Relativistic Density Functional Theory for atomic nucleus and neutron star

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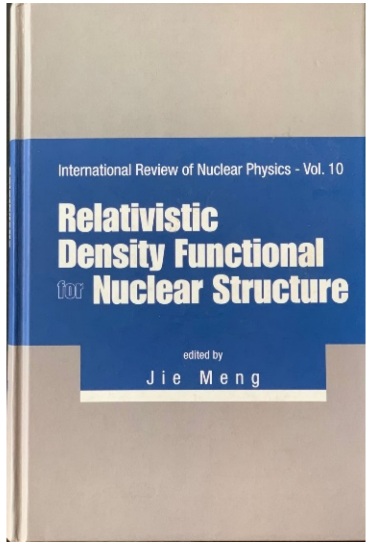
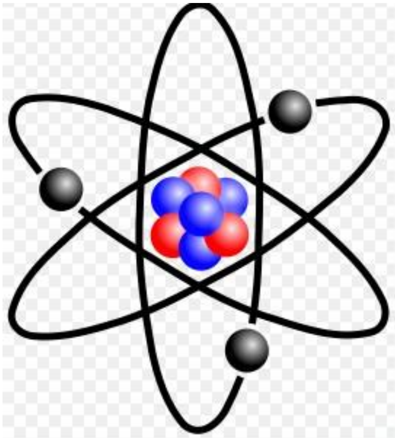
1. Nucleus : relativistic or nonrelativistic system
2. Advantage of Relativistic Theory
3. Solve a Schrödinger equation numerically
4. Solve a Dirac equation numerically
5. Nuclear matter
6. Nuclear ground state properties
7. Nuclear excited state properties
8. Interface with astrophysics and fundamental physics

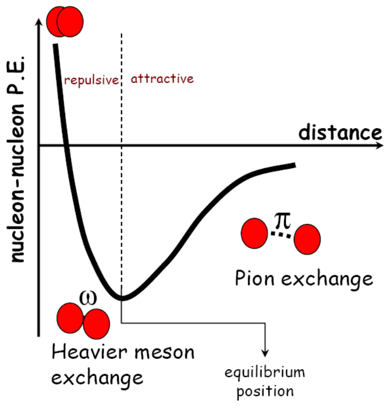


Milestone toward the nuclear model

During the hundred years' struggling, in the development of nuclear physics itself, there emerged a lot of significant milestones, including



The discovery of neutron by Chadwick which verified the composition of nucleus as protons and neutrons



The meson-exchange theory for the interaction between nucleons by Yukawa

H. Euler, Z. Physik 105, 553 (1937)

Heisenberg's student who calculated the nuclear matter in 2nd order perturbation theory

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Why Covariant?

P. Ring Physica Scripta, T150, 014035 (2012)

Spin-orbit automatically included

Lorentz covariance restricts parameters

Pseudo-spin Symmetry

Connection to QCD: big V/S ~ ±400 MeV

Consistent treatment of time-odd fields

Relativistic saturation mechanism

Liang, Meng, Zhou, Physics Reports **570** : 1-84 (2015).

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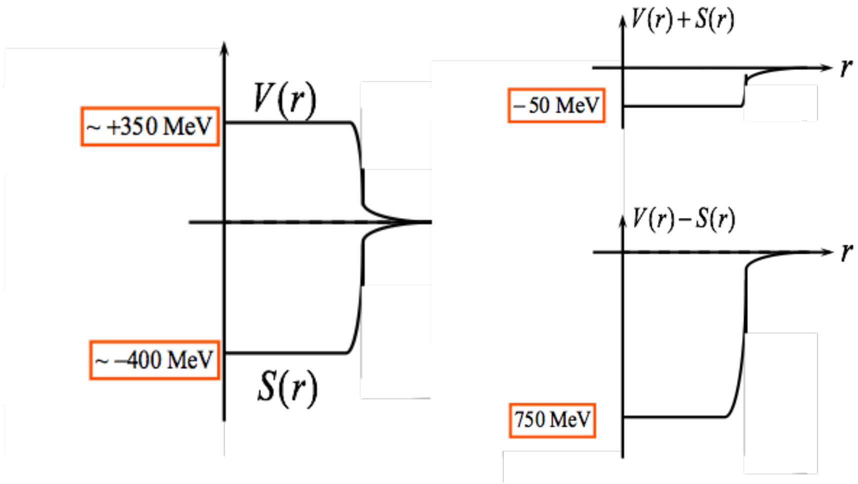
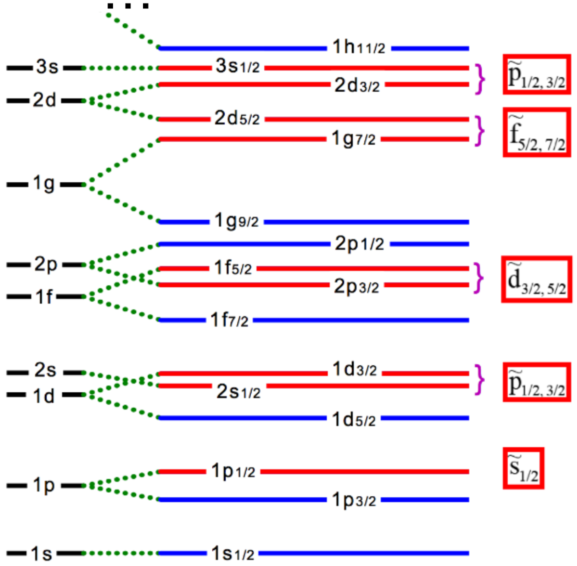


Pseudospin symmetry



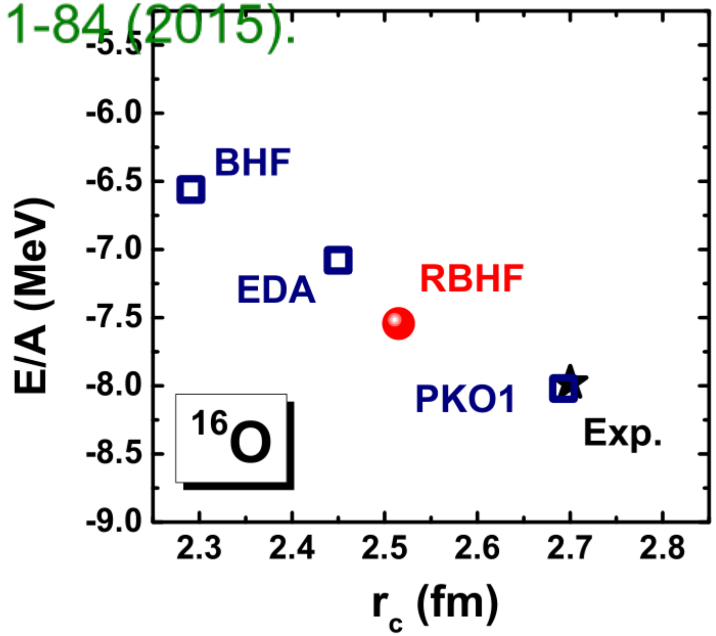
$$\begin{array}{lll} n-1, & l+2, & j=l+3/2 \\ n, & l, & j=l+1/2 \end{array}$$

$$\begin{array}{lcl} \text{pseudo-orbit} & : & \tilde{l}=l+1 \\ \text{pseudo-spin} & : & \tilde{s}=1/2 \end{array}$$

Hecht & Adler NPA137(1969)129

Arima, Harvey & Shimizu PLB 30(1969)517

Ginocchio PRL 78, 436



Shen et al Chin. Phys. Lett. 33 (2016) 102103

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Brief introduction of CDFT

CDFT： Relativistic quantum many-body theory based on DFT and effective field theory for strong interaction

