Great ideas around 1950s

Approach!

- Skyrme (1958): model with zero range: two-body, three-body, tensor
- Arima & Horie (1954): first configuration mixing calculations
- BCS (1957)...
- Bogoliubov (1958)...
- 1960s，Particle Number Conserving (PNC) method for pairing correction by Li-Ming Yang and Jin-Yan Zeng 杨立铭, 曾谨言, 物理学报. 1964, **20**: 846-862
- 1965, Coherent effect with short range interaction, Min Yu and Zong-Ye Zhang et al 张宗烨, 余友文, 朱熙泉, 李清润,于敏, 科学通报, 1965, 10: 1-7
- …

Nuclear theory

- *Ab inito*

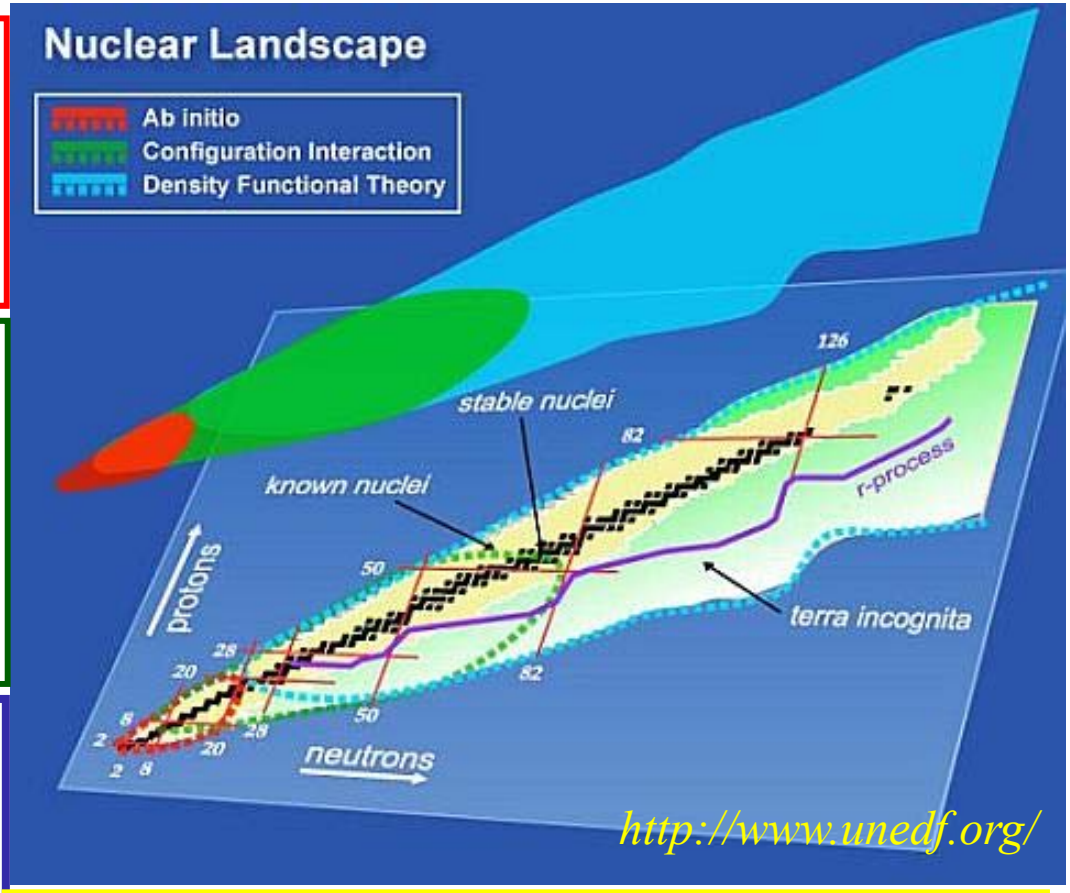
  Navratil, Vary, Barrett Phys. Rev. Lett. 84 (2000) 5728
  Bogner, Furnstahl, Schwenk
  Prog. Part. Nucl. Phys. 65 (2010) 94
  …

- Shell model

  Caurier, Martínez-Pinedo, Nowacki, Poves, Zuker,
  Rev. Mod. Phys. 77 (2005) 427
  Otsuka, Honma, Mizusaki, Shimizu, Utsuno,
  Prog. Part. Nucl. Phys.47(2001)319
  Brown, Prog. Part. Nucl. Phys. 47 (2001) 517
  …

- **Density functional theory**

  Jones and Gunnarsson,
  Rev. Mod. Phys., 61 (1989) 689
  Bender, Heenen, Reinhard,
  Rev. Mod. Phys., 75 (2003) 121
  Ring, Prog. Part. Nucl. Phys.37(1996)193
  Meng, Toki, Zhou, Zhang, Long, Geng,
  Prog. Part. Nucl. Phys. 57 (2006) 470
  …



密度泛函理论有希望给出核素图上所有原子核性质的统一描述

Relativistic Density Functional for Nuclear Structure，International Review of Nuclear Physics Vol 10（World Scientific, 2016）

Hohenberg-Kohn theorem (1964)

The exact energy of a quantum mechanical many body system is a functional of the local density $\rho(\mathbf{r})$

$$E[\rho] = \langle \Psi | H | \Psi \rangle$$

This functional is universal. It does not depend on the system, only on the interaction.

One obtains the exact density $\rho(\mathbf{r})$ by a variation of the functional with respect to the density

note:

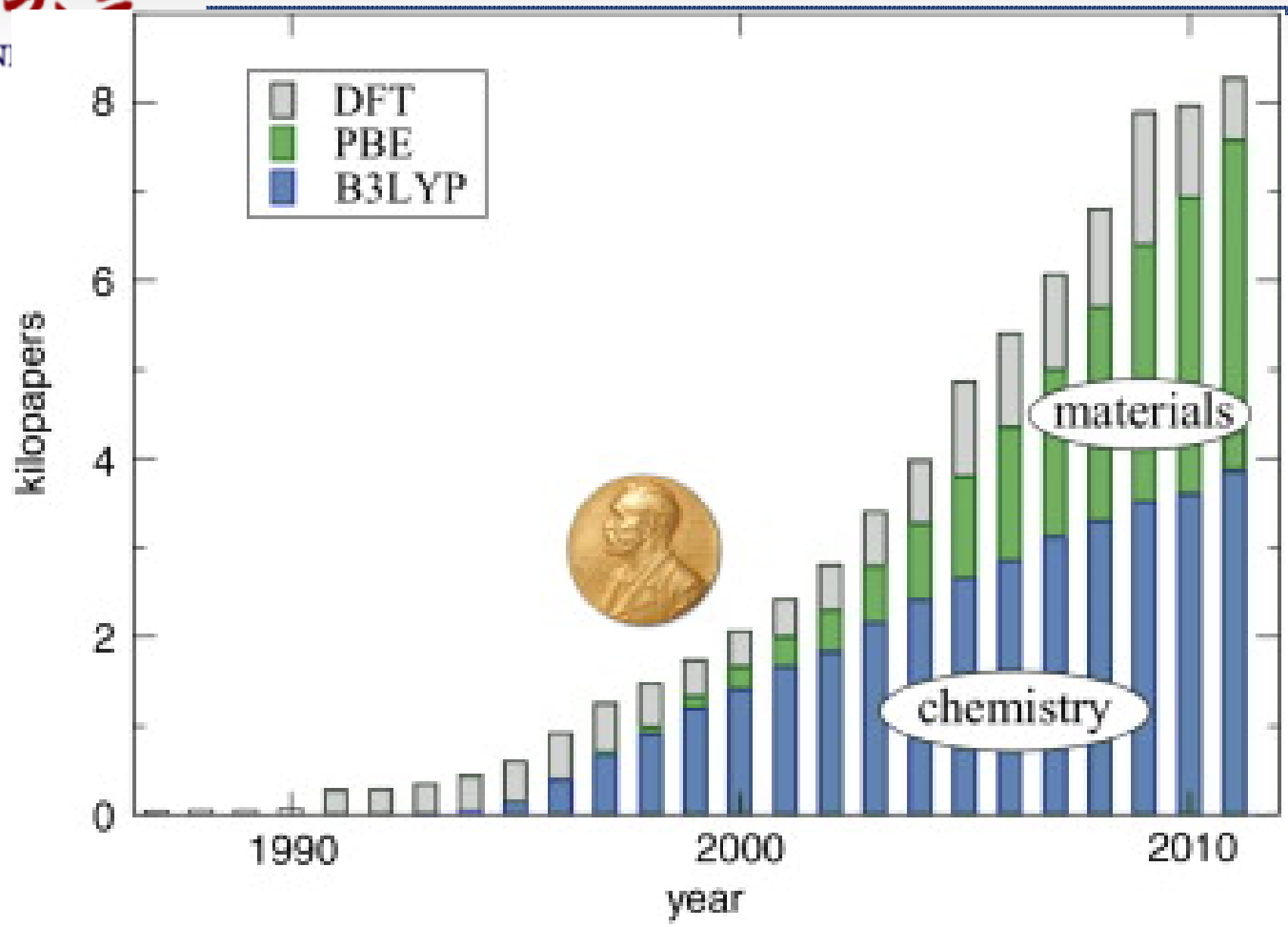
$\rho(\mathbf{r})$ is a function of 3 variables.

$\Psi(\mathbf{r}_1 \ldots \mathbf{r}_N)$ is a function of $3N$ variables.

Hohenberg

Kohn

 Nobel Prize in Chemistry 1998



The numbers of papers (in kilopapers) corresponding to the search of a topic “DFT” in Web of Knowledge (grey) for different and the most popular density functional potentials: B3LYP citations (blue), and PBE citations (green, on top of blue).

K. Burke, Perspective on density functional theory, J. Chem. Phys., 136 (2012) 150901 [1-9]

Density functional theory in nuclei

Nuclear DFT has been introduced by **effective Hamiltonians**: by Vautherin and Brink (1972) using the Skyrme model as a vehicle

$$E = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff}(\hat{\rho}) | \Phi \rangle = E[\hat{\rho}]$$

Based on the philosophy of Bethe, Goldstone, and Brueckner one has a density dependent interaction in the nuclear interior G(ρ)

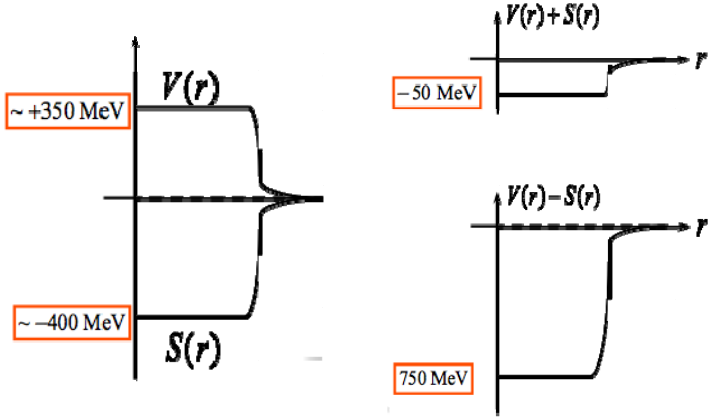
At present, the ansatz for E(ρ) is phenomenological:

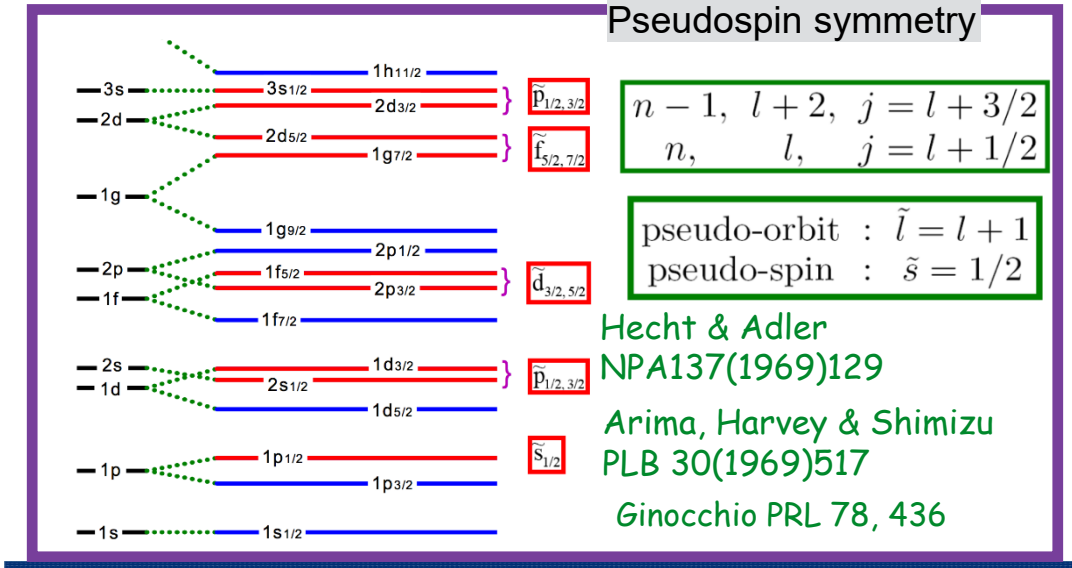
- Skyrme: non-relativistic, zero range
- Gogny: non-relativistic, finite range (Gaussian)
- CDFT: Covariant density functional theory

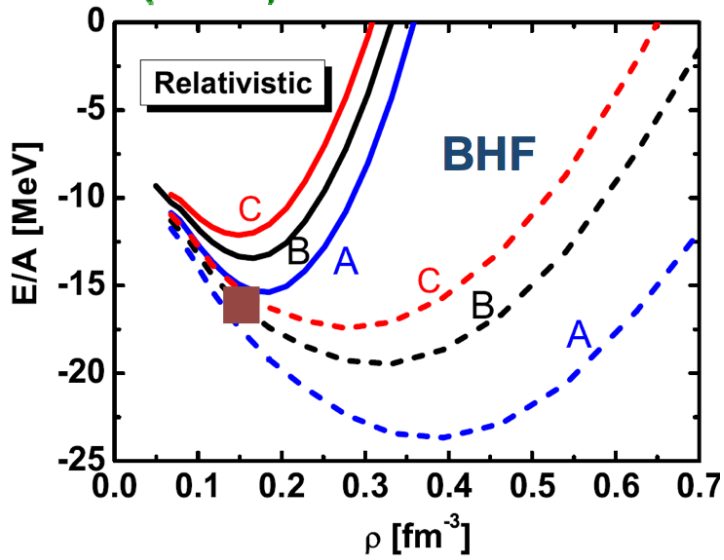
Why Covariant?

