

Interdisciplinary symposium on modern density functional theory

http://indico2.riken.jp/indico/event/iDFT June 19-23, 2017 Okochi hall, RIKEN (Wako Campus)

Covariant density functional theory for nuclear

structure and nuclear astrophysics

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Existence Limit of nucleus



2

2017/7/3



Birth of nuclear physics

The Nobel Prize in Physics 1903 Henri Becquerel, Pierre Curie, Marie Curie



Antoine Henri Becquerel



Pierre Curie



Marie Curie, née Sklodowska

Around the turn of Nineteenth and Twentieth centuries, the discoveries of radioactivity by Becquerel and the Curies and the existence of a compact nucleus at the center of an atom by Rutherford et al. opened the door of nuclear science. These achievements conceived the birth of quantum mechanics, promoted the exploitation and utilization of nuclear energy and nuclear technology, and brought about a huge impact on human life.











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



Shell model & Collective model

The independent particle shell model of nucleus by Mayer and Jensen *et al.*, and the collective Hamiltonian for nuclear rotation and vibration by Bohr and Mottelson, etc. However, since 1950s, nuclear physics stepped into a more challenging stage.

- Although the independent particle shell model could describe the singleparticle motion in a nucleus with a phenomenological mean potential, it cannot provide even a qualitative description for the nuclear bulk properties.
- On the contrary, a unified phenomenological description of nuclear vibration and rotation can be achieved by the collective Hamiltonian whereas it is helpless in understanding the motion of a single nucleon.





J. H. D. Jensen

M. G. Mayer

E. P. Wigner

Nobel Prize in Physics 1963



A. N. Bohr B. R. Mottelson J. Rainwater Nobel Prize in Physics 1975



Shell model & Collective model



Strong spin-orbit interaction **Great for:**

magic numbers
ground state properties
some low lying excited states

Lead to deformed Nilsson model

S. G. Nilsson, Mat. Fys. Medd. Dan. Vid. Selsk. 29, No.16(1955). S. G. Nilssion, et al., Nucl. Phys. A131(1969) 1.

Totally fails for nuclear bulk properties



Strutinsky Shell correction calculation

Compromise between Shell model and collective model

Great success for FRDM WS4 ...





V.M. Strutinsky,

Shell effects in nuclear masses and deformation energies, Nuclear Physics A 95 (1967) 420 Times Cited: 1,664

"Shells" in deformed nuclei, Nuclear Physics A 122 (1968) 1 Times Cited: 1,040



Finite-Range Droplet Model (FRDM)

P. Möller, J.R. Nix, W.D. Myers, W.J. Swiatecki, At. Data Nucl. Data Tables 59, 185 (1995). Times Cited: 2,385 Error of the mass model is 0.669 MeV

Weizsäcker-Skyrme (WS) formula

"Isospin for S-O & E_sym + mirror nuclei"

inspired by the Skyrme energy-density functional and a macroscopicmicroscopic mass formula, with an rms deviation of 336 keV with respect to

the 2149 measured masses in 2003 Atomic Mass Evaluation.

N. Wang, M. Liu and X. Z. Wu, Phys. Rev. C 81, 044322 (2010). N. Wang, Z. Y. Liang, M. Liu and X. Z. Wu, Phys. Rev. C 82, 044304 (2010). M. Liu, N. Wang, Y. G. Deng, and X. Z. Wu, Phys. Rev. C 84, 014333 (2011).

Taking into account the surface diffuseness effect, the rms deviation with 2353 known masses falls to 298 keV.

N. Wang, M. Liu, X. Z. Wu and J. Meng, Phys. Lett. B 734, 215 (2014).



How to achieve microscopically and self-consistently a unified description of the single-nucleon and collective motions of nucleus based on the strong interaction theory is a crucial question to be answered by nuclear scientists.





Many-body problems

$$\hat{H} \Psi = \left[-\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i>j} V_{ij} \right] \Psi = E \Psi$$

$$\hat{H} = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U(r_i) \right] + \sum_{i>j} V_{ij} - \sum_i U(r_i)$$
Mean field potential
Residual interaction

The self-consistent mean-field approach to nuclear structure is analogous to Kohn-Sham Density Functional Theory.

Density functional theory (DFT), with the name comes from the use of functionals of the particle density, is aquantum mechanical theory used in physics and chemistry to investigate the structure (mainly the ground state) of many-particle systems.