Strong force: Meson-exchange of the nuclear force

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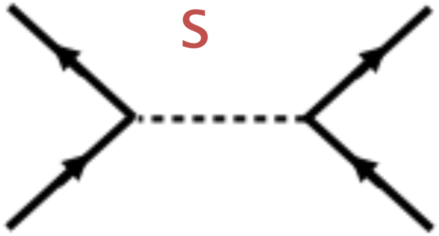
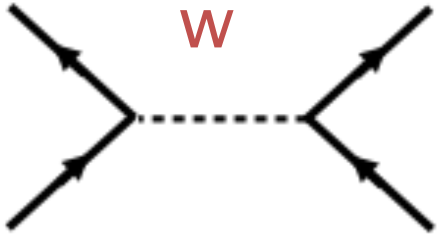


(Jp T)=(0+0)

Sigma-meson:
attractive scalar field

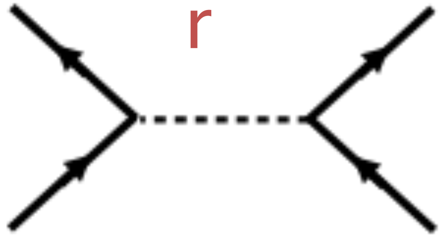
w



(Jp T)=(1−0)

Omega-meson:
Short-range repulsive

r



(Jp T)=(1−1)

Rho-meson:
Isovector field

Electromagnetic force: The photon

Brief introduction of CDFT

Lagrangian:

$$L = \bar{\psi}[i\gamma^{\mu}\partial_{\mu} - M - g_{\sigma}\sigma - \gamma^{\mu}(g_{\omega}\omega_{\mu} + g_{\rho}\vec{\tau}\bullet\vec{\rho}_{\mu} + e\tfrac{1-\tau_3}{2}A_{\mu}) - \tfrac{f_{\pi}}{m_{\pi}}\gamma_5\gamma^{\mu}\partial_{\mu}\vec{\pi}\bullet\vec{\tau}]\psi$$

$$+\frac{1}{2}\partial^{\mu}\sigma\partial_{\mu}\sigma - \frac{1}{2}m_{\sigma}^2\sigma^2 - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_{\omega}^2\omega_{\mu}\omega^{\mu} - \frac{1}{4}\vec{R}_{\mu\nu}\bullet\vec{R}^{\mu\nu}$$

$$+\frac{1}{2}m_{\rho}^2\vec{\rho}^{\mu}\Box\vec{\rho}_{\mu} + \frac{1}{2}\partial_{\mu}\vec{\pi}\bullet\partial^{\mu}\vec{\pi} - \frac{1}{2}m_{\pi}^2\vec{\pi}\bullet\vec{\pi} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$$

$$\Omega^{\mu\nu} = \partial^{\mu}\omega^{\nu} - \partial^{\nu}\omega^{\mu}$$

$$\vec{R}^{\mu\nu} = \partial^{\mu}\vec{\rho}^{\nu} - \partial^{\nu}\vec{\rho}^{\mu}$$

$$F^{\mu\nu} = \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu}$$

Hamiltonian:

$$H = \bar{\psi}(-i\boldsymbol{\gamma}\bullet\nabla + M)\psi + \frac{1}{2}\int d^4y \sum_{i=\sigma,\omega,\rho,\pi,A} \bar{\psi}(x)\bar{\psi}(y)\Gamma_i D_i(x,y)\psi(y)\psi(x)$$

$$= T + V$$

$$\Gamma_{\sigma}(1,2) \equiv -g_{\sigma}(1)g_{\sigma}(2), \qquad \Gamma_{\rho}(1,2) \equiv +(g_{\rho}\gamma_{\mu}\vec{\tau})_1\Box(g_{\rho}\gamma^{\mu}\vec{\tau})_2,$$

$$\Gamma_{\omega}(1,2) \equiv +(g_{\omega}\gamma_{\mu})_1(g_{\omega}\gamma_{\mu})_2, \quad \Gamma_{\pi}(1,2) \equiv -(\tfrac{f_{\pi}}{m_{\pi}}\vec{\tau}\gamma_5\gamma_{\mu}\partial^{\mu})_1\Box(\tfrac{f_{\pi}}{m_{\pi}}\vec{\tau}\gamma_5\gamma_{\nu}\partial^{\nu})_2$$

$$\Gamma_{\mathrm{em}}(1,2) \equiv +\frac{e^2}{4}(\gamma_{\mu}(1-\tau_3))_1(\gamma^{\mu}(1-\tau_3))_2$$

Brief introduction of CDFT

$$H = T + \sum_{i=\sigma,\omega,\rho,\pi,A} V_i$$

$$\psi(x) = \sum_i [f_i(\mathbf{x}) e^{-i\varepsilon_i t} c_i + g_i(\mathbf{x}) e^{i\varepsilon_i' t} d_i^\dagger]$$

$$\psi^\dagger(x) = \sum_i [f_i^\dagger(\mathbf{x}) e^{i\varepsilon_i t} c_i^\dagger + g_i^\dagger(\mathbf{x}) e^{-i\varepsilon_i' t} d_i]$$

$$T = \int d\mathbf{x} \sum_{\alpha\beta} \bar{f}_\alpha (-i\gamma \cdot \nabla + M) f_\beta c_\alpha^\dagger c_\beta ,$$

Hartree

$$V_i = \frac{1}{2} \int d\mathbf{x}_1 d\mathbf{x}_2 \sum_{\alpha\beta;\alpha'\beta'} c_\alpha^\dagger c_\beta^\dagger c_{\beta'} c_{\alpha'} \bar{f}_\alpha(1) \bar{f}_\beta(2) \Gamma_i(1,2) D_i(1,2) f_{\beta'}(2) f_{\alpha'}(1)$$

Foc

k

Energy density functional:

$$|\Phi_0\rangle = \prod_\alpha c_\alpha^\dagger |0\rangle$$

$$E = \langle \Phi_0 | H | \Phi_0 \rangle = \langle \Phi_0 | T | \Phi_0 \rangle + \sum_{i=\sigma,\omega,\rho,\pi,A} \langle \Phi_0 | V_i | \Phi_0 \rangle$$

$$= E_k + E_\sigma^D + E_\sigma^E + E_\omega^D + E_\omega^E + E_\rho^D + E_\rho^E + E_\pi + E_{\text{em}}^D + E_{\text{em}}^E$$

Equations of motion

For system with time invariance:

$$\left[\alpha\cdot\boldsymbol{p}+V(\boldsymbol{r})+\beta\left(M+S(\boldsymbol{r})\right)\right]\psi_i=\varepsilon_i\psi_i$$

Same footing for

- Deformation
- Rotation
- Pairing
  (RHB,BCS,SLAP)
- …

$$\begin{cases} V(\boldsymbol{r})=g_\omega\omega(\boldsymbol{r})+g_\rho\tau_3\rho(\boldsymbol{r})+e\dfrac{1-\tau_3}{2}A(\boldsymbol{r}) \\ S(r)=g_\sigma\sigma(\boldsymbol{r}) \end{cases}$$

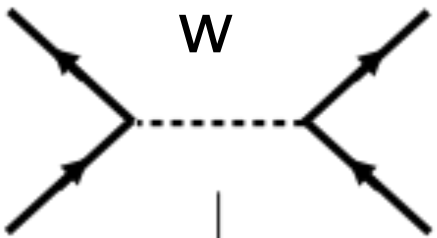
$$\left[-\Delta+m_\sigma^2\right]\sigma=-g_\sigma\rho_s-g_2\sigma^2-g_3\sigma^3$$

$$\left[-\Delta+m_\omega^2\right]\omega=g_\omega\rho_b-c_3\omega^3$$

$$\left[-\Delta+m_\rho^2\right]\rho=g_\rho\left[\rho_b^{(n)}-\rho_b^{(p)}\right]-d_3\rho^3$$

$$\begin{cases} \rho_s(\boldsymbol{r})=\sum_{i=1}^{A}\bar{\psi}_i(\boldsymbol{r})\psi_i(\boldsymbol{r}) \\ \rho_v(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\psi_i(\boldsymbol{r}) \\ \rho_3(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\tau_3\psi_i(\boldsymbol{r}) \\ \rho_c(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\dfrac{1-\tau_3}{2}\psi_i(\boldsymbol{r}) \end{cases}$$

