perey
central
Coulomb
central+Coulomb
Potential Energy (MeV)
Radius (fm)
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
0
2
4
6
8
10
12
14
16


Shifted Harmonic Oscillator
Neutron states of Perey Potential
Single Particle Energy (MeV)
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
$0I_{13/2}$
$0H_{11/2}$
$0G_{9/2}$
$0F_{7/2}$
$0D_{5/2}$
$0P_{1/2}$
$0P_{3/2}$
$0S_{1/2}$
$\hbar\Omega = 7.5$ MeV

Note that the Experimental gs spin is 3/2+ and there is a 1/2+ at 77 keV and an 11/2- isomer at 409 keV. <u>Why are the neutrons not easily excited?</u>



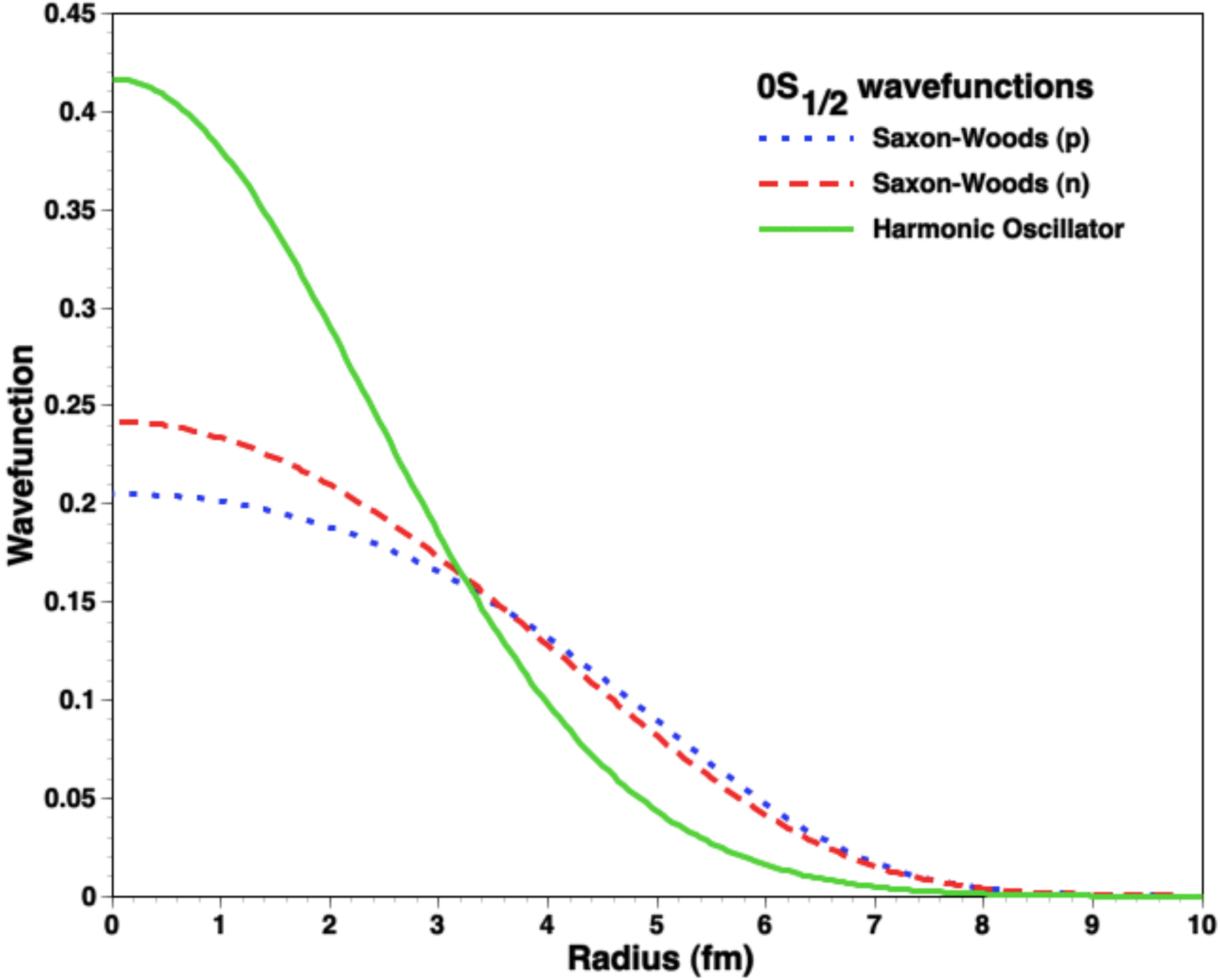
Survey of the single-particle wavefunctions

