

## Density Dependent Hartree-Fock (DDHF)

### The 3-body zero-range Density Dependent Skyrme Int.

$$\begin{aligned} V_{Sk} &= t_0(1 + x_0 P_\sigma) \delta(\mathbf{r}_i - \mathbf{r}_j) \\ &+ \frac{1}{2} t_1 (1 + x_1 P_\sigma) \{ p_{12}^2 \delta(\mathbf{r}_i - \mathbf{r}_j) + \delta(\mathbf{r}_i - \mathbf{r}_j) p_{12}^2 \} \\ &+ t_2 (1 + x_2 P_\sigma) p_{12} \cdot \delta(\mathbf{r}_i - \mathbf{r}_j) p_{12} \\ &+ \frac{1}{6} t_3 (1 + x_3 P_\sigma) \rho^\alpha(\bar{\mathbf{r}}) \delta(\mathbf{r}_i - \mathbf{r}_j) \\ &+ i W_0 (\sigma_i + \sigma_j) \cdot p_{12} \times \delta(\mathbf{r}_i - \mathbf{r}_j) p_{12} \end{aligned}$$

$p_{12} = p_i - p_j$  is the relative momentum

$P_\sigma \rightarrow$  Spin Exchange Operator  $\sigma_i \leftrightarrow \sigma_j$

$\sigma \rightarrow$  Spin Pauli Matrices

$$\bar{r} = \frac{1}{2}(r_i + r_j)$$

$t_3 \rightarrow$  3 – Body Contact Interaction Term

$W_o \rightarrow$  Spin – Orbit Term

**Advantage: Expectation value of E wrt Slater Determinant (Mean Field) WF  
 $\rightarrow$  In Analytical Form**

**The Total Energy Functional  $E \rightarrow$  Skyrme, Coulomb, Pairing Parts + Spurious CM Motion**

$$E = E_{Sk} + E_{Coul} + E_{Pair} - E_{c.m.}$$

**Spherical Nuclei  $\rightarrow$  s.p. WF**

$$\varphi_{\beta}(\mathbf{r}) = \frac{R_{\beta}(r)}{r} \mathcal{Y}_{j_{\beta} l_{\beta} m_{\beta}}(\theta, \phi)$$

**and**

$$\mathcal{Y}_{j_{\beta} l_{\beta} m_{\beta}} (= [Y_{l_{\beta}} \times \chi_{1/2}]_{j_{\beta} m_{\beta}})$$

**Are Spinor Spherical Harmonics**

$$E_{Sk} =$$

$$\begin{aligned}
& 4\pi \int dr r^2 \left\{ \frac{\hbar^2}{2m} \tau + \frac{1}{2} t_0 (1 + \frac{1}{2} x_0) \rho^2 - \frac{1}{2} t_0 (\frac{1}{2} + x_0) \sum_q \rho_q^2 \right. \\
& + \frac{1}{4} [t_1 (1 + \frac{1}{2} x_1) + t_2 (1 + \frac{1}{2} x_2)] \rho \tau \\
& - \frac{1}{4} [t_1 (\frac{1}{2} + x_1) - t_2 (\frac{1}{2} + x_2)] \sum_q \rho_q \tau_q \\
& + \frac{1}{16} [3t_1 (1 + \frac{1}{2} x_1) + t_2 (1 + \frac{1}{2} x_2)] \sum_q \rho_q \nabla^2 \rho_q \\
& - \frac{1}{16} [3t_1 (1 + \frac{1}{2} x_1) - t_2 (1 + \frac{1}{2} x_2)] \rho \nabla^2 \rho \\
& \left. - \frac{1}{2} W_0 [\rho \nabla \cdot \mathbf{J} + \sum_q \rho_q \nabla \cdot \mathbf{J}_q] \right\}
\end{aligned}$$

$$\nabla^2 = \partial_r^2 + \frac{2}{r}\partial_r \quad , \quad \partial_r \rightarrow \frac{\partial}{\partial r}$$

**The Spherical Densities and Currents are**

$$\rho_q(r) = \sum_{n_\beta j_\beta l_\beta} n_\beta^q \frac{2j_\beta + 1}{4\pi} \left(\frac{R_\beta}{r}\right)^2$$

$$\tau_q(r) = \sum_{n_\beta j_\beta l_\beta} n_\beta^q \frac{2j_\beta + 1}{4\pi} \left[ \left(\partial_r \frac{R_\beta}{r}\right)^2 + \frac{l(l+1)}{r^2} \left(\frac{R_\beta}{r}\right)^2 \right]$$

$$\nabla \mathbf{J}_q(r) = \left(\partial_r + \frac{2}{r}\right) J_q(r)$$

$$J_q(\mathbf{r}) = \sum_{n_\beta j_\beta l_\beta} n_\beta^q \frac{2j_\beta + 1}{4\pi} (j_\beta(j_\beta + 1) - l_\beta(l_\beta + 1) - \frac{3}{4}) \frac{2}{r} \left(\frac{R_\beta}{r}\right)^2$$

**The Occupation Probabilities  $n_{\beta}^q \rightarrow$   
Independent of  $m_{\beta}$  .  $q$  Runs over n and p**

$$\rho = \rho_p + \rho_n \quad \tau = \tau_p + \tau_n$$
$$\nabla \cdot \mathbf{J} = \nabla \cdot \mathbf{J}_p + \nabla \cdot \mathbf{J}_n$$

**The Variation of E wrt  $R_{\beta} \rightarrow$  HF Equations**

$$h_q R_{\beta} = \epsilon_{\beta} R_{\beta}$$

**The Mean Field Hamiltonian**

$$h_q = \partial_r \mathcal{B}_q \partial_r + U_q + U_{ls,q} \mathbf{l} \sigma$$

$$\mathcal{B}_q = \frac{\hbar^2}{2m_q} + \frac{1}{8}[t_1(1 + \frac{1}{2}x_1) + t_2(1 + \frac{1}{2}x_2)]\rho - \frac{1}{8}[t_1(\frac{1}{2} + x_1) - t_2(\frac{1}{2} + x_2)]\rho_q$$

$$U_{ls,q} = \frac{1}{4}W_o(\rho + \rho_q) + \frac{1}{8}(t_1 - t_2)J_q - \frac{1}{8}(x_1t_1 + x_2t_2)J$$

$$\begin{aligned}
U_q &= t_0(1 + \frac{1}{2}x_0)\rho - t_0(\frac{1}{2} + x_0)\rho_q \\
&+ \frac{1}{12}t_3\rho^\alpha[(2 + \alpha)(1 + \frac{1}{2}x_3)\rho \\
&- 2(\frac{1}{2} + x_3)\rho_q - \alpha(\frac{1}{2} + x_3)\frac{\rho_p^2 + \rho_n^2}{\rho}] \\
&+ \frac{1}{4}[t_1(1 + \frac{1}{2}x_1) + t_2(1 + \frac{1}{2}x_2)]\tau \\
&- \frac{1}{4}[t_1(\frac{1}{2} + x_1) - t_2(\frac{1}{2} + x_2)]\tau_q \\
&- \frac{1}{8}[3t_1(1 + \frac{1}{2}x_1) - t_2(1 + \frac{1}{2}x_2)]\nabla^2\rho \\
&+ \frac{1}{8}[3t_1(\frac{1}{2} + x_1) + t_2(\frac{1}{2} + x_2)]\nabla^2\rho_q \\
&- \frac{1}{2}W_o(\nabla \cdot \mathbf{J} + \nabla \cdot \mathbf{J}_q) + \delta_{q1/2} U_{Coul}
\end{aligned}$$



$U_{Coul} \rightarrow$  Direct + Exchange Terms.

Direct Term is Trivial, Exchange Term is Taken As

$$U_{coul}(exchange) = \left(-\frac{3}{\pi}\right)^{1/3} 4\pi \int dr r^2 \rho_p^{4/3}$$

$$E_{c.m.} = \frac{\langle P_{c.m.}^2 \rangle}{2AM}$$

For H.O. s.p. Basis  $E_{c.m.} = \frac{3}{4} \hbar \omega$

BCS Type Occupation Probabilities are obtained Through Gap and Number Equations. Then

$$E_{Pair} = - \sum_q G_q \left[ \sum_{\beta \in q} \sqrt{n_{\beta}^q (1 - n_{\beta}^q)} \right]^2$$