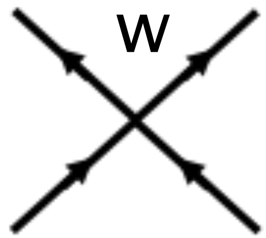
Effective Point-Coupling interaction



$$H = \bar{\psi}_i\left(-i\gamma \bullet \nabla + M\right)\psi_i + \frac{1}{4}F^{i\nu}F_{i\nu}$$
$$+\frac{1}{2}((\nabla\sigma)^2 + m_\sigma^2\sigma^2) + g_\sigma\sigma\rho_s + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4$$
$$+\frac{1}{2}g_\omega\omega_0\rho_v + \frac{1}{2}g_\rho\vec{\rho}_0\rho_3$$

$$g_\omega\omega = \frac{1}{1-\Delta/m_\omega^2}\frac{g_\omega^2}{m_\omega^2}\rho_v = \frac{g_\omega^2}{m_\omega^2}\rho_v + \frac{g_\omega^2}{m_\omega^4}\Delta\rho_v + \cdots \approx \alpha_v\rho_v + \delta_v\Delta\rho_v$$

$$H = \bar{\psi}_i\left(-i\gamma\square\nabla + M\right)\psi_i + \frac{1}{4}F^{i\nu}F_{i\nu}$$
$$+\frac{1}{2}\alpha_S\rho_S^2 + \frac{1}{2}\delta_S\rho_S\Delta\rho_S + \frac{1}{3}\beta_S\rho_S^3 + \frac{1}{4}\gamma_S\rho_S^4$$
$$+\frac{1}{2}\alpha_V\rho_V^2 + \frac{1}{2}\delta_V\rho_V\Delta\rho_V + \frac{1}{2}\alpha_{TV}\rho_{TV}^2 + \frac{1}{2}\delta_{TV}\rho_{TV}\Delta\rho_{TV}$$



Equations of motion

For system with time invariance:

$$\left[\alpha\cdot\boldsymbol{p}+V(\boldsymbol{r})+\beta\left(M+S(\boldsymbol{r})\right)\right]\psi_i=\varepsilon_i\psi_i$$

$$\begin{cases} V(\boldsymbol{r})=\alpha_V\rho_V(\boldsymbol{r})+\gamma_V\rho_V^3(\boldsymbol{r})+\delta_V\Delta\rho_V(\boldsymbol{r})+\alpha_{TV}\rho_{TV}(\boldsymbol{r})+\delta_{TV}\Delta\rho_{TV}(\boldsymbol{r})+e\dfrac{1-\tau_3}{2}A(\boldsymbol{r}) \\ S(r)=\alpha_S\rho_S+\beta_S\rho_S^2+\gamma_S\rho_S^3+\delta_S\Delta\rho_S \end{cases}$$

Without Klein-Gordon equation

$$\begin{cases} \rho_s(\boldsymbol{r})=\sum_{i=1}^{A}\bar{\psi}_i(\boldsymbol{r})\psi_i(\boldsymbol{r}) \\ \rho_v(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\psi_i(\boldsymbol{r}) \\ \rho_3(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\tau_3\psi_i(\boldsymbol{r}) \\ \rho_c(\boldsymbol{r})=\sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\dfrac{1-\tau_3}{2}\psi_i(\boldsymbol{r}) \end{cases}$$

Covariant Density Functional Theory

Elementary building blocks

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \qquad \mathcal{O}_\tau \in \{1, \tau_i\} \qquad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

Densities and currents

Isoscalar-scalar $\rho_S(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\psi_k(\mathbf{r})$

Isoscalar-vector $j_\mu(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\gamma_\mu\psi_k(\mathbf{r})$

Isovector-scalar $\vec{\rho}_S(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\vec{\tau}\psi_k(\mathbf{r})$

Isovector-vector $\vec{j}_\mu(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\vec{\tau}\gamma_\mu\psi_k(\mathbf{r})$

Energy Density Functional

$$E_{kin} = \sum_k v_k^2 \int \bar{\psi}_k \left(-\gamma\nabla + m\right)\psi_k d\mathbf{r}$$

$$E_{2nd} = \frac{1}{2}\int (\alpha_S\rho_S^2 + \alpha_V\rho_V^2 + \alpha_{tV}\rho_{tV}^2)d\mathbf{r}$$

$$E_{hot} = \frac{1}{12}\int (4\beta_S\rho_S^3 + 3\gamma_S\rho_S^4 + 3\gamma_V\rho_V^4)d\mathbf{r}$$

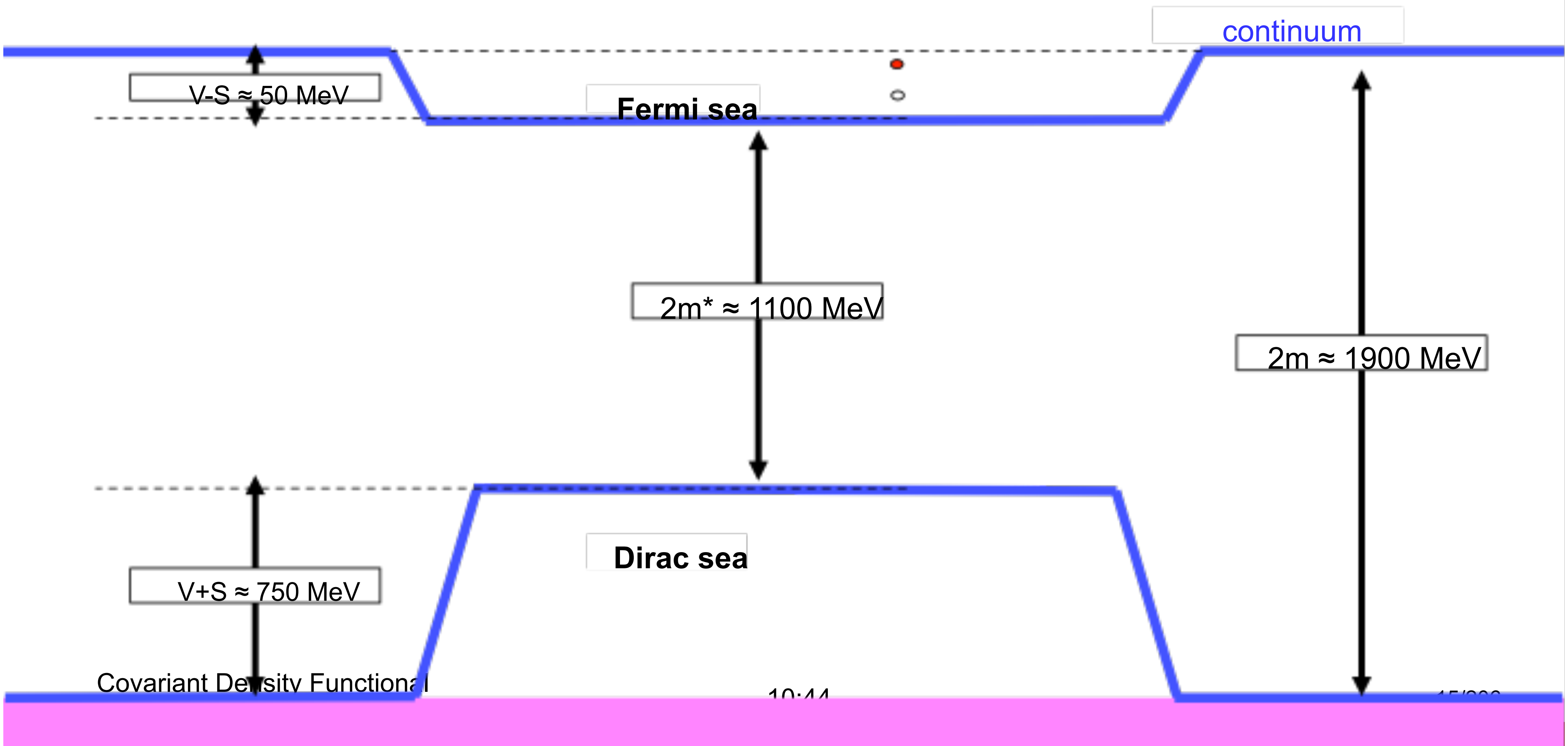
$$E_{der} = \frac{1}{2}\int (\delta_S\rho_S\triangle\rho_S + \delta_V\rho_V\triangle\rho_V + \delta_{tV}\rho_{tV}\triangle\rho_{tV})d\mathbf{r}$$