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).







Brockmann & Machleidt, PRC42, 1965 (1990)

History of CDFT

- Meson theory of nuclear force. Yukawa 1935.
- Relativistic field theory of nuclear many-body system based on baryon and classic scalar meson; nuclear saturation may come from strong nonlinear self-interaction of scalar field. Schiff 1951.
- Nuclear saturation mechanism from linear theory. Teller 1955.
- Calculated nuclear structure with relativistic Hartree method. Rozsnayi 1961.
- Strong nonlinear coupling of meson fields may result in abnormal nuclear matter. Lee and Wick 1974.
- Renormalizable RMF with scalar and vector meson fields. Walecka 1974.
- Incompressibility: nonlinear coupling terms of σ. Boguta and Bodmer 1977.
- Introducing ρ and π meson field, and apply to finite nuclei. Serot 1979.

Nuclear relativistic mean field theory with σ, ω, and ρ mesons was founded!

History of CDFT

- **Full relativistic Brueckner Hartree-Fock calculations to determine the properties of symmetric nuclear matter at various densities.**

  Brockmann and Toki 1992.

- **Parameter sets:**

  nonlinear coupling: NLl Reinhard1986, NLSH Sharma1993, TM1 Sugahara1994, NL3 Lalazissis1997, PK1 Long2004

  density-dependent: TW99 Typel1999, DD-ME1 Niksic2002, PKDD Long2004

  … PKO1 Long2006 … PC-PK1 Zhao2010

- **Deformed nucleus**

  S.-J. Lee et al., Phys. Rev. Lett. 57, 2916 (1986)
  - **Comment: R. J. Furnstahl, et al, Phys. Rev. Lett. 60, 162 (1988).**
  - **Reply: Suk-Joon Lee, Phys. Rev. Lett. 60, 163 (1988).**
  - **Erratum: Phys. Rev. Lett. 59, 1171 (1987).**

  W. Pannert, P. Ring, and J. Boguta, Phys. Rev. Lett. 59, 2420 (1987)
  C. E. Price and G. E. Walker, Phys. Rev. C 36, 354 (1987).

History of CDFT

- **Coordinate space**
- **Spherical: Spherical nucleus:**

  Meng & Ring, PRL77,3963 (96); 80,460 (1998)

  Meng, NPA 635, 3-42 (1998)

- **Deformed: in grid or coupled channel equations**

  Price, and Walker, Phys. Rev. C 36, 354 (1987).

  Zhou, Meng, and Ring, in Nuclear Physics Trends,AIP Conf. Proc., Vol. 865, edited by Y.-G. Ma and A. Ozawa (AIP, 2006), p. 90.

- **3D lattice:**

  Hagino and Tanimura, Phys. Rev. C 82, 057301 (2010).

  Tanimura, Hagino, and Liang, Prog. Theor. Exp. Phys. (2015) 073D01.

  Ren, Zhang, and Meng, Phys. Rev. C 95, 024313 (2017)

History of CDFT

Numerical technology

- **H.O. : matrix diagonalization**

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

- **Woods-Saxon basis: spherical nucleus**

  Zhou, Meng, and Ring, Phys. Rev. C 68, 034323 (2003). RH

  Long, Van Giai, and Meng, Phys. Lett. B640, 150 (2006). RHF

  Long, Ring, Meng, and Van Giai, PRC81 , 031302 (2010). RHFB

- **Woods-Saxon basis: Deformed nucleus**

  Zhou, Meng, Ring and Zhao, Phys. Rev. C 82, 011301 (2010)

  Li, Meng, Ring, Zhao, and Zhou, Phys. Rev. C 85, 024312 (2012)

  Chen, Li, Liang, and Meng, Phys. Rev. C 85, 067301 (2012)

  Li, Meng, Ring, Zhao, and Zhou, Chin. Phys. Lett. 29, 042101 (2012).

- **Woods-Saxon basis: triaxial deformed nucleus**

  …

History of CDFT

Single-particle resonant states

- **Scattering phase shift method**

  Cao and Ma, Phys. Rev. C 66, 024311 (2002).

- **Analytic continuation in the coupling constant**

  Yang, J. Meng, and S.-G. Zhou, Chin. Phys. Lett. 18, 196 (2001).

- **Box discretization approach**

  Zhang, Zhou, Meng, and Zhao, Phys. Rev. C77, 014312 (2008).

- **complex scaling method**

  Guo, Fang, Jiao, Wang, and Yao, Phys.Rev. C 82, 034318 (2010).

- **Jost function approach**

  Lu, Zhao, and Zhou, Phys. Rev. Lett. 109,072501 (2012).

- **Green's function method**

  Sun, Zhang, Zhang, Hu, and Meng, Phys. Rev. C 90, 054321 (2014)

  …..

History of CDFT

Nuclear ground states

- **Breaking the axial symmetrys**

  Meng, Peng, Zhang, and Zhou, Phys. Rev. C 73, 037303 (2006).
  Peng, Sagawa, Zhang, Yao, Zhang, and Meng, Phys. Rev. C 77, 024309 (2008).
  Yao, Qi, Zhang, Peng, Wang, and Meng, Phys. Rev. C 79, 067302 (2009).
  Li, Zhang, and Meng, Phys. Rev. C 83, 037301 (2011).
  Lu, Zhao, Zhou, Phys. Rev. C 84, 014328 (2011).

- **Breaking the reflection symmetry**

  Rutz, Maruhn, Reinhard, and Greiner, Nucl. Phys. A 590, 680 (1995).

  Geng, Meng, and Toki, Chin. Phys. Lett. 24, 1865 (2007).

- **Breaking the axial and the reflection symmetries**

  Lu, Zhao, Zhou, PRC 85, 011301 (2012)
  Zhao, Lu, Zhao, Zhou, PRC 86, 057304 (2012)
  Lu, Zhao, Zhao, Zhou, PRC 89, 014323 (2014)
  Zhao, Lu, Vretenar, Zhao, Zhou, PRC 91, 014321 (2015)

History of CDFT

Among the mesons which mediate the nucleon interaction, the π meson might be one of the most important. However, the one π exchange cannot be taken into account if we exclude the exchange (Fock) terms.

- **RHF without meson self-interactions**
  Bouyssy, Marcos, Mathiot and Van Giai; Phys. Rev. Lett. (1985)
  Bouyssy, Mathiot, van Giai and Marcos, Phys. Rev. C (1987)
- **RHF with the nonlinear self-coupling terms**
  Bernardos, Fomenko, Giai, Quelle, Marcos, Niembro,and Savushkin, Phys. Rev. C (1993).
  Marcos, Savushkin, Fomenko, Lopez-Quelle and Niembro J. Phys. G (2004).
- **DDRHF & DDRHFB**
  Long, Van Giai and Meng, Phys. Lett. B (2006)
  Long, Ring, Van Giai and Meng, Phys. Rev. C (2010)

P. Ring: Should everything be recalculated with Fock terms?

Liang, Zhao, Ring, Roca-Maza and Meng, Phys. Rev. C 86, 021302(R) (2012)
Localized form of Fock terms in nuclear covariant density functional theory

History of CDFT

- **Rotating nucleus**

  Koepf and Ring NPA (1989)
  Kaneko, Nakano, and Matsuzaki PLB (1993)

- **Superdeformed rotating nucleus and identical bands**

  Koepf and Ring NPA (1990), Konig and Ring NPA (1993)

- **Magnetic rotation**

  Madokoro, Meng, Matsuzaki, and Yamaji PRC (2000)
  Peng, Meng, Ring, and Zhang PRC (2008)
  Zhao, Zhang, Peng, Liang, Ring , and Meng PLB (2011)

- **Antimagnetic rotation**

  Zhao, Peng, Liang, Ring, and Meng PRL (2011)
  Zhao, Peng, Liang, Ring, and Meng PRC (2012)

- **Isotope shift in Pb**

  Sharma, Lalazissis and Ring (1993)

- **Pseudospin symmetry**

  Ginocchio PRL (1997) Liang, Meng and Zhou Phys. Rep. (2015)

History of CDFT

Dynamical calculations:

- **Time-Dependent Relativistic Theory**
  D. Vretenar, H. Berghammer, and P. Ring, Phys. Lett. B (1993), Nucl. Phys. A (1995)

- **Small Amplitude Oscillations (RPA)**
  - **Linear σ–ω RMF model:** lack of non-linear terms?
    M. L'Huillier, Van Giai, Phys. Rev. C (1989)
  - **With nonlinear self-interaction terms:** different from TD RMF?
    Ma, Van Giai, Toki, M. L'Huillier, Phys. Rev. C (1997)
    Ma, Toki, Van Giai, Nucl. Phys. A (1997)
  - **With negative-energy states in the Dirac sea:** equivalent to TD RMF
    Ring, Ma, Van Giai, Vretenar, Wandelt, and Cao (2001)
  - **With pairing (RHB+QRPA)**
    Paar, Ring, Niksic, and Vretenar, Phys. Rev. C (2003), (2004)
  - **With temperature**
    Y. Niu, Paar, Vretenar, and Meng, Phys. Lett. B (2009), Phys. Rev. C (2011)
  - **With Fock (DDRHF(B)+(Q)RPA):** self-consistency is achieved
    Liang, Van Giai, and Meng, Phys. Rev. Lett. 101, 122502 (2008)
    Niu, Niu, Liang, Long, Niksic, Vretenar, and Meng, Phys. Lett. B723, 172 (2013)

History of CDFT

To describe nuclear spectroscopy, one has to go beyond the mean-field approximation, namely to restore the broken symmetry and mix the different shape configurations, especially for the transitional nuclei with the soft potential.

- **Angular momentum projection+generator coordinator method (3DAMP+GCM)**

  Yao, Meng, Pena Arteaga, Ring, Chin. Phys. Lett. 25 (2008) 3609.
  Yao, Meng, Ring, Pena Arteaga, Phys. Rev. C 79 (2009) 044312
  Yao, Meng, Ring, Vretenar, Phys. Rev. C 81 (2010) 044311
  Yao, Mei, Chen, Meng, Vretenar, Ring, Phys. Rev. C 83 (2011) 014308
  Yao, Meng, Ring, Li, Li, Hagino, Phys. Rev. C 84 (2011) 024306

- **EDF-based 5-dimensional collective Hamiltonian**

  Niksic, Li, Vretenar, Prochniak, Meng, Ring, Phys. Rev. C 79 (2009) 034303
  Li, Nikšic, Vretenar, Meng, Lalazissis, Ring, Phys. Rev. C 79 (2009) 054301
  Li, Nikšic, Vretenar, Meng, Phys. Rev. C 80 (2009) 061301(R)
  Li, Nikšic, Vretenar, Meng, Phys. Rev. C 81 (2010) 034316
  Li, Nikšic, Vretenar, Chen, Meng, Phys. Rev. C 84 (2011) 054304
  Li, Li, Xiang, Yao, Meng, Phys. Lett. B 717 (2012) 470

History of CDFT

Relativistic Brueckner Hartree-Fock calculation for finite nucleus

- **Relativistic Brueckner–Hartree–Fock Theory for Finite Nuclei**

  Shen, Hu, Liang, Meng, Ring, Zhang, Chin. Phys. Lett. 33 (2016) 102103

- **Fully self-consistent relativistic Brueckner-Hartree-Fock theory for finite nuclei.**

  Shen, Liang, Meng, Ring, Zhang, Phys. Rev. C 96, 014316 (2017)

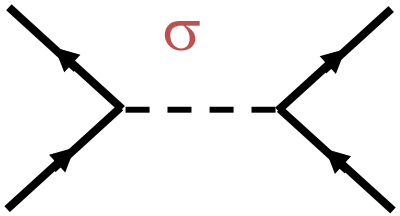
Relativistic Density Functional Theory

- Brief History
- Covariant Density Functional Theory
- Numerical details
- Nuclear ground state properties
- Nuclear excited state properties
- Interface with astrophysics and standard model
- Summary & Perspectives