## Illustration:

### Skyrme Int. Parameters

$$t_o = -1057, t_1 = 235.9, t_2 = -100, t_3 = 14463.5,$$

$$W_o = 120, x_o = 0.56, x_1 = x_2 = 0.0, x_3 = 1.0$$

$$\alpha = 1$$

### **Gap Parameter:**

$$\Delta_q = 11.2 \text{ MeV} / \sqrt{A} \quad A = A_p + A_n$$

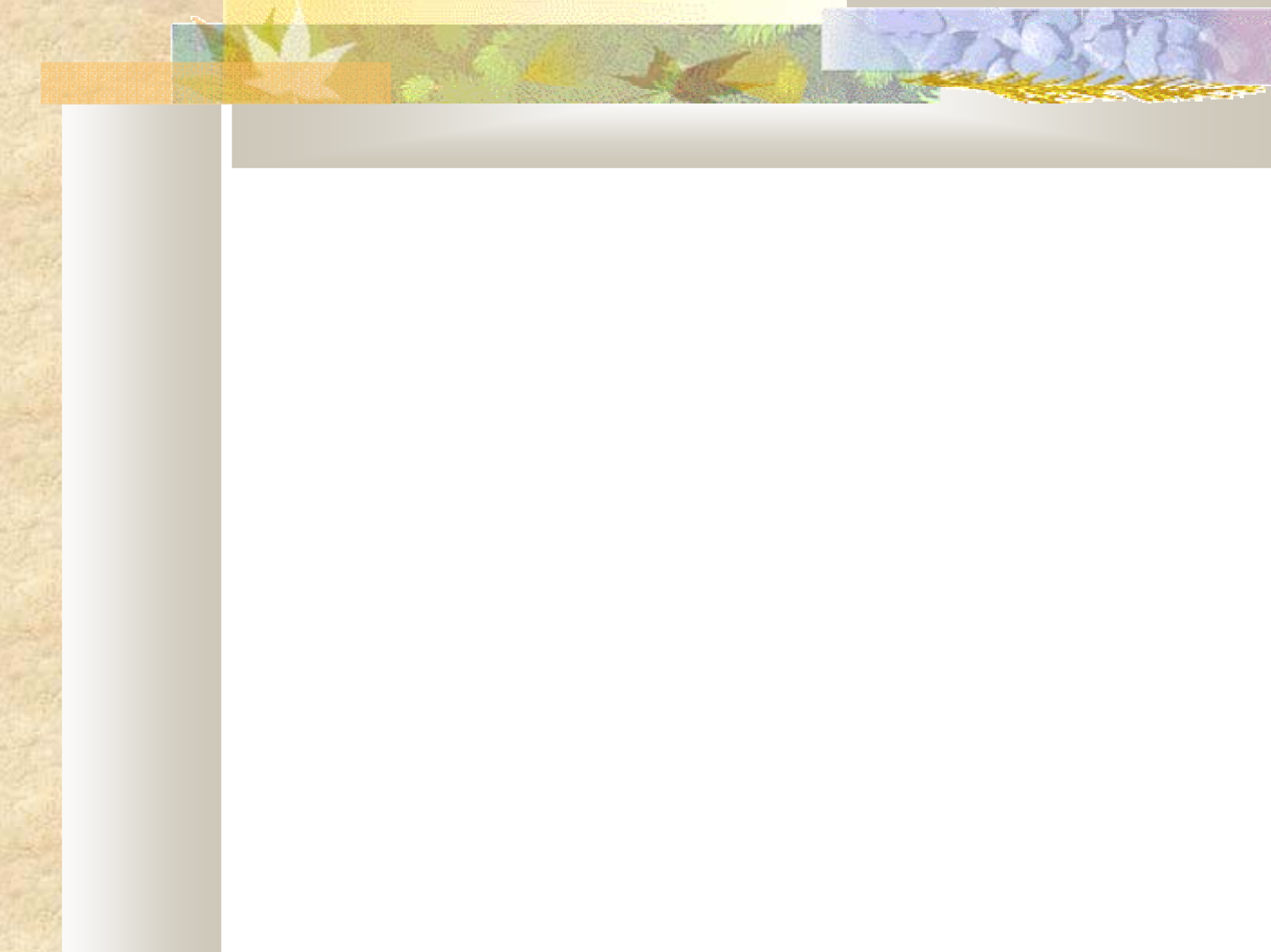
$$r_c = \sqrt{r_p^2 + 0.64}$$

•

$$r_m = \left[ \frac{(Zr_p^2 + Nr_n^2)}{(Z+N)} \right]^{1/2}$$

	$^{16}_8O$	$^{40}_{20}Ca$	$^{48}_{20}Ca$	$^{90}_{40}Zr$	$^{208}_{82}Pb$
BE/A	-8.22 (-7.98)	-8.64 (-8.55)	-8.93 (-8.67)	-8.81 (-8.71)	-7.89 (-7.87)
$r_c$	2.68 (2.73)	3.41 (3.49)	3.46 (3.48)	4.22 (4.27)	5.44 (5.50)
$r_m$	2.55	3.29	3.43	4.17	5.45

**Calculations Reproduce Expt. Well.**





## Relativistic Mean Field (RMF) Approach


**Non-Relativistic Analysis Indicates That**

$$U \sim 50 \text{ MeV} \ll mc^2 (\sim 1000 \text{ MeV}).$$

**Question: Why Relativistic Formulation?**

**Reasons::**

**\*\* Nuclear l.s splitting is 30 Times Larger and is of Opposite Sign as That of Atomic Case|**



**\*\* Conventional Optical Model (OPM) Fails to Describe Spin Observables in the Intermediate Energy Polarized Proton – Nucleus (p-A) Scattering.**

**Dirac Phenomenology: Use of Dirac Eq. With Lorentz Scalar and Vector Potentials in Place of Schrodinger Eq. Remarkably Successful. Scalar Pot.  $U$  and Vector Pot.  $V$  are of the Order of  $-400$  and  $350$  MeV – Their Diff. Yields Required  $50$  MeV. This Success Triggered the Application of RMF to Nuclear Structure.**

## RMF-Formulation:

**Nucleon Interacts With the Meson ( $\sigma, \omega$  and  $\rho$ ) and e.m. ( $\gamma$ ) Fields.  
The Lagrangian : Free Baryon ( $L_B$ ), Mesons ( $L_M$ ) and the INT. ( $L_{BM}$ ) Terms.**

$$L_B = \bar{\psi}_i (\nu \gamma^\mu \partial_\mu - M) \psi_i$$

$$L_M = \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - U(\sigma) \\ - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_\omega^2 \omega^\mu \omega_\mu \\ - \frac{1}{4} \vec{R}^{\mu\nu} \vec{R}_{\mu\nu} + \frac{1}{2} m_\rho^2 \vec{\rho}^\mu \vec{\rho}_\mu - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}$$



$$\begin{aligned}
 \mathbf{L}_{\text{MB}} = & -g_\sigma \bar{\psi}_i \psi_i \sigma \\
 & -g_\omega \bar{\psi}_i \gamma^\mu \psi_i \omega_\mu \\
 & -g_\rho \bar{\psi}_i \gamma^\mu \vec{\tau} \psi_i \vec{\rho}_\mu \\
 & -e \bar{\psi}_i \gamma^\mu \frac{(1 + \tau_3)}{2} \psi_i A_\mu
 \end{aligned}$$


**With**

$$U(\sigma) = \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4$$

**The Field Tensors**

$$\begin{aligned}
 \Omega^{\mu\nu} &= \partial^\mu \omega^\nu - \partial^\nu \omega^\mu \\
 \vec{R}^{\mu\nu} &= \partial^\mu \vec{\rho}^\nu - \partial^\nu \vec{\rho}^\mu - g_\rho (\vec{\rho}^\mu \times \vec{\rho}^\nu) \\
 \mathbf{F}^{\mu\nu} &= \partial^\mu A^\nu - \partial^\nu A^\mu
 \end{aligned}$$





**The Classical Variation Principle  
Gives the EQS. Of Motion.  
Replacing the Fields By Their  
Expectation Values →  
Dirac EQ. With Pot. Terms for  
Nucleons and KG Type EQS. With  
Sources For Meson and the Photon**

# Non Linear Walecka Model

## Relativistic Mean Field: RMF

Ann. Phys. 198 (1990) 132  
Gambhir, Ring and Thimet

### Nucleons Interact With Meson Fields

$\sigma, \omega, \rho$  and  $\gamma$

**Lagrangian**

Masses:  $M, m_\sigma, m_\omega, m_\rho$   
Couplings:  $g_\sigma, g_\omega, g_\rho$   
 $g_2, g_3$

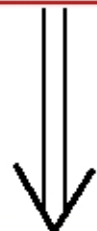
Classical  $\Downarrow$  Variation Principle

**Equations of Motion**

Approx: Field Operators  $\Rightarrow$  C - Numbers

**Dirac Equation: Nucleons**  
**K. G. Equation: Mesons & Photon**

For: **Static Case** + **Charge Conserv** + **Time Reversal**



Dirac Eqn:

**Scalar + Time like vector**

$$\mathbf{M}^* = \mathbf{M} + \sigma \mathbf{g}_\sigma ; \omega^0, \rho^{00}, \mathbf{A}^0$$

K. G. Eqn:

**Sources: Baryon  
Densities and Currents**

**Closed Set of Equations  
(RMF Equations)**

**⇒ To be solved  
Self – Consistently**

## The Dirac Eq.:

$$\left( -i\alpha \cdot \nabla + \beta (M + g_\sigma \sigma) + g_\omega \omega^0 + g_\rho \tau_3 \rho_3^0 + e \frac{1 + \tau_3}{2} A^0 \right) \psi_i = \epsilon_i \psi_i.$$

## The KG Eqs.:

$$\left\{ -\nabla^2 + m_\sigma^2 \right\} \sigma = -g_\sigma \rho_s - g_2 \sigma^2 - g_3 \sigma^3$$

$$\left\{ -\nabla^2 + m_\omega^2 \right\} \omega^0 = g_\omega \rho_v$$

$$\left\{ -\nabla^2 + m_\rho^2 \right\} \rho_3^0 = g_\rho \rho_3$$

$$-\nabla^2 A^0 = e \rho_c$$

$m_\sigma (g_\sigma), m_\omega (g_\omega), m_\rho (g_\rho)$  are Meson  
Masses (Coupling Constants)  
 $g_2 (g_3)$  : Coupling Constants of Cubic  
(Quartic) Non-Linear Terms

**Currents and Densities are:**

$$\rho_s = \sum_i n_i \bar{\psi}_i \psi_i$$

$$\rho_v = \sum_i n_i \psi_i^\dagger \psi_i$$

$$\rho_3 = \sum_i n_i \psi_i^\dagger \tau_3 \psi_i$$

$$\rho_c = \sum_i n_i \psi_i^\dagger \left( \frac{1 + \tau_3}{2} \right) \psi_i$$

**Pairing:**

**Important**

- **Constant Gap Approx.**

$\Delta_n$  ( $\Delta_p$ ) Fixed  $\Rightarrow$

**Simple BCS Type**

- **Self Consistent:**

**Bogoliubov Transform**  $\Rightarrow$

**Relativistic Hartree**

**Bogoliubov (RHB) Equations**

## RHB Equations:

$$\begin{pmatrix} h_D - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -h_D^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k \begin{pmatrix} U \\ V \end{pmatrix}_k$$

$h_D$ : Dirac Hamiltonian

$\hat{\Delta}$ : Pairing Field

$U_k, V_k$  : Dirac Super-Spinors



## Dirac Hamiltonian:

$$\mathbf{h}_D = -i\boldsymbol{\alpha} \cdot \nabla + \beta (\mathbf{M} + \mathbf{g}_\sigma \boldsymbol{\sigma}) + g_\omega \omega^0 + g_\rho \tau_3 \rho_3^0 + e \frac{1 - \tau_3}{2} A^0$$

$$\int \left( U_k^\dagger U_{k'} + V_k^\dagger V_{k'} \right) = \delta_{kk'}$$



**Kernel** of Pairing Field  $\hat{\Delta}$  is:

$$\Delta_{ab}(\mathbf{r}, \mathbf{r}') = \frac{1}{2} \sum_{c,d} V_{abcd}^{pp}(\mathbf{r}, \mathbf{r}') \kappa_{cd}(\mathbf{r}, \mathbf{r}')$$