$$\psi_\alpha = \psi_{nljm_j} = \frac{R_{nlj}(r)}{r}[Y_{lm_l}(\vartheta,\varphi)\chi_{sm_s}]_{jm_j}$$

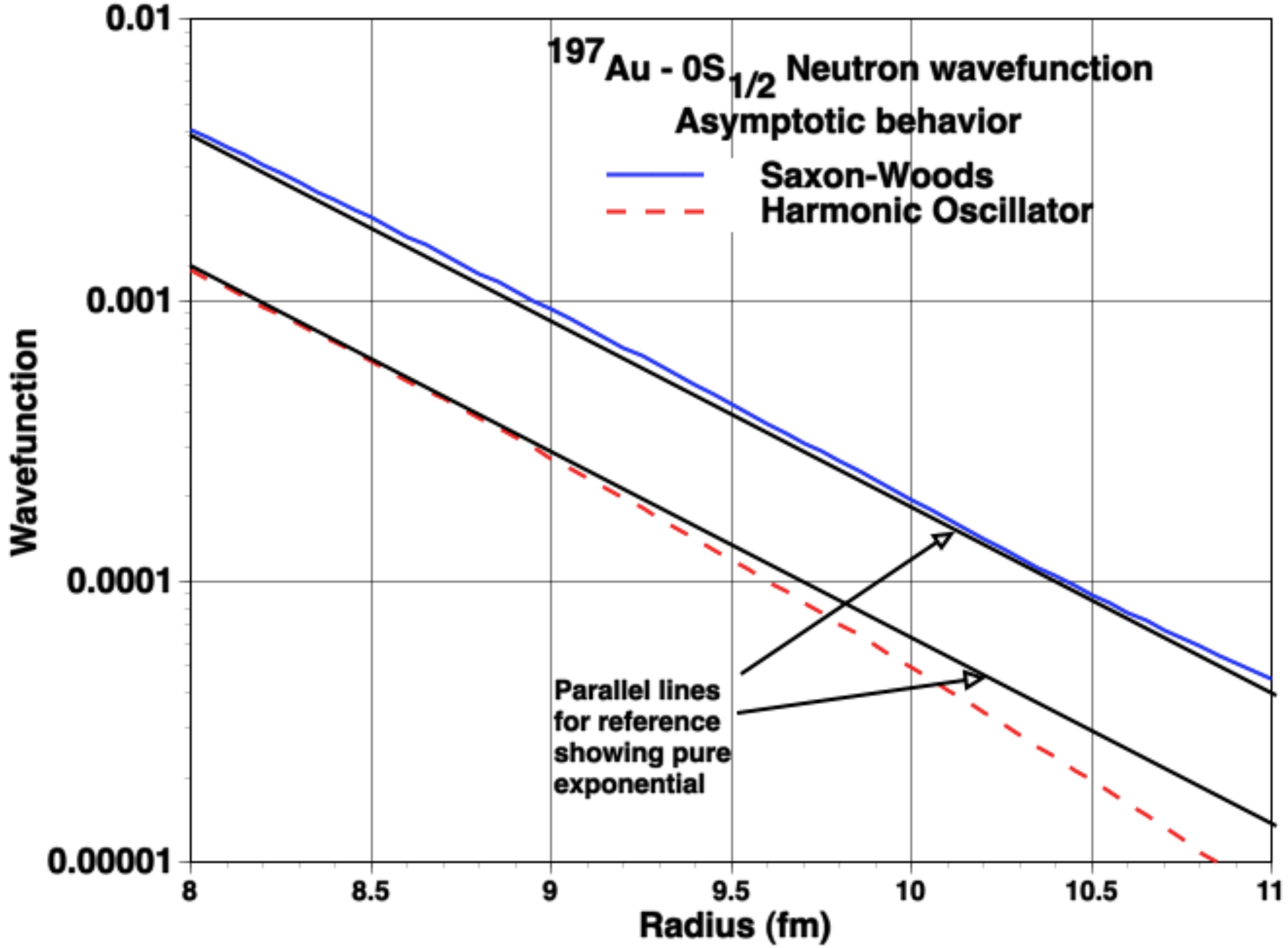
$$e_\alpha = e_{nlj} \ \leftarrow \text{degeneracy in } m_j$$