$$E_{em} = \frac{e}{2}\int j_\mu^p A^\mu d\mathbf{r}$$

$$\begin{pmatrix} m+S+V & \boldsymbol{\sigma}(\boldsymbol{p}-\boldsymbol{V}) \\ \boldsymbol{\sigma}(\boldsymbol{p}-\boldsymbol{V}) & -m-S+V \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix} = \varepsilon \begin{pmatrix} f \\ g \end{pmatrix}$$

scalar potential: $S(r) \approx -400$ MeV

vector potential: $V(r) \approx 350$ MeV



Equation of motion in spherical nucleus

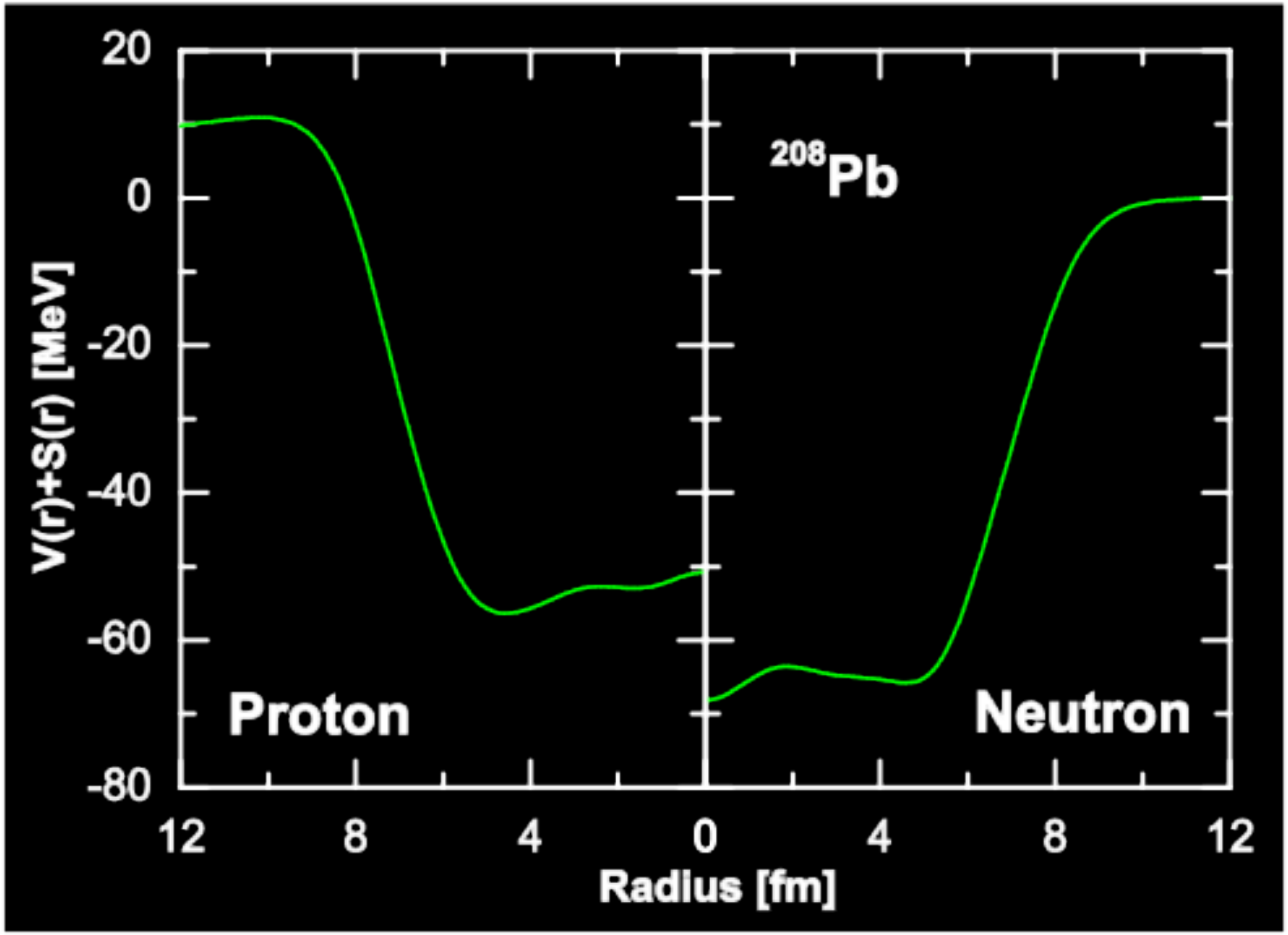
In spherical cases:

$$\psi_{\alpha\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} i\, G_\alpha^\kappa(r)\, Y_{jm}^{l}(\Omega) \\ -F_\alpha^\kappa(r)\, Y_{jm}^{\tilde{l}}(\Omega) \end{pmatrix} \chi_{t_\alpha}(t) \qquad \begin{cases} j = l \pm 1/2 \\ \kappa = (-)^{j+l+1/2}(j+1/2) \\ \tilde{l} = l + (-)^{j+l-1/2} \end{cases}$$

$$\begin{cases} \varepsilon_\alpha G_\alpha^\kappa(r) = \left(-\dfrac{\partial}{\partial r} + \dfrac{\kappa}{r}\right) F_\alpha^\kappa(r) + \left[M + S(r) + V(r)\right] G_\alpha^\kappa(r) \\ \varepsilon_\alpha F_\alpha^\kappa(r) = \left(+\dfrac{\partial}{\partial r} + \dfrac{\kappa}{r}\right) G_\alpha^\kappa(r) - \left[M + S(r) - V(r)\right] F_\alpha^\kappa(r) \end{cases}$$