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)



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

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

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.

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



Hohenberg







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]



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 $G(\rho)$

At present, the ansatz for $E(\rho)$ is phenomenological:

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

Why Covariant?

- ✓ Spin-orbit automatically included
- Lorentz covariance restricts parameters
- Pseudo-spin Symmetry
- ✓ Connection to QCD: big V/S ~ \pm 400 MeV
- Consistent treatment of time-odd fields
- ✓ Relativistic saturation mechanism
 - Liang, Meng, Zhou, Physics Reports 570 : 1-84 (2015).







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



Brief introduction of CDFT

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

field theory for strong interaction

Strong force: Meson-exchange of the nuclear force



Sigma-meson: attractive scalar field Omega-meson: Short-range repulsive

Rho-meson: Isovector field

Electromagnetic force: The photon



Brief introduction of CDFT

Lagrangian:

$$\begin{split} L &= \overline{\psi}[i\gamma^{\mu}\partial_{\mu} - M - g_{\sigma}\sigma - \gamma^{\mu}(g_{\omega}\omega_{\mu} + g_{\rho}\vec{\tau} \bullet \vec{\rho}_{\mu} + e^{\frac{1-\tau_{3}}{2}}A_{\mu}) - \frac{f_{\pi}}{m_{\pi}}\gamma_{5}\gamma^{\mu}\partial_{\mu}\vec{\pi} \bullet \vec{\tau}]\psi \\ &+ \frac{1}{2}\partial^{\mu}\sigma\partial_{\mu}\sigma - \frac{1}{2}m_{\sigma}^{2}\sigma^{2} - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega_{\mu}\omega^{\mu} - \frac{1}{4}\vec{R}_{\mu\nu} \bullet \vec{R}^{\mu\nu} \\ &+ \frac{1}{2}m_{\rho}^{2}\vec{\rho}^{\mu}\Box\vec{\rho}_{\mu} + \frac{1}{2}\partial_{\mu}\vec{\pi} \bullet \partial^{\mu}\vec{\pi} - \frac{1}{2}m_{\pi}^{2}\vec{\pi} \bullet \vec{\pi} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\ \Omega^{\mu\nu} &= \partial^{\mu}\omega^{\nu} - \partial^{\nu}\omega^{\mu} \\ \mathbf{Hamiltonian:} & F^{\mu\nu} &= \partial^{\mu}\vec{\rho}^{\nu} - \partial^{\nu}\vec{\rho}^{\mu} \\ H &= \vec{\psi}(-i\gamma \bullet \nabla + M)\psi + \frac{1}{2}\int d^{4}y \sum_{i=\sigma,\omega,\rho,\pi,A}\vec{\psi}(x)\vec{\psi}(y)\Gamma_{i}D_{i}(x,y)\psi(y)\psi(x) \\ &= T + V & \Gamma_{\sigma}(1,2) \equiv -g_{\sigma}(1)g_{\sigma}(2), \quad \Gamma_{\rho}(1,2) \equiv +(g_{\rho}\gamma_{\mu}\vec{\tau})_{1}\Box(g_{\rho}\gamma^{\mu}\vec{\tau})_{2}, \end{split}$$

$$\Gamma_{\omega}(1,2) \equiv +(g_{\omega}\gamma_{\mu})_{1}(g_{\omega}\gamma_{\mu})_{2}, \Gamma_{\pi}(1,2) \equiv -(\frac{f_{\pi}}{m_{\pi}}\vec{\tau}\gamma_{5}\gamma_{\mu}\partial^{\mu})_{1}\Box(\frac{f_{\pi}}{m_{\pi}}\vec{\tau}\gamma_{5}\gamma_{\nu}\partial^{\nu})_{2}$$

$$\Gamma_{\rm em}(1,2) \equiv +\frac{e^{2}}{4}(\gamma_{\mu}(1-\tau_{3}))_{1}(\gamma^{\mu}(1-\tau_{3}))_{2}$$



Brief introduction of CDFT

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

$$\psi(x) = \sum_{i} [f_{i}(\mathbf{x})e^{-i\varepsilon_{i}t}c_{i} + g_{i}(\mathbf{x})e^{i\varepsilon_{i}t}d_{i}^{\dagger}]$$

$$\psi^{\dagger}(x) = \sum_{i} [f_{i}^{\dagger}(\mathbf{x})e^{i\varepsilon_{i}t}c_{i}^{\dagger} + g_{i}^{\dagger}(\mathbf{x})e^{-i\varepsilon_{i}^{\dagger}t}d_{i}]$$