Examine these plots of $R_{nlj}(r)/r$ and comment on the QM properties seen:

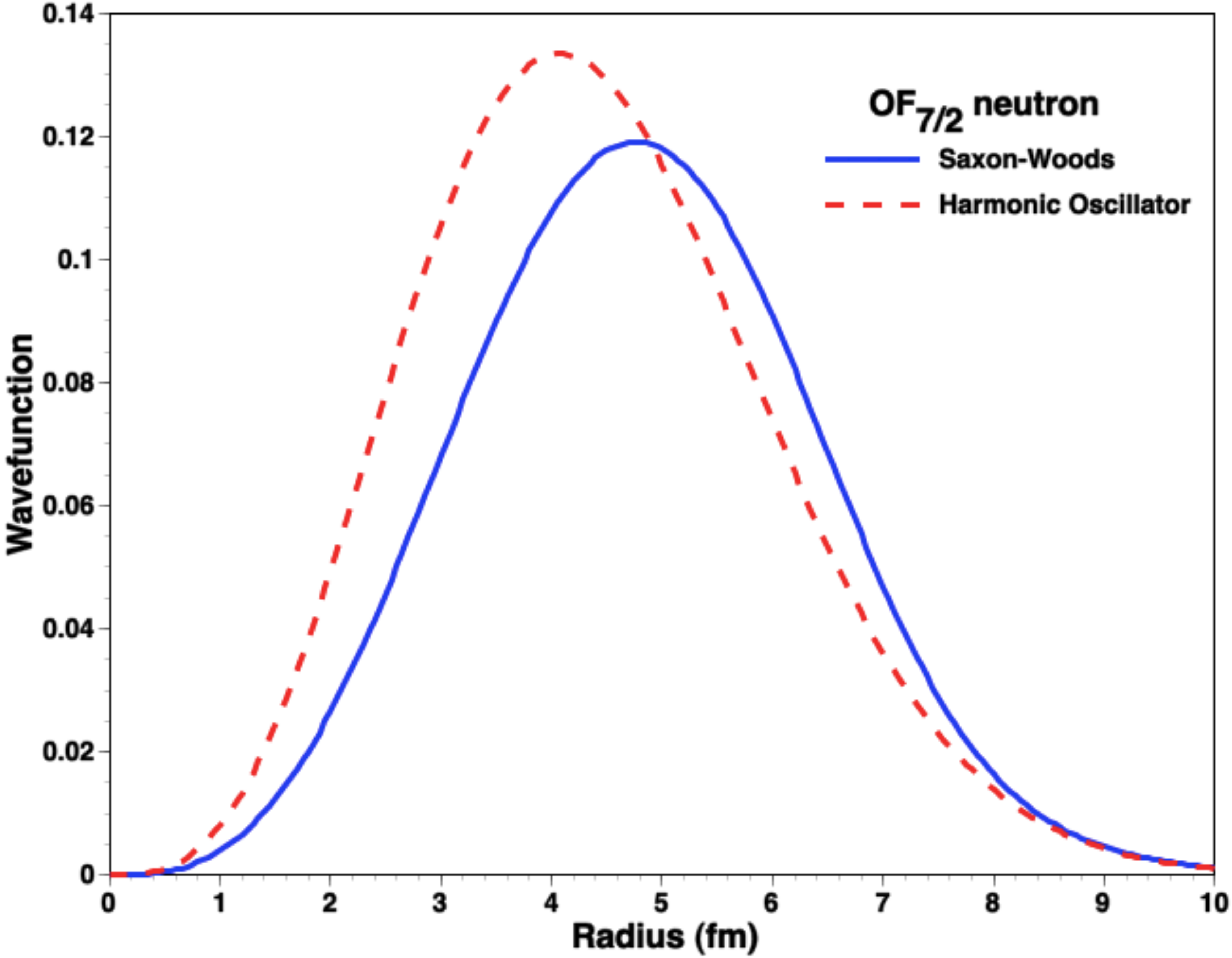
- Harmonic oscillator versus Saxon-Woods
- As a function of binding energy
- As a function of angular momentum
- Near the origin and in the tail region
- Other features anticipated/observed