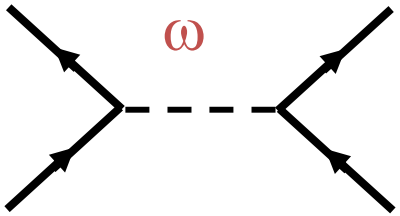
Brief introduction of CDFT

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

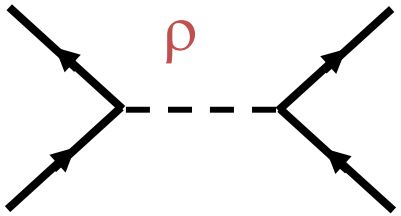
Strong force: Meson-exchange of the nuclear force



$(J^{\pi}\ T)=(0^{+}0)$



$(J^{\pi}\ T)=(1^{-}0)$



$(J^{\pi}\ T)=(1^{-}1)$

Sigma-meson:
attractive scalar field

Omega-meson:
Short-range repulsive

Rho-meson:
Isovector field

Electromagnetic force: The photon

Brief introduction of CDFT

Lagrangian:

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

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

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

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

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

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

Hamiltonian:

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

$$=T+V$$

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

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

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

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

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

Fock

Energy density functional:

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

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

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

Equations of motion

For system with time invariance:

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

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

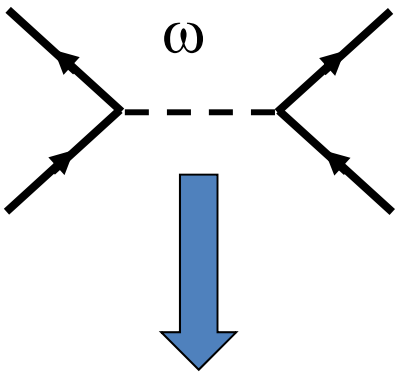
Same footing for

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

$$\left[-\Delta+m_\sigma^2\right]\sigma=-g_\sigma\rho_s-g_2\sigma^2-g_3\sigma^3$$
$$\left[-\Delta+m_\omega^2\right]\omega=g_\omega\rho_b-c_3\omega^3$$
$$\left[-\Delta+m_\rho^2\right]\rho=g_\rho\left[\rho_b^{(n)}-\rho_b^{(p)}\right]-d_3\rho^3$$

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

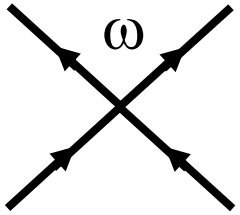
Effective Point-Coupling interaction



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

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

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



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

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

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

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

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

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

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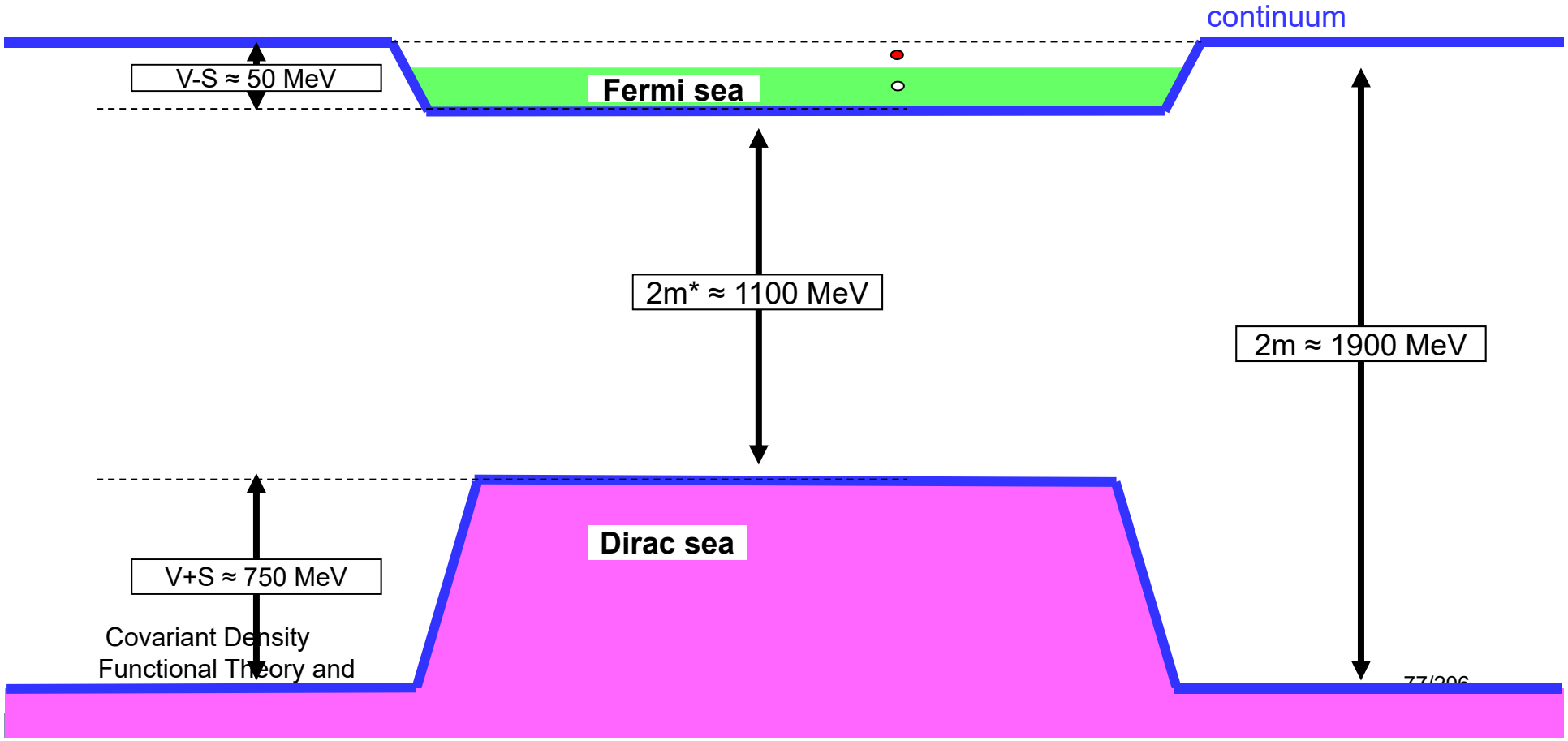
$$\begin{pmatrix} m+S+V & \boldsymbol{\sigma}(\boldsymbol{p}-\boldsymbol{V}) \\ \boldsymbol{\sigma}(\boldsymbol{p}-\boldsymbol{V}) & -m-S+V \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \varepsilon \begin{pmatrix} f \\ g \end{pmatrix}$$

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

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



Covariant Density Functional Theory and

Covariant density functional

Meson Exchange

Nonlinear parameterizations:

$$M, m_\sigma, m_\omega, m_\rho, g_\sigma, g_\omega, g_\rho, g_2, g_3, c_3, d_3$$

NL3, NLSH, TM1, TM2, PK1, …

Density dependent parameterizations:

$$M, m_\sigma, m_\omega, m_\rho, g_\sigma(\rho), g_\omega(\rho), g_\rho(\rho)$$

TW99, DD-ME1, DD-ME2, PKDD, …

Point Coupling

Nonlinear parameterizations:

$$M, \alpha_S, \alpha_V, \alpha_{TV}, \delta_S, \delta_V, \delta_{TV}, \beta_S, \gamma_S, \gamma_V$$

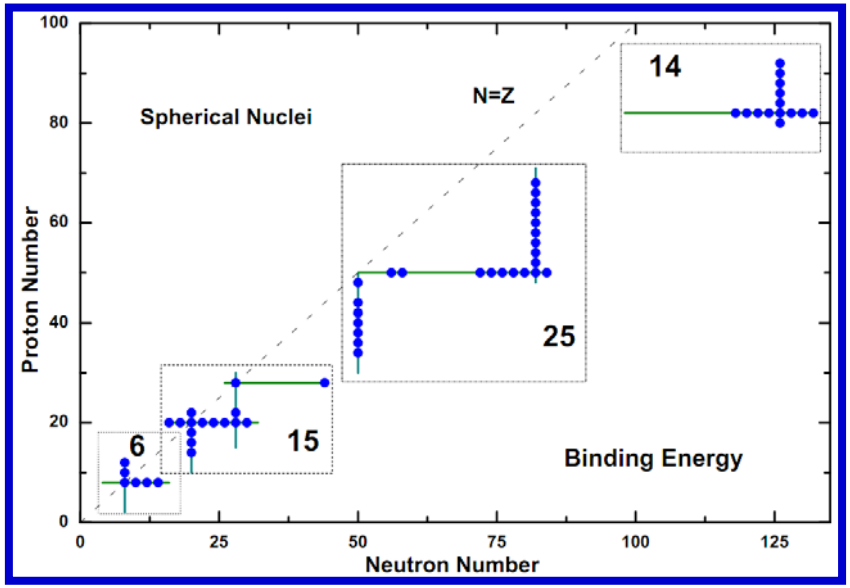
PC-LA, PC-F1, PC-PK1 …

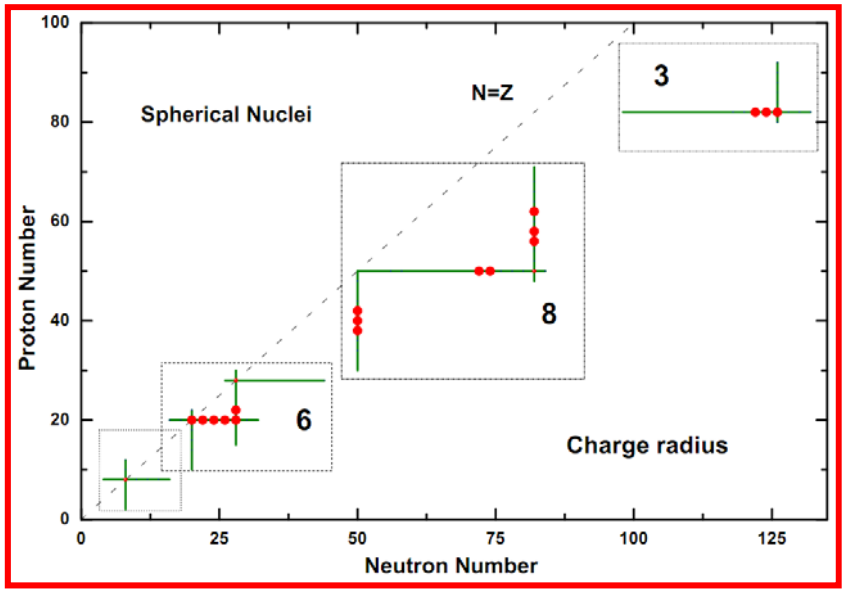
Density dependent parameterizations:

$$M, \delta_S, \alpha_S(\rho), \alpha_V(\rho), \alpha_{TV}(\rho)$$

DD-PC1, …

Covariant density functional PC-PK1





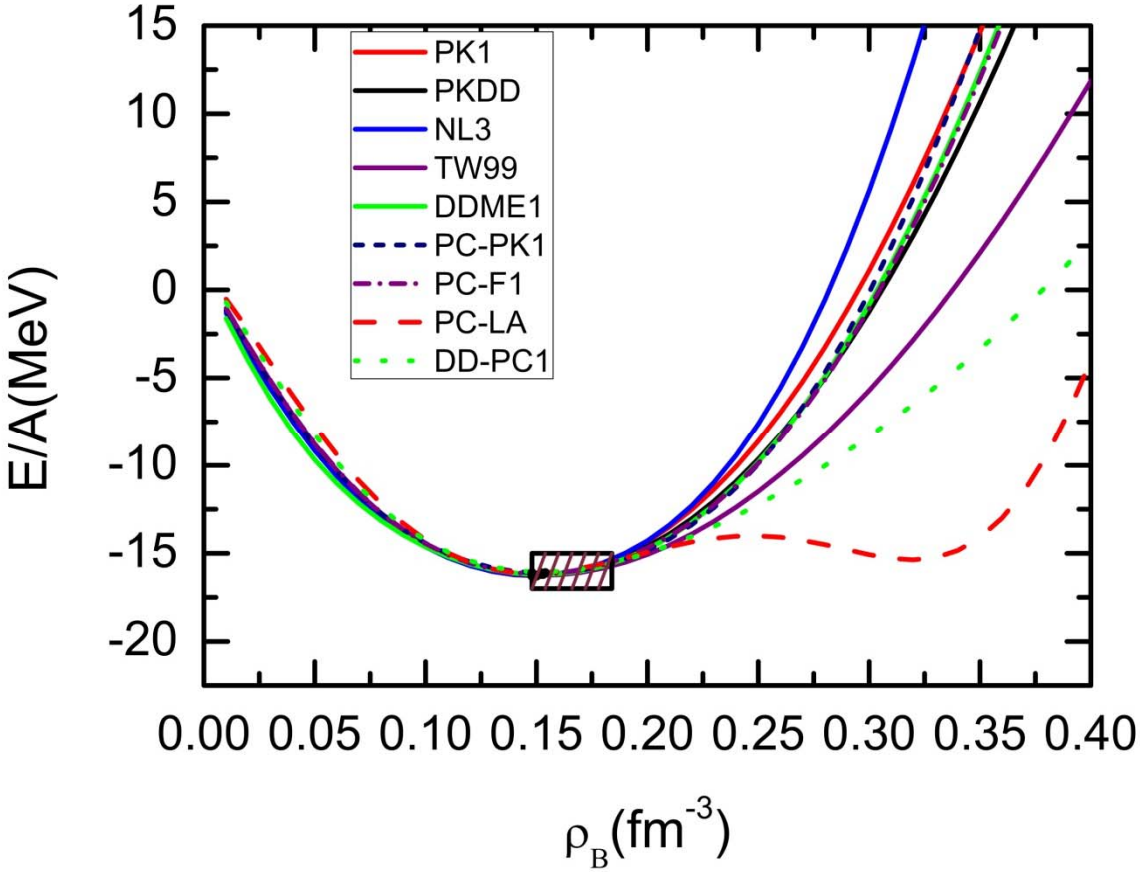
Coupl.	Cons.	PC-PK1	Dimension
α_S	$[10^{-4}]$	-3.96291	MeV^{-2}
β_S	$[10^{-11}]$	8.66530	MeV^{-5}
γ_S	$[10^{-17}]$	-3.80724	MeV^{-8}
δ_S	$[10^{-10}]$	-1.09108	MeV^{-4}
α_V	$[10^{-4}]$	2.69040	MeV^{-2}
γ_V	$[10^{-18}]$	-3.64219	MeV^{-8}
δ_V	$[10^{-10}]$	-4.32619	MeV^{-4}
α_{TV}	$[10^{-5}]$	2.95018	MeV^{-2}
δ_{TV}	$[10^{-10}]$	-4.11112	MeV^{-4}
V_n	$[10^{0}]$	-349.5	$\mathrm{MeV\ fm}^3$
V_p	$[10^{0}]$	-330	$\mathrm{MeV\ fm}^3$

Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)

Nuclear matter properties

Binding energy per nucleon:

$$E/A = \varepsilon/\rho - M$$



EOS of symmetric nuclear matter

Nuclear matter properties

Saturation point: $p(\rho_0) = 0$

- **Compressibility**

$$K(\alpha) \approx K_0 + K_{asy}\alpha^2, \alpha = (\rho_n - \rho_p)/(\rho_n + \rho_p)$$

$$K_0 = 9\rho_0^2 \left[\frac{\partial^2(\varepsilon/\rho)}{\partial\rho^2}\right]_{\rho_0}$$

$$K_{asy} = K_{sym} - 6L$$

- **Symmetry energy**

$$E_{sym}(\rho) = E_{sym}(\rho_0) + \frac{L}{3}\left(\frac{\rho-\rho_0}{\rho_0}\right) + \frac{K_{sym}}{18}\left(\frac{\rho-\rho_0}{\rho_0}\right)^2$$

$$E_{sym}(\rho) = \frac{1}{2}\left(\frac{\partial^2(\varepsilon/\rho)}{\partial t^2}\right)_{t=0}, t = \frac{\rho_n - \rho_p}{\rho_n}$$

$$L = 3\rho_0\left(\frac{\partial E_{sym}(\rho)}{\partial\rho}\right)_{\rho_0}, K_{sym} = 9\rho_0^2\left(\frac{\partial^2 E_{sym}(\rho)}{\partial\rho^2}\right)_{\rho_0}$$

- **Effective masses**

$$M_D^* = M^* = M + S$$

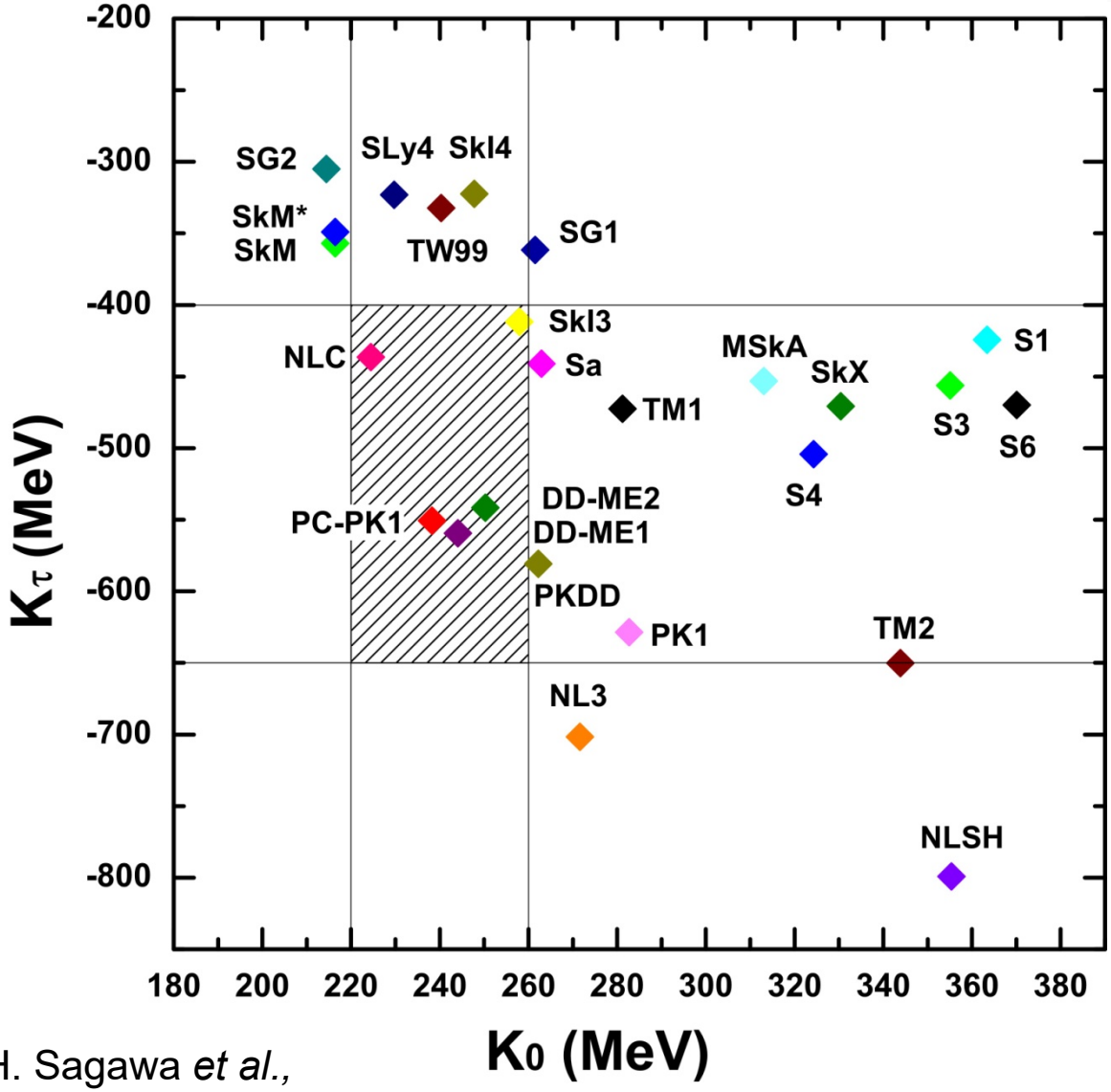
$$M_L^* = \sqrt{(M_D^*)^2 + k_F^2}$$

CDFT for Nuclear matter

Saturation properties:

Model	ρ_0 (fm^{-3})	E/A (MeV)	M_D^*/M	M_L^*/M	E_{sym} (Mev)	L (MeV)	K_{sym} (MeV)	K_0 (MeV)	K_{asy} (MeV)
Empirical	0.166	-16	$0.55-0.60$	0.8	~ 32	88		240	-550
	± 0.018	± 1		± 0.1		± 25		± 20	± 100
NL3	0.148	-16.25	0.59	0.65	37.4	119	101	272	-611
PK1	0.148	-16.27	0.61	0.66	37.6	116	55	283	-640
TW99	0.153	-16.25	0.55	0.62	32.8	55	-125	240	-457
DD-ME1	0.152	-16.2	0.58	0.64	33.1	56	-101	245	-435
PKDD	0.15	-16.27	0.57	0.63	36.8	90	-81	262	-622
PC-LA	0.148	-16.13	0.58	0.64	37.2	108	-61	264	-711
PC-F1	0.151	-16.17	0.61	0.67	37.8	117	74	255	-628
PC-PK1	0.153	-16.12	0.59	0.65	35.6	113	95	238	-582
DD-PC1	0.152	-16.06	0.58	0.64	33	70	-108	230	-529

$$K_T = K_{T,V} + K_{T,S} A^{-1/3}$$



We know K_A from E_{GMR}:

$$E_{GMR} = \hbar\sqrt{\frac{K_A}{m\langle r^2\rangle}}$$

In an approximate way, K_A may be expressed as

$$K_A \sim K_\infty\,(1 + cA^{-1/3}) + K_\tau\,((N-Z)/A)^2 + K_{Coul}\,Z$$

Data from from Umesh Garg, also H. Sagawa *et al.*, *Phys. Rev. C* ***76, 034327 (2007)***

Neutron star properties in CDFT

The predictions given by DDRHF with the PKO series and RMF with PK1, TM1, DD-ME1, DD-ME2, and PKDD fulfill all the *M-R* constraints.

Sun, Long, Meng and Lombardo, PRC **78**, 065805(2008)

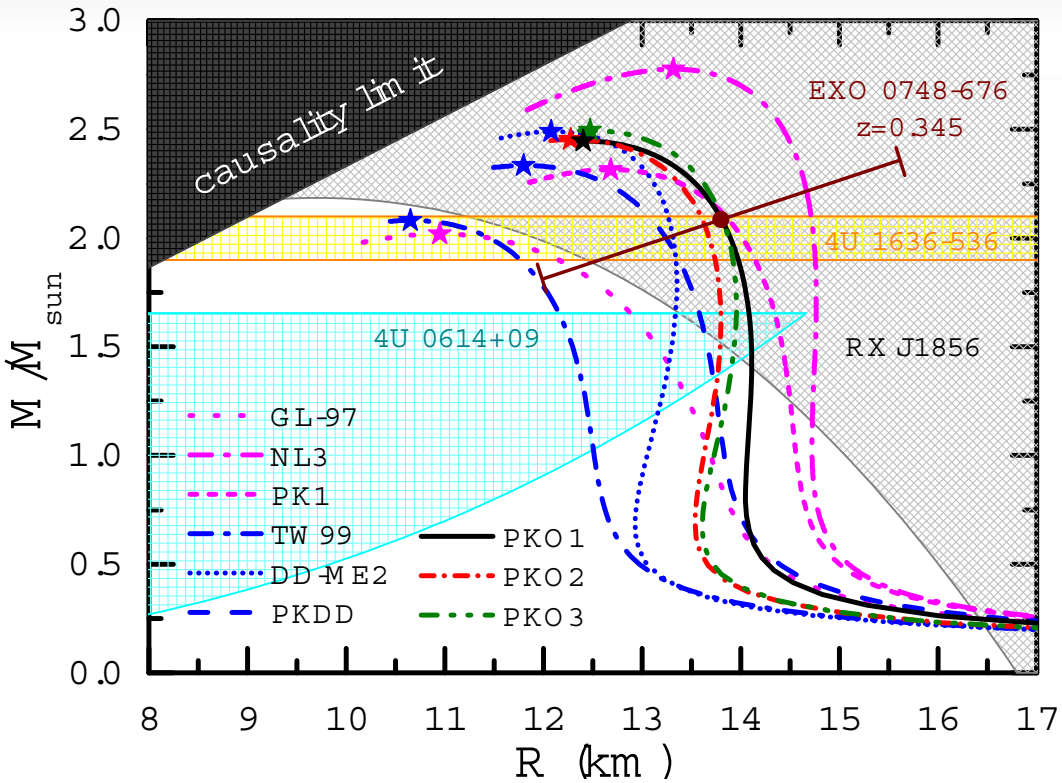


TABLE VI. The criteria of the *M-R* constraints: (1) the isolated neutron star RX J1856, (2) EXO 0748-676, (3) the low-mass X-ray binary 4U 0614 + 09, (4-u) 4U 1636-536 with its upper mass limits, and (4-l) 4U 1636-536 with its lower mass limits. Fulfillment (violation) of a constraint is indicated with + (−) and the marginal cover is marked with δ. See the text for details.

