“2020绵阳原子核结构理论研讨会(2020.01.10-01.14)

协变密度泛函理论
对原子核磁矩和磁偶极跃迁的研究

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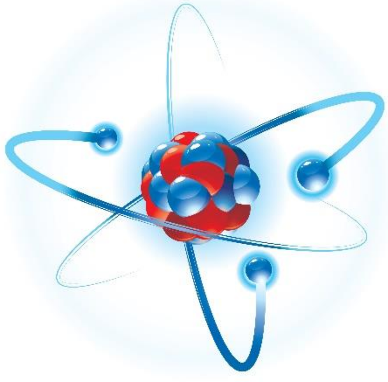
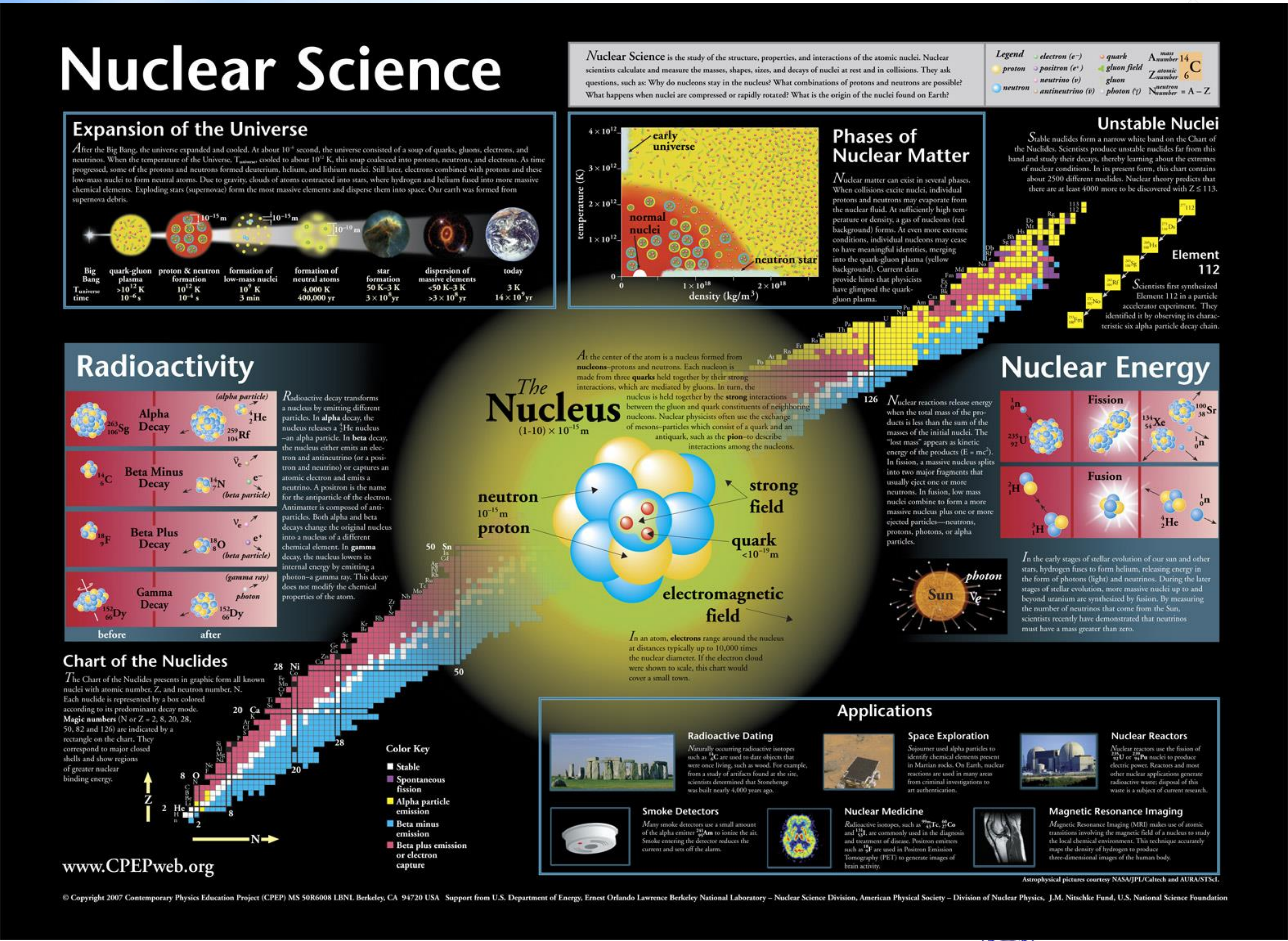


主要内容

- 协变密度泛函理论

- 核磁矩
  - 球形奇A核
  - 形变奇A核

- 磁偶极跃迁
  - 集体转动
  - 集体振动


Nuclear Science
Nuclear Science is the study of the structure, properties, and interactions of the atomic nuclei. Nuclear scientists calculate and measure the masses, shapes, sizes, and decays of nuclei at rest and in collisions. They ask questions, such as: Why do nucleons stay in the nucleus? What combinations of protons and neutrons are possible? What happens when nuclei are compressed or rapidly rotated? What is the origin of the nuclei found on Earth?
Legend
proton
neutron
electron (e^-)
positron (e^+)
neutrino (ν)
antineutrino ($\bar{\nu}$)
quark
gluon field
gluon
photon (γ)
A mass number
Z atomic number
$^{14}_{6}C$
N neutron number = A – Z
Expansion of the Universe
After the Big Bang, the universe expanded and cooled. At about 10^{-6} second, the universe consisted of a soup of quarks, gluons, electrons, and neutrinos. When the temperature of the Universe, $T_{universe}$, cooled to about 10^{12} K, this soup coalesced into protons, neutrons, and electrons. As time progressed, some of the protons and neutrons formed deuterium, helium, and lithium nuclei. Still later, electrons combined with protons and these low-mass nuclei to form neutral atoms. Due to gravity, clouds of atoms contracted into stars, where hydrogen and helium fused into more massive chemical elements. Exploding stars (supernovae) form the most massive elements and disperse them into space. Our earth was formed from supernova debris.
10^{-15} m
10^{-15} m
10^{-10} m
Big Bang
$T_{universe}$
time
quark-gluon plasma $>10^{12}$ K 10^{-6} s
proton & neutron formation 10^{12} K 10^{-4} s
formation of low-mass nuclei 10^{9} K 3 min
formation of neutral atoms 4,000 K 400,000 yr
star formation 50 K–3 K 3×10^{8} yr
dispersion of massive elements <50 K–3 K $>3\times10^{8}$ yr
today 3 K 14×10^{9} yr
temperature (K)
4×10^{12}
3×10^{12}
2×10^{12}
1×10^{12}
0
early universe
normal nuclei
neutron star
0
1×10^{18}
2×10^{18}
density (kg/m^3)
Phases of Nuclear Matter
Nuclear matter can exist in several phases. When collisions excite nuclei, individual protons and neutrons may evaporate from the nuclear fluid. At sufficiently high temperature or density, a gas of nucleons (red background) forms. At even more extreme conditions, individual nucleons may cease to have meaningful identities, merging into the quark-gluon plasma (yellow background). Current data provide hints that physicists have glimpsed the quark-gluon plasma.
Unstable Nuclei
Stable nuclides form a narrow white band on the Chart of the Nuclides. Scientists produce unstable nuclides far from this band and study their decays, thereby learning about the extremes of nuclear conditions. In its present form, this chart contains about 2500 different nuclides. Nuclear theory predicts that there are at least 4000 more to be discovered with Z ≤ 113.
Element 112
Scientists first synthesized Element 112 in a particle accelerator experiment. They identified it by observing its characteristic six alpha particle decay chain.
Radioactivity
Alpha Decay
$^{263}_{106}Sg$
(alpha particle)
$^{4}_{2}He$
$^{259}_{104}Rf$
Beta Minus Decay
$^{14}_{6}C$
$\bar{\nu}_e$
e^-
$^{14}_{7}N$
(beta particle)
Beta Plus Decay
$^{18}_{9}F$
ν_e
e^+
$^{18}_{8}O$
(beta particle)
Gamma Decay
$^{152}_{66}Dy$
(gamma ray)
photon
$^{152}_{66}Dy$
before
after
Radioactive decay transforms a nucleus by emitting different particles. In alpha decay, the nucleus releases a $^{4}_{2}He$ nucleus –an alpha particle. In beta decay, the nucleus either emits an electron and antineutrino (or a positron and neutrino) or captures an atomic electron and emits a neutrino. A positron is the name for the antiparticle of the electron. Antimatter is composed of antiparticles. Both alpha and beta decays change the original nucleus into a nucleus of a different chemical element. In gamma decay, the nucleus lowers its internal energy by emitting a photon–a gamma ray. This decay does not modify the chemical properties of the atom.
The Nucleus
(1-10) × 10^{-15} m
At the center of the atom is a nucleus formed from nucleons–protons and neutrons. Each nucleon is made from three quarks held together by their strong interactions, which are mediated by gluons. In turn, the nucleus is held together by the strong interactions between the gluon and quark constituents of neighboring nucleons. Nuclear physicists often use the exchange of mesons–particles which consist of a quark and an antiquark, such as the pion–to describe interactions among the nucleons.
neutron
10^{-15} m
proton
strong field
quark
$<10^{-19}$ m
electromagnetic field
In an atom, electrons range around the nucleus at distances typically up to 10,000 times the nuclear diameter. If the electron cloud were shown to scale, this chart would cover a small town.
Nuclear Energy
126
Nuclear reactions release energy when the total mass of the products is less than the sum of the masses of the initial nuclei. The "lost mass" appears as kinetic energy of the products (E = mc^2). In fission, a massive nucleus splits into two major fragments that usually eject one or more neutrons. In fusion, low mass nuclei combine to form a more massive nucleus plus one or more ejected particles—neutrons, protons, photons, or alpha particles.
Fission
$^{1}_{0}n$
$^{235}_{92}U$
$^{134}_{54}Xe$
$^{100}_{38}Sr$
$^{1}_{0}n$
Fusion
$^{2}_{1}H$
$^{3}_{1}H$
$^{4}_{2}He$
$^{1}_{0}n$
Sun
photon
ν_e
In the early stages of stellar evolution of our sun and other stars, hydrogen fuses to form helium, releasing energy in the form of photons (light) and neutrinos. During the later stages of stellar evolution, more massive nuclei up to and beyond uranium are synthesized by fusion. By measuring the number of neutrinos that come from the Sun, scientists recently have demonstrated that neutrinos must have a mass greater than zero.
Chart of the Nuclides
The Chart of the Nuclides presents in graphic form all known nuclei with atomic number, Z, and neutron number, N. Each nuclide is represented by a box colored according to its predominant decay mode. Magic numbers (N or Z = 2, 8, 20, 28, 50, 82 and 126) are indicated by a rectangle on the chart. They correspond to major closed shells and show regions of greater nuclear binding energy.
Z
N
Color Key
Stable
Spontaneous fission
Alpha particle emission
Beta minus emission
Beta plus emission or electron capture
Applications
Radioactive Dating
Naturally occurring radioactive isotopes such as $^{14}_{6}C$ are used to date objects that were once living, such as wood. For example, from a study of artifacts found at the site, scientists determined that Stonehenge was built nearly 4,000 years ago.
Space Exploration
Sojourner used alpha particles to identify chemical elements present in Martian rocks. On Earth, nuclear reactions are used in many areas from criminal investigations to art authentication.
Nuclear Reactors
Nuclear reactors use the fission of $^{235}_{92}U$ or $^{239}_{94}Pu$ nuclei to produce electric power. Reactors and most other nuclear applications generate radioactive waste; disposal of this waste is a subject of current research.
Smoke Detectors
Many smoke detectors use a small amount of the alpha emitter $^{241}_{95}Am$ to ionize the air. Smoke entering the detector reduces the current and sets off the alarm.
Nuclear Medicine
Radioactive isotopes, such as $^{99m}_{43}Tc$, $^{60}_{27}Co$ and $^{131}_{53}I$, are commonly used in the diagnosis and treatment of disease. Positron emitters such as $^{18}_{9}F$ are used in Positron Emission Tomography (PET) to generate images of brain activity.
Magnetic Resonance Imaging
Magnetic Resonance Imaging (MRI) makes use of atomic transitions involving the magnetic field of a nucleus to study the local chemical environment. This technique accurately maps the density of hydrogen to produce three-dimensional images of the human body.
Astrophysical pictures courtesy NASA/JPL/Caltech and AURA/STScI.
www.CPEPweb.org
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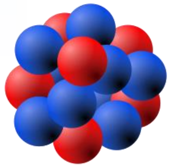
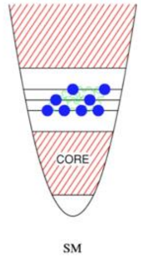
如何理解原子核?