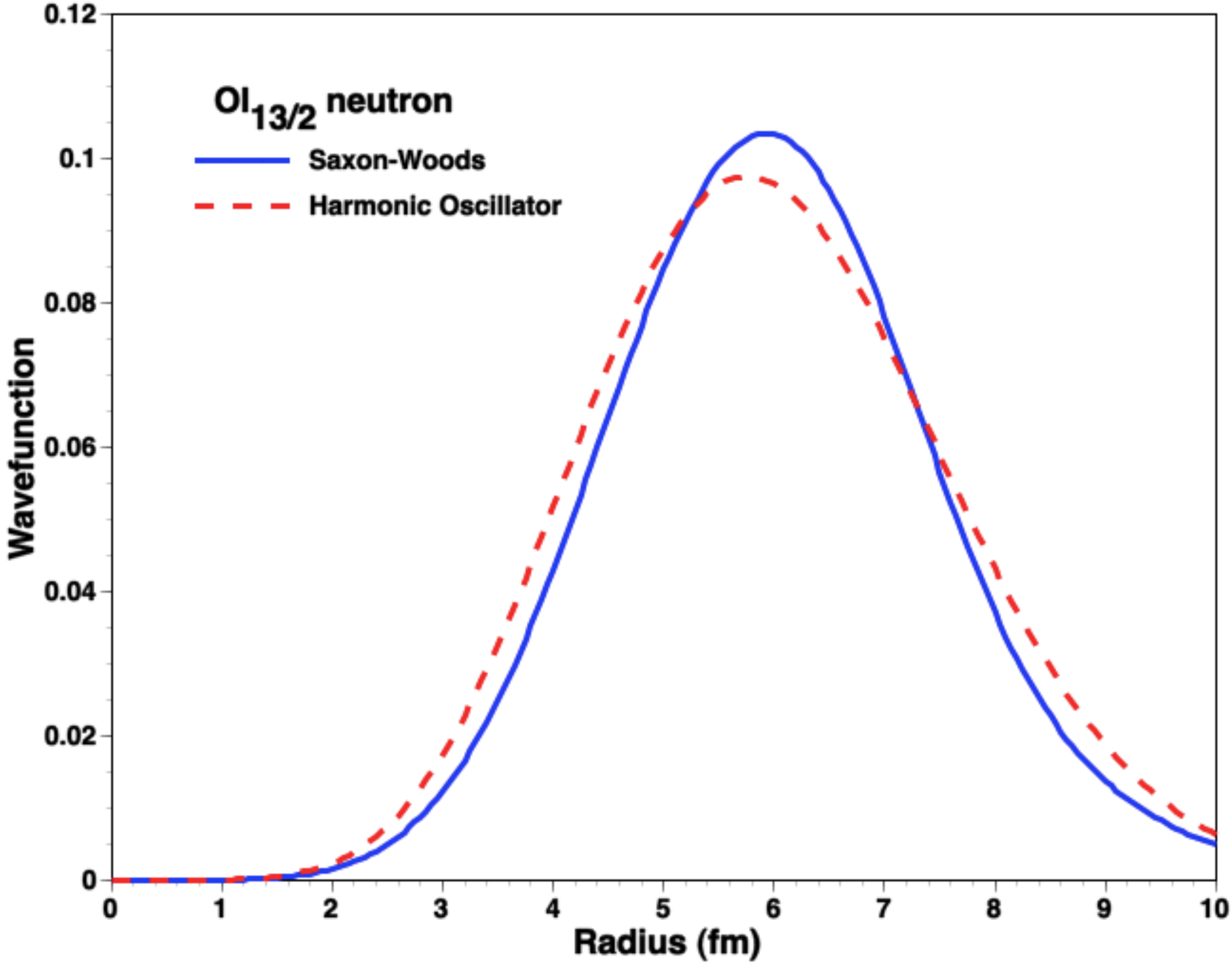
$0S_{1/2}$ wavefunctions
Saxon-Woods (p)
Saxon-Woods (n)
Harmonic Oscillator
Wavefunction
Radius (fm)
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7 8 9 10