$\kappa$  : Pairing Tensor  $\rightarrow$

$$\kappa_{cd}(\mathbf{r}, \mathbf{r}') = \sum_{E_k > 0} U_{ck}^*(\mathbf{r}) V_{dk}(\mathbf{r}')$$

$V^{pp}$ : Interaction in *pp* channel

## Constant Gap Approximation:

$\hat{\Delta}$  Diagonal

RHB  $\rightarrow$  RMF with FROZEN  
GAP:

Occupancies: given by BCS  
equation:

$$n_k = v_k^2 = \frac{1}{2} \left[ 1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right]$$

$\lambda \rightarrow$  Lagrange Multiplier

$\Delta \rightarrow$  Pairing Gap

$\epsilon_k \rightarrow$  Single Particle Energies

# **RMF / RHB Calculations**

**Input:**

**Lagrangian Parameter Set (NL3)**

**$\Delta$  / Pairing Interaction**

**$\Delta$ : Odd – Even Mass Difference**

**OR**

**Determine so as to Reproduce**

**RHB Proton / Neutron Pairing Energies  
With Gogny D1S Interaction**

# **RMF / RHB Calculations**

**Output:**

**Dirac Spinors / Mesonic Fields**

**Single Particle Energies**

**Binding Energies**

**Densities**

**Radii**

### NL3 Parameter Set

<b>Masses (MeV)</b>	<b>m</b>	<b>939</b>	<b><math>m_\sigma</math></b>	<b>508.194</b>
	<b><math>m_\omega</math></b>	<b>782.501</b>	<b><math>m_\rho</math></b>	<b>763.0</b>
<b>Coupling Constants</b>	<b><math>g_\sigma</math></b>	<b>10.217</b>	<b><math>g_\omega</math></b>	<b>12.868</b>
	<b><math>g_\rho</math></b>	<b>4.474</b>	<b><math>g_2</math></b>	<b>-10.431</b>
	<b><math>g_3</math></b>	<b>-28.885</b>		<b>(fm<sup>-1</sup>)</b>

• **Zero Range Density Dependent:**

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4} V_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) (1 - \sigma_1 \sigma_2) \left( 1 - \frac{\rho(r)}{\rho_0} \right)$$

$$\rho_0 = 0.152 \text{ fm}^{-3}$$

$$V_0 \approx -700 \text{ MeV-fm}^{-3}$$



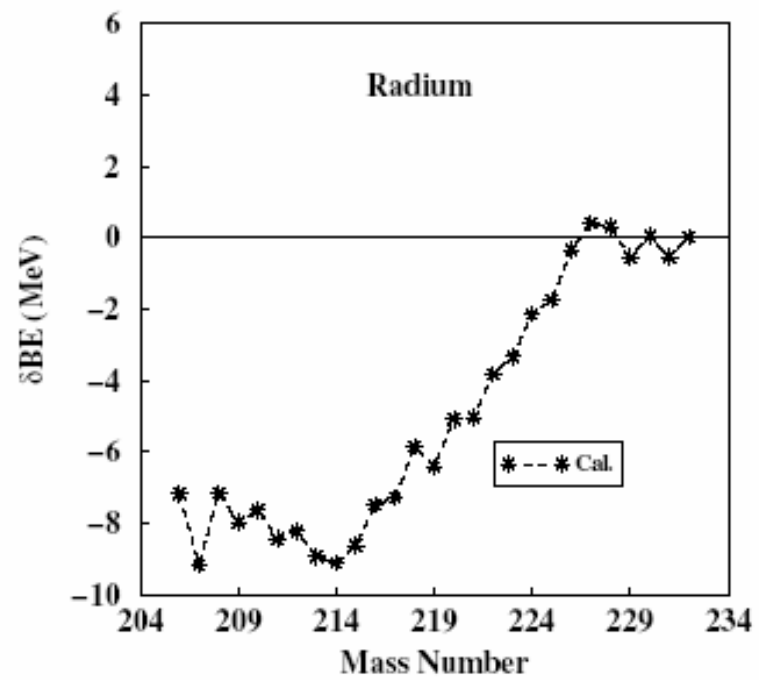
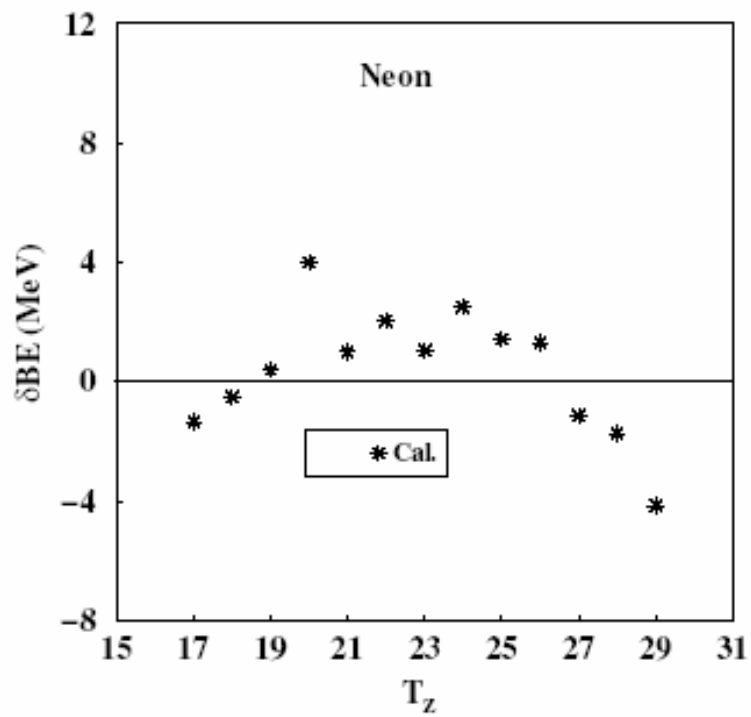
$V^{pp}(\mathbf{r}, \mathbf{r}')$ : Non Relativistic:

• Gogny D1S:

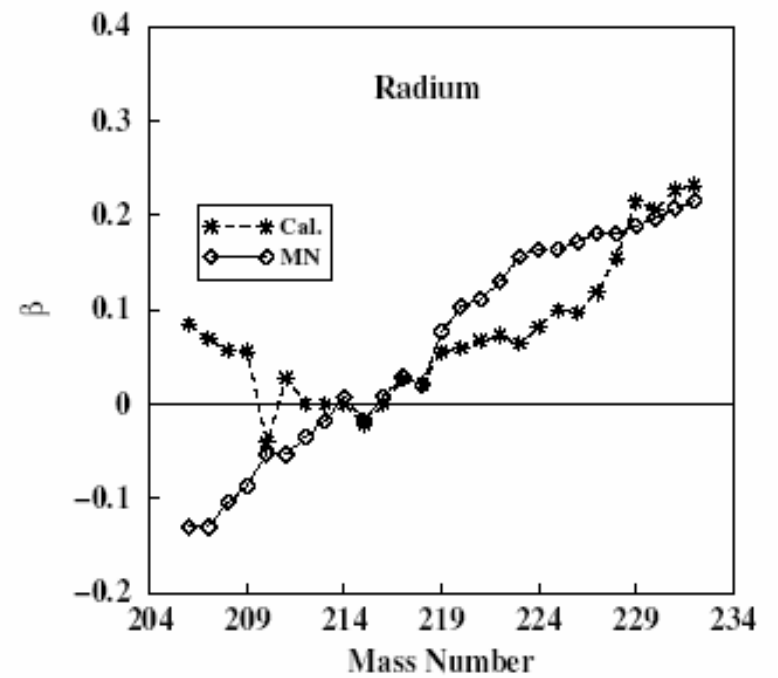
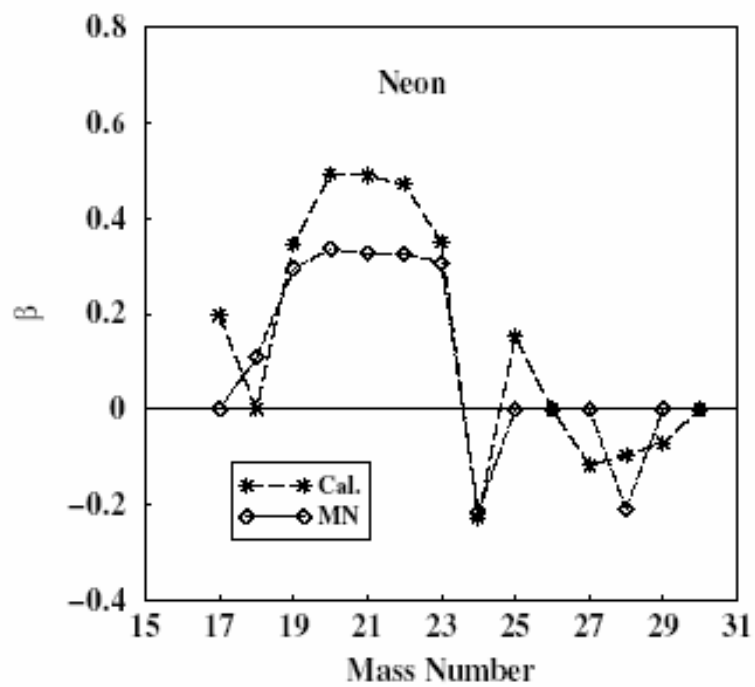
$$V(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1,2} e^{-\{(\mathbf{r}_1 - \mathbf{r}_2)/\mu_i\}^2} (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau)$$