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

$$Hartree$$

$$V_{i} = \frac{1}{2} \int d\mathbf{x}_{1} d\mathbf{x}_{2} \sum_{\alpha\beta;\alpha'\beta'} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\beta'} c_{\alpha'} \overline{f}_{\alpha} (1) \overline{f}_{\beta} (2) \Gamma_{i} (1, 2) D_{i} (1, 2) f_{\beta'} (2) f_{\alpha'} (1)$$
Fock

Energy density functional:

$$\left|\Phi_{0}\right\rangle = \prod_{\alpha} c_{\alpha}^{\dagger} \left|0\right\rangle$$

$E = \langle \Phi_0 | H | \Phi_0 \rangle = \langle \Phi_0 | T | \Phi_0 \rangle + \sum \langle \Phi_0 | V_i | \Phi_0 \rangle$ $i=\sigma.\omega.\rho.\pi.A$

 $= E_k + E_{\sigma}^D + E_{\sigma}^E + E_{\omega}^D + E_{\omega}^E + E_{\rho}^D + E_{\rho}^E + E_{\pi} + E_{\rm em}^D + E_{\rm em}^E$ 2017/7/3



For system with time invariance:

$$\left[\alpha \cdot \boldsymbol{p} + V(\boldsymbol{r}) + \beta \left(M + S(\boldsymbol{r})\right)\right] \boldsymbol{\psi}_{i} = \varepsilon_{i} \boldsymbol{\psi}_{i}$$

$$\begin{cases} V(\boldsymbol{r}) = g_{\omega}\omega(\boldsymbol{r}) + g_{\rho}\tau_{3}\rho(\boldsymbol{r}) + e\frac{1-\tau_{3}}{2}A(\boldsymbol{r}) \\ S(\boldsymbol{r}) = g_{\sigma}\sigma(\boldsymbol{r}) \end{cases}$$

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

$$\begin{bmatrix} -\Delta + m_{\sigma}^{2} \end{bmatrix} \sigma = -g_{\sigma}\rho_{s} - g_{2}\sigma^{2} - g_{3}\sigma^{3}$$
$$\begin{bmatrix} -\Delta + m_{\omega}^{2} \end{bmatrix} \omega = g_{\omega}\rho_{b} - c_{3}\omega^{3}$$
$$\begin{bmatrix} -\Delta + m_{\rho}^{2} \end{bmatrix} \rho = g_{\rho} \left[\rho_{b}^{(n)} - \rho_{b}^{(p)}\right] - d_{3}\rho^{3}$$

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



Effective Point-Coupling interaction

$$H = \overline{\psi}_{i} \left(-i\gamma \cdot \nabla + M\right) \psi_{i} + \frac{1}{4} F^{i\nu} F_{i\nu}$$

$$+ \frac{1}{2} ((\nabla \sigma)^{2} + m_{\sigma}^{2} \sigma^{2}) + g_{\sigma} \sigma \rho_{s} + \frac{1}{3} g_{2} \sigma^{3} + \frac{1}{4} g_{3} \sigma^{4}$$

$$+ \frac{1}{2} g_{\omega} \omega_{0} \rho_{\nu} + \frac{1}{2} g_{\rho} \overline{\rho}_{0} \rho_{3}$$

$$g_{\omega} \omega = \frac{1}{1 - \Delta / m_{\omega}^{2}} \frac{g_{\omega}^{2}}{m_{\omega}^{2}} \rho_{\nu} = \frac{g_{\omega}^{2}}{m_{\omega}^{2}} \rho_{\nu} + \frac{g_{\omega}^{2}}{m_{\omega}^{4}} \Delta \rho_{\nu} + \cdots \approx \alpha_{\nu} \rho_{\nu} + \delta_{\nu} \Delta \rho_{\nu}$$

$$H = \overline{\psi}_{i} \left(-i\gamma \Box \nabla + M\right) \psi_{i} + \frac{1}{4} F^{i\nu} F_{i\nu}$$

$$+ \frac{1}{2} \alpha_{s} \rho_{s}^{2} + \frac{1}{2} \delta_{s} \rho_{s} \Delta \rho_{s} + \frac{1}{3} \beta_{s} \rho_{s}^{3} + \frac{1}{4} \gamma_{s} \rho_{s}^{4}$$

$$\frac{1}{2} \alpha_{\nu} \rho_{\nu}^{2} + \frac{1}{2} \delta_{\nu} \rho_{\nu} \Delta \rho_{\nu} + \frac{1}{2} \alpha_{T\nu} \rho_{V}^{2} + \frac{1}{3} \beta_{\sigma} \rho_{T\nu} \Delta \rho_{T\nu}$$