原子核：质子和中子(统称核子)组成的有限量子多体系统。

处理量子多体问题的方法：

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

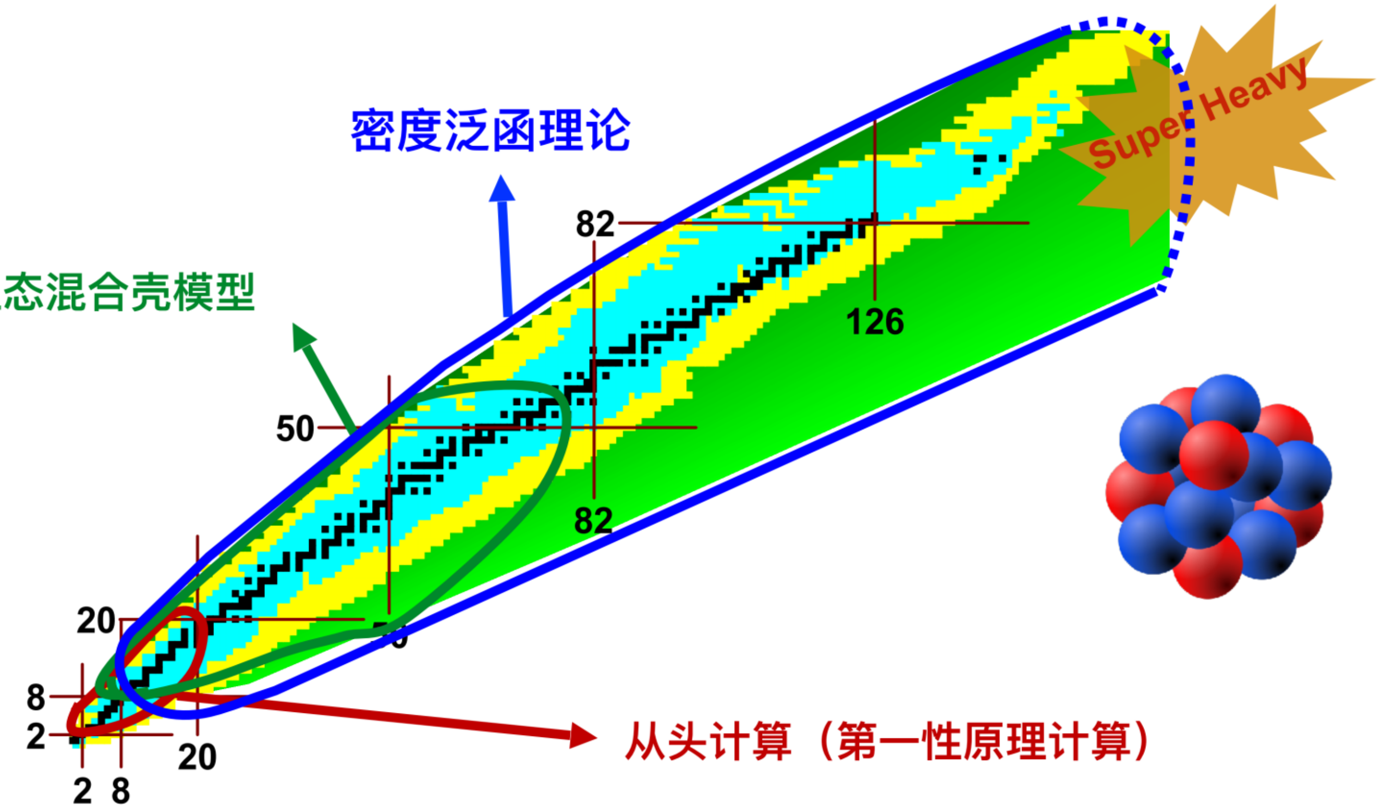


$$\hat{H}=\sum_i\left[-\frac{\hbar^2}{2m}\nabla_i^2+U(r_i)\right]+\sum_{i>j}V_{ij}-\sum_i U(r_i)$$

平均势场

剩余相互作用

核理论方法前沿热点



密度泛函理论(DFT)：量子多体系统最成功的方法之一，包含有限个数参数，成功地描述核素图上近乎所有原子核基态和激发态性质。

密度泛函理论(Density Functional Theory)

The many-body problem is mapped onto a one-body problem

Kohn-Sham DFT

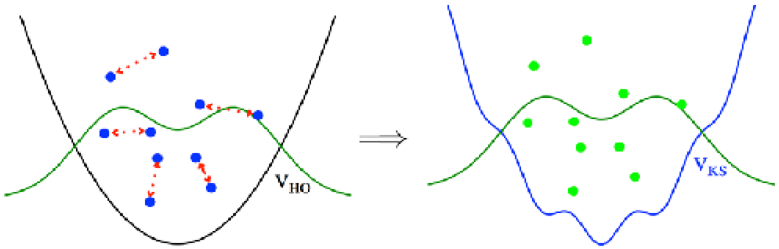


Figure from Drut PPNP 2010

Hohenberg-Kohn Theorem

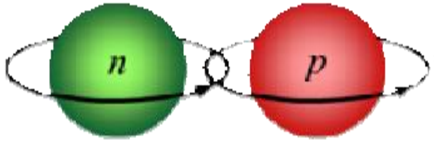
The exact ground-state energy of a quantum mechanical many-body system is a universal functional of the local density.

$$E[\rho] \Rightarrow \boxed{\hat{h} = \frac{\delta E}{\delta \rho}} \Rightarrow \boxed{\hat{h}\varphi_i = \varepsilon_i \varphi_i} \Rightarrow \boxed{\rho = \sum_{i=1}^{A} |\varphi_i|^2}$$

The practical usefulness of the Kohn-Sham theory depends entirely on whether an **Accurate Energy Density Functional** can be found!

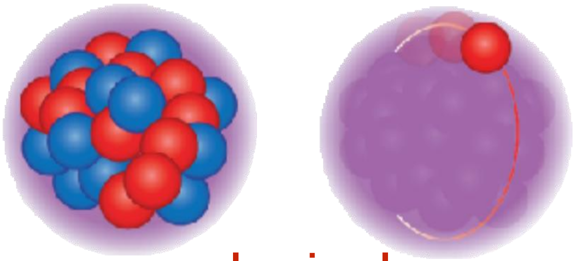
原子核的密度泛函理论

✓ The nuclear force is complicated



✓ More degrees of freedom: spin, isospin, pairing, …

✓ Nuclei are self-bound systems



DFT for the intrinsic density

✓ At present, all successful functionals are phenomenological not connected to any NN- or NNN-interaction

✓ Adjust to properties of nuclear matter and/or finite nuclei, and (in future) to ab-initio results

Nowadays, the ansatz for E(ρ) is phenomenological:

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

为什么要“协变”？

- ✓ Large mean fields S≈-400 MeV, V≈350 MeV
- ✓ Large spin-orbit splitting automatically included
- ✓ Pseudo-spin Symmetry
- ✓ Success of Relativistic Brueckner
- ✓ Consistent treatment of time-odd fields
- ✓ Relativistic saturation mechanism

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$$(-i\vec{\alpha}\cdot\nabla+\beta(m+S)+V)\psi_i=\varepsilon_i\psi_i$$

$$\begin{pmatrix} m+S+V & -i\vec{\sigma}\cdot\nabla \\ -i\vec{\sigma}\cdot\nabla & -m-S+V \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}=(m+\varepsilon)\begin{pmatrix} f \\ g \end{pmatrix}$$

Strong spin-orbit interaction

$$\left\{-\nabla\frac{1}{2m_{eff}}\nabla+V_{pot}+\boxed{\frac{1}{2m^2}\nabla V_{ls}\cdot(\vec{p}\times\vec{s})}\right\}f=\varepsilon f,$$

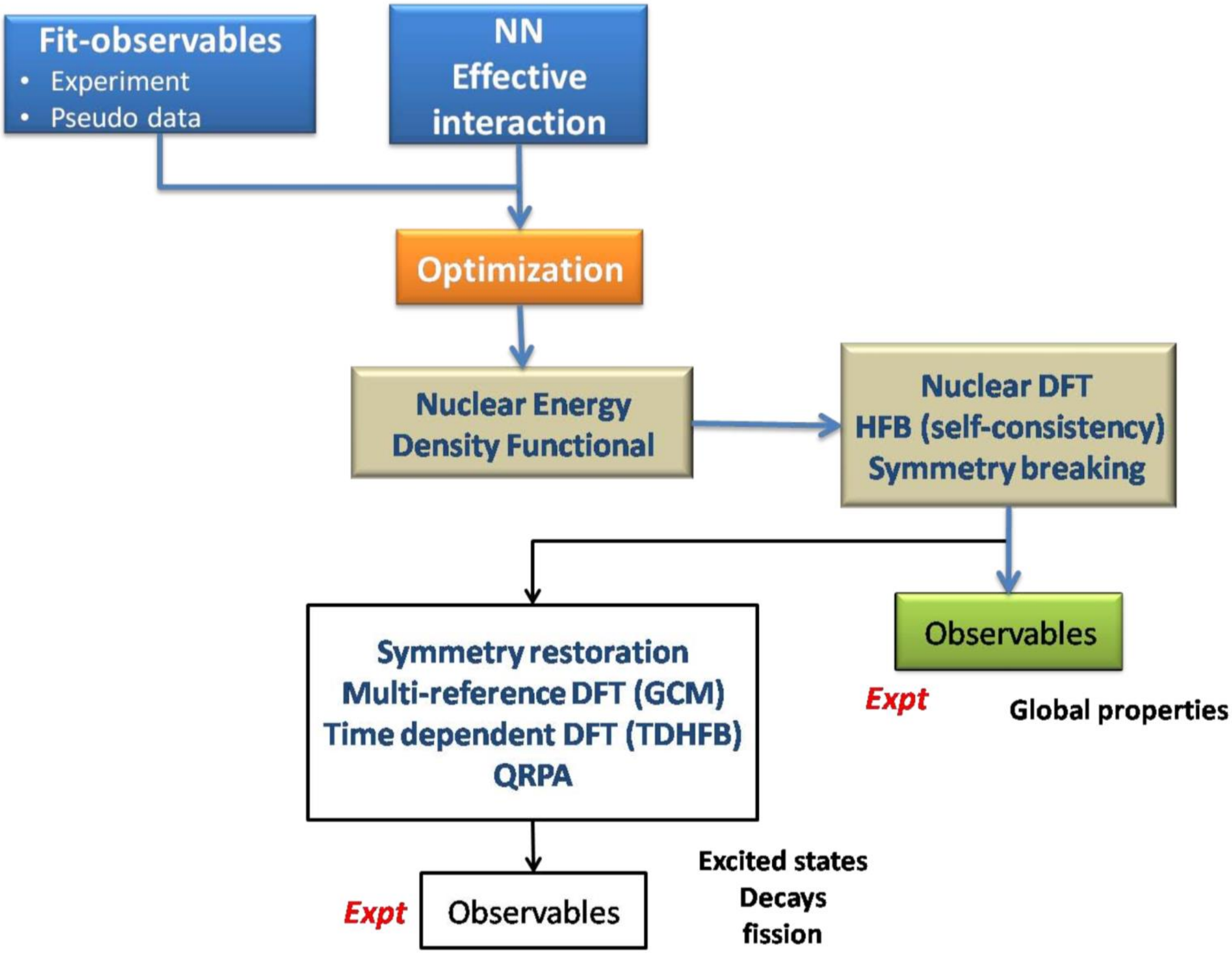
$$\boxed{\frac{1}{2m^2}\left(\frac{1}{r}\frac{\partial V_{ls}(r)}{\partial r}\right)\vec{l}\cdot\vec{s}}$$