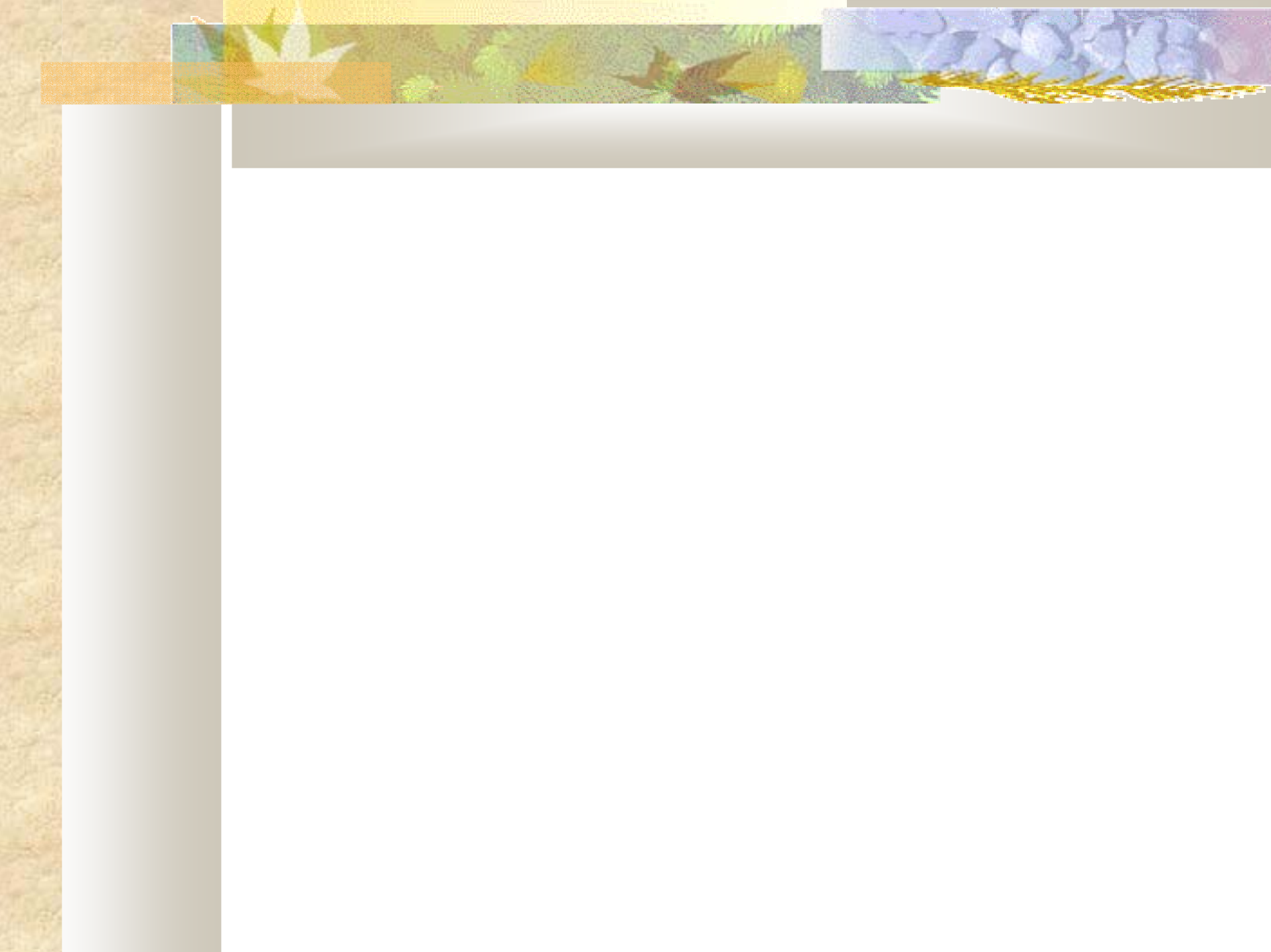
D1S Parameters:

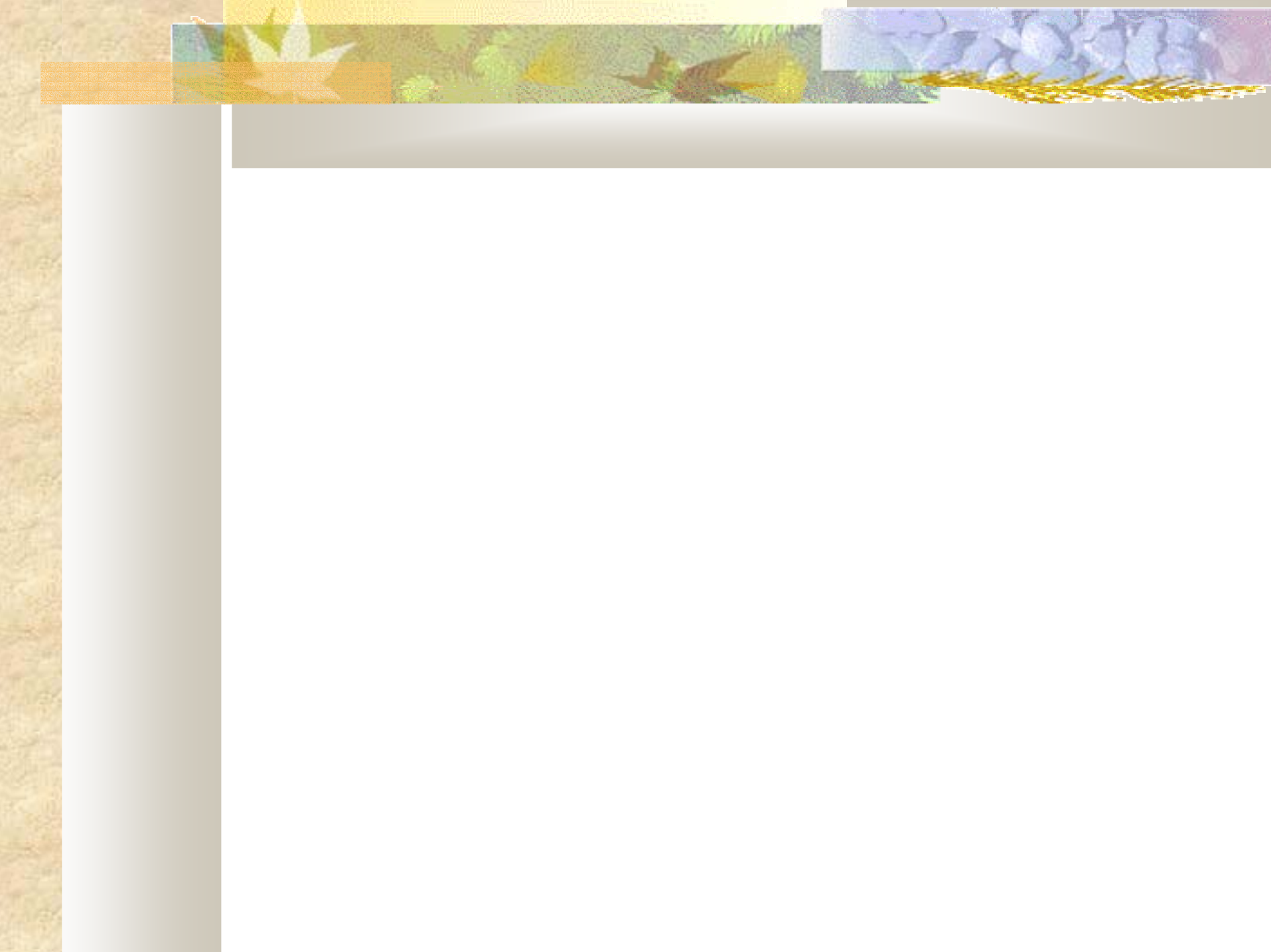
Parameter	$i = 1$	$i = 2$
$\mu_i$	0.7	1.2
$W_i$	-1720.30	103.64
$B_i$	1300.00	-163.48
$H_i$	-1813.53	162.81
$M_i$	1397.60	-223.93