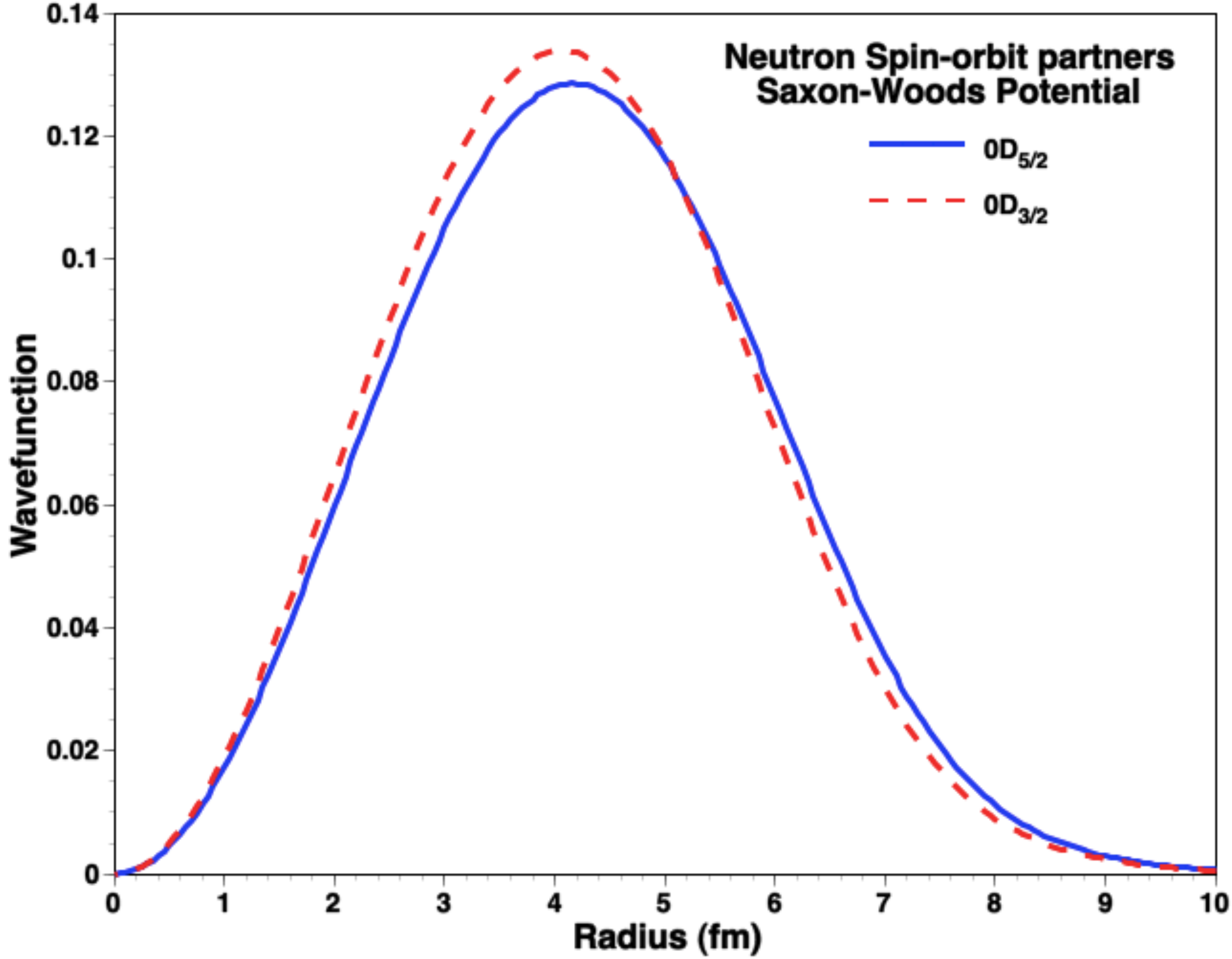
^{197}Au - 0S$_{1/2}$ Neutron wavefunction
Asymptotic behavior
Saxon-Woods
Harmonic Oscillator
Parallel lines for reference showing pure exponential
Wavefunction
Radius (fm)
0.01
0.001
0.0001
0.00001
8
8.5
9
9.5
10
10.5
11