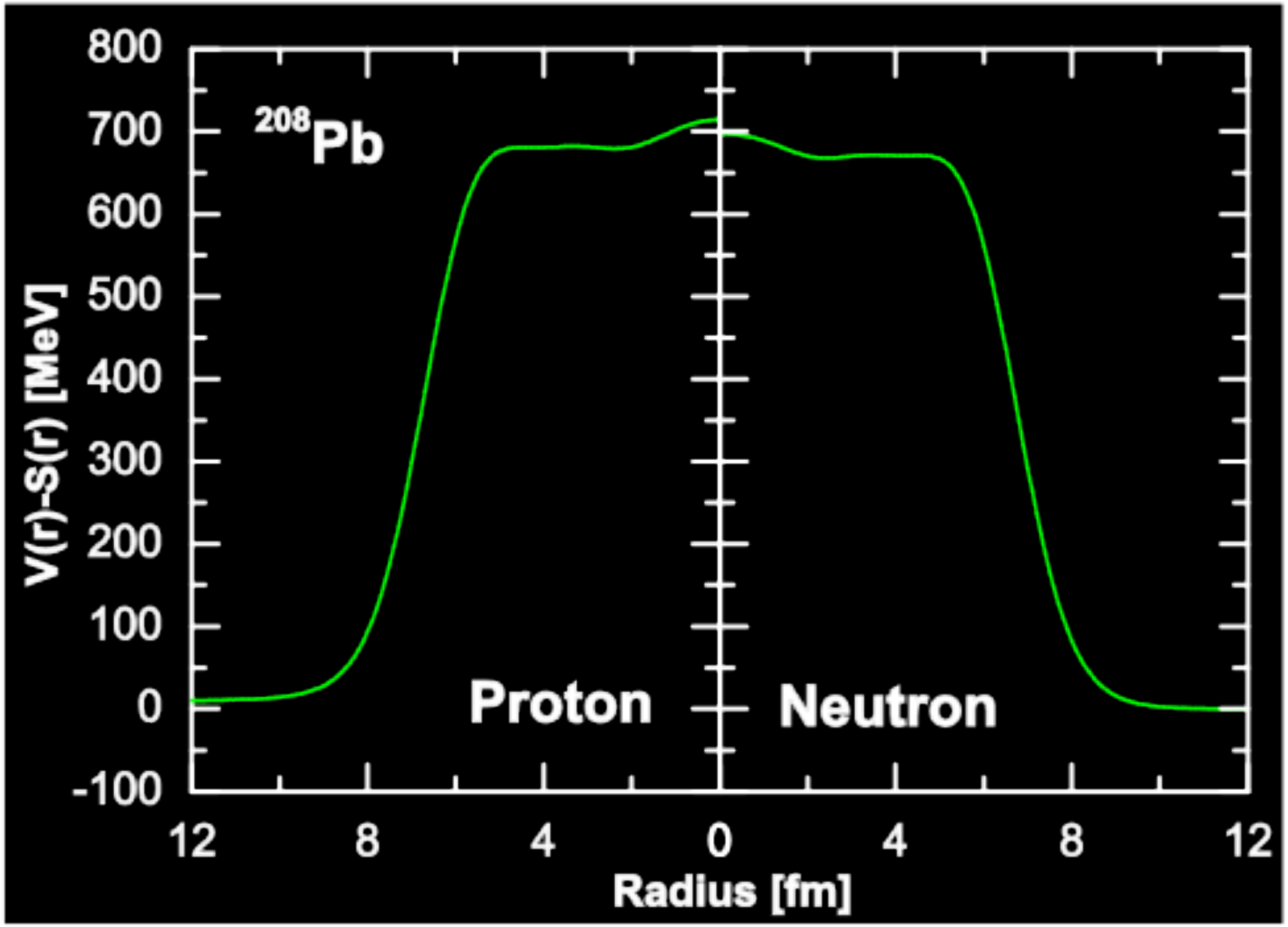
Example: double magic nucleus 208Pb

Sum of the scalar and vector potentials in the radial Dirac equation: potentials for the nucleon.



Example: double magic nucleus 208Pb

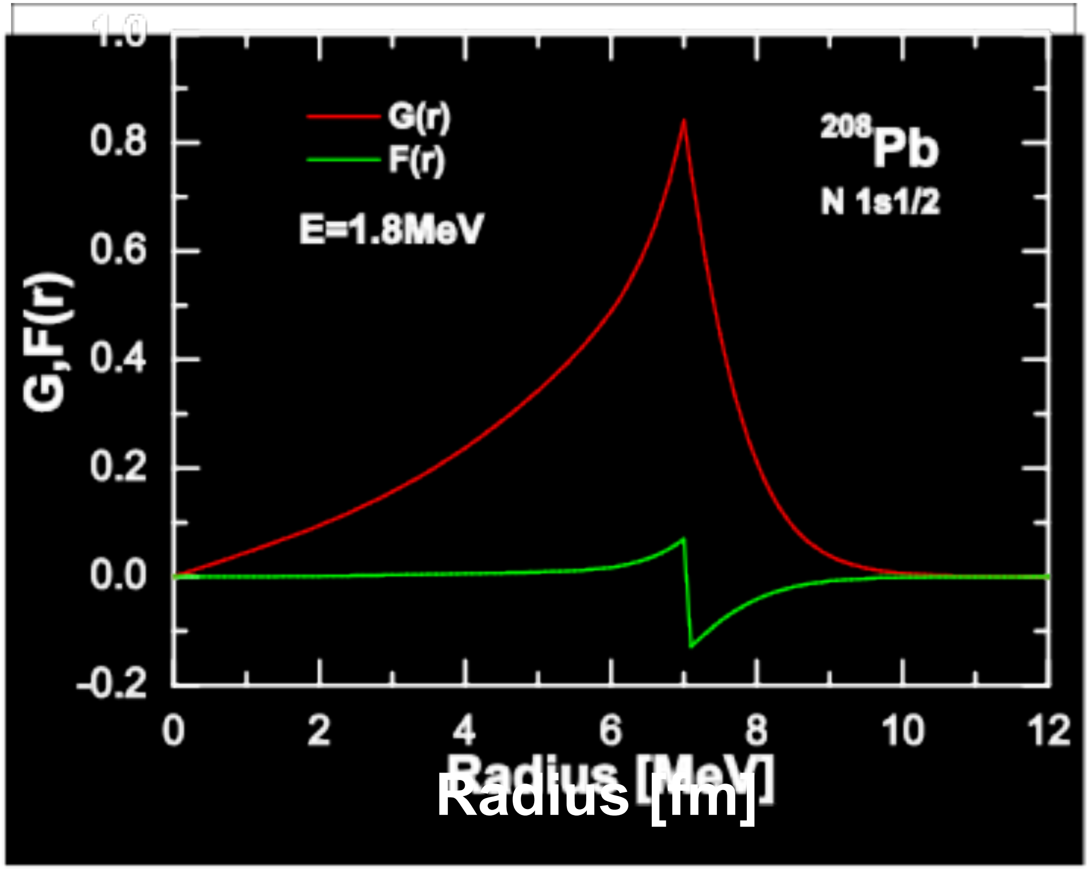
Difference of the scalar and vector potentials in the radial Dirac equation: potentials for the anti-nucleon.