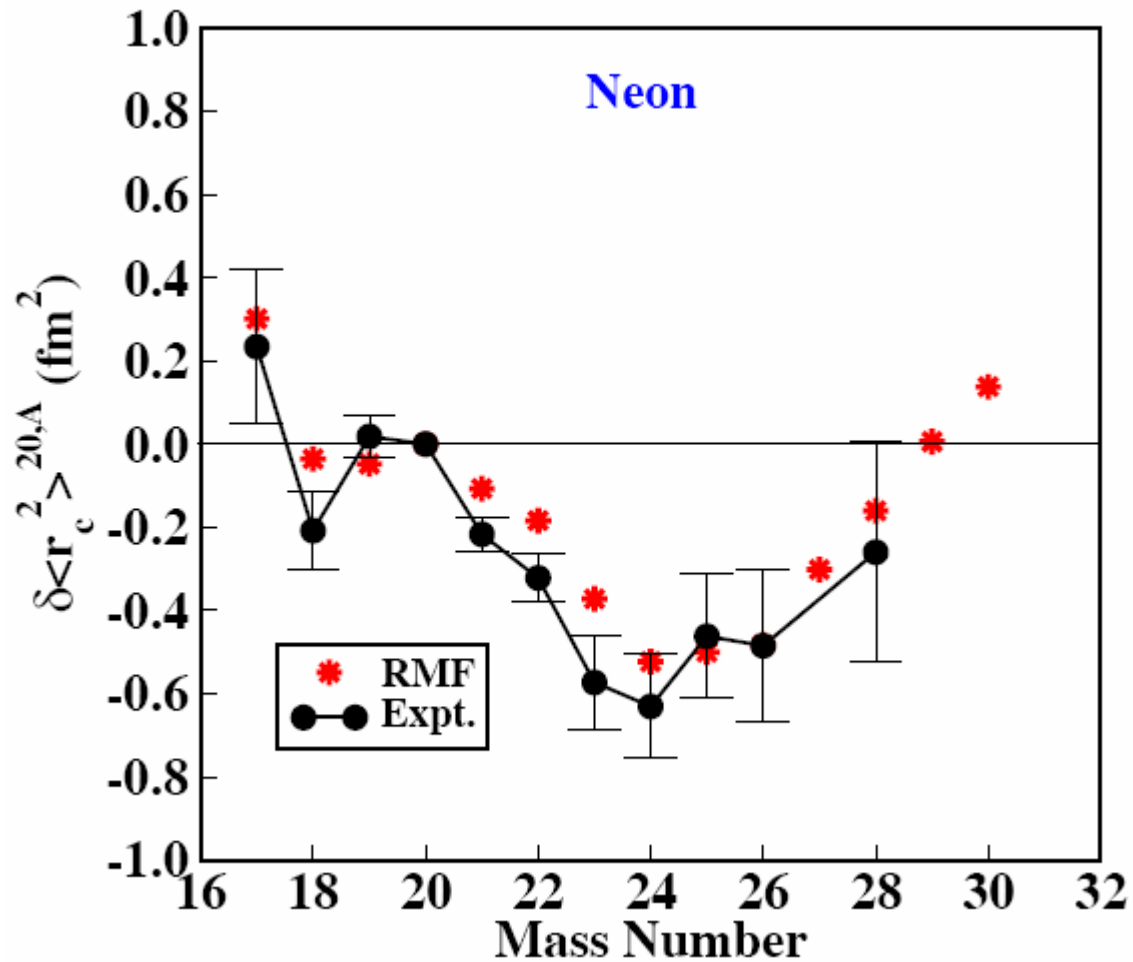


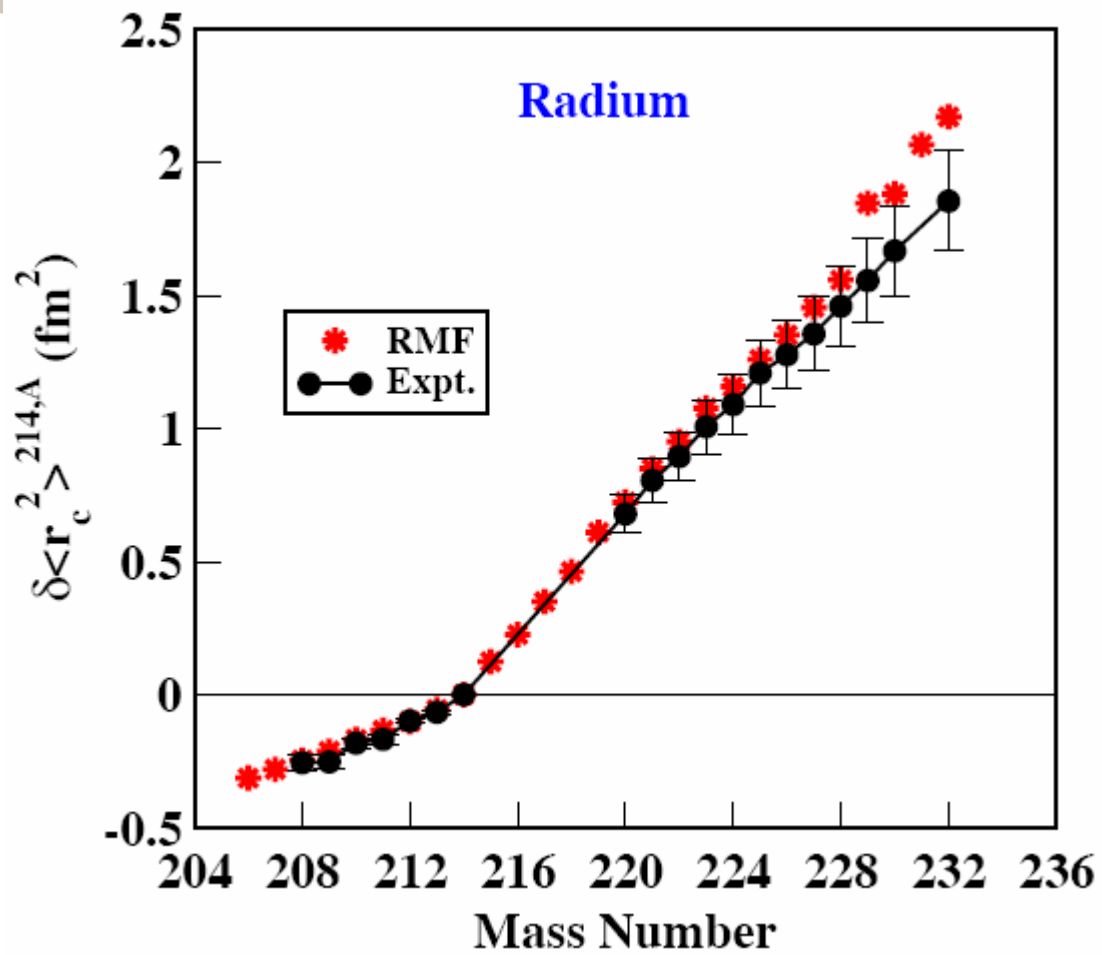






# Ground State Properties





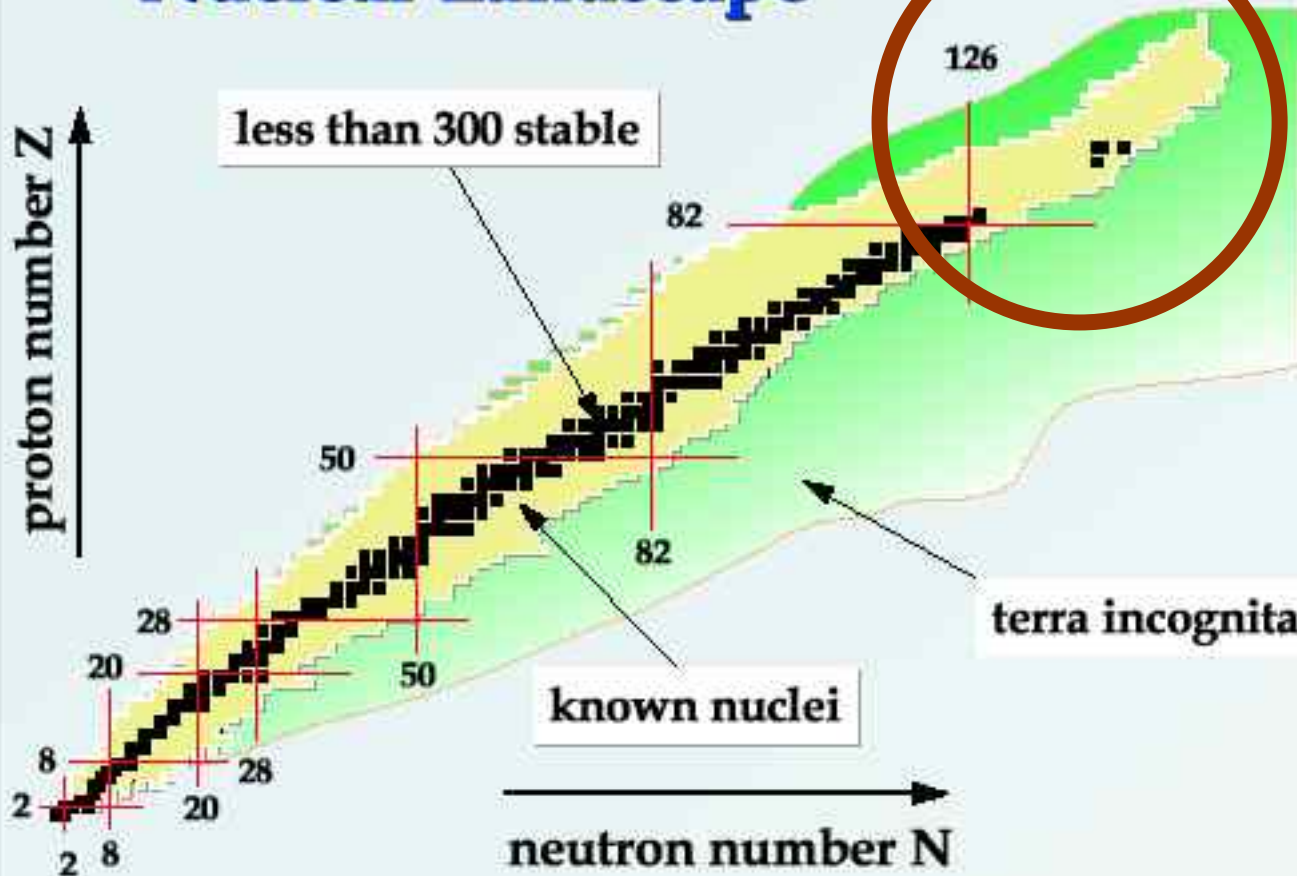
# Ground State Properties

- **Binding Energies: Well Reproduced**  
**~ 0.25% of Expt. (On the Average)**
- **$\beta$ : Reasonable: Consistent with**  
**Moller – Nix Systematics**
- **Charge Radii: Upto 2<sup>nd</sup> Decimal**
- **Isotopic Shifts: Reproduced**