$$m_{eff}=m-\frac{1}{2}(V-S),$$

$$V_{pot}=V+S,\quad V\approx 350MeV,\quad S\approx -400MeV,$$

$$V_{ls}=\frac{m}{m_{eff}}(V-S).$$

原子核协变密度泛函理论理论步骤



研究领域和综述文章

- ★ 奇特原子核结构
- ★ 高速转动原子核
- ★ 原子核的奇异形状
- ★ 原子核质量与寿命
- ★ 超重元素与新核素
- ★ 核天体物理
- ★ 超核物理
- ★ 其他交叉学科

J. Meng, H. Toki, S.-G. Zhou, S.Q. Zhang, W.H. Long, and L.S. Geng, Prog. Part. Nucl. Phys. 57 (2006) 470-563

孟杰, 郭建友, 李剑, 李志攀, 梁豪兆, 龙文辉, 牛一斐, 牛中明, 尧江明, 张颖, 赵鹏巍, 周善贵, 原子核物理中的协变密度泛函理论, 物理学进展, 第31卷04期 (2011) 199-336

J. Meng, J. Peng, S.Q. Zhang, and P.W. Zhao, Front. Phys. 8 (2013) 55-79

H. Z. Liang, J. Meng, and S.-G. Zhou, Physics Reports 570 (2015) 1-84

J. Meng and S.-G. Zhou, J. Phys. G42 (2015) 093101

J. Meng (ed.), Relativistic Density Functional for Nuclear Structure (World Scientific, Singapore, 2016)

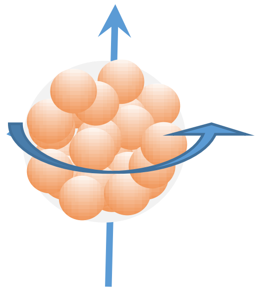
主要内容

- ❑ 协变密度泛函理论
- ❑ 核磁矩
- ❑ 磁偶极跃迁

原子核磁矩

核磁矩：核子固有自旋及在核内的运动

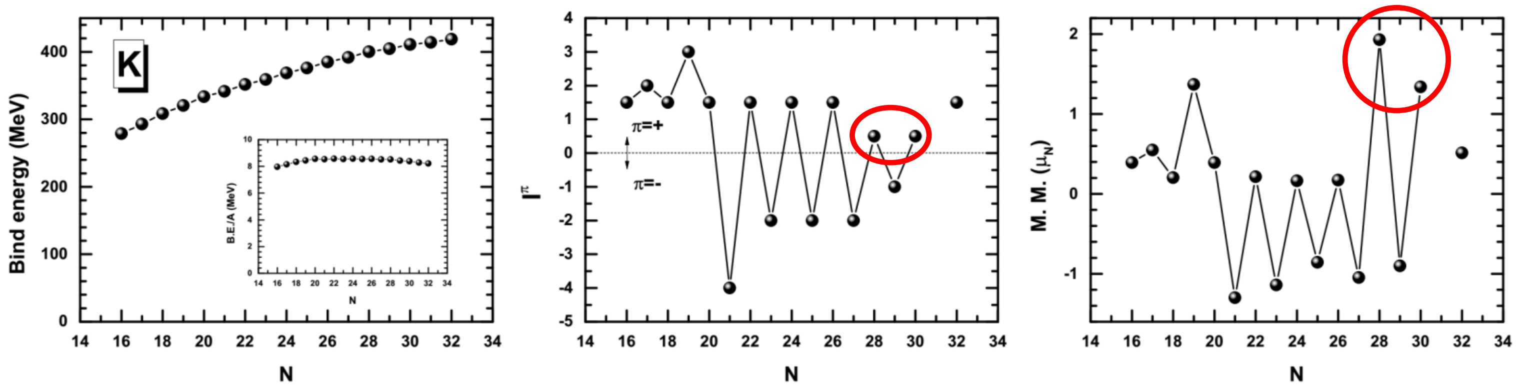
$$\mu = \langle IM|\hat{\mu}_z|IM\rangle_{M=I}$$



❖ **最重要核观测量之一**，反映丰富的核结构信息，如壳结构演化等；

❖ 联系**原子谱学的精细结构**信息

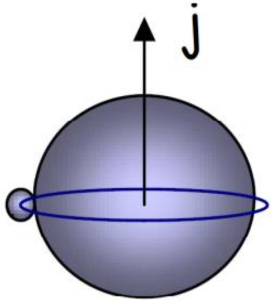
➢ 核磁矩的理论描述**非常困难**：(1)首先正确再现自旋和宇称；(2)对原子核波函数非常敏感



K同位素链原子核结合能，自旋、宇称和磁矩

Schmidt磁矩——极端单粒子壳模型

- 原子核的磁矩仅由最后一个未配对价核子决定

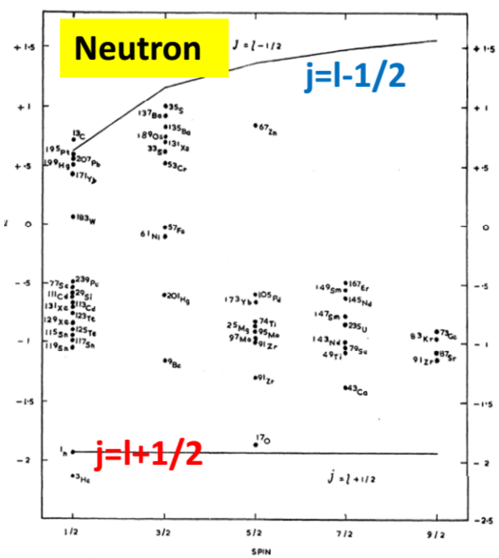


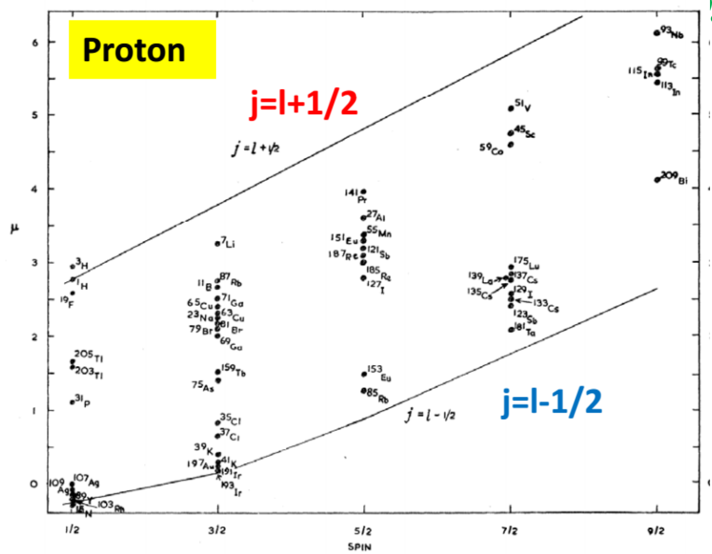
$$\mu = \begin{cases} g_l l + \dfrac{1}{2} g_s, & j = l + 1/2 \\ \dfrac{j}{j+1}\left[g_l (l+1) - \dfrac{1}{2} g_s \right], & j = l - 1/2. \end{cases}$$

质子(中子)轨道和自旋g因子: $g_l = 1(0), g_s = 5.587(-3.826)$

- 几乎所有奇 A 核实验磁矩值都在两条Schmidt 线之间

Blin-Stoyle, Rev. Mod. Phys. 56)





- 介子交换流效应
- 组态混合效应

Arima, Adv. Nucl. Phys. (1987), Towner, Phys. Rep. (1987)

协变密度泛函理论中的磁矩问题

Covariant density functional theory (CDFT), i.e., Relativistic mean-field (RMF) theory: great success in describing nuclear properties but not for nuclear magnetic moments. *Ring, PPNP(1996), Vretenar, Phys. Rep. (2005), Meng, PPNP (2006).*

It was a surprise and for a long time an open problem, that relativistic theories containing only a scalar potential (σ) and the time-like component of a Lorentz vector field ω could not reproduce the corresponding Schmidt values. *Miller_Ann. Phys. (1975), Serot_PLB_(1981).*

Magnetic Moments of ^{15}N and ^{15}O

$\Delta E_{so} = 6.9$	^{15}N			^{15}O		
	Anomalous	Dirac	Total	Anomalous	Dirac	Total
$M1$	−0.623	0.716	0.093	0.665	0.0	0.665
$M2$	−0.613	0.566	−0.047	0.654	0.0	0.654
$M3$	−0.610	0.349	−0.261	0.651	0.0	0.651
Schmidt	−0.598	0.333	−0.265	0.637	0.0	0.637
Experiment			−0.28			0.72

Dirac磁矩增强——协变密度泛函理论

The problem is easy to understand: the large scalar potential required by the spin-orbit force significantly reduces the effective mass of valence nucleon, thus increasing its electromagnetic current and the (Dirac) magnetic moment.

- From Gordon identity, the spatial part of the Dirac current

$$\mathbf{j}_D = \frac{Q}{M^*}\bar{\psi}(\mathbf{r})\mathbf{p}\psi(\mathbf{r}) + \frac{Q}{2M^*}\nabla \times [\psi^+(\mathbf{r})\beta\mathbf{\Sigma}\psi(\mathbf{r})],$$

  where the effective (scalar) mass $M^* = M + S \approx 0.6M$

- The corresponding nuclear magnetic moments, $\mu = \frac{1}{2}\int d\mathbf{r}\ [\mathbf{r}\times\mathbf{J}]_z$

$$\boldsymbol{\mu} = \boldsymbol{\mu}_D + \boldsymbol{\mu}_A = \underbrace{Q\int d\mathbf{r}\frac{M}{M^*}\bar{\psi}[\mathbf{L}+\mathbf{\Sigma}]\psi}_{\mu_D} + \underbrace{\int d\mathbf{r}\kappa\bar{\psi}\mathbf{\Sigma}\psi}_{\mu_A}$$

- Compared with the magnetic moment in non-relativistic theory

$$\boldsymbol{\mu} = g_l\mathbf{l} + g_s\mathbf{s} = g_l\mathbf{l} + \frac{g_s}{2}\boldsymbol{\sigma} = \underbrace{g_l(\mathbf{l}+\boldsymbol{\sigma})}_{\mu_D} + \underbrace{(\frac{g_s}{2} - g_l)\boldsymbol{\sigma}}_{\mu_A}.$$

- Dirac magnetic moment in RMF theory is enhanced.