	PKO1	PKO2	PKO3	GL-97	NL1	NL3	NLSH	TM1	PK1	TW99	DD-ME1	DD-ME2	PKDD
1	+	+	+	−	+	+	+	+	+	−	+	+	+
2	+	+	+	+	+	+	+	+	+	Δ	+	+	+
3	+	+	+	+	Δ	Δ	−	+	+	+	+	+	+
4-u	+	+	+	−	+	+	+	+	+	Δ	+	+	+
4-l	+	+	+	+	+	+	+	+	+	+	+	+	+

Ground state properties

CDFT, implemented with self-consistency and taking into account various correlations by spontaneously broken symmetries, provide an excellent description for the ground-state properties including

- Total energy and other physical observables as the expectation values of local one-body operators.
- Open shell nuclei with pairing correlations properly treated by generalized CDFT based on BCS or HFB approach.
- Exotic nuclei with extreme neutron or proton numbers, where novel phenomena such as halos may appear.
- …

1. Meng, Toki, Zhou, Zhang, Long, Geng, Prog. Part. Nucl. Phys. 57 (2006) 470
2. Meng and Zhou, J. Phys. G: Nucl. Part. Phys. 42 (2015) 093101

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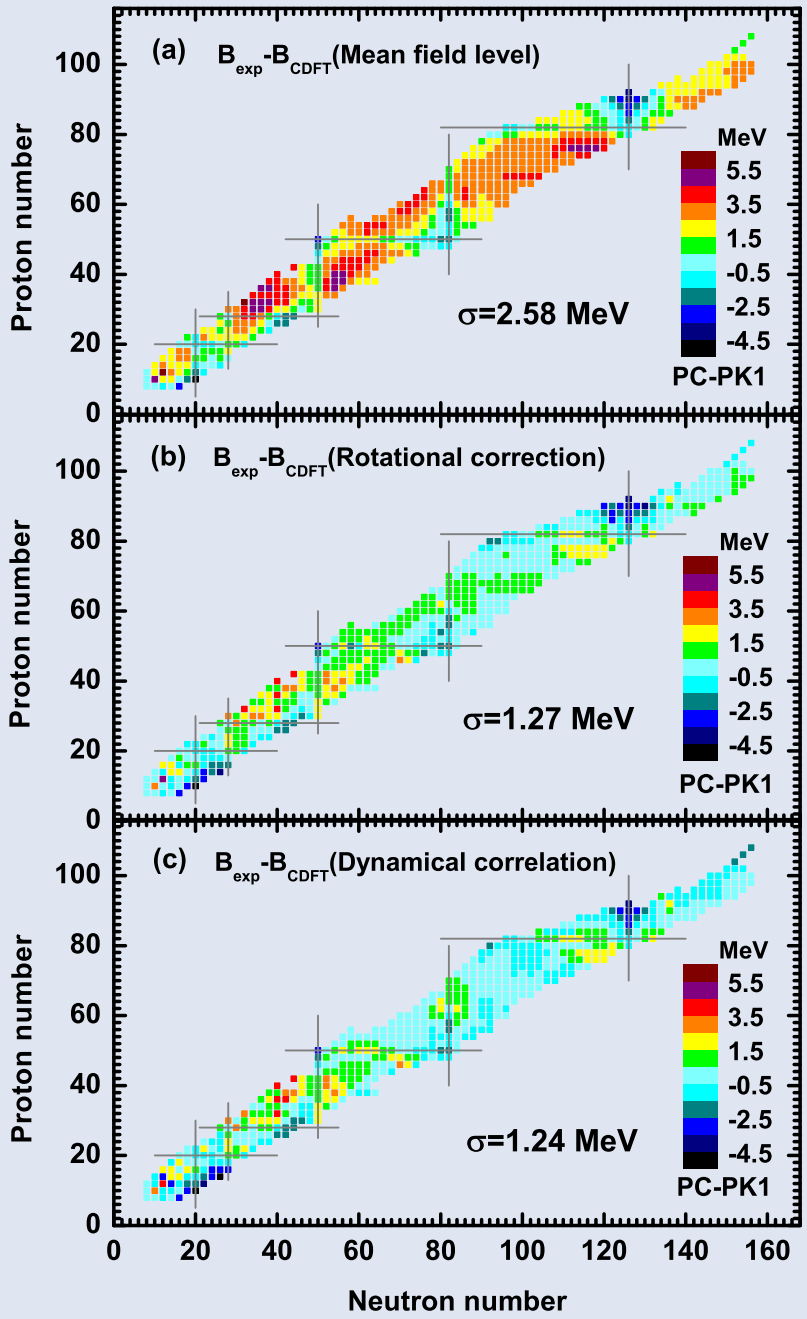
CDFT calculated binding energies by PC-PK1 with the data for 575 even–even nuclei:

(a) the binding energies of the lowest mean-field states;

(b) including the rotational correction energies;

(c) the full dynamical correlation Energies.

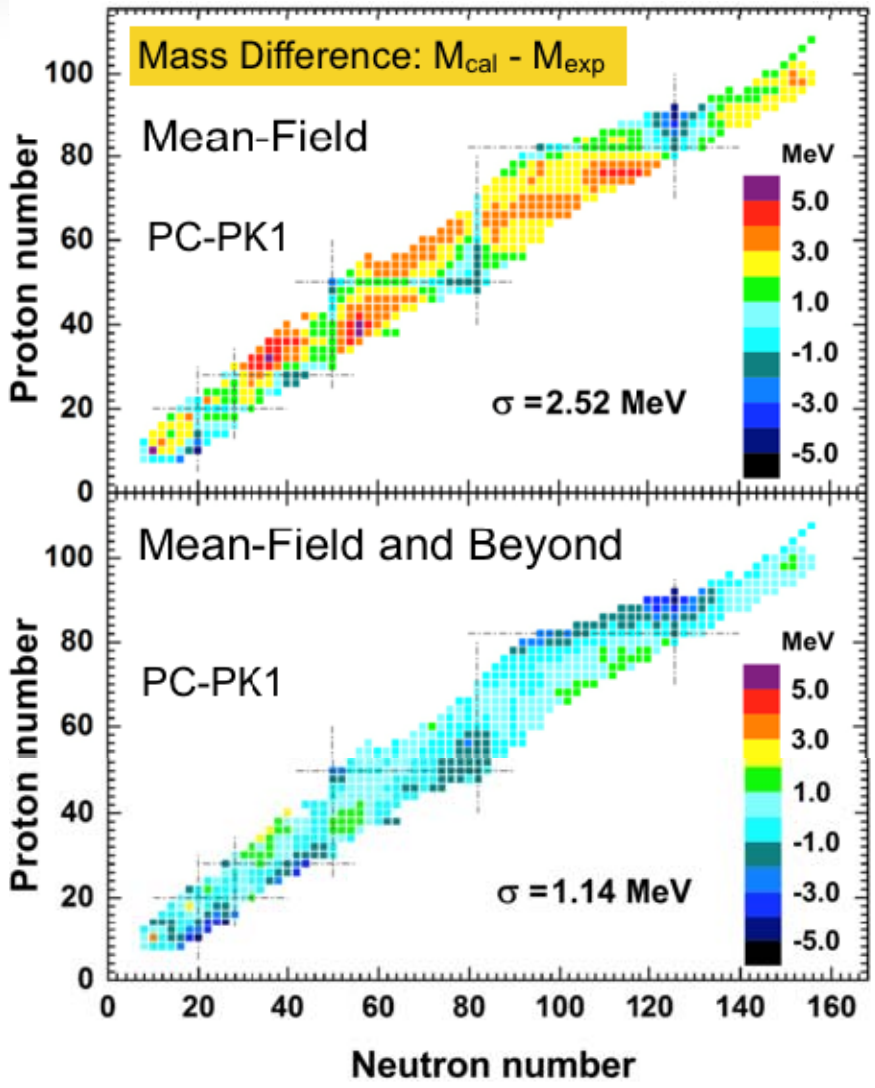
Zhang, Niu, Li, Yao, Meng, Front. Phys. 9(2014) 529

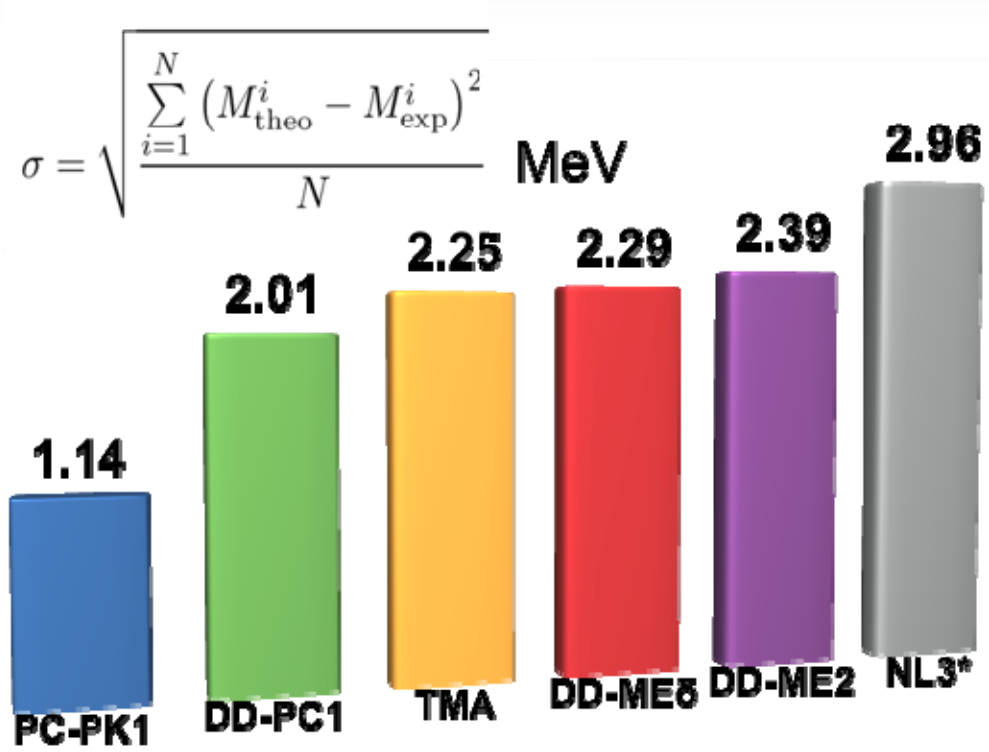


PC-PK1

Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)

Nuclear Masses





Agbemava PRC 2014
Geng PTP 2005

Zhao, Li, Yao, Meng, PRC 82, 054319 (2010)
Zhang, Niu, Li, Yao, Meng, Front. Phys. 9 (2014) 529
Lu, Li, Li, Yao, Meng PRC 91 (2015) 027304

Best density-functional description for nuclear masses so far!

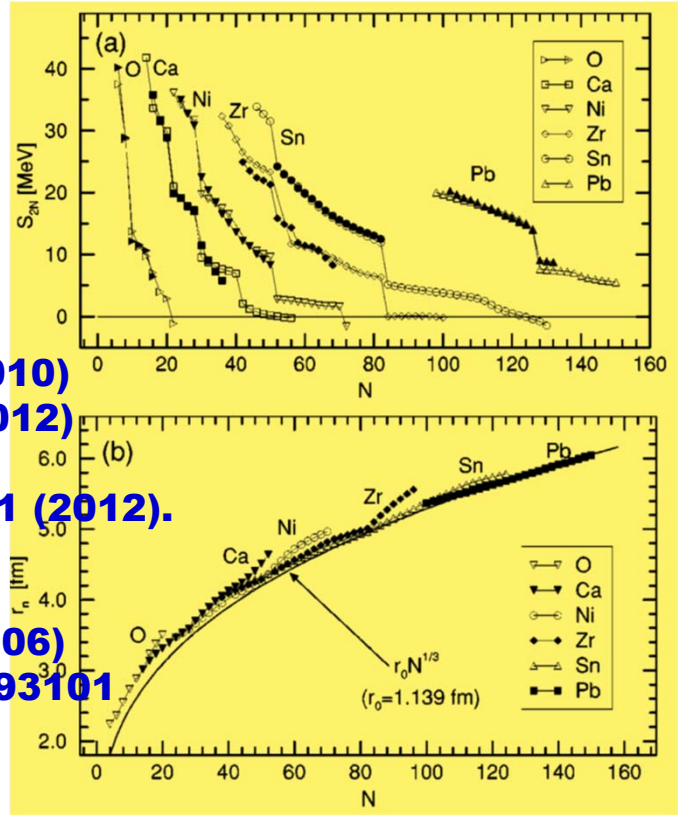
Relativistic Continuum Hartree-Bogoliubov theory

Spherical nucleus: continuum & pairing
Meng & Ring, PRL77,3963 (96)
Meng & Ring, PRL80,460 (1998)
Meng, NPA 635, 3-42 (1998) Meng, Tanihata, & Yamaji, PLB 419, 1(1998)
Meng, Toki, Zeng, Zhang & Zhou, PRC65, 041302R

Spherical nucleus but in DDRHFB: Fock term
Long, Ring, Meng & Van Giai, PRC81 , 031302
Wang, Dong, Long, PRC 87, 047301(2013).
Lu, Sun, Long, PRC 87, 034311 (2013).

Deformed nucleus: deformation & blocking
Zhou, Meng, Ring & Zhao, Phys. Rev. C 82, 011301 (R)(2010)
Li, Meng, Ring, Zhao & Zhou, Phys. Rev. C 85, 024312 (2012)
Chen, Li, Liang & Meng, Phys. Rev. C 85, 067301 (2012)
Li, Meng, Ring, Zhao & Zhou, Chin. Phys. Lett. 29, 042101 (2012).