Example: double magic nucleus 208Pb

Shooting method

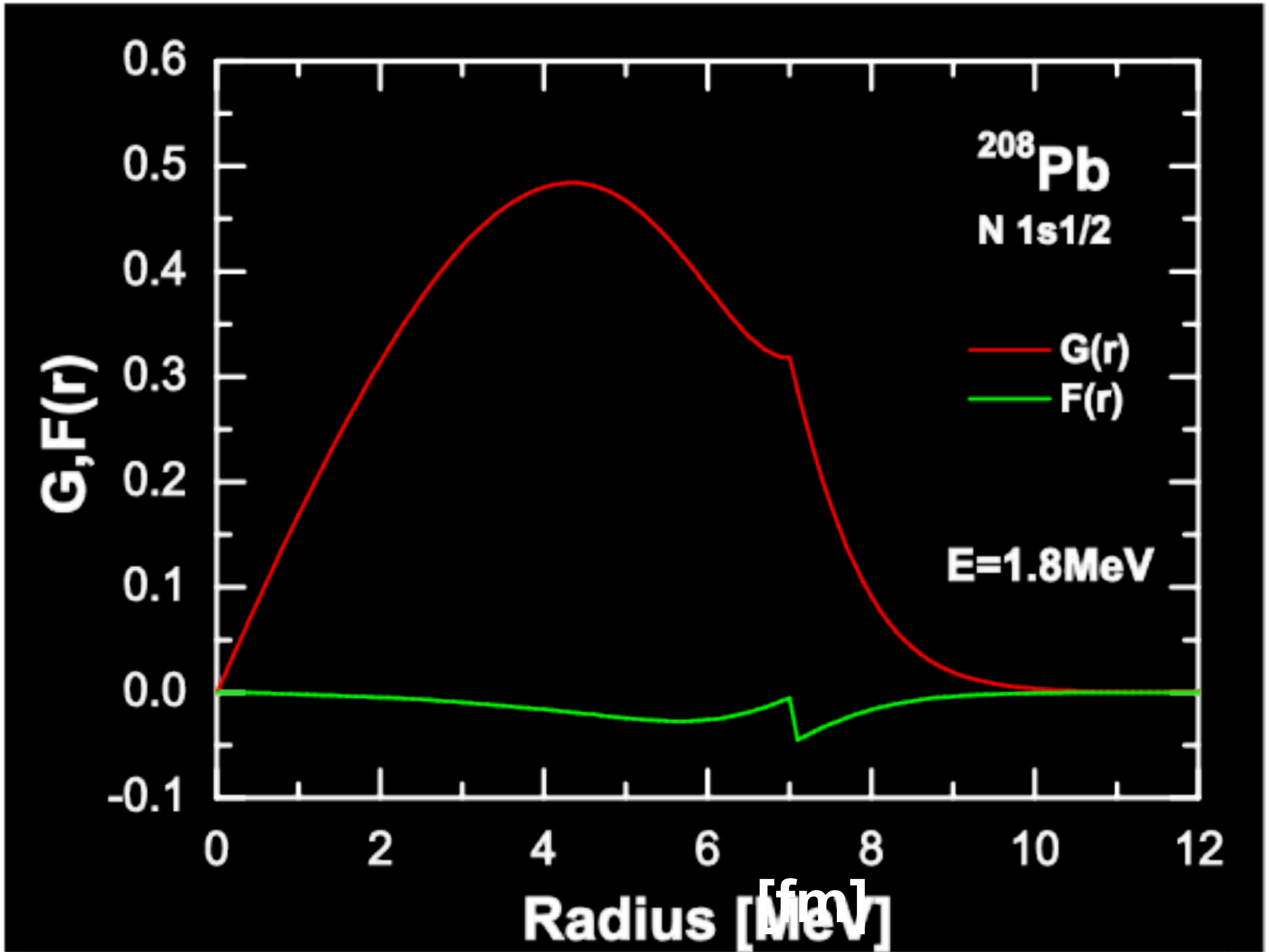
A fourth-order Runge-Kutta algorithm



1. For given energy E, numerical integrated the Dirac equation from r=0 outward and r=∞ inwards to r=rmatch.
2. Rescale the wave function F and G, and GL(r match.)=GR(r match.). If FL(r match.) ≠ FR(r match.), change the energy E by ΔE ~ ΔF (r match.) .
3. Repeating the process until ΔE satisfy the required accuracy.
4. Renormalize the wave function.

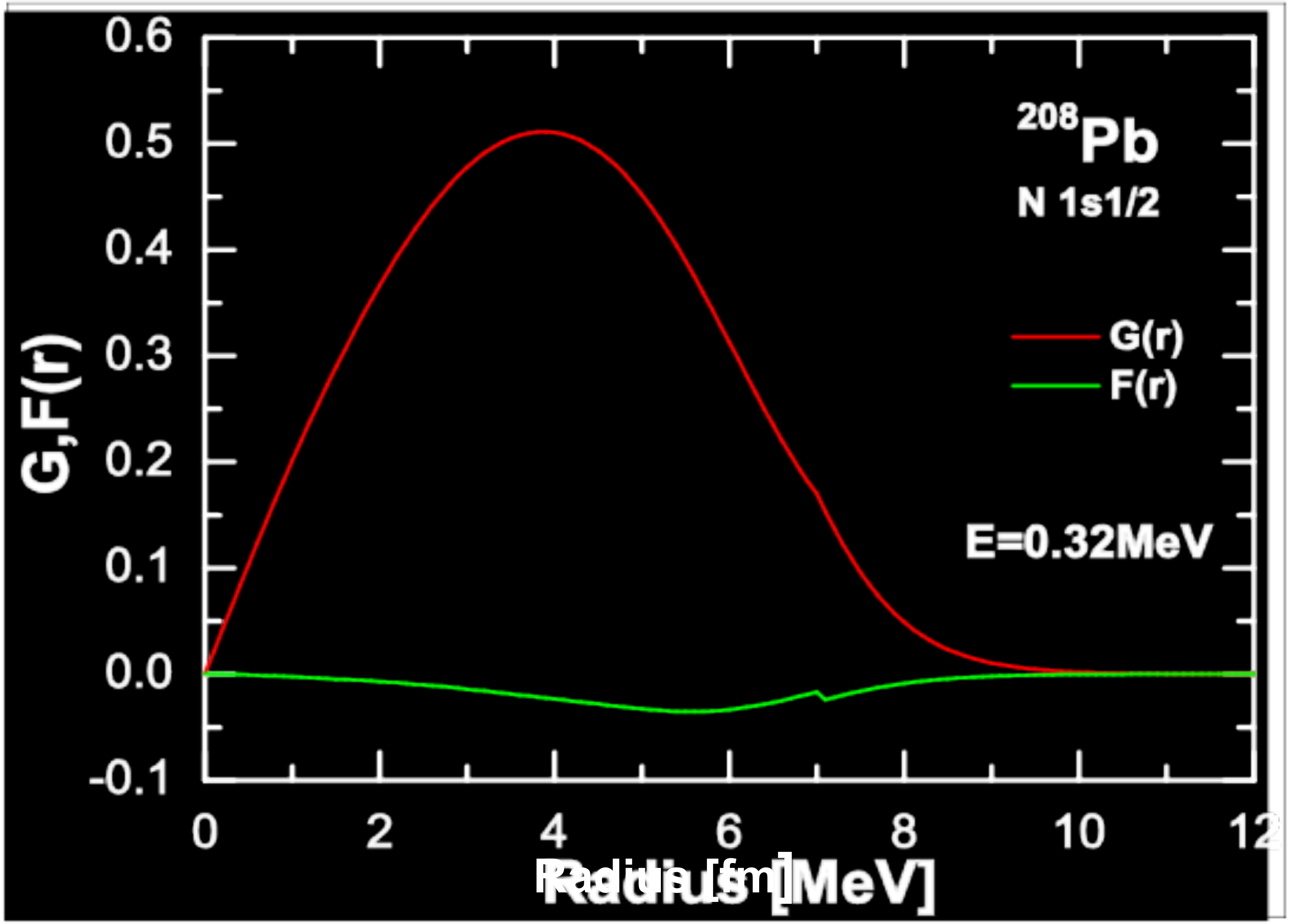
Example: double magic nucleus 208Pb

4-th iteration !