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磁矩问题解决方法

Although the valence-particle approximation is reasonable in a non-relativistic calculation, it is simply wrong in a relativistic calculation. This puzzle can be resolved by including the polarization of the core by external particle.

- ✓ Random Phase Approximation (RPA) and the corresponding linear response theory

  Mcneil(1986), Furnastahl(1987), Ichii(1987), Shepard(1988)

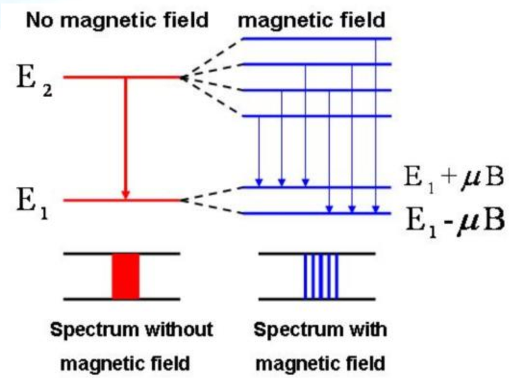
- ✓ Self-consistent deformed RMF theory with the baryon currents of both valence nucleon and the core. Hofmann(1988), Furnstahl(1989), Yao(2006)

  The spatial components of vector meson field **V**, (i.e., time-odd fields or magnetic potential), break the time-reversal symmetry of wavefunctions in the core, thus producing a non-zero contribution to the Dirac current.

Finally, agreement with Schmidt values and the isoscalar magnetic moments are also well reproduced.

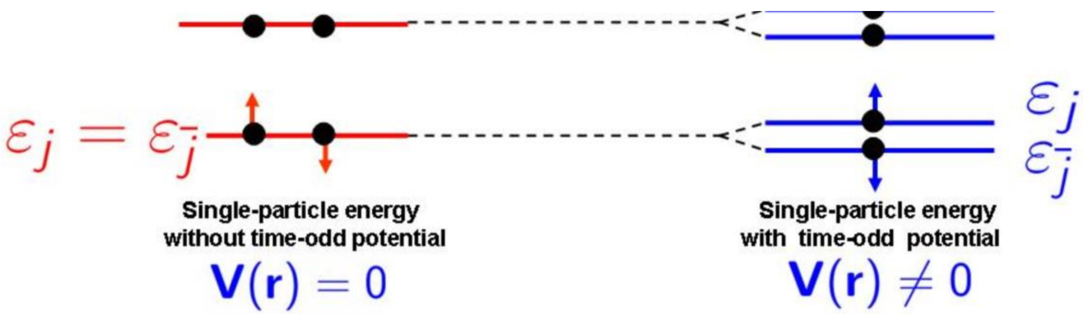
奇时间场效应

Time-odd field V ($\hat{T}V\hat{T}^{-1} = -V$) :important in atomic and nuclear physics: zeeman effect, hyperfine structure.



Dirac equation with time-odd field $\mathbf{V}(\mathbf{r})$

$$\{-i\boldsymbol{\alpha}\cdot\nabla - \boldsymbol{\alpha}\cdot\mathbf{V}(\mathbf{r}) + V_0(\mathbf{r}) + \beta[M + S(\mathbf{r})]\}\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$



- ✓ Sph. RMF: Without polarization
- ✓ Def. RMF: With polarization
- ☐ Dirac M.M is reduced.
- ☐ Total M.M: in agreement with the Schmidt value & greatly improved.

^{15}N	μ	μ_D	μ_A
exp.	-0.28		
Schmidt	-0.26	0.33	-0.60
Sph.RMF	-0.03	0.59	-0.62
Axi.RMF	-0.29	0.44	-0.73

磁矩：包含介子交换流和组态混合效应

- Magnetic moment operator

$$\hat{\mu} = \hat{\mu}_{\rm free} + \hat{\mu}_{\rm mec}$$

- Ground-state wave function with mixing of particle-hole (p-h) configurations:

$$|\tilde{j}\rangle = |j\rangle + \sum C_{\rm 1p-1h}|j \otimes \text{1p-1h}; j\rangle + \sum C_{\rm 2p-2h}|j \otimes \text{2p-2h}; j\rangle + \cdots\cdots$$

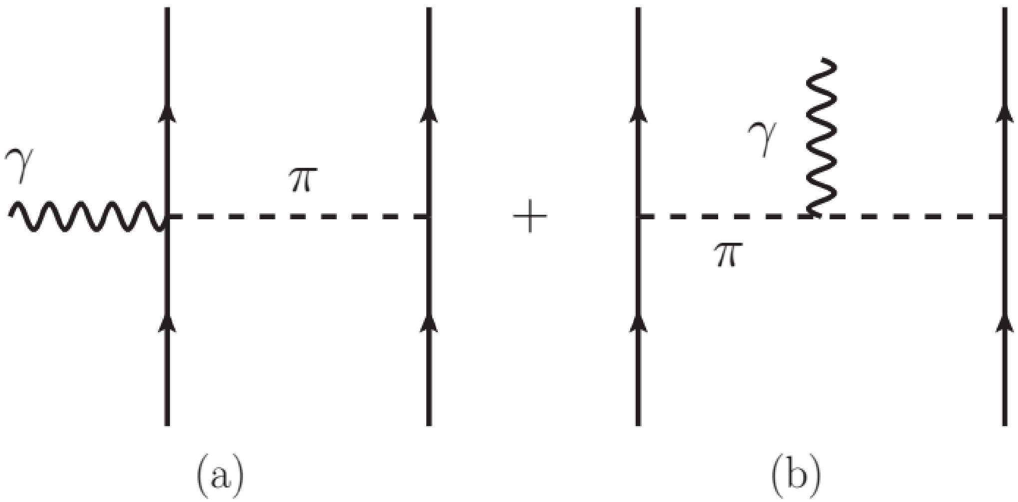
- Magnetic moments after including meson exchange current and configuration mixing.

$$\begin{aligned} \mu_{\rm Total} &= \langle\tilde{j}|\hat{\mu}_{\rm free} + \hat{\mu}_{\rm mec}|\tilde{j}\rangle \\ &= \langle j|\hat{\mu}_{\rm free}|j\rangle + \langle\tilde{j}|\hat{\mu}_{\rm mec}|\tilde{j}\rangle + \langle\tilde{j}|\hat{\mu}_{\rm free}|\tilde{j}\rangle - \langle j|\hat{\mu}_{\rm free}|j\rangle \\ &= \mu_{\rm MF} + \mu_{\rm MEC} + \mu_{\rm CM} \end{aligned}$$

- $\mu_{\rm MF}(\mu_{\rm RMF}) \longleftarrow$ **deformed RMF theory with time-odd fields**
- $\mu_{\rm MEC}$: meson exchange current corrections
  $\langle j|\hat{\mu}_{\rm mec}(1\pi)|j\rangle \longleftrightarrow$ **one-pion exchange current corrections**
- $\mu_{\rm CM}$: configuration mixing corrections
  Perturbation theory $\Longrightarrow$ first- and second-order CM (1st, 2nd)

单pi介子交换流

- In Hartree approximation, pion field is zero.
- Exchange of virtual charged pions between two nucleons
  $\Rightarrow$ MEC corrections to magnetic moments. Morse, PLB (1990)



(a) **Seagull**: a photon $\leftrightarrow$ nucleon + pion at a single vertex.
(b) **In Flight**: a photon $\leftrightarrow$ pion being exchanged.

$$\boldsymbol{\mu}_{\rm MEC} = \frac{1}{2}\int d\mathbf{r}\, \mathbf{r} \times [\,\mathbf{j}^{\rm seagull}(\mathbf{r}) + \mathbf{j}^{\rm in-flight}(\mathbf{r})\,].$$

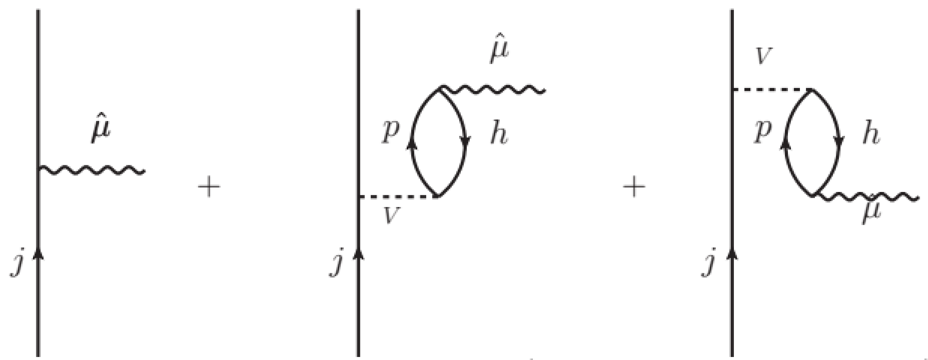
一阶组态混合效应

The ground-state wave function with mixing of particle-hole configurations,

$$|\tilde{j}\rangle = |j\rangle + \sum C_{1\mathrm{p}-1\mathrm{h}} |j \otimes 1\text{p-}1\text{h}; j\rangle + \sum C_{2\mathrm{p}-2\mathrm{h}} |j \otimes 2\text{p-}2\text{h}; j\rangle$$

In perturbation theory, the **first-order corrections**

$$\delta\mu_{1\mathrm{st}}^{\mathrm{cm}} = \langle \tilde{j}|\hat{\mu}|\tilde{j}\rangle - \langle j|\hat{\mu}|j\rangle = \sum C_{1\mathrm{p}-1\mathrm{h}} [\langle j|\hat{\mu}|j \otimes 1\text{p-}1\text{h}; j\rangle + \langle j \otimes 1\text{p-}1\text{h}; j|\hat{\mu}|j\rangle].$$



$$\langle j|\hat{\mu}|j\rangle \quad + \quad \underbrace{C_{1\mathrm{p}-1\mathrm{h}}\langle j|\hat{\mu}|j \otimes ph^{-1}(1^+); j\rangle \ + \ C_{1\mathrm{p}-1\mathrm{h}}\langle j \otimes ph^{-1}(1^+); j|\hat{\mu}|j\rangle}_{\delta\mu_{1\mathrm{cm}}}$$

j is valence particle state, and V residual interaction.

$$\delta\mu_{\mathrm{cm}}^{1\mathrm{st}} = \sum_{j_p j_h J} \frac{2\langle j_h \| \boldsymbol{\mu} \| j_p\rangle}{\Delta E_j} (-1)^{j_h+j+J} \hat{j}^{-1} \sqrt{\frac{j}{j+1}} (2J+1) \begin{Bmatrix} j_h & j_p & 1 \\ j & j & J \end{Bmatrix} \langle j j_p; JM | V | j j_h; JM\rangle .$$

二阶组态混合效应

The ground-state wave function with mixing of particle-hole configurations:

$$|\tilde{j}\rangle = |j\rangle + \sum C_{\mathrm{1p-1h}} |j \otimes \text{1p-1h}; j\rangle + \sum C_{\mathrm{2p-2h}} |j \otimes \text{2p-2h}; j\rangle$$

In perturbation theory, the **second-order corrections** Shimizu, NPA (1974):

$$\delta\mu^{\mathrm{2nd}}_{\mathrm{cm}} = \langle j|V \frac{P}{E_j - H_0} \mu \frac{P}{E_j - H_0} V|j\rangle - \langle j|\mu|j\rangle \langle j|V \frac{P}{(E_j - H_0)^2} V|j\rangle$$

P: projection operator, $\sum |\text{1p-1h}\rangle\langle\text{1p-1h}|$, $\sum |\text{2p-2h}\rangle\langle\text{2p-2h}|$, etc.
$|j\rangle$ and E_j: unperturbed ground-state wavefunction and energy.
V: two-body residual interaction.