For system with time invariance:

 $\left[\alpha \cdot \boldsymbol{p} + V(\boldsymbol{r}) + \beta \left(M + S(\boldsymbol{r})\right)\right] \boldsymbol{\psi}_{i} = \varepsilon_{i} \boldsymbol{\psi}_{i}$

$$V(\mathbf{r}) = \alpha_V \rho_V(\mathbf{r}) + \gamma_V \rho_V^3(\mathbf{r}) + \delta_V \Delta \rho_V(\mathbf{r}) + \alpha_{TV} \rho_{TV}(\mathbf{r}) + \delta_{TV} \Delta \rho_{TV}(\mathbf{r}) + e \frac{1 - \tau_3}{2} A(\mathbf{r})$$

$$S(\mathbf{r}) = \alpha_S \rho_S + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \Delta \rho_S$$

Without Klein-Gordon equation

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

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

Isoscalar-vector

Isovector-scalar

Isovector-vector

$$egin{aligned} &
ho_S(\mathbf{r}) = \sum_k^{occ} ar{\psi}_k(\mathbf{r}) \psi_k(\mathbf{r}) \ &j_\mu(\mathbf{r}) = \sum_k^{occ} ar{\psi}_k(\mathbf{r}) \gamma_\mu \psi_k(\mathbf{r}) \ &ar{
ho}_S(\mathbf{r}) = \sum_k^{occ} ar{\psi}_k(\mathbf{r}) ec{ au} \psi_k(\mathbf{r}) \ &ec{ extsf{j}}_\mu(\mathbf{r}) = \sum_k^{occ} ar{\psi}_k(\mathbf{r}) ec{ au} \psi_k(\mathbf{r}) \end{aligned}$$

Energy Density Functional

$$egin{aligned} E_{kin} &= \sum_k v_k^2 \int ar{\psi}_k \left(-\gamma
abla + m
ight) \psi_k d\mathbf{r} \ E_{2nd} &= rac{1}{2} \int (lpha_S
ho_S^2 + lpha_V
ho_V^2 + lpha_{tV}
ho_{tV}^2) d\mathbf{r} \ E_{hot} &= rac{1}{12} \int (4 eta_S
ho_S^3 + 3 \gamma_S
ho_S^4 + 3 \gamma_V
ho_V^4) d\mathbf{r} \ E_{der} &= rac{1}{2} \int (\delta_S
ho_S riangle_{PS} + \delta_V
ho_V riangle_{PV} + \delta_{tV}
ho_{tV} riangle_{hV}) d\mathbf{r} \ E_{em} &= rac{e}{2} \int j_\mu^p A^\mu d\mathbf{r} \end{aligned}$$





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:

$$M, \alpha_{\scriptscriptstyle S}, \alpha_{\scriptscriptstyle V}, \alpha_{\scriptscriptstyle TV}, \delta_{\scriptscriptstyle S}, \delta_{\scriptscriptstyle V}, \delta_{\scriptscriptstyle TV}, \beta_{\scriptscriptstyle S}, \gamma_{\scriptscriptstyle S}, \gamma_{\scriptscriptstyle V}$$

PC-LA, PC-F1, PC-PK1 ...

Density dependent parameterizations:

 $M, \delta_{s}, \alpha_{s}(\rho), \alpha_{v}(\rho), \alpha_{TV}(\rho)$

DD-PC1, ...