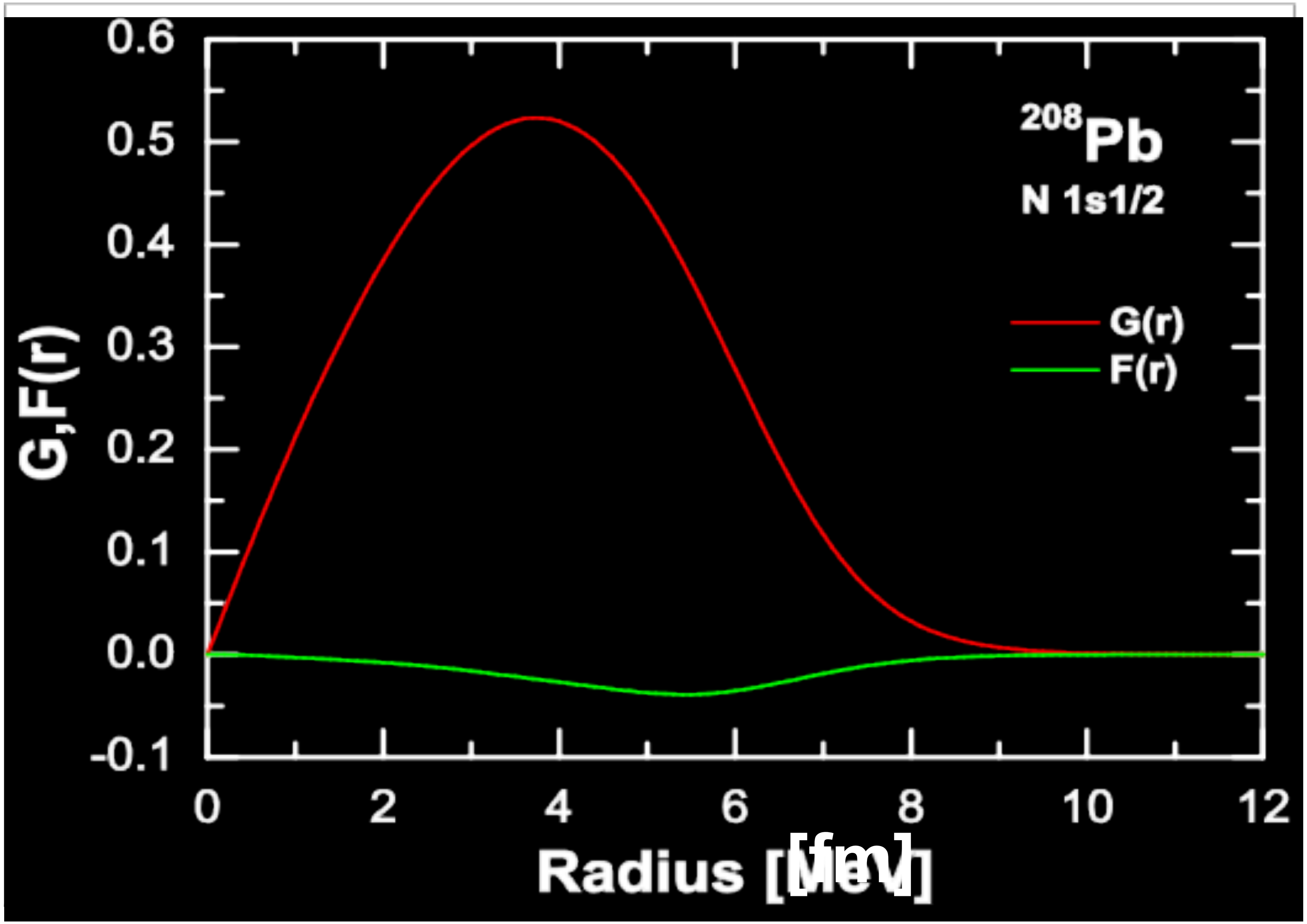
Example: double magic nucleus 208Pb

6-th iteration !

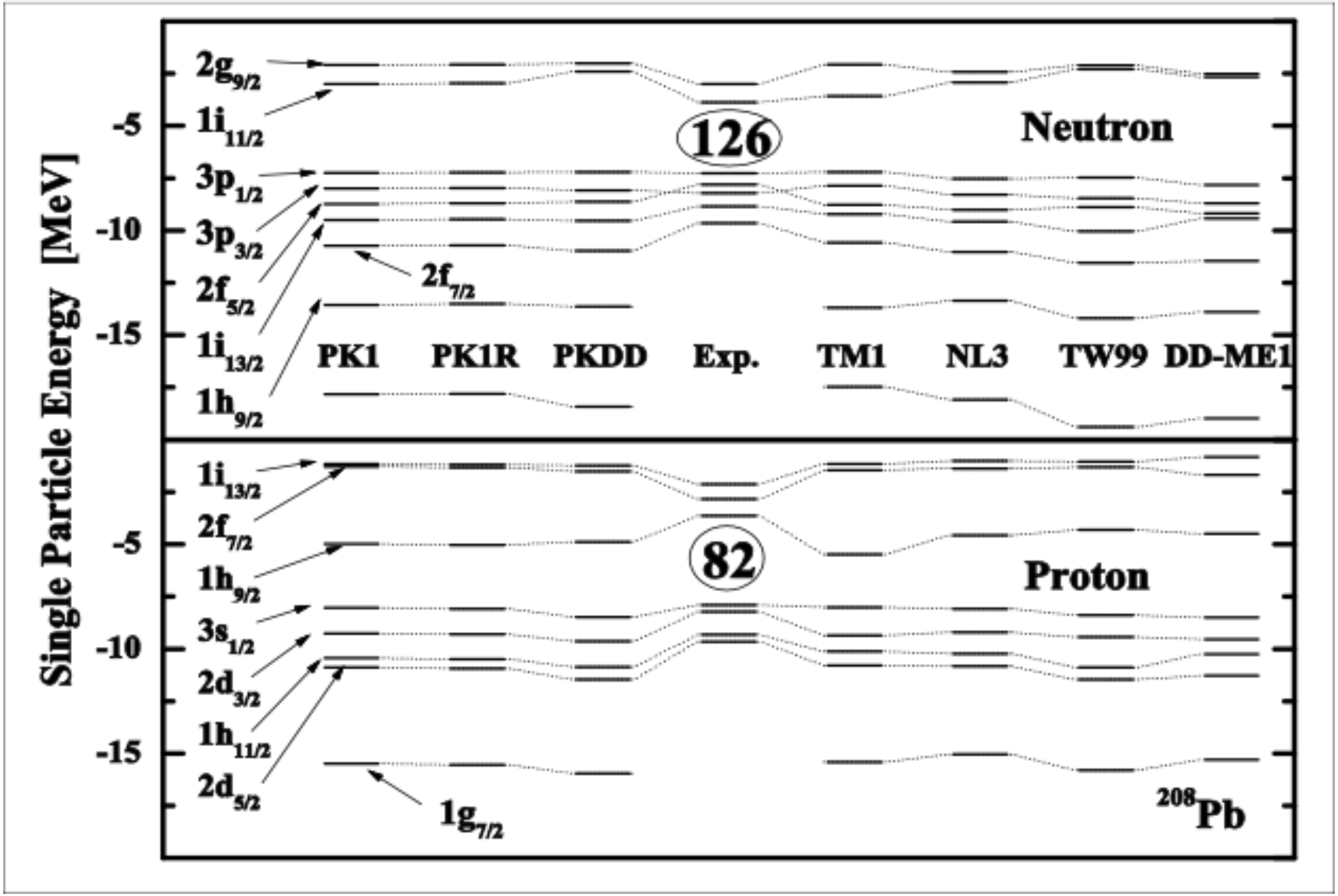


Example: double magic nucleus 208Pb

Convergent wave function ~10 iteration !



Example: double magic nucleus 208Pb



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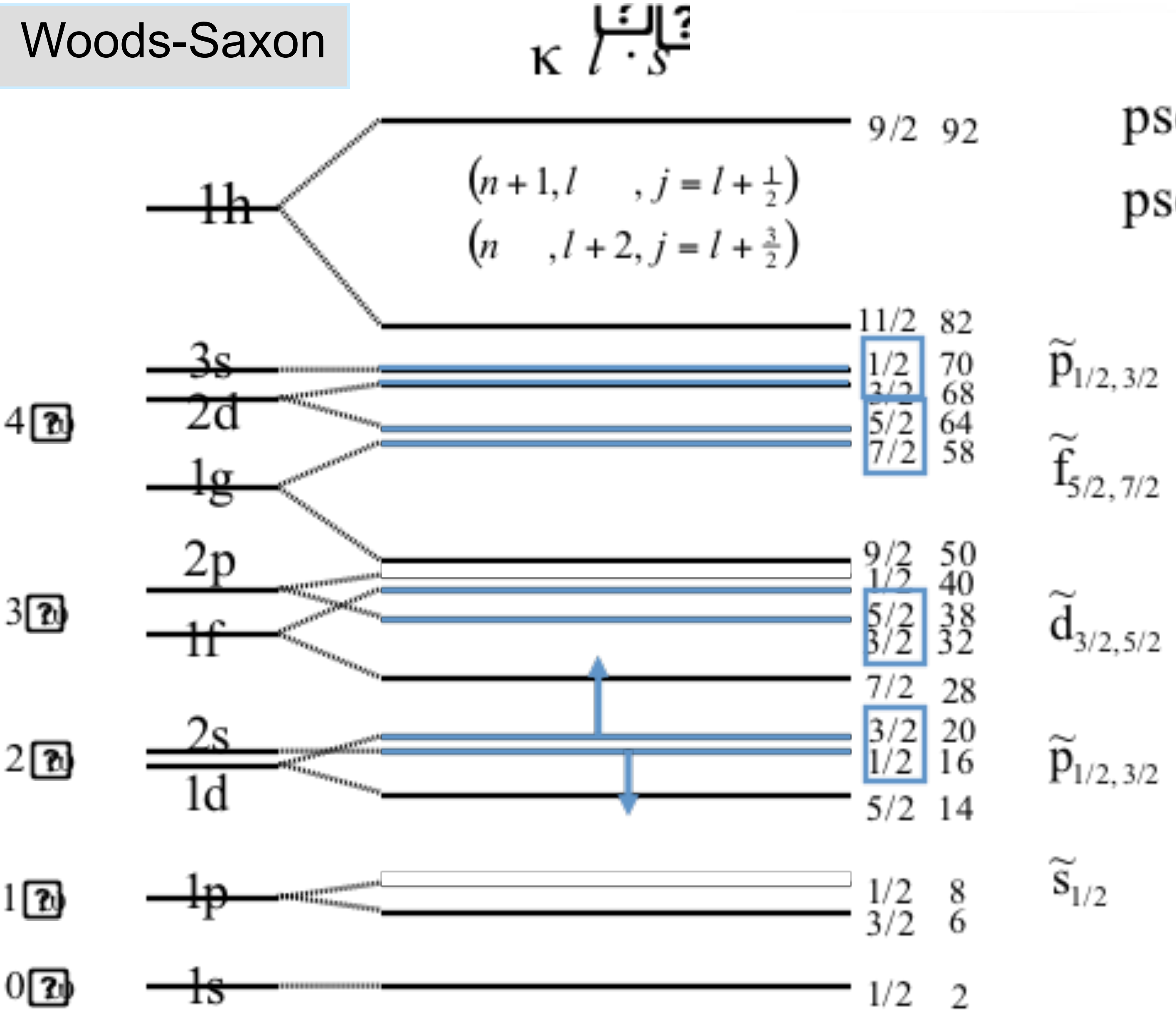
Spin and pseudospin symmetry