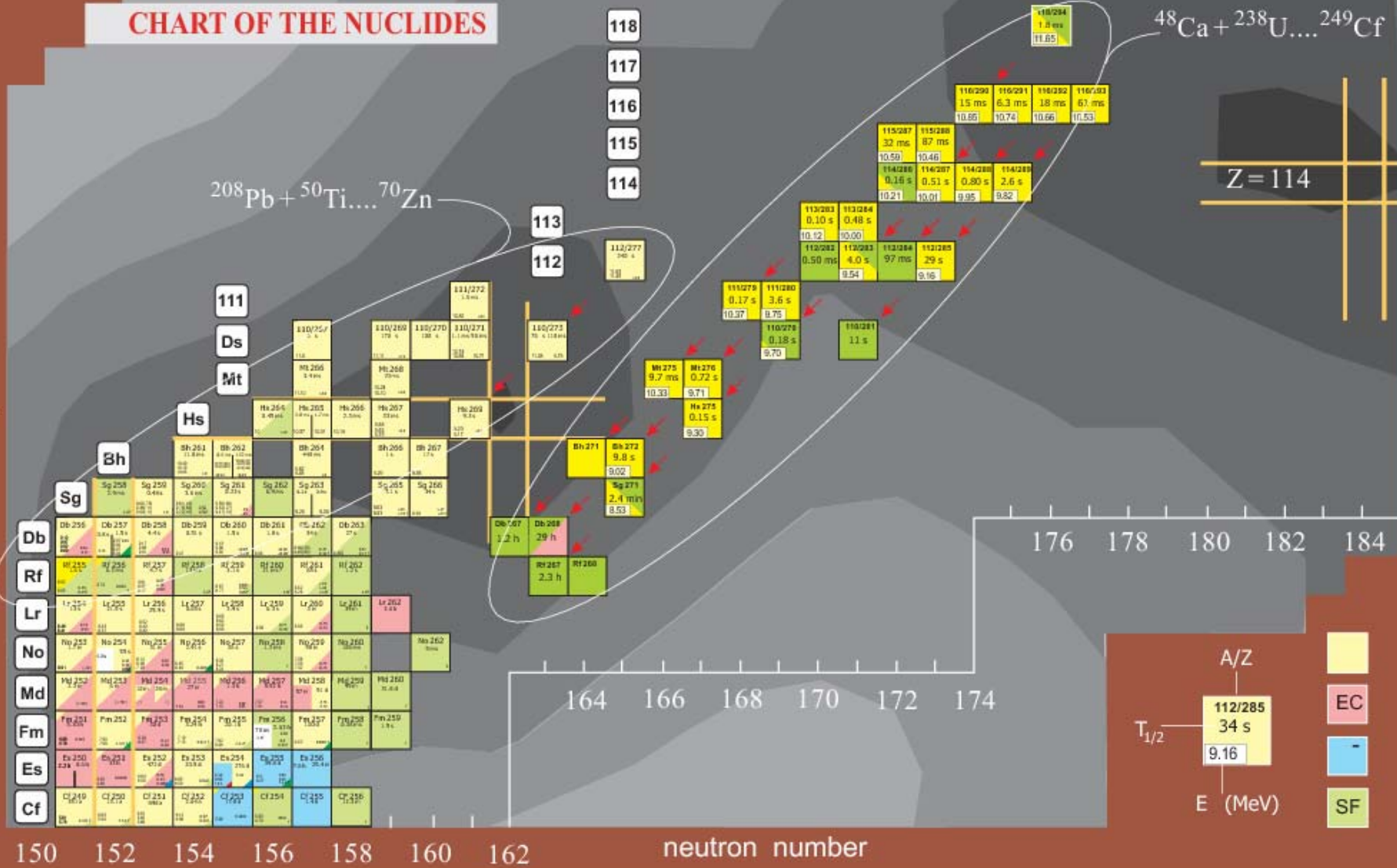
# Nuclear Landscape

proton number Z



# CHART OF THE NUCLIDES

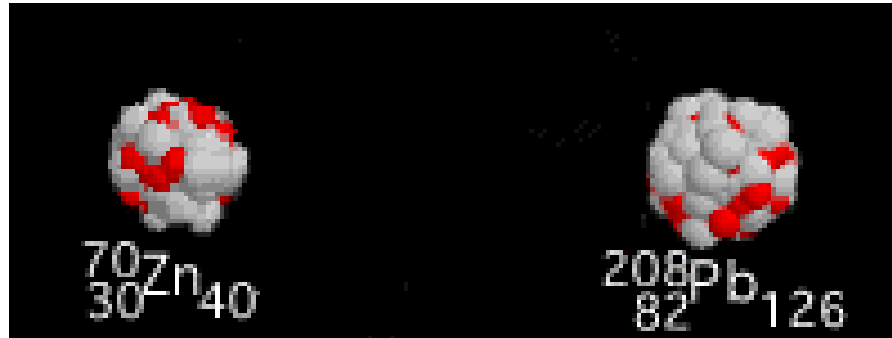
proton number



Yu. Ts. Oganessian *et al.*, JINR Preprint E7-2004-160



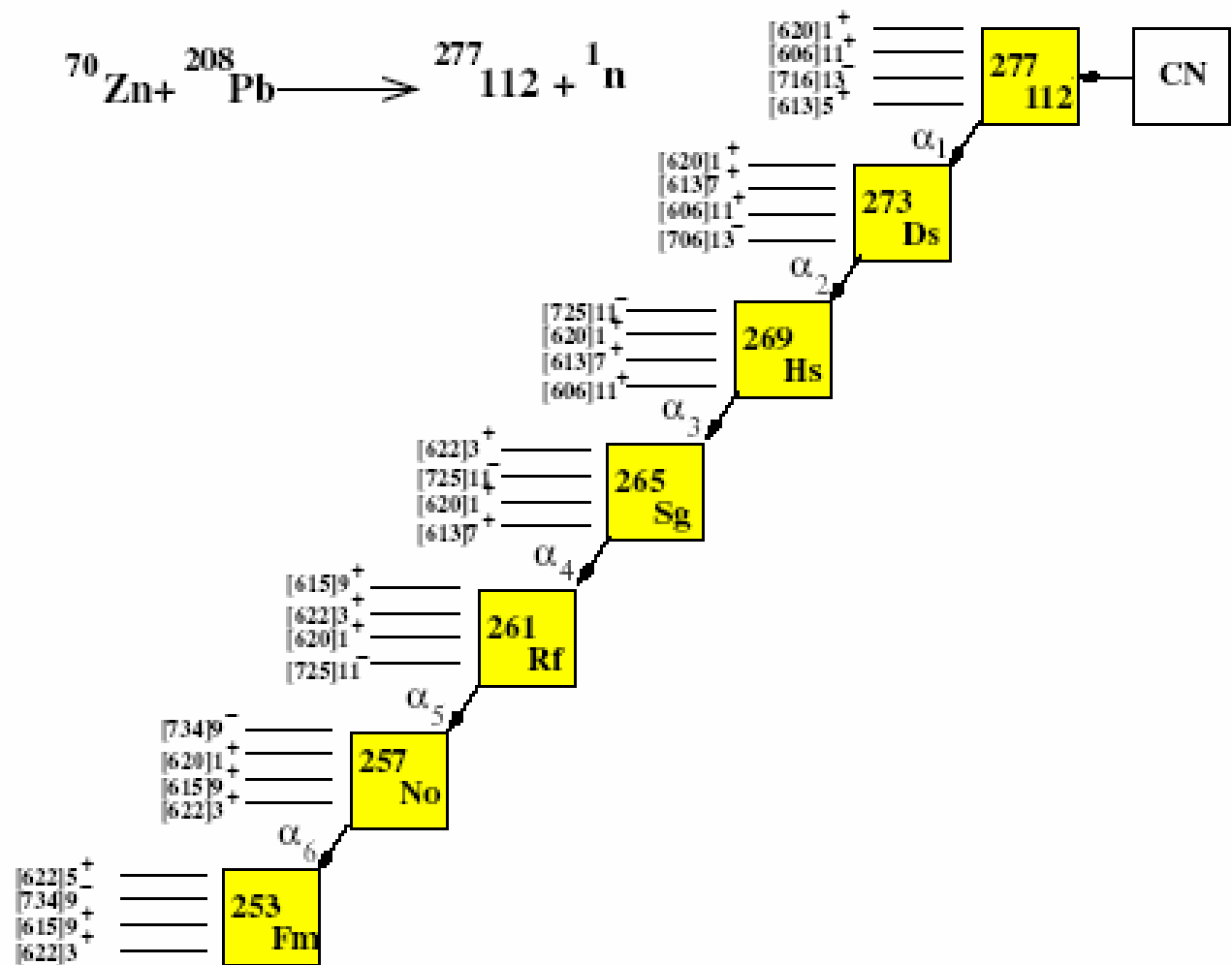
# Production: (Cold Fusion)