2017/7/3



Covariant density functional PC-PK1





Coup	. Cons.	PC-PK1	Dimension
$lpha_S$	$[10^{-4}]$	-3.96291	MeV^{-2}
eta_S	$[10^{-11}]$	8.66530	${\rm MeV}^{-5}$
γ_S	$[10^{-17}]$	-3.80724	${\rm MeV^{-8}}$
δ_S	$[10^{-10}]$	-1.09108	${\rm MeV}^{-4}$
$lpha_V$	$[10^{-4}]$	2.69040	MeV^{-2}
γ_V	$[10^{-18}]$	-3.64219	${\rm MeV^{-8}}$
δ_V	$[10^{-10}]$	-4.32619	${\rm MeV}^{-4}$
$lpha_{TV}$	$[10^{-5}]$	2.95018	${\rm MeV}^{-2}$
δ_{TV}	$[10^{-10}]$	-4.11112	${\rm MeV}^{-4}$
V_n	$[10^0]$	-349.5	$MeV fm^3$
V_p	$[10^0]$	-330	$MeV fm^3$

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

2017/7/3



Nuclear matter properties

Binding energy per nucleon:



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

EOS of symmetric nuclear matter



Nuclear matter properties

Compressibility

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

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

$$K_{0}=9{
ho_{0}}^{2}iggl[rac{\partial^{2}igl(arepsilon/
hoigr)}{\partial {
ho}^{2}}iggr]_{
ho_{0}}$$

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

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

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

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



Saturation properties:

Model	$ ho_0$	E/A	M_D^*/M	M_L^*/M	E_{sym}	L	K_{sym}	K_0	K_{asy}
	(fm^{-3})	(MeV)			(Mev)	(MeV)	(MeV)	(MeV)	(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)** 2017/7/3



Neutron star properties in CDFT





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	+	+	+	+	+	+	+	+	+	+	+	+	+



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



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) ⁰ ²⁰ ⁴⁰ ⁶⁰ ⁸⁰ ¹⁰⁰ ¹²⁰ Li, Meng, Ring, Zhao & Zhou, Phys. Rev. C 85, 024312 (2012) Chen, Li, Liang & Meng, Phys. Rev. C 85, 067301 (2012) ⁶⁰ ^(b) ⁵⁰ ^(b) ⁵¹ ^(c)

Reviews:

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





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







Drip-lines in variant models

PEKING UNIVERSITY The number of bound nuclides with between 2 and 120 protons is around 7,000 28JUNE2012|VOL486|NATURE|509



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





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 β_{λμ} with even μ included
 Triaxial & octupole shapes both crucial around the outer barrier



Figure: Potential energy curve of ²⁴⁰Pu

- 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)



courtesy of B.N. LU



Electric and Magnetic Rotation



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



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

NUCLE PHYSIC



Nuclear Physics A 617 (1997) 131-147

Tilted rotation of triaxial nuclei

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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. (c) 1997 Elsevier Science B.V.

PACS:

Keywords: Tilted axis cranking; Triaxiality; Chirality

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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^o





First Observations of the Chiral doublets bands

VOLUME 86, NUMBER 6

PHYSICAL REVIEW LETTERS

5 FEBRUARY 2001

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

K. Starosta,^{1,*} T. Koike,¹ C. J. Chiara,¹ D. B. Fossan,¹ D. R. LaFosse,¹ A. A. Hecht,² C. W. Beausang,² M. A. Caprio,² J. R. Cooper,² R. Krücken,² J. R. Novak,² N. V. Zamfir,^{2,†} K. E. Zyromski,² D. J. Hartley,³ D. L. Balabanski,^{3,‡} Jing-ye Zhang,³ S. Frauendorf,⁴ and V. I. Dimitrov^{4,‡}

¹Department of Physics and Astronomy, SUNY at Stony Brook, Stony Brook, New York 11794 ²Wright Nuclear Structure Laboratory, Yale University, New Haven, Connecticut 06520 ³Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996 ⁴Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556 and Institute for Nuclear and Hadronic Physics, Research Center Rossendorf, 01314 Dresden, Germany (Received 24 July 2000)

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 ¹³⁰Cs, ¹³²La, and ¹³⁶Pm from the current study, and for ¹³⁴Pr 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.

Observed in 2001



PHYSICAL REVIEW C 73, 037303 (2006)

Possible existence of multiple chiral doublets in ¹⁰⁶Rh

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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 (M χ D), i.e., more than one pair of chiral doublet bands in one single nucleus, is suggested for ¹⁰⁶Rh based on the triaxial deform corresponding proton and neutron configurations.