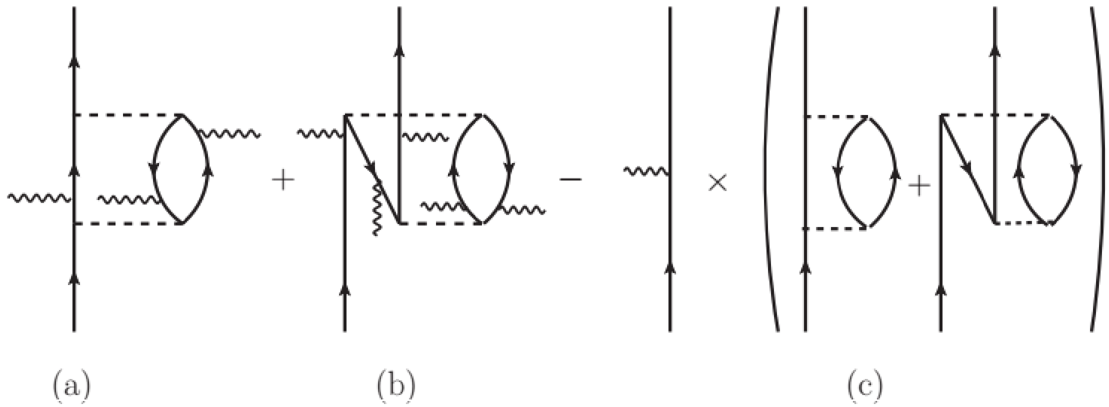


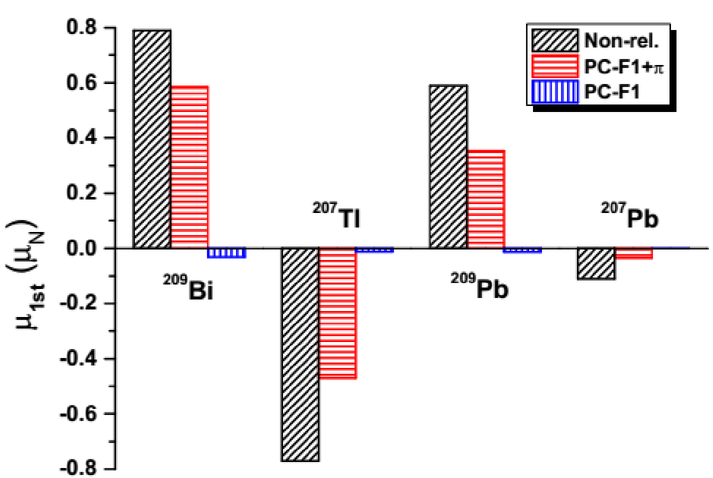
Figure 1: Diagrams representation for 1p-1h mode (a), 2p-2h mode (b) and wavefunction renormalization

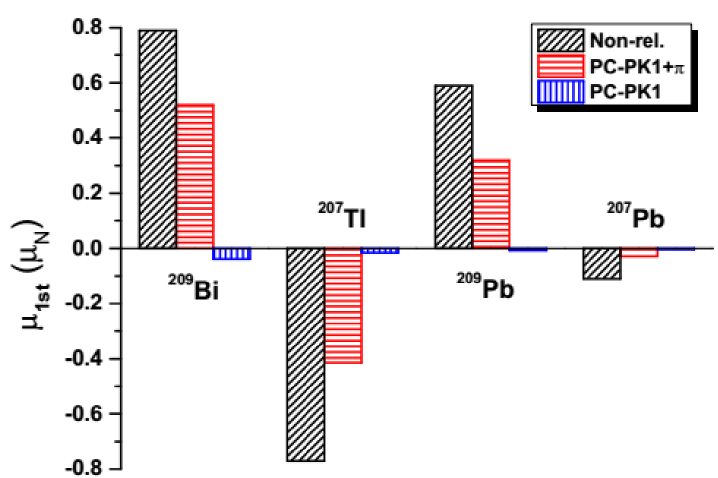
一阶组态混合效应

Table 1: First-order (1st) corrections to magnetic moments of ^{209}Bi.

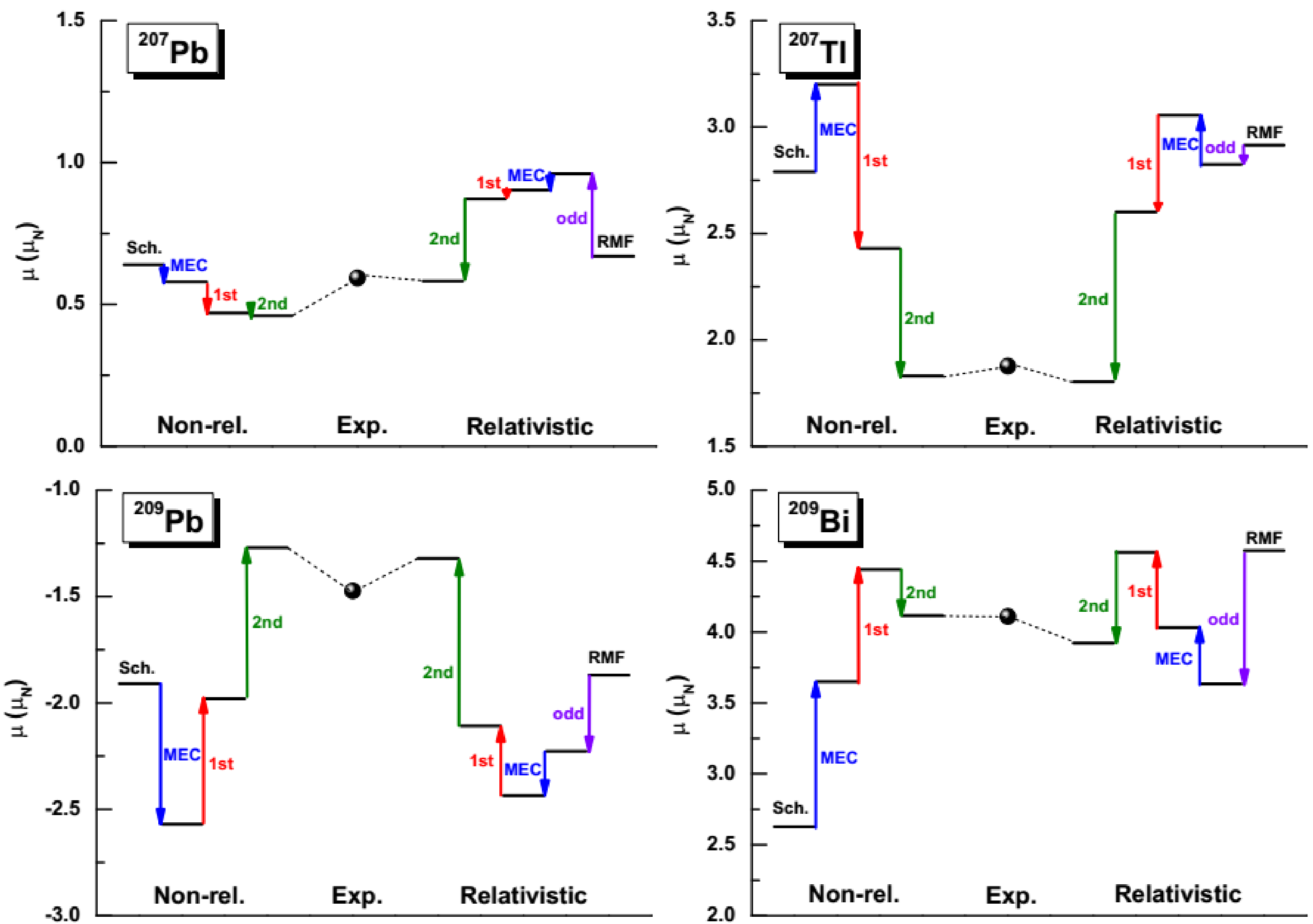
	Non-rel.								Rel.			
Interactions	KK	Gillet	KR. I	KR. II	Brueckner	HJ	Kuo	M3Y†	PC-F1	PC-PK1	PC-F1*	PC-PK1*
Ref.	[1]	[2]					[3]				with π	
$(1h_{\frac{9}{2}}1h_{\frac{11}{2}}^{-1})_\pi$	0.37	0.46	0.53	0.70	0.71	0.55		0.43	-0.10	-0.11	0.23	0.19
$(1i_{\frac{11}{2}}1i_{\frac{13}{2}}^{-1})_\nu$	0.15	-0.02	0.00	-0.06	0.04	0.25		0.24	0.07	0.07	0.36	0.33
Total	0.52	0.43	0.53	0.64	0.75	0.80	0.79	0.68	-0.03	-0.04	0.59	0.52

[1] Mavromatis, NP (1966).
[2] Mavromatis, NPA (1967).
[3] Arima and Huang-Lin, PLB (1972).
† The interaction matrix elements are taken from Bertsch and Schaeffer, NPA (1977).