Woods-Saxon



$$\text{pseudo-orbit}: \tilde{l} = l + 1$$

$$\text{pseudo-spin}: \tilde{s} = 1/2$$

Hecht & Adler
NPA137(1969)129

Arima, Harvey & Shimizu
PLB30(1969)517

A. Bohr, I. Hamamoto, and B. R. Mottelson, Phys. Scr. 26,267 198

Pseudo quantum numbers

$$\psi^{N}_{n\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} i\ G_{n\kappa}(r)\, Y^{l}_{jm}(\Omega) \\ -F_{\tilde{n}\kappa}(r)\, Y^{\tilde{l}}_{jm}(\Omega) \end{pmatrix}$$

$$\begin{cases} j = l \pm 1/2 \\ \kappa = (-)^{j+l+1/2}(j+1/2) \\ \tilde{l} = l + (-)^{j+l-1/2} \end{cases}$$

$$n = \text{node number} + 1$$

$$(2s_{1/2}, 1d_{3/2}) \Rightarrow (\tilde{p}_{1/2,3/2}) \qquad (\tilde{n} = 2)\,\tilde{p}_{1/2,3/2}$$

$$2s_{1/2} = \begin{pmatrix} n = 2,\ l = 0,\ j = l + \frac{1}{2} \\ \tilde{n} = 2, \tilde{l} = 1, j = \tilde{l} - \frac{1}{2} \end{pmatrix} \quad 1d_{3/2} = \begin{pmatrix} n = 1,\ l = 2,\ j = l - \frac{1}{2} \\ \tilde{n} = 2, \tilde{l} = 1, j = \tilde{l} + \frac{1}{2} \end{pmatrix}$$

Pseudo quantum numbers are nothing
but the quantum numbers of the lower component.

Ginocchio
PRL78(97)436

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Nuclear matter

Infinite nuclear matter:

- **Neglecting the coulomb field**
- **Baryon wave function is the eigenstate of momentum *k***
- **Source currents are independent of the spatial coordinate *x***

The equations of motion can be simplified as:

$$\varepsilon_B(k) = g_{\omega B}\omega^0 + g_{\rho B}\tau_3\rho_{0,3} + \sum_{0B}^{R} + \sqrt{k^2 + m_B^{*2}}$$

$$\begin{cases} m_\sigma^2\sigma = -g_\sigma\rho_s - g_2\sigma^2 - g_3\sigma^3 \\ m_\omega^2\omega = g_\omega\rho_b - c_3\omega^3 \end{cases}$$

$$\begin{cases} \rho_s(\boldsymbol{r}) = \sum_{i=1}^{A}\bar{\psi}_i(\boldsymbol{r})\psi_i(\boldsymbol{r}) = \dfrac{2k_F^3}{3\pi^2} \\ \rho_v(\boldsymbol{r}) = \sum_{i=1}^{A}\psi_i^+(\boldsymbol{r})\psi_i(\boldsymbol{r}) = \sum_{\sigma,\tau}\int_0^{k_F}\dfrac{d^3k}{(2\pi)^3}\dfrac{m_B^*}{\sqrt{k^2+m_B^{*2}}} \end{cases}$$

Nuclear matter

The energy density and pressure of nuclear matter:

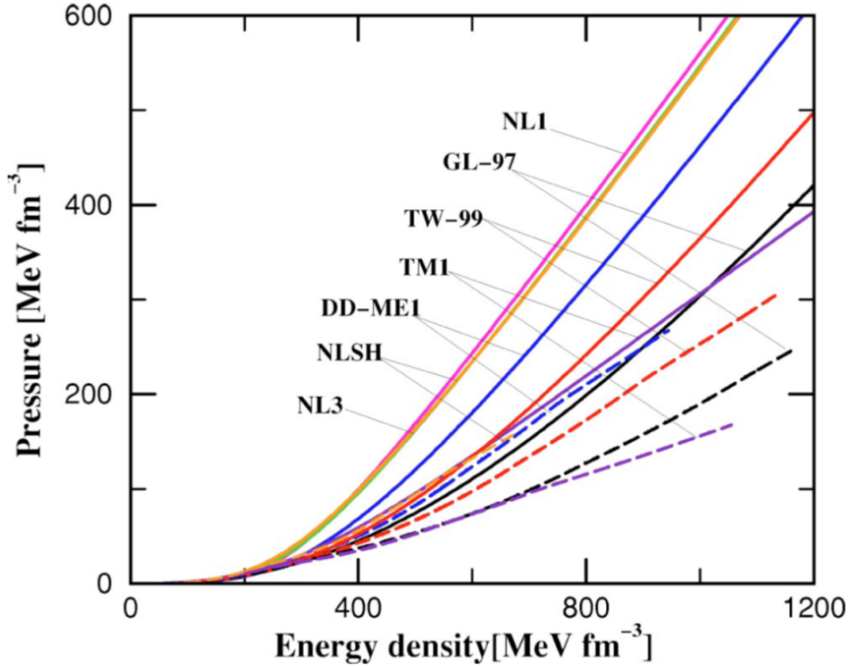
$$\varepsilon = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{2}m_\omega^2\omega^0\omega^0 + \frac{1}{2}m_\rho^2\rho^0\rho^0 + \frac{g_2}{3}\sigma^3 + \frac{g_3}{4}\sigma^4 + 3\Lambda_v g_\rho^2 g_\omega^2(\rho^0\omega^0)^2$$

$$+\frac{1}{\pi}\left\{\int_0^{k_n} k^2 dk\sqrt{k^2 + (M + g_\sigma\sigma)} + \int_0^{k_p} k^2 dk\sqrt{k^2 + (M + g_\sigma\sigma)}\right\}$$

$$P = -\frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{2}m_\omega^2\omega_0^2 + \frac{1}{2}m_\rho^2\rho_{0,3}^2 + \sum_B \rho_B\Sigma_{0l}^R$$

$$+\frac{1}{3\pi^2}\sum_B\int_0^{k_B}\frac{k^4}{\sqrt{k^2 + m_B^{*2}}}dk.$$

EOS of neutron stars



Ban, et al., Phys. Rev. C 69, 045805 (2004).