# Decay: ( $\alpha$ Emission)



<http://ie.lbl.gov/education/glossary/glossaryf.htm>



S. Hofmann et al, Z. Phys. A 354 (1996) 229.

# **:Superheavy Nuclei: (Half Lives)**

## **Calculation:**

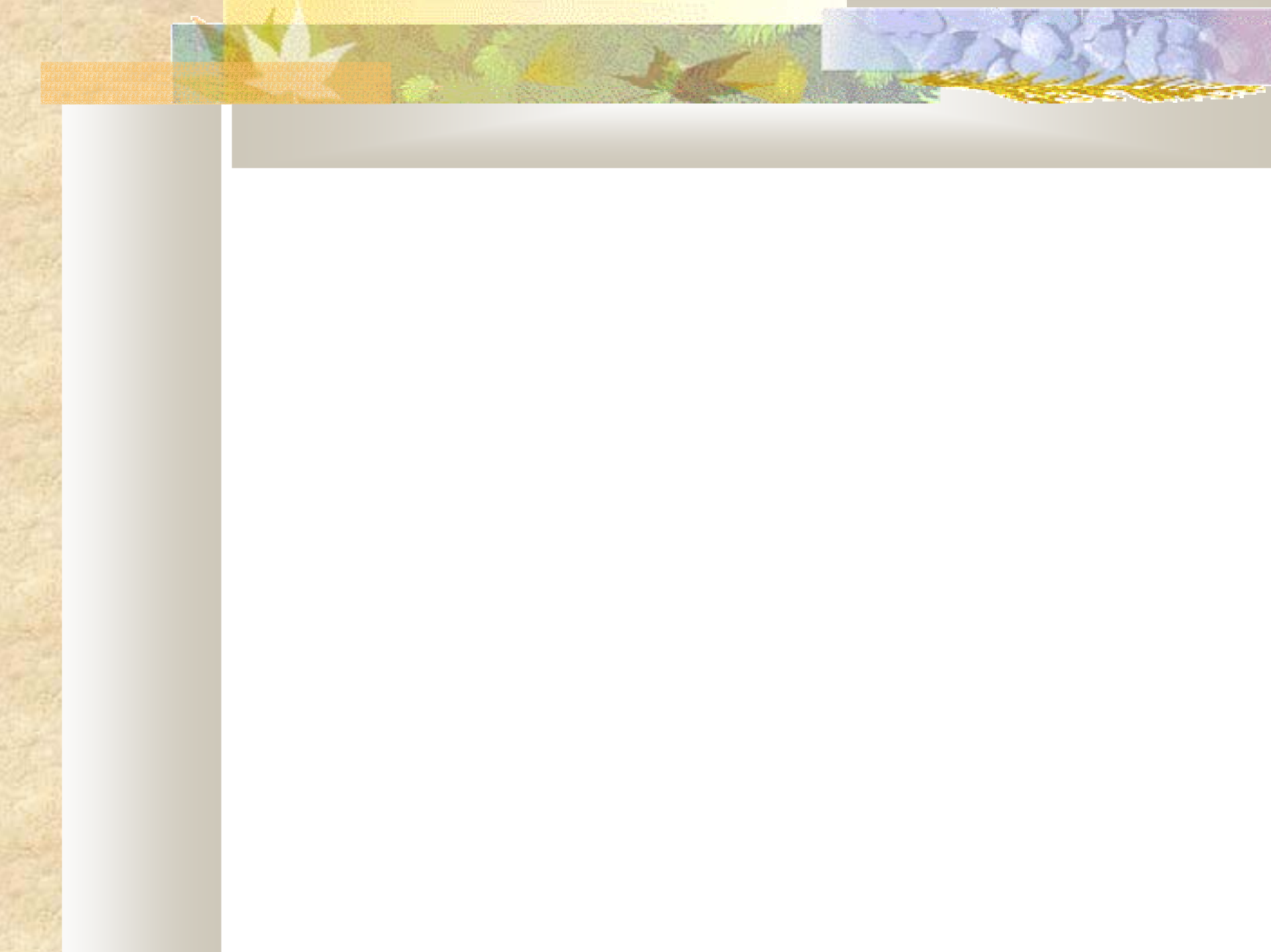
**Ground State Properties: RMF**

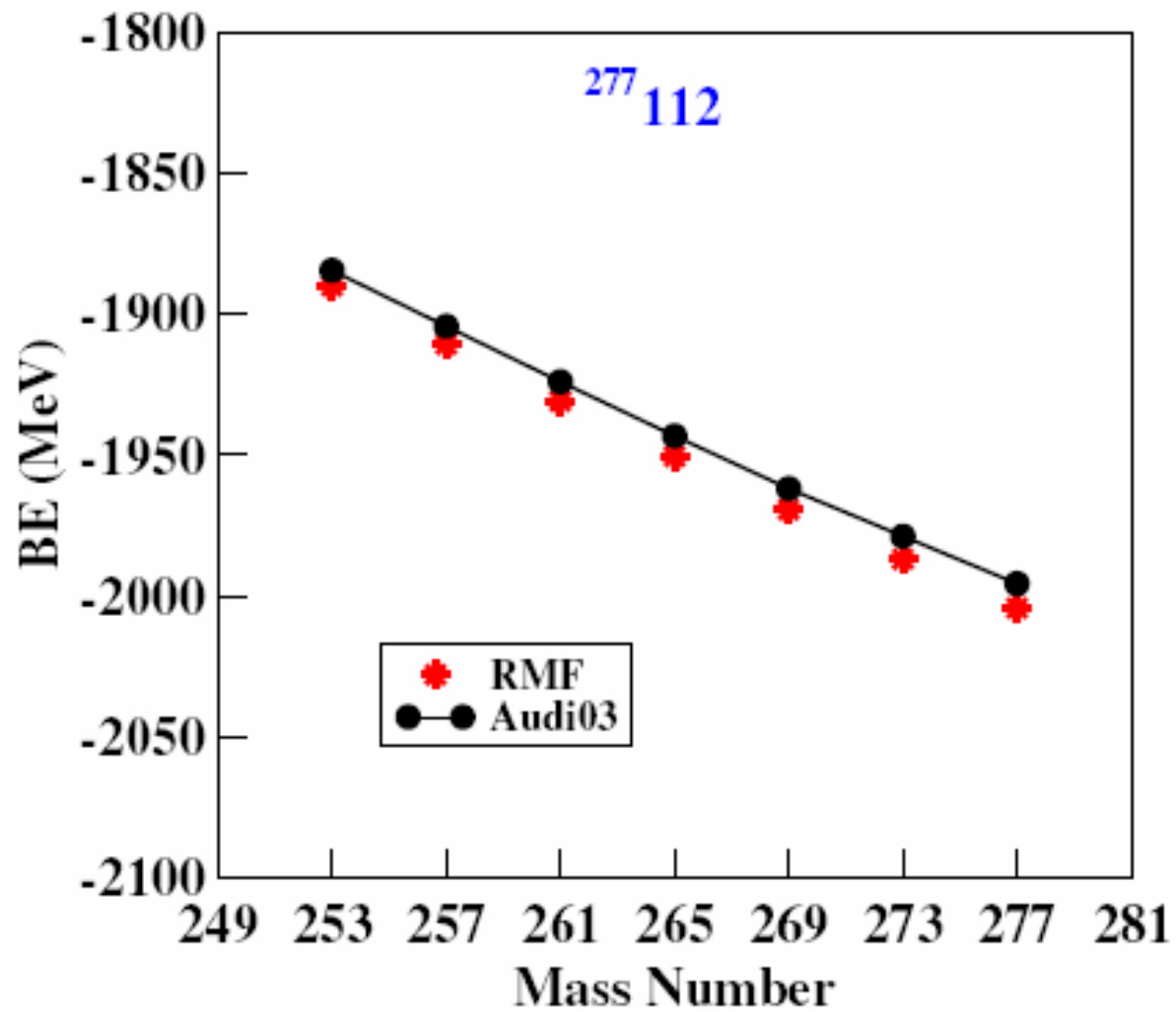
**-- Well Reproduced (BE,  $\beta$ , etc.)**