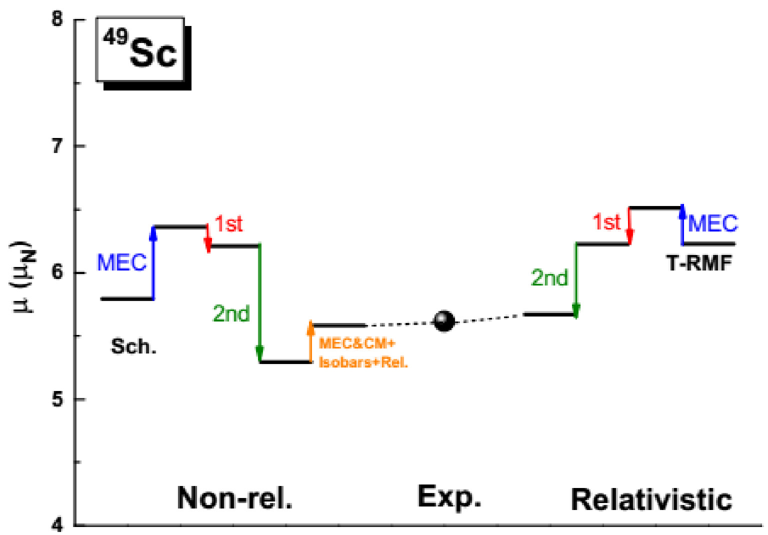


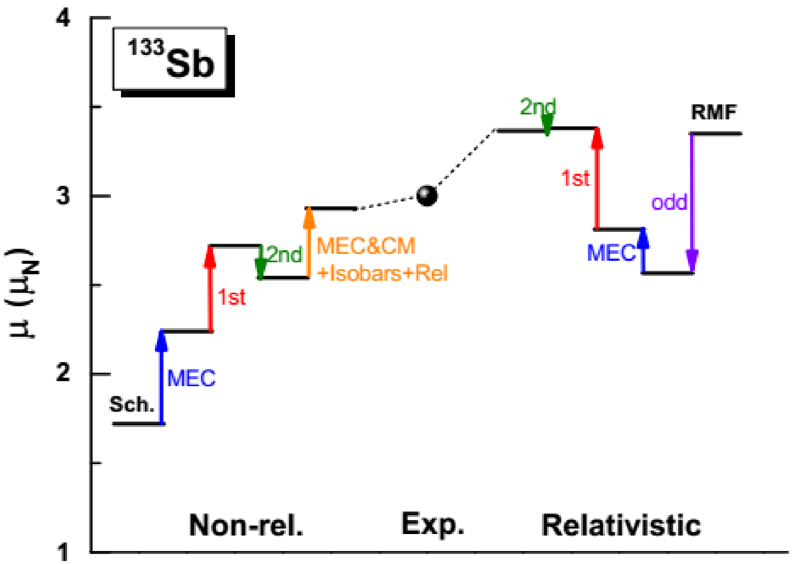
^{208}Pb附近原子核的磁矩



考虑单π介子交换流、一阶和二阶核芯极化效应后, 协变密度泛函理论很好磁矩描述，**误差6.1%也好于非相对论理论结果13.2%.**

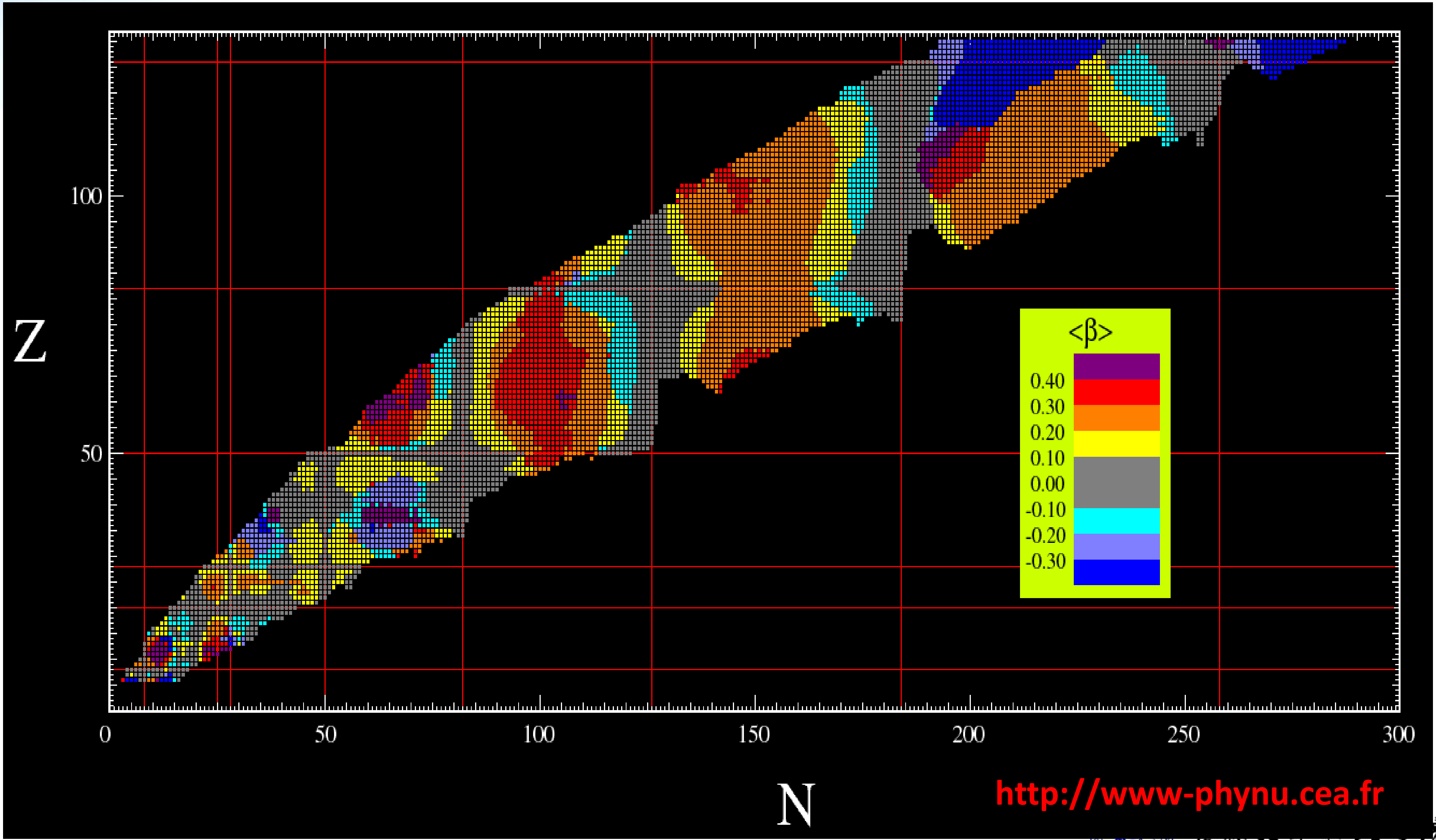
^{49}Sc和^{133}Sb磁矩





原子核形变

Quadrupole deformation of nuclear chart



http://www-phynu.cea.fr

形变奇A核的磁矩

- Magnetic moments of deformed odd-A nuclei: **valence nucleon approximation is out of work**.

Spherical　　　　Deformed

- ✓ The contribution from core would be significant: perturbation is invalid.
- ✓ Total angular momentum: not good quantum number (the rotational symmetry is broken in mean field theory).

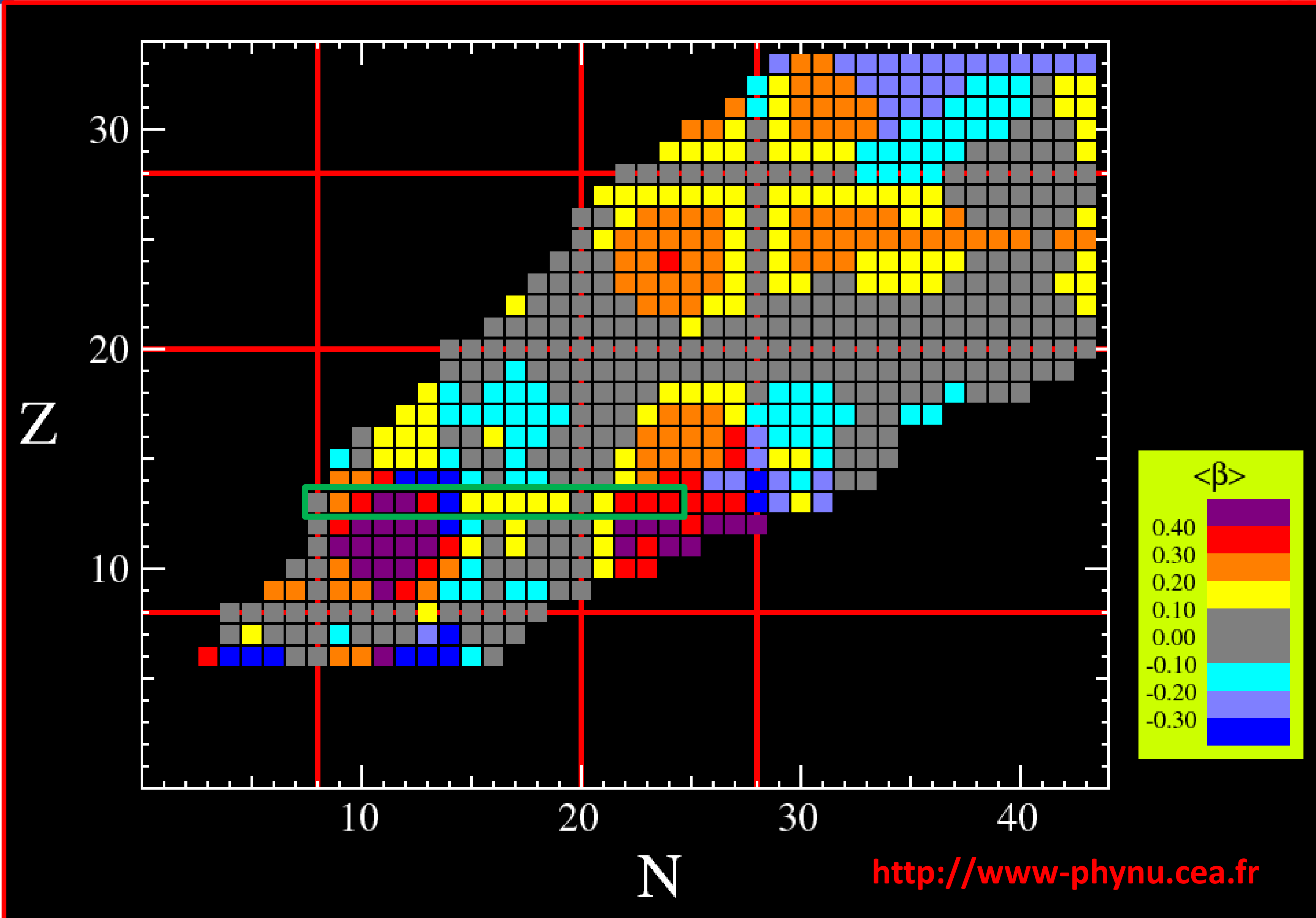
- Rotational coupling between **axially deformed core (collective rotational motion)** and **odd nucleon (intrinsic nucleonic motion)**

Collective g factor

$$\mu = \frac{I}{I+1}(g_R + g_k I) = \frac{I}{I+1}(g_R + \mu_{intri.})$$

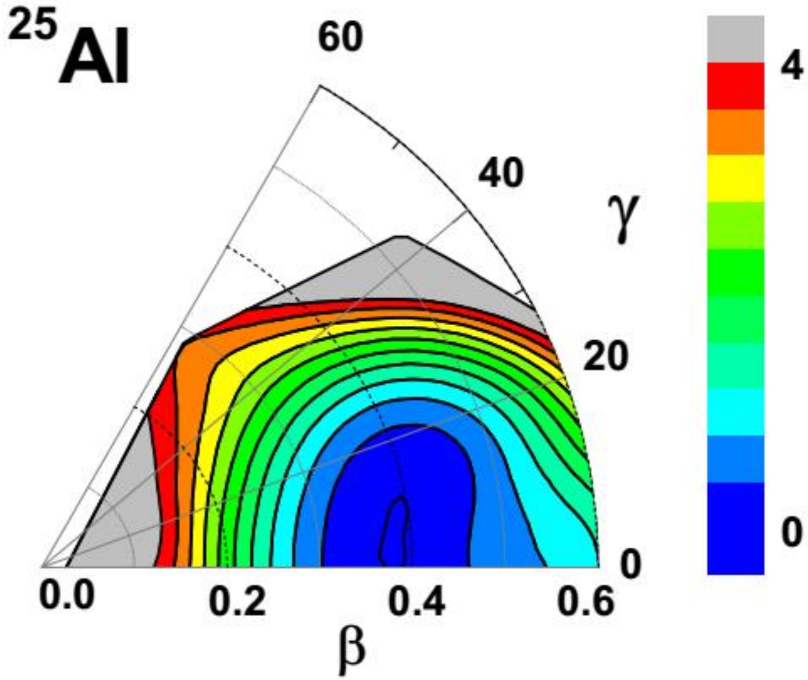
Intrinsic mean field M.M.