DOI: 10.1103/PhysRevC.73.037303

PACS number(s): 21.10.Re, 21.60.Jz, 21



The investigation followed by:

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



First observation of the $M\chi D$ bands

week ending PHYSICAL REVIEW LETTERS PRL 110, 172504 (2013) 26 APRIL 2013 Evidence for Multiple Chiral Doublet Bands in ¹³³Ce A. D. Ayangeakaa,¹ U. Garg,¹ M. D. Anthony,¹ S. Frauendorf,¹ J. T. Matta,¹ B. K. Nayak,^{1,*} D. Patel,¹ Q.B. Chen (陈启博),² S.Q. Zhang (张双全),² P.W. Zhao (赵鹏巍),² B. Qi (亓斌),³ J. Meng (孟杰),^{2,4,5} R. V. F. Janssens,⁶ M. P. Carpenter,⁶ C. J. Chiara,^{6,7} F. G. Kondev,⁸ T. Lauritsen,⁶ D. Seweryniak,⁶ S. Zhu,⁶ S. S. Ghugre,⁹ and R. Palit^{10,11} ¹Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA ²State Key Laboratory of Nuclear Physics and Technology, School of Pi -O- Band 5 (Exp) -O- Band 2 (Exp) -Band 6 (Exp) -D-Band 3 (Exp) Energy (MeV) ²⁰(10⁵) Sum of triple gates on Band 6 ···· Band 5 (TPRN ····· Band 2 (TPRM Counts Band 6 (TPF Band 3 (TPRN) 'yl Band 5 Band Sum of triple gates on Band 5 ounts (10⁴) a $\xi = 0.7$ $\xi = 1.0$ Band 6 20 856 20 S(I) [keV/ħ] [12 200 300 500 600 700 800 d Energy (keV) Band 4 10 Band 3 $\xi = 1.0$ $\xi = 0.7$ 16 $B(M1)/B(E2) [(\mu_N/eb)^2]$ ^{133}C 12 ¹³³Ce 16 24 8 10 12 16

Level Scheme

Theoretical description



Exploration of M_XD in ⁷⁸Br

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





- 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 timedependent single-particle problem.
- The corresponding single-particle field is not only timedependent, but also depends on the single-particle density with its full time dependence, i.e., it includes memory effects.



- For vibrations with small amplitude, it can be expanded in the vicinity of the ground state and a connection to the static energy density functional can be found.
- In the adiabatic approximation, i.e. by neglecting the memory effects and the energy dependence in Fourier space, one ends up with the RPA with a residual interaction derived as the second derivative of the static energy functional with the density.
- RPA provides a successful description of the mean energies of giant resonances in nuclei, but not able to reproduce the decay width of these excitations.
- For the decay width and the fragmentation of single-particle states, one has to go beyond mean field and to consider the energy dependence of the self-energy. This can be done within the particle-vibrational coupling (PVC) model.

Paar, Vretenar, Khan, Colo, Rep. Prog. Phys. 70, 691 (2007).

RHB+QRPA: Nuclear β⁺/EC-decay half-lives

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► RHB+QRPA: well reproduces the experimental half-lives for neutron-deficient Ar, Ca, Ti, Fe, Ni, and Zn isotopes by a universal *T*=0 pairing strength.

▶ FRDM+QRPA: systematically overestimates the nuclear half-lives the pp residual interactions in the *T*=0 channel are not considered.



Nuclear β^+ /EC-decay half-lives calculated in RHB+QRPA model with the PC-PK1 parameter set. **Niu et al., PRC 87, 051303(R) (2013)**



HB+QRPA/PC-PK1: Nuclear β-decay half-lives



Z. Y. Wang, Z. M. Niu, Y. F. Niu, J. Y. Guo <u>arXiv:1503.01222</u> Nuclear \$β\$-decay half-lives in the relativistic point-coupling model



- Many-body energy takes the form of a functional of all transition density matrices between the various Slater determinants of different deformation and orientation. Mixing of these different configurations allows the restoration of symmetries and to take into account fluctuations around the mean-field equilibrium solution.
- In full space and with deformation degrees of freedom, such calculations require considerable numerical efforts, at the limit of present computer capabilities.
- A considerable simplification is by using the constraint calculations for the derivation of a collective Hamiltonian in these degrees of freedom.



7D GCM: two deformation parameters + projection 3DAM and 2PN



 ♦ The low-energy spectrum in ⁷⁶Kr are well reproduced after including triaxiality in the full microscopic
 GCM+ PN3DAMP calculation based on the CDFT using PC-PK1.