Reviews:
Meng,Toki, Zhou, Zhang, Long & Geng, PPNP 57. 460 (2006)
Meng and Zhou, J. Phys. G: Nucl. Part. Phys. 42 (2015) 093101



Drip-lines in variant models

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The number of bound nuclides with between 2 and 120 protons is around 7,000

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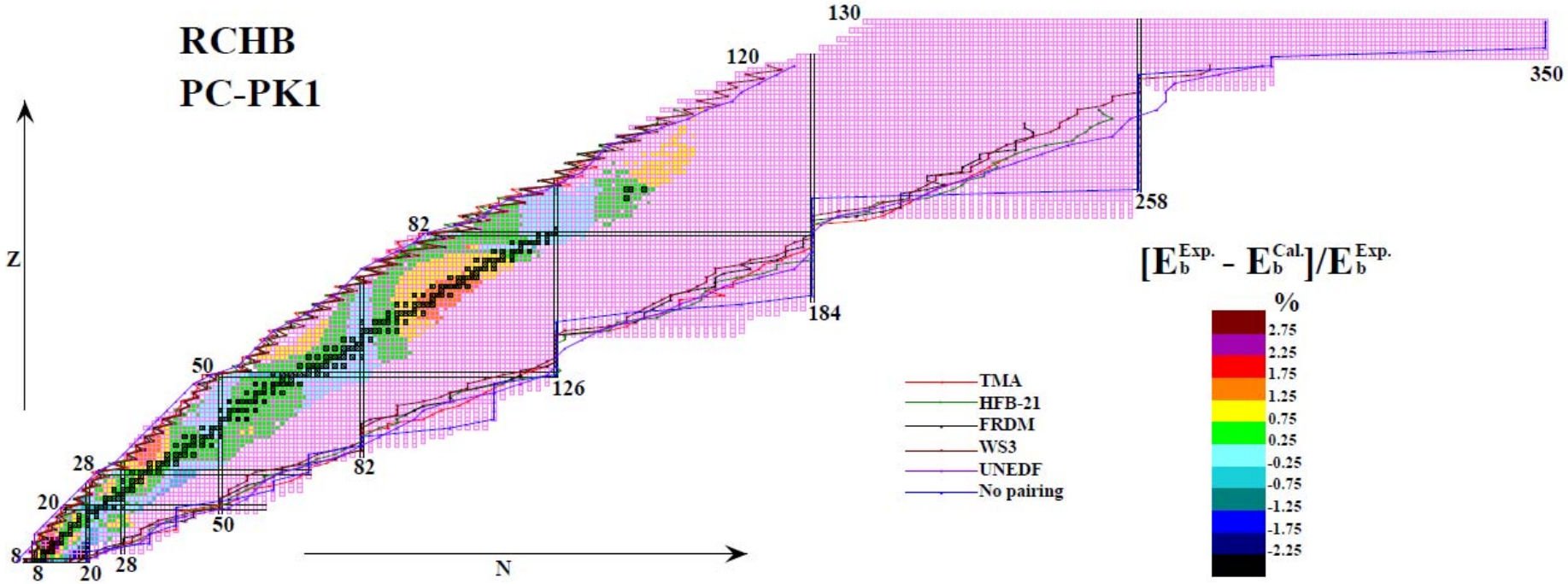
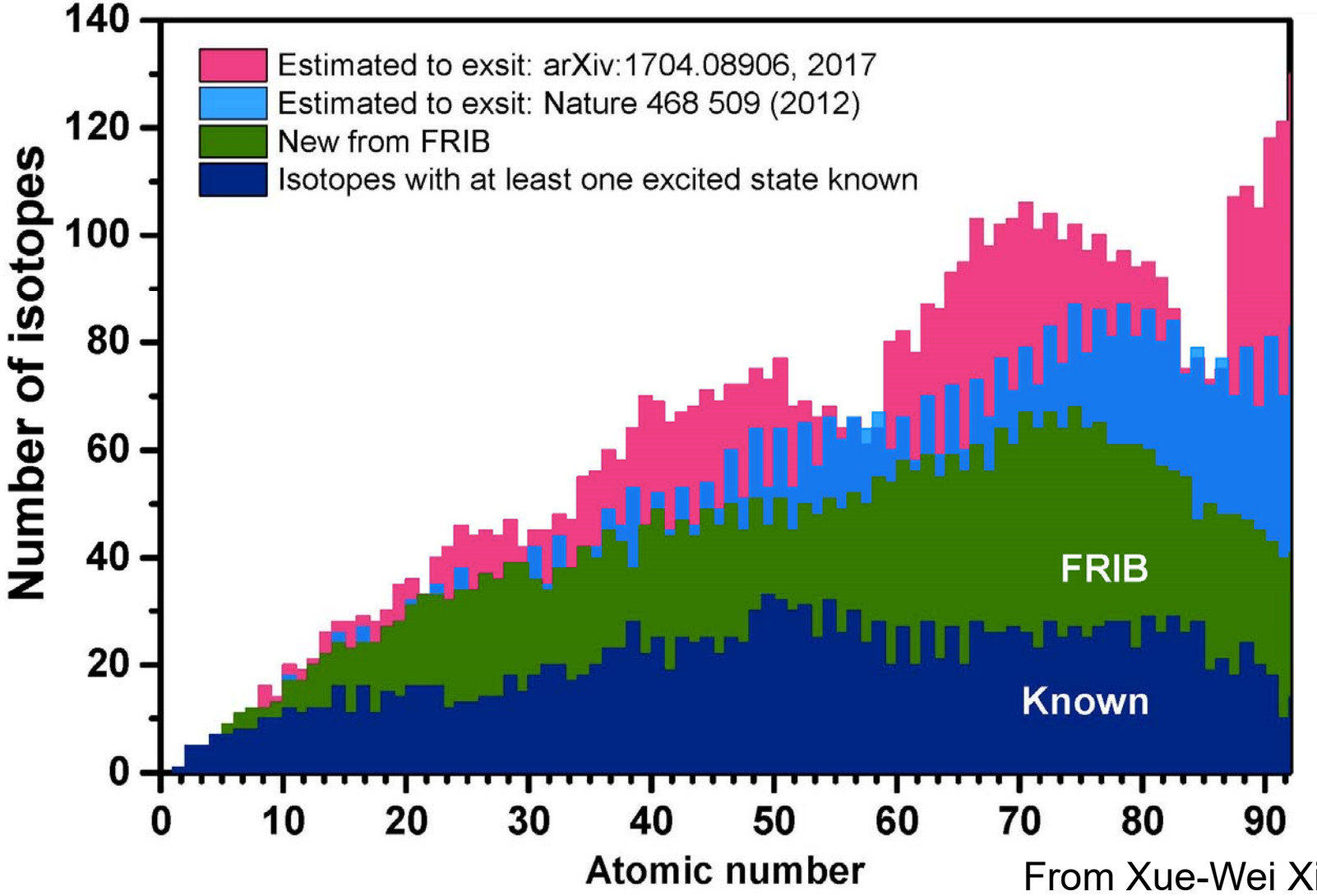


Figure: 10532 bound nuclei from Z=8 to Z=130 predicted by RCHB theory with PC-PK1. For 2227 nuclei with data, binding energy differences between data and calculated results are shown in different color. The nucleon drip-lines predicted TMA, HFB-21, WS3, FRDM , UNEDF and without pairing correlation are plotted for comparison.

See also: Afanasjev, Agbemava, Ray, Ring, PLB726(2013)680

Rare Isotope Beams Facilities



From Xue-Wei Xia

FRIB will be able to make most of all possible isotopes

CDFT in a static external field

CDFT in a static external field includes:

- Constrained CDFT is a powerful tool to investigate the shape evolution, shape isomers, shape-coexistence, and fission landscapes.
- Cranking CDFT obtained by transforming from the laboratory to the intrinsic frame is widely used to describe rotational spectra in near spherical, deformed, superdeformed, and triaxial nuclei.

Review on cranking CDFT:

1. Vretenar, Afanasjev, Lalazissis, Ring, Physics Reports 409 (2005)101-260
2. Meng, Peng, Zhang, Zhao, Front. Phys. 8 (2013) 55-79

Multidimentionally constrained CDFT

- MDC-CDFT: all $\beta_{\lambda\mu}$ with even μ included
- Triaxial & octupole shapes both crucial around the outer barrier

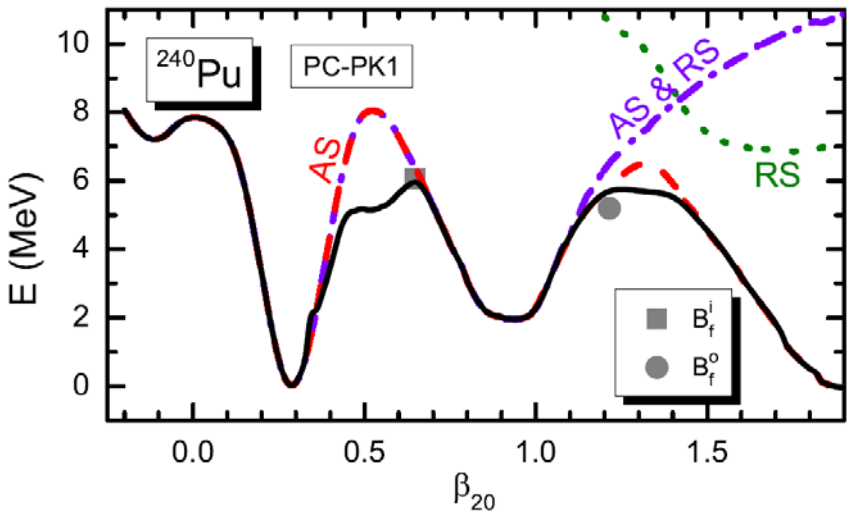


Figure: Potential energy curve of ^{240}Pu

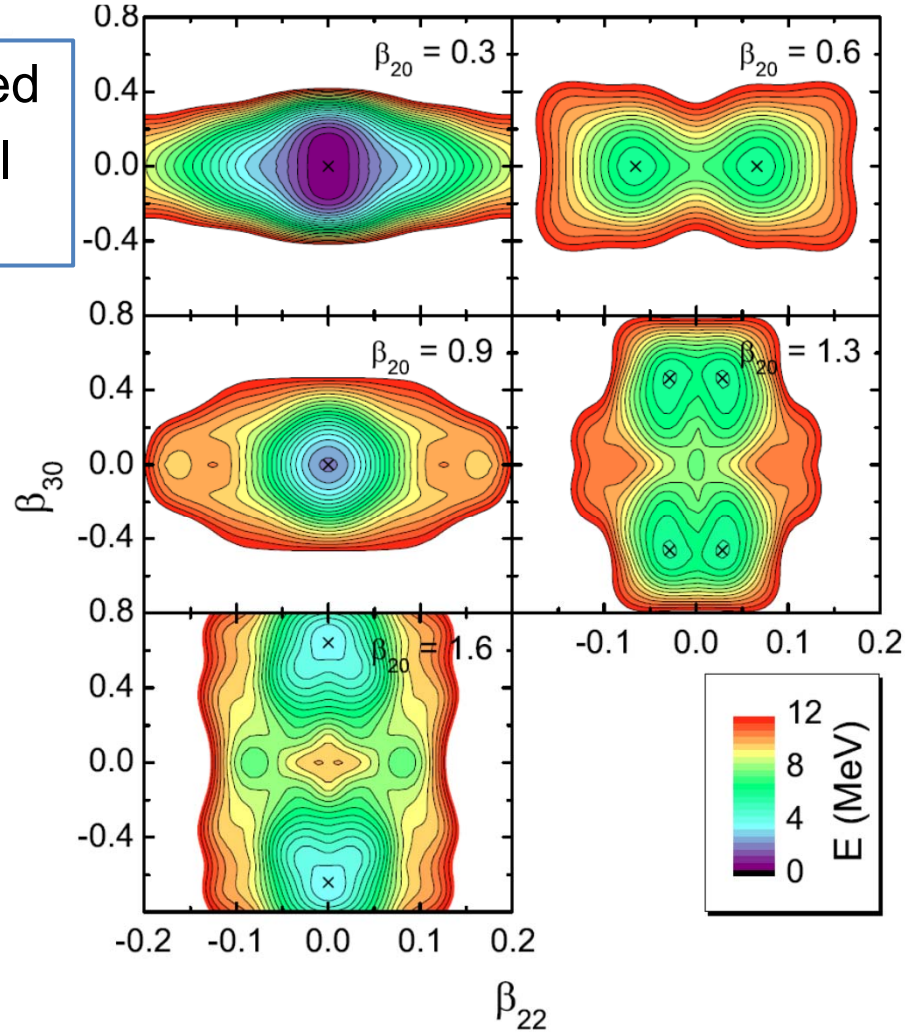


Figure: 3D PES of ^{240}Pu

courtesy of B.N. LU

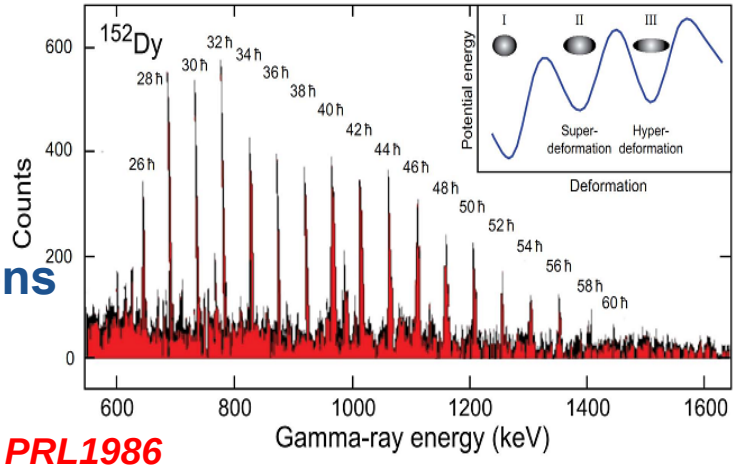
1. Lu, Zhao, Zhou, PRC 85, 011301 (2012)
2. Zhao, Lu, Zhao, Zhou, PRC 86, 057304 (2012)
3. Lu, Zhao, Zhao, Zhou, PRC 89, 014323 (2014)
4. Zhao, Lu, Vretenar, Zhao, Zhou, arXiv:1404.5466 (2014)