0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
Wavefunction
0
1
2
3
4
5
6
7
8
9
10
Radius (fm)
$OF_{7/2}$ neutron
Saxon-Woods
Harmonic Oscillator



0.12
0.1
0.08
0.06
0.04
0.02
0
Wavefunction
0
1
2
3
4
5
6
7
8
9
10
Radius (fm)
0I13/2 neutron
Saxon-Woods
Harmonic Oscillator


Neutron Spin-orbit partners
Saxon-Woods Potential
0D5/2
0D3/2
Wavefunction
Radius (fm)
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0
1
2
3
4
5
6
7
8
9
10

Additional questions to ponder

- How does one measure radial charge densities and radial mass densities?
- Are the oscillations in the ESPSM densities reasonable and how would residual interactions be likely to change them?
- How does the measured charge density of 197-Au compare with the ESPSM result.
- How do the experimental spectra of 197-Au compare with the excitations of the ESPSM near the Fermi Surface?

Planned Extensions

- Density of nucleons in the Harmonic Oscillator model to compare with the Perey and Perey model densities
- Simple spin-orbit potential added to Harmonic Oscillator and matched to experimental single-particle spectra
- Single particle electromagnetic transition matrix elements: B(E1), B(M1), etc.,
- Newer phenomenological shell model potentials - A.J. Koning & J.P. Delaroche, Nucl. Phys. A 713, 231 (2003).
- Deformed single particle basis states

Beyond the ESPSM: Interactions among the nucleons

- Shell model with phenomenological (fit) interactions - recent review articles of Alex Brown, Andres Zuker, et al.
- Shell model with derived (G-matrix) interactions - recent review article of Morten Hjorth-Jenssen, et al.
- Ab-initio No-Core Shell Model (NCSM) = Our focus here, based on the theory of effective operators - Goal is to derive the nuclear shell model from "first principles" = "ab-initio"

Topics in Next Lecture

- Renormalization schemes for NN + NNN interactions
- Applications of ab-initio NCSM
- Advanced computational issues

Acknowledgements

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- Support from DOE (DE-FG02-87ER-40371 & DE-FC02-09ER41582)
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