♦ This study answers the important question of dynamic correlations and triaxiality in shape-coexistence nucleus ⁷⁶Kr and provides the first benchmark for the EDF based collective Hamiltonian method.

Yao, Hagino, Li, Meng, Ring, Phys. Rev. C 89, 054306 (2014)

Benchmark for the collective Hamiltonian in five dimensions



5DCH Calculations based on CDFT PC-PK1 indicate a simultaneous quantum shape phase transition from spherical to prolate shapes, and from reflection symmetric to octupole shapes.





Relativistic description of nuclear matrix elements in neutrinoless double-β decay

Editors' Suggestion

Phys. Rev. C 90, 054309 – Published 10 November 2014 Song, Yao, Ring, and Meng

Relativistic description of nuclear matrix elements in neutrinoless double- β decay

L. S. Song, J. M. Yao, P. Ring, and J. Meng Phys. Rev. C **90**, 054309 (2014) – Published 10 November 2014



Phys. Rev. C 91, 024316 (2015) Yao, Song, Hagino, Ring, and Meng

TABLE II. The calculated NME $M^{0\nu}$ of the $0\nu\beta\beta$ decay with the REDF (PC-PK1), in comparison with those by the NREDF (D1S), RQRPA, PHFB, ISM, and IBM2. Only the results considering the short-range correlation (SRC) effect by UCOM, except for the IBM2 where CCM is used and using the parameter $R = 1.2A^{1/3}$ fm are adopted for comparison. The values in the parentheses are the results with additional pairing fluctuations.

	1 0						
S	Models $g_A(0)$	REDF(PC-PK1) 1.254	NREDF(D1S) 1.25	RQRPA (Tübingen) 1.254	PHFB 1.254	ISM 1.25	IBM2 1.269
2	$\label{eq:48} \begin{array}{l} {}^{48}\text{Ca} \rightarrow {}^{48}\text{Ti} \\ {}^{76}\text{Ge} \rightarrow {}^{76}\text{Se} \\ {}^{82}\text{Se} \rightarrow {}^{82}\text{Kr} \\ {}^{96}\text{Zr} \rightarrow {}^{96}\text{Mo} \\ {}^{100}\text{Mo} \rightarrow {}^{100}\text{Ru} \\ {}^{116}\text{Cd} \rightarrow {}^{116}\text{Sn} \\ {}^{124}\text{Sn} \rightarrow {}^{124}\text{Te} \\ {}^{130}\text{Te} \rightarrow {}^{130}\text{Xe} \end{array}$	2.94 6.13 5.40 6.47 6.58 5.52 4.33 4.98	$\begin{array}{c} 2.37 \ (2.23) \\ 4.60 \ (5.55) \\ 4.22 \ (4.67) \\ 5.65 \ (6.50) \\ 5.08 \ (6.59) \\ 4.72 \ (5.35) \\ 4.81 \ (5.79) \\ 5.13 \ (6.40) \end{array}$	5.17 5.32 1.77 3.88 3.21 4.07	3.32 7.22 4.66	0.85 2.81 2.64 2.62 2.65	2.38 6.16 4.99 3.00 4.50 3.29 4.02 4.61
		4.32 5.60	4.20 (4.77) 1.71 (2.19)	2.54	3.24	2.19	3.79 2.88

The authors report a fully relativistic des based on a state-of-the-art nuclear struct and electric quadrupole transitions in both double- β decay experiments.



Application of CDFT in Nuclear astrophysics





The effective interaction in current CDFT is not derived from the basic theory of the strong interaction --- QCD. As indicated by the successes achieved by the covariant density functional, the feasibility of a unified selfconsistent description of nuclear ground state and excitation properties starting from an effective nucleon-nucleon interaction is anticipated.

In future, one needs to obtain properly the nucleon-nucleon interaction in nuclear medium starting from the quantum chromo-dynamics, eventually to build the standard model of nuclear structure that can implement the ab initio exploration for all nuclei in the nuclear chart.



Thank you for your attention!

Le & Jab initio covariant investigations of heavy nuclei

CHIN. PHYS. LETT. Vol. 33, No. 10 (2016) 102103

Express Letter

Relativistic Brueckner–Hartree–Fock Theory for Finite Nuclei *

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