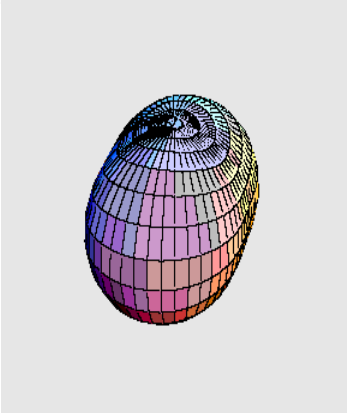
Abusara, Afanasjev, and Ring, PRC 85, 024314 (2012)

Electric and Magnetic Rotation

ΔI = 2

E2 Transitions



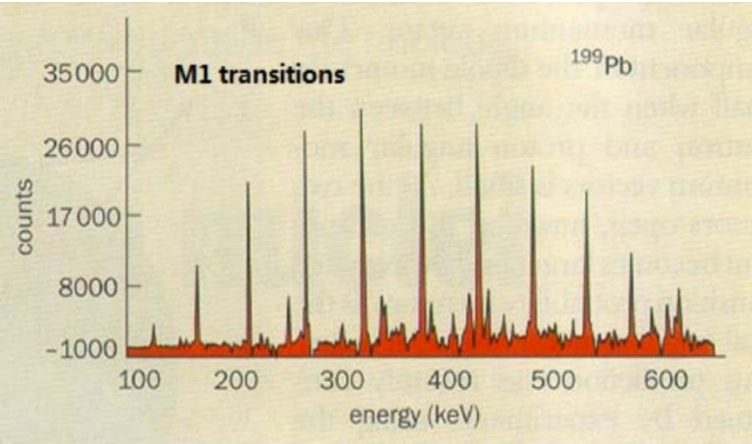


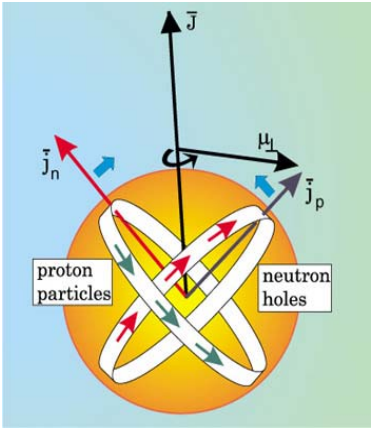
Twin PRL1986

Vretenar, Afanasjev, Lalazissis, Ring, Physics Reports 409 (2005)101

ΔI = 1

M1 Transitions



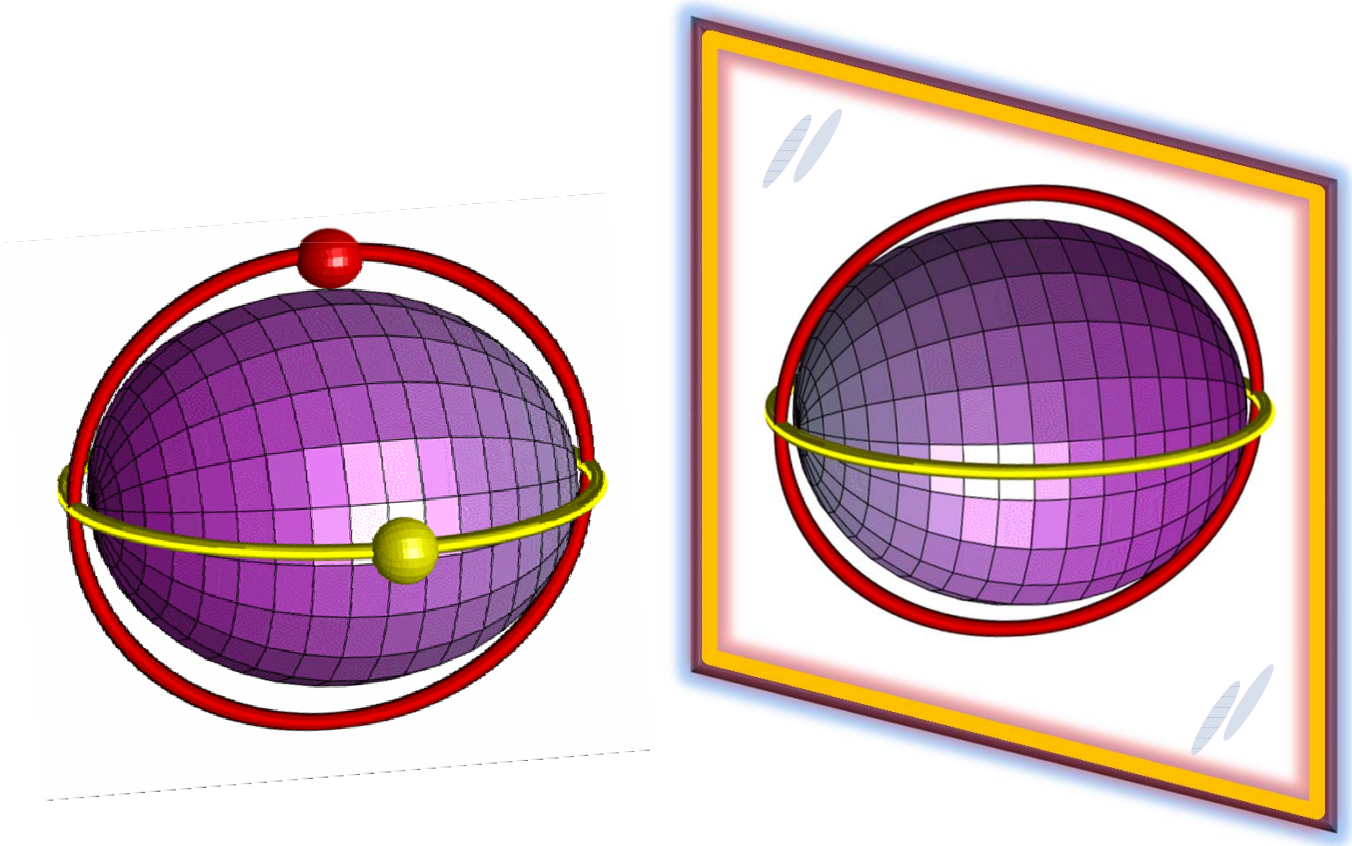


Frauendorf RMP2001 Hübel PPNP2005

Meng, Peng, Zhang, Zhao, Front. Phys. 8 (2013) 55-79

Zhao, Peng, Liang, Ring, Meng, PRL 107, 122501 (2011) - Anti-magnetic

Chiral Rotation



courtesy of X.H. Wu

Chiral symmetry breaking in intrinsic frame

Chiral symmetry in atomic nuclei

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Nuclear Physics A 617 (1997) 131–147

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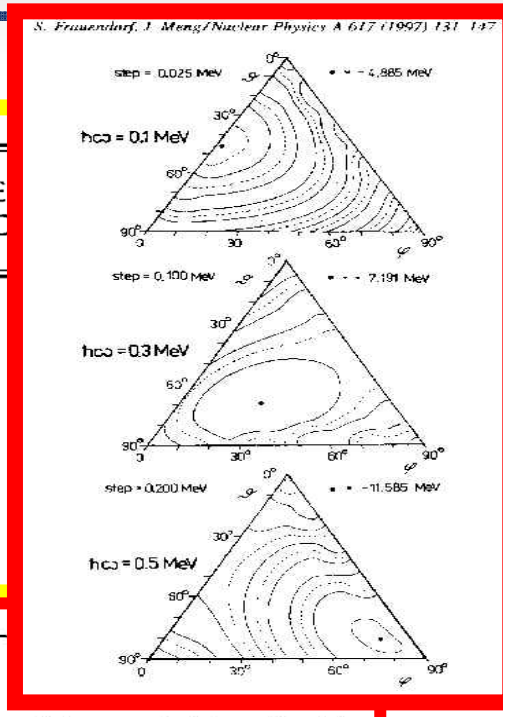
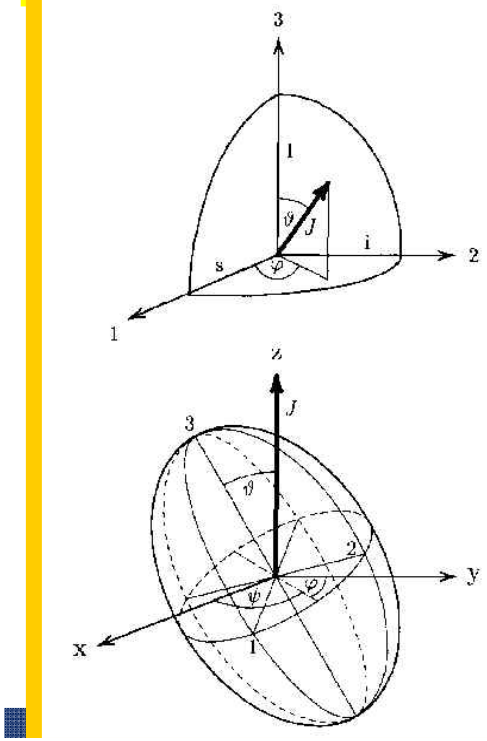
Tilted rotation of triaxial nuclei

S. Frauendorf, Jie Meng [1]

Institut für Kern- und Hadronenphysik, Forschungszentrum Rossendorf e.V., PF 510119, 01314 Dresden, Germany





Abstract

The Tilted Axis Cranking theory is applied to the model of two particles coupled to a triaxial rotor. Comparing with the exact quantal solutions, the interpretation and quality of the mean field approximation is studied. Conditions are discussed when the axis of rotation lies inside or outside the principal planes of the triaxial density distribution. The planar solutions represent $\Delta I = 1$ bands, whereas the aplanar solutions represent pairs of identical $\Delta I = 1$ bands with the same parity. The two bands differ by the chirality of the principal axes with respect to the angular momentum vector. The transition from planar to chiral solutions is evident in both the quantal and the mean field calculations. Its physical origin is discussed. © 1997 Elsevier Science B.V.

PACS: ...

Keywords: Tilted axis cranking; Triaxiality; Chirality

[1] Also at Institute of Theoretical Physics, Chinese Academy of Science, Beijing 100080, PR China. Present address: Alexander von Humboldt fellow, Physik-Department der Technischen Universität München, D-85747 Garching, Germany.

Chiral symmetry in atomic nuclei

Nuclear Chirality: Based on the geometry for one particle and one hole coupled to a triaxial rotor with gamma=30^0

1. nearly degenerate doublet bands
2. S(I) independent of spin
3. identical spin alignments
4. identical B(M1), B(E2) values
5. staggering of B(M1)/B(E2) ratios
6. interband B(E2)=0 at high spin

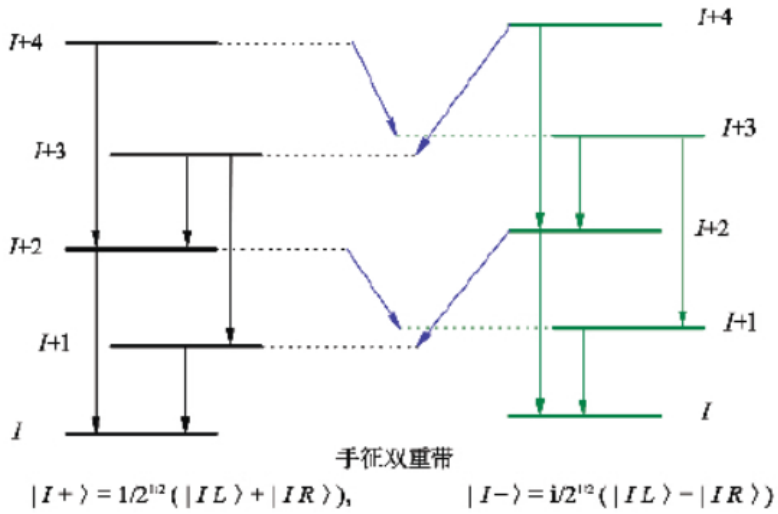
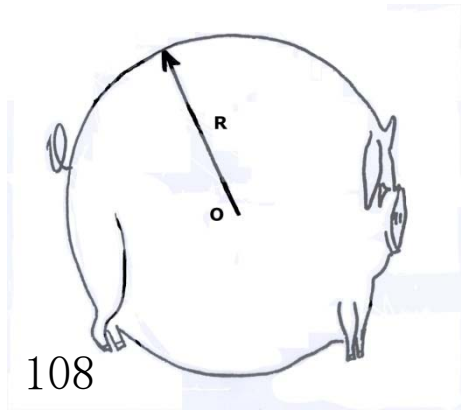


图2 原子核手性的实验信号之一：实验上观测到宇称相同的和在一定自旋范围内近简并的两条 $\Delta I = 1$ 的转动带（L 和 R 分别表示左手性和右手性的量子数）



S.Y. Wang, S.Q. Zhang, B. Qi, and J. Meng, Chinese Physics Letters 24 (2007) 664

孟杰 物理 38（2009）108

First Observations of the Chiral doublets bands

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Observed in 2001

VOLUME 86, NUMBER 6 PHYSICAL REVIEW LETTERS 5 FEBRUARY 2001

Chiral Doublet Structures in Odd-Odd $N = 75$ Isotones: Chiral Vibrations

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New sideband partners of the yrast bands built on the $\pi h_{11/2}\nu h_{11/2}$ configuration were identified in $_{55}$Cs, $_{57}$La, and $_{61}$Pm $N = 75$ isotones of ^{134}Pr. These bands form with ^{134}Pr unique doublet-band systematics suggesting a common basis. Aplanar solutions of 3D tilted axis cranking calculations for triaxial shapes define left- and right-handed chiral systems out of the three angular momenta provided by the valence particles and the core rotation, which leads to spontaneous chiral symmetry breaking and the doublet bands. Small energy differences between the doublet bands suggest collective chiral vibrations.