奇质量数Al核的磁矩



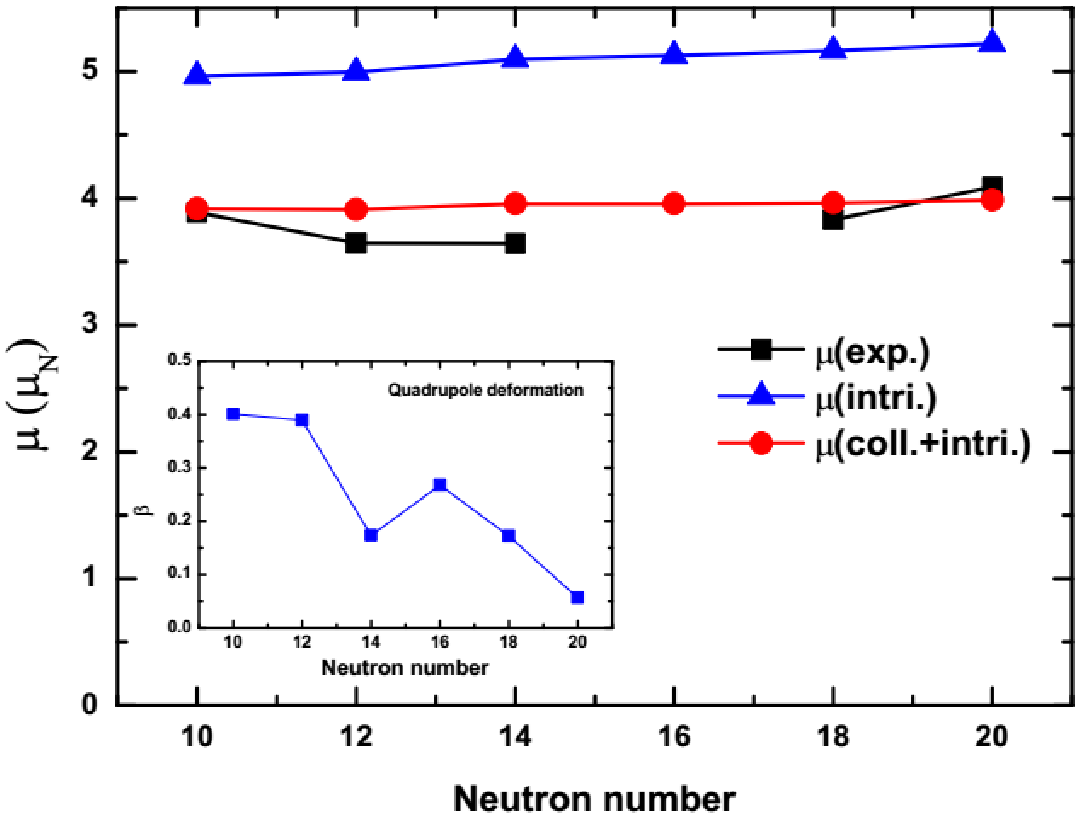
Z
30
20
10
10
20
30
40
N
<β>
0.40
0.30
0.20
0.10
0.00
-0.10
-0.20
-0.30
http://www-phynu.cea.fr

奇质量数Al核的磁矩



- The constrained calculations in deformed RMF theory with time-odd fields by PK1 parameter set indicates the ground state of ^{25}Al: prolate deformation with $\beta = 0.39$, $\mu_{intri.} = 5.00\mu_N$, intrinsic configuration $\pi[202\ 5/2]$.
- The final calculated magnetic moment: $\mu_{cal.} = 3.91\mu_N$, well reproduces the data $\mu_{exp.} = 3.65\mu_N$.

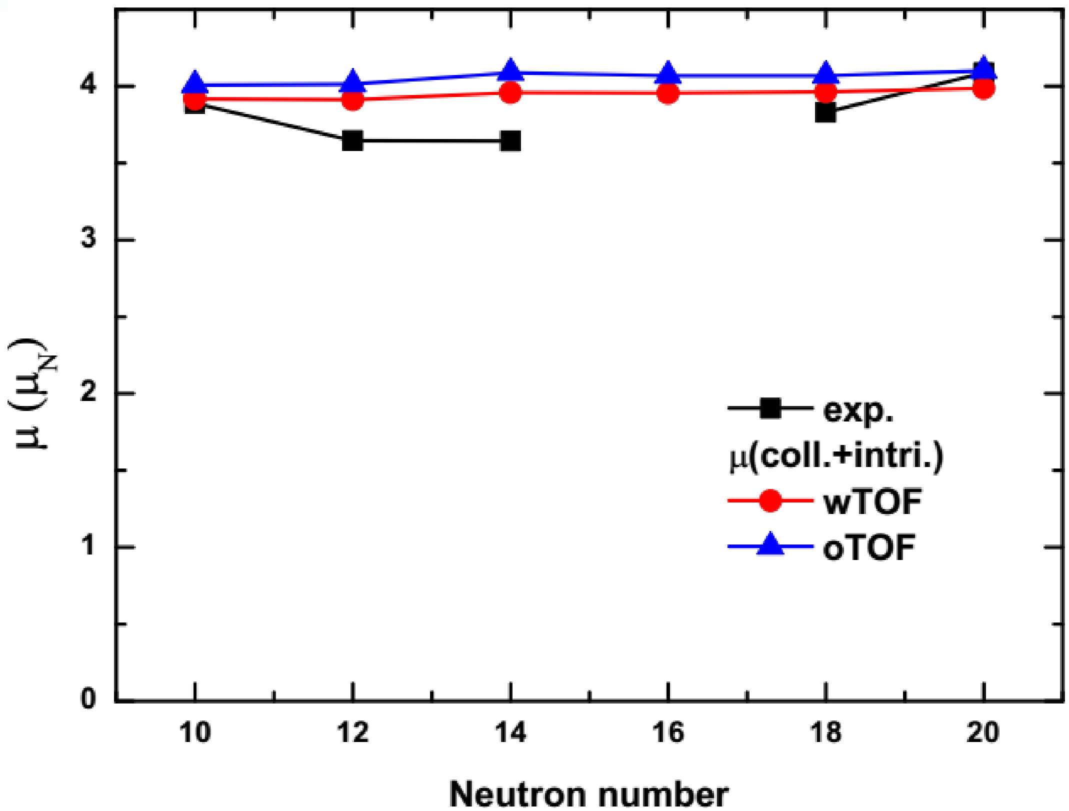
奇质量数Al核的磁矩



Magnetic moments are calculated with the intrinsic configuration $\pi[202\ 5/2]$.

- The intrinsic (mean-field) magnetic moments are around $5\mu_N$, close to the Schmidt value $4.79\mu_N$ of $\pi 1d_{5/2}$. (sensitive to the configuration, not deformation)
- The experimental magnetic moments are well reproduced after including the coupling of collective rotation and intrinsic s.p. motion.

奇质量数Al核的磁矩



Different results are compared:

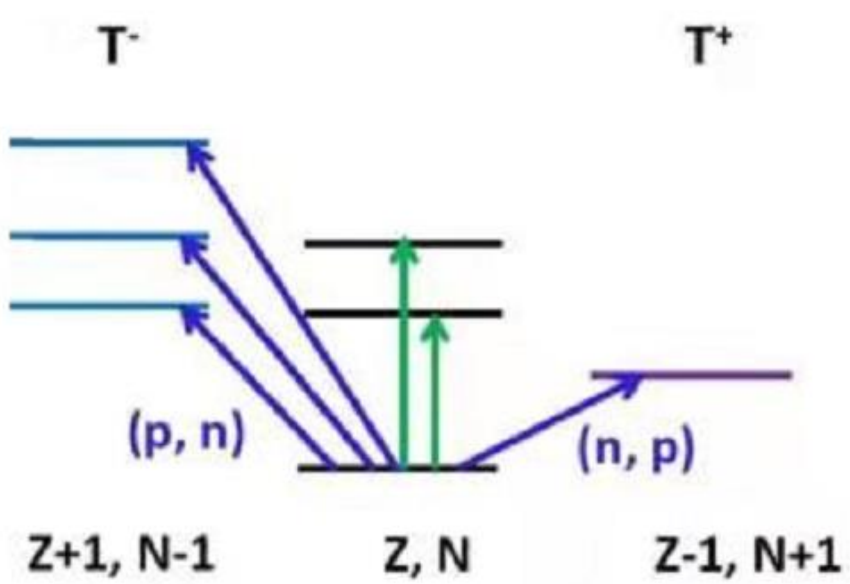
- After including the time-odd fields (TOF), the theoretical descriptions are improved.

主要内容

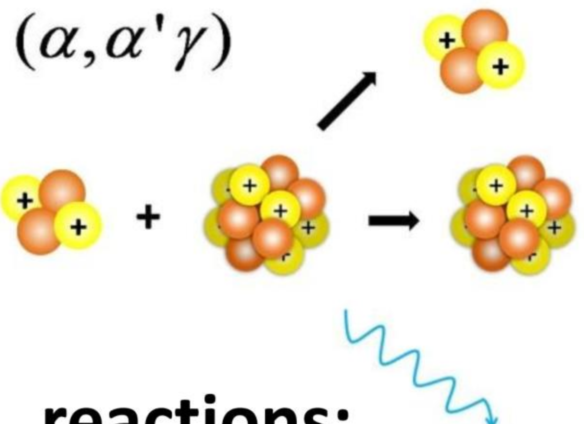
- ❑ 协变密度泛函理论
- ❑ 核磁矩
- ❑ 磁偶极跃迁

原子核磁偶极跃迁

磁偶极(M1)激发：核激发的基本模式，核结构信息的探针



非电荷交换激发



reactions:

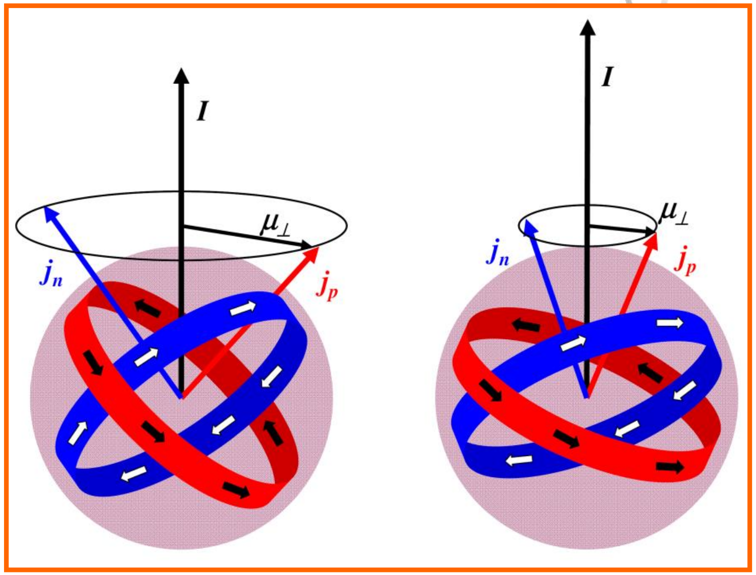
(α, α’ γ),

(γ, γ’), (γ, n) ,(e, e’)

集体转动激发中的磁偶极跃迁——磁转动

- In earlier 1990s, the rotational-like sequences of strongly enhanced M1 transitions were surprisingly observed in several light-mass Pb isotopes, which are known to be spherical or near-spherical.
- The explanation of such bands was given in terms of the shears mechanism.