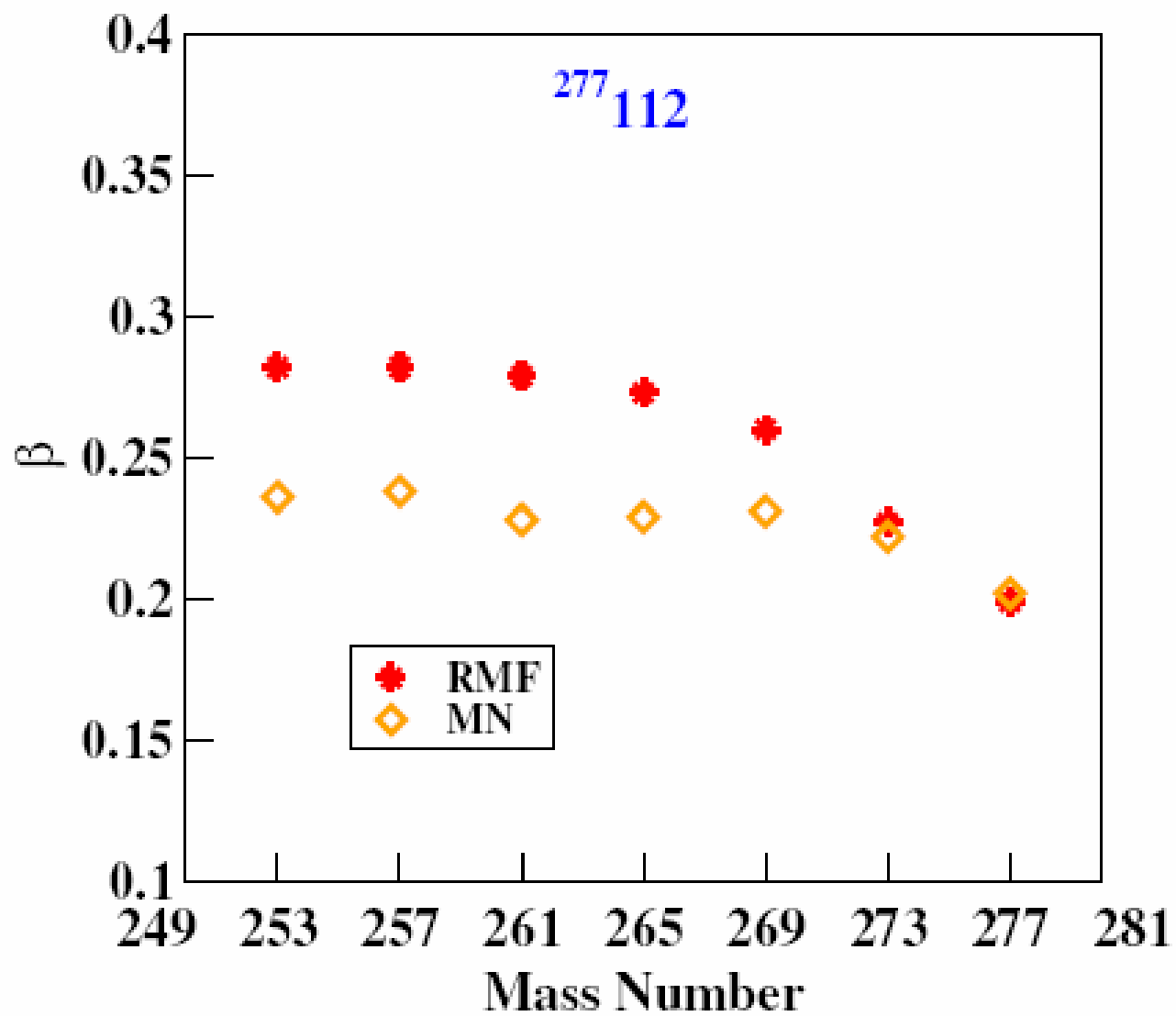
**Half Lives: WKB Approximation**

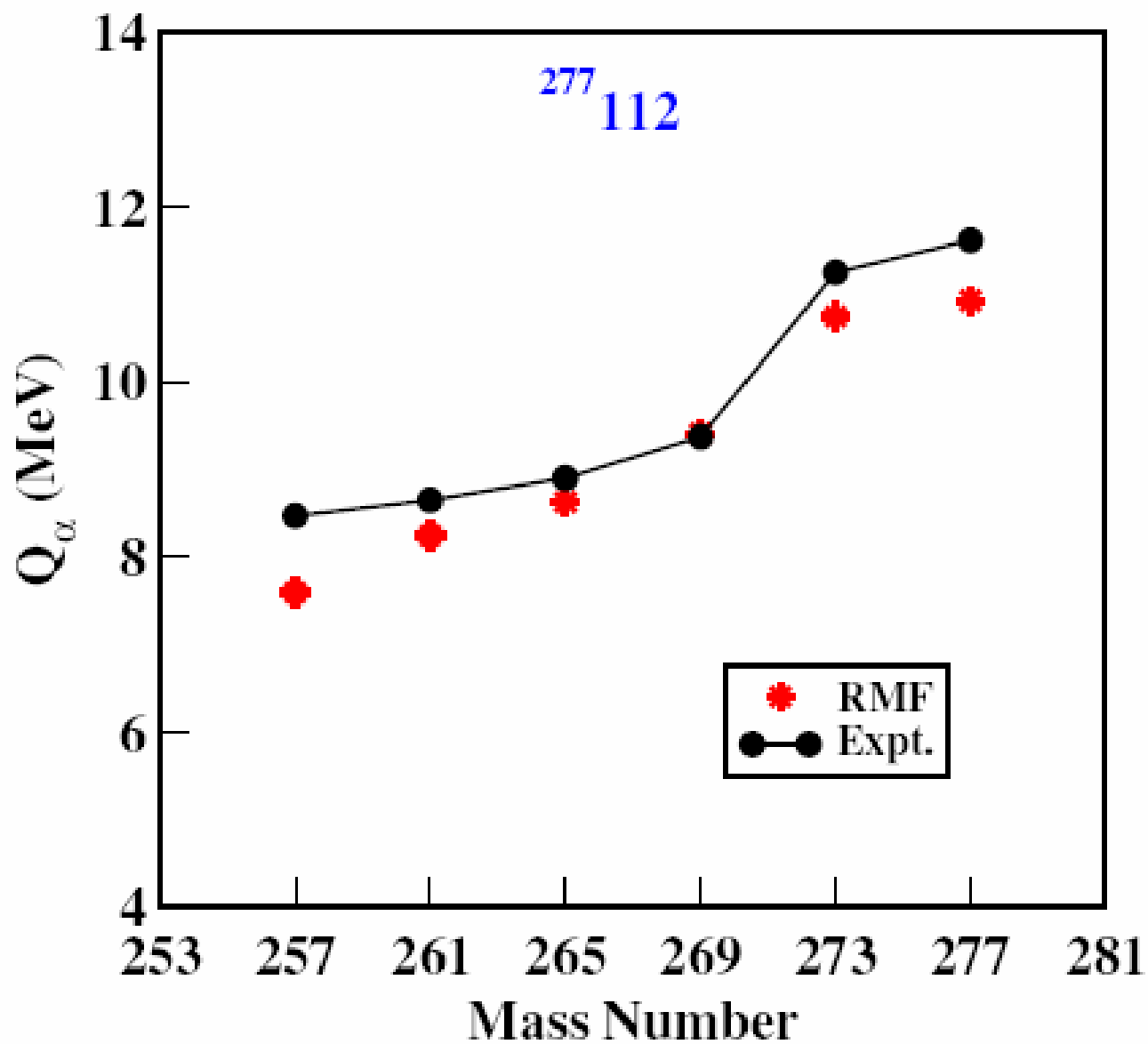
**-- Requires: Q Values + Potentials**

**→  $\alpha$  - Daughter Interaction Potentials  
(Double Folding Model)**

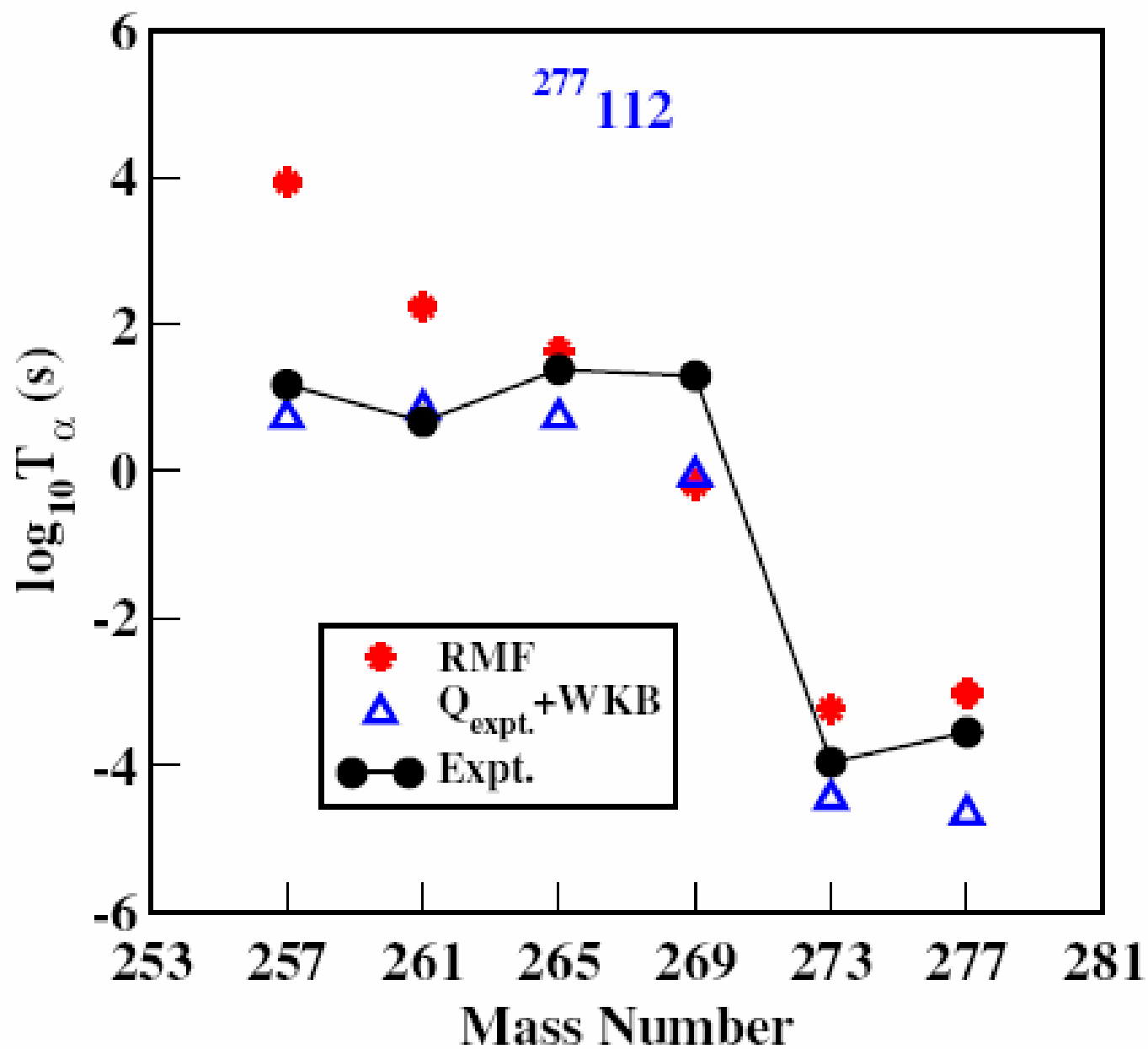












## Summary & Conclusions

- **Q Values: Well Reproduced**
- **Experimental Q values + WKB → Reproduces half lives well → Double Folding Potential Reliable**
- **Half Lives Depend Sensitive on Q values**



**RMF IS SUCCESSFUL**





## **Recent Developments:**

### **Large Shell-Model Calculations:**

**Large Dimensions  
Effective Interaction**

**ANTOINE (E.Courier, Strasburg, France)**

**OXBASH (B.A.Brown; Michigan, USA)**

**DUSM (Vallieres + Novoselsky, Phil., USA)**

**sd – shell ( $^{16}\text{O}$  Core)  $\rightarrow$  Good**

**pf – shell ( $^{40}\text{Ca}$  Core)  $\rightarrow$   
Yet to be Achieved Fully**

**Limits:  $10^7$  –  $10^8$  Basis States**

**How Much Dependence on Effective Interaction?**

**What can we Learn from Eigenvectors with  
Billions of Components?**



**Exotic Nuclei: Asymptotics is Important**  
**Continuum Shell Model**

**Ab – Initio : No Core Shell Model (NCSM)**  
**With nn, nnn Interaction**

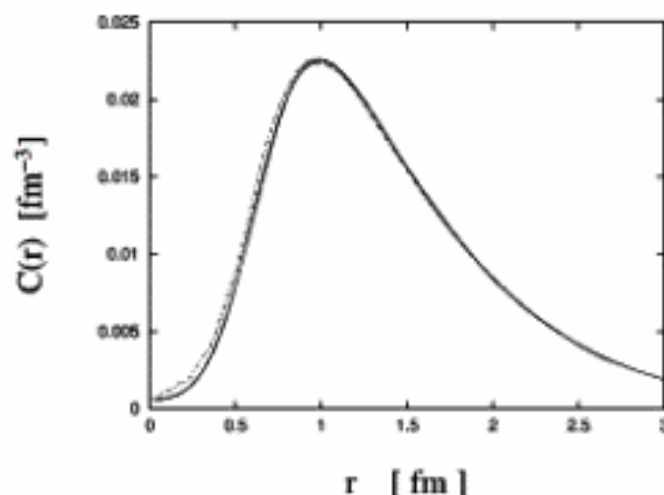
- Hyperspherical harmonic variational:
- Green's function Monte Carlo:  $A \leq 7$
- No-core shell model:  $A \leq 12$

# Benchmark calculation for $A=4$

- Test calculation with realistic interaction: all methods agree.

$$\langle \Psi | \sum_{k < l}^4 \delta(r - r_{kl}) | \Psi \rangle$$

Method	$\langle T \rangle$	$\langle V \rangle$	$E_b$	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	-128.33(10)	-25.94(5)	1.485(3)
CRCGV	102.30	-128.20	-25.90	1.482
SVM	102.35	-128.27	-25.92	1.486
HH	102.44	-128.34	-25.90(1)	1.483
GFMC	102.3(1.0)	-128.25(1.0)	-25.93(2)	1.490(5)
NCSM	103.35	-129.45	-25.80(20)	1.485
EIHH	100.8(9)	-126.7(9)	-25.944(10)	1.486



- But  $E_{\text{expt}} = -28.296 \text{ MeV} \Rightarrow$  need for three-nucleon interaction.





**$^{16}\text{O}$  Calculations  
in  
2010!**

binding energy difference (MeV)