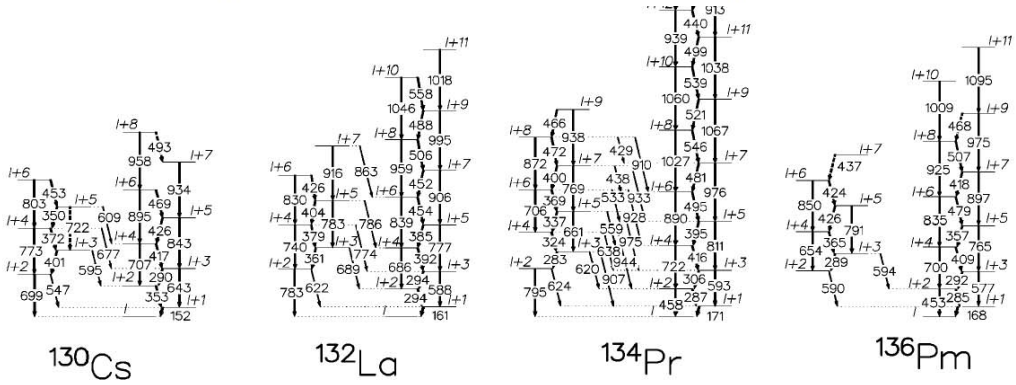

FIG. 2. Partial level schemes presenting the $\pi h_{11/2}\nu h_{11/2}$ bands and newly identified sidebands of ^{130}Cs, ^{132}La, and ^{136}Pm from the current study, and for ^{134}Pr from Ref. [3]. For each $N = 75$ isotone, the yrast $\Delta I = 1$ $\pi h_{11/2}\nu h_{11/2}$ band is shown on the right while the $\Delta I = 1$ sideband is shown on the left side of each level scheme.

MχD proposed in 2006

PHYSICAL REVIEW C **73**, 037303 (2006)

Possible existence of multiple chiral doublets in ^{106}Rh

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Adiabatic and configuration-fixed constrained triaxial relativistic mean field (RMF) approaches are developed for the first time. A new phenomenon, the existence of multiple chiral doublets (MχD), i.e., more than one pair of chiral doublet bands in one single nucleus, is suggested for ^{106}Rh based on the triaxial deform corresponding proton and neutron configurations.

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The investigation followed by:

- ***Prediction for other odd-odd Rh isotopes:*** **J. Peng et al., PRC77, 024309 (2008)**
- ***Confirmed with time-odd fields included:*** **J. M. Yao et al., PRC79, 067302 (2009)**
- ***Prediction for the odd-A Rh isotopes:*** **J. Li et al., PRC83, 037301 (2011)**

First observation of the MχD bands

PRL **110,** 172504 (2013) PHYSICAL REVIEW LETTERS week ending 26 APRIL 2013

Evidence for Multiple Chiral Doublet Bands in ^{133}Ce

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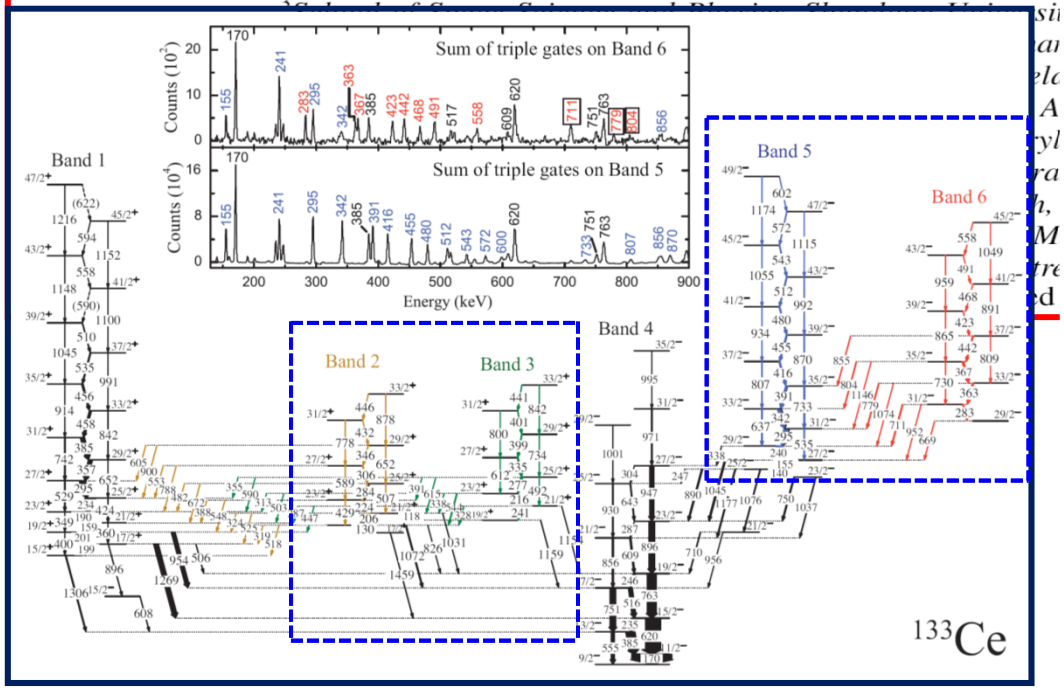
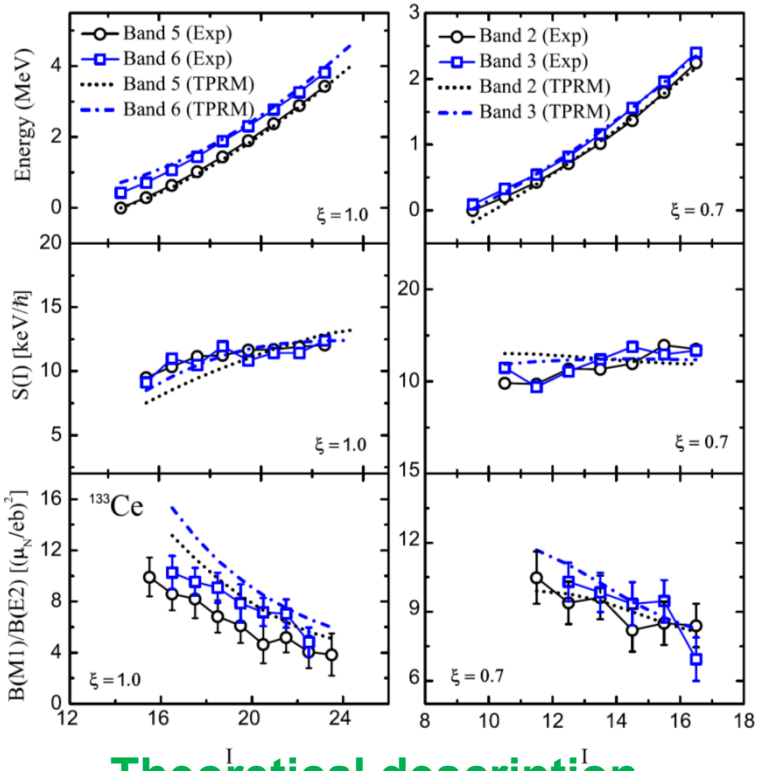


Level Scheme



Theoretical description

Exploration of MχD in ^{78}Br

Spontaneous chiral and reflection symmetry breaking

PRL 116, 112501 (2016) PHYSICAL REVIEW LETTERS week ending 18 MARCH 2016

Evidence for Octupole Correlations in Multiple Chiral Doublet Bands

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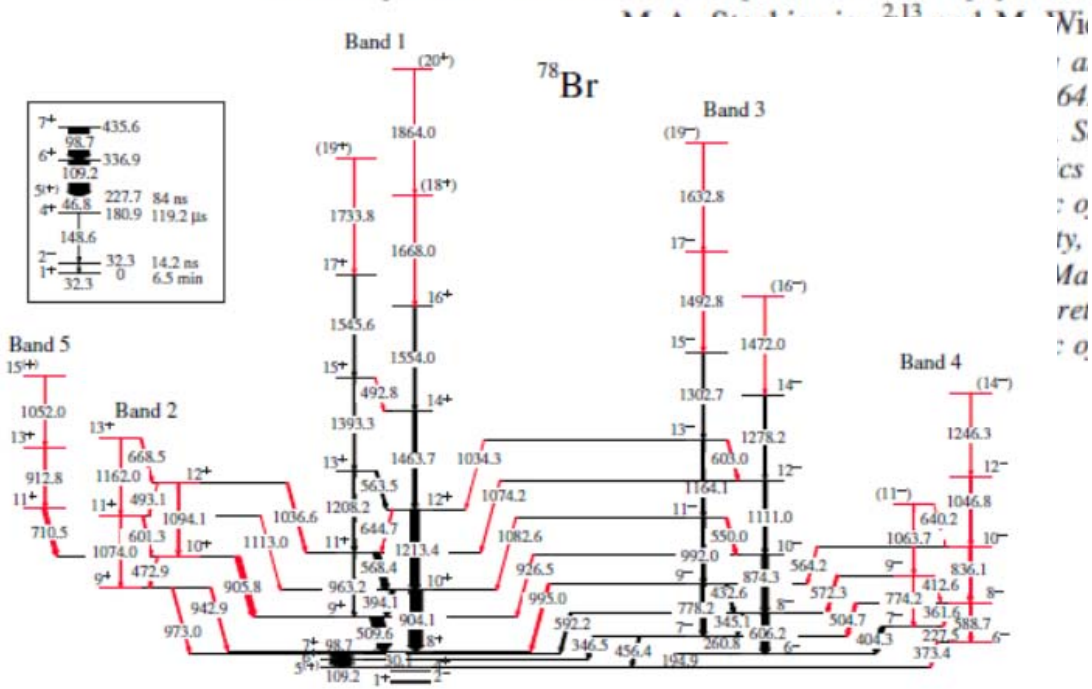

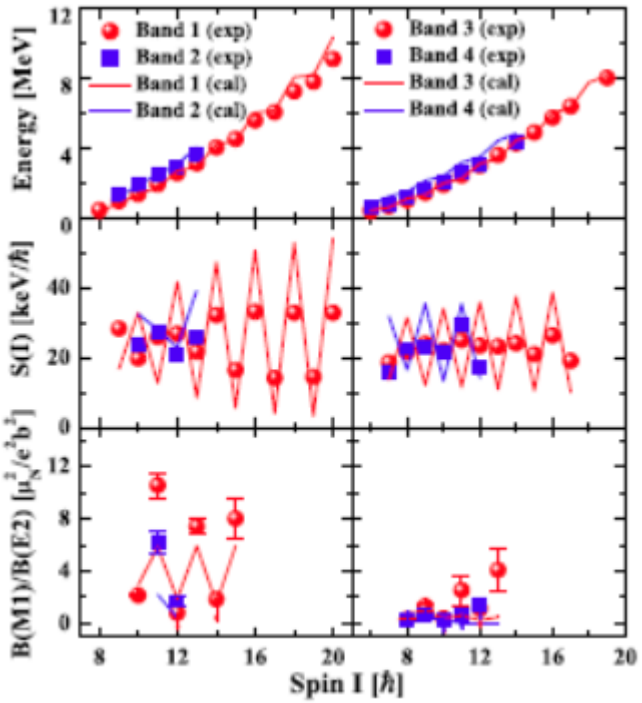

Time-dependent CDFT

- For excited states, a proper method is time-dependent CDFT.
- In analogy to the Hohenberg-Kohn theorem, there exists the Runge-Gross theorem.
- Runge-Gross theorem provides an exact mapping of the full time-dependent many-body problem onto a time-dependent single-particle problem.
- The corresponding single-particle field is not only time-dependent, but also depends on the single-particle density with its full time dependence, i.e., it includes memory effects.