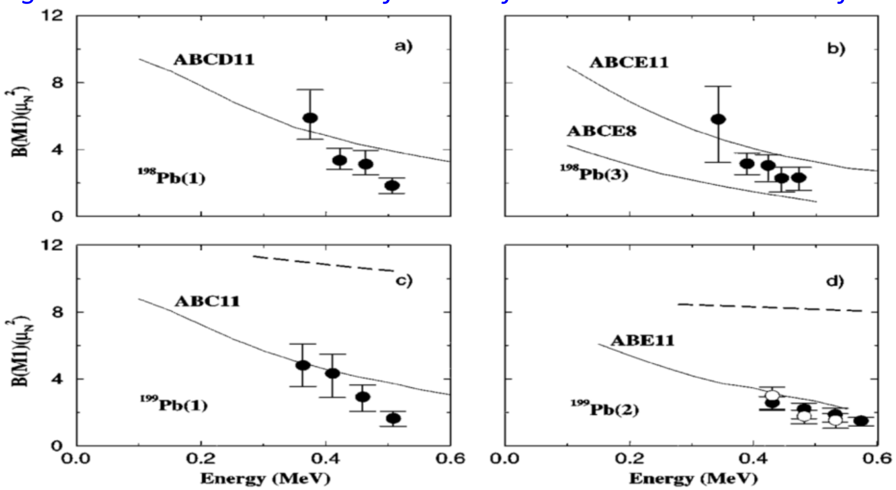
Frauendorf NPA557, 259 (1993)
Frauendorf_Meng_Reif, Proceedings of the Conference on Physics From Large γ -Ray Detector Arrays p.52 (1994).

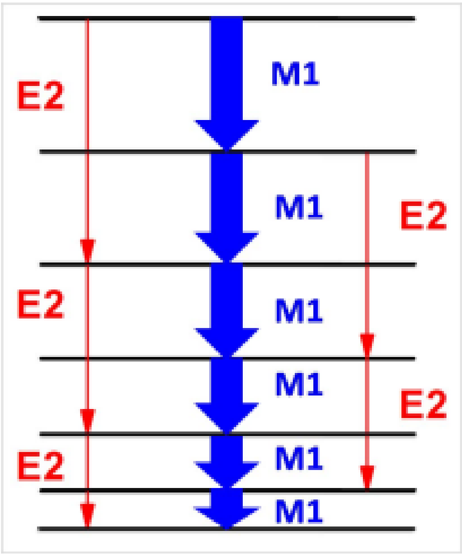


- ✓ rotational bands with $\Delta I = 1$
- ✓ near spherical or weakly deformed nuclei
- ✓ strong M1 and very weak E2 transitions
- ✓ B(M1) decreases with the increase of spin

□ Experimental confirmation   Clark_et al, PRL78, 1868(1997)

Evidence for "Magnetic Rotation" in Nuclei: Lifetimes of States in the M1 bands of 198,199Pb

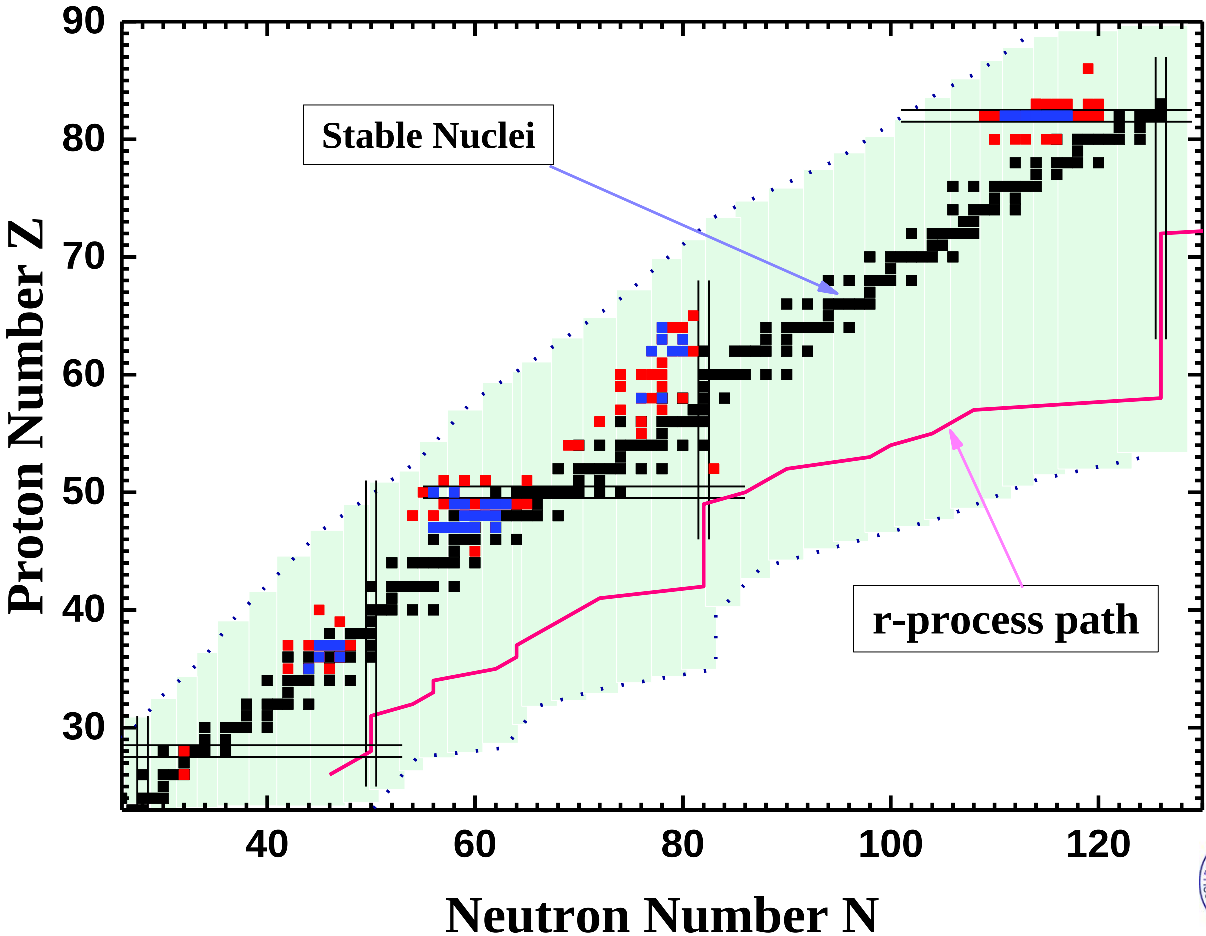




磁转动实验进展

- So far, nearly 200 MR candidates in around 100 nuclei have been found in *A* ~ 60,80,110,140 and 190 regions.

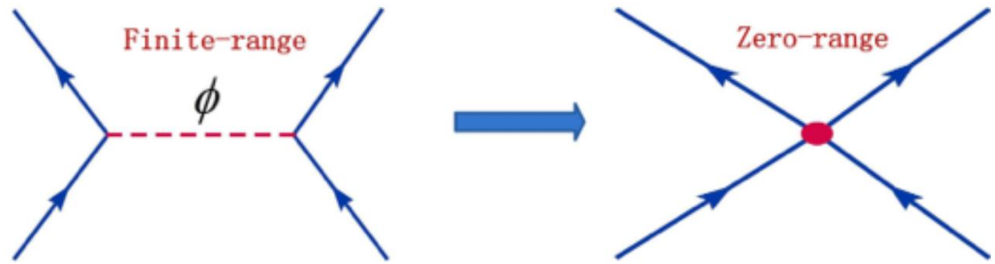
- *Clark & Macchiavelli, Annu. Rev. Nucl. Part. Sci., 50 (2000) 1,Frauendorf, Rev. Mod. Phys., 73 (2001) 463, Meng, et al., Front. Phys. 8 (2013) 55, Relativistic Density Functional for Nuclear Structure, Edited by Jie Meng Singapore: World Scientific, (2016)*



Tilted axis cranking CDFT

General Lagrangian density

$$
\begin{aligned}
L =& \bar{\psi}(i\gamma_\mu \partial^\mu - m)\psi \\
&-\frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
&-\frac{1}{2}\alpha_{TV}(\bar{\psi}\vec{\tau}\gamma_\mu\psi)(\bar{\psi}\vec{\tau}\gamma^\mu\psi) - \frac{1}{3}\beta_S(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_S(\bar{\psi}\psi)^4 \\
&-\frac{1}{4}\gamma_V[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)]^2 - \frac{1}{2}\delta_S\partial_\nu(\bar{\psi}\psi)\partial^\nu(\bar{\psi}\psi) - \frac{1}{2}\delta_V\partial_\nu(\bar{\psi}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\gamma^\mu\psi) - \frac{1}{2}\delta_{TV}\partial_\nu(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\
&-e\frac{1-\tau_3}{2}\bar{\psi}\gamma^\mu\psi A_\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}
\end{aligned}
$$

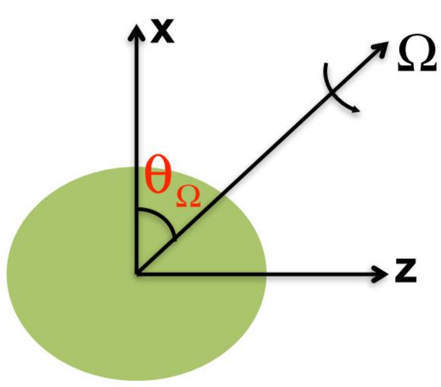


$$\frac{-g_\phi^2}{-\nabla^2 + m_\phi^2} \qquad \frac{-g_\phi^2}{m_\phi^2} + \frac{-g_\phi^2}{m_\phi^4}\nabla^2$$

Transform to the frame rotating with a uniform velocity

$$\Omega = (\Omega_x, 0, \Omega_z) = (\Omega\cos\theta_\Omega, 0, \Omega\sin\theta_\Omega)$$

$$x^\alpha = \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix} \to \tilde{x}^\alpha = \begin{pmatrix} \tilde{t} \\ \tilde{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \mathbf{R} \end{pmatrix} \begin{pmatrix} t \\ \mathbf{x} \end{pmatrix}$$



Koepf NPA1989; Kaneko PLB1993; Madokoro PRC1997

观测量计算

Binding energy

$$
\begin{aligned}
E_{\text{tot}} = \sum_{k=1}^{A}\epsilon_k - \int d^3r\Big\{ & \frac{1}{2}\alpha_S\rho_S^2 + \frac{1}{2}\alpha_V j_V^{\mu}(j_V)_{\mu} \\
& + \frac{1}{2}\alpha_{TV} j_{TV}^{\mu}(j_{TV})_{\mu} + \frac{2}{3}\beta_S\rho_S^3 + \frac{3}{4}\gamma_S\rho_S^4 \\
& + \frac{3}{4}\gamma_V\left(j_V^{\mu}(j_V)_{\mu}\right)^2 + \frac{1}{2}\delta_S\rho_S\Delta\rho_S + \frac{1}{2}\delta_V(j_V)_{\mu}\Delta j_V^{\mu} \\
& + \frac{1}{2}\delta_{TV} j_{TV}^{\mu}\Delta(j_{TV})_{\mu} + \frac{1}{2}e j_p^0 A_0\Big\} + \sum_{k=1}^{A}\langle k|\boldsymbol{\Omega}\hat{\boldsymbol{J}}|k\rangle \\
& + E_{\text{c.m.}}.
\end{aligned}
$$

Angular momentum

$$J = \sqrt{\langle \hat{J}_x\rangle^2 + \langle \hat{J}_z\rangle^2} \equiv \sqrt{I(I+1)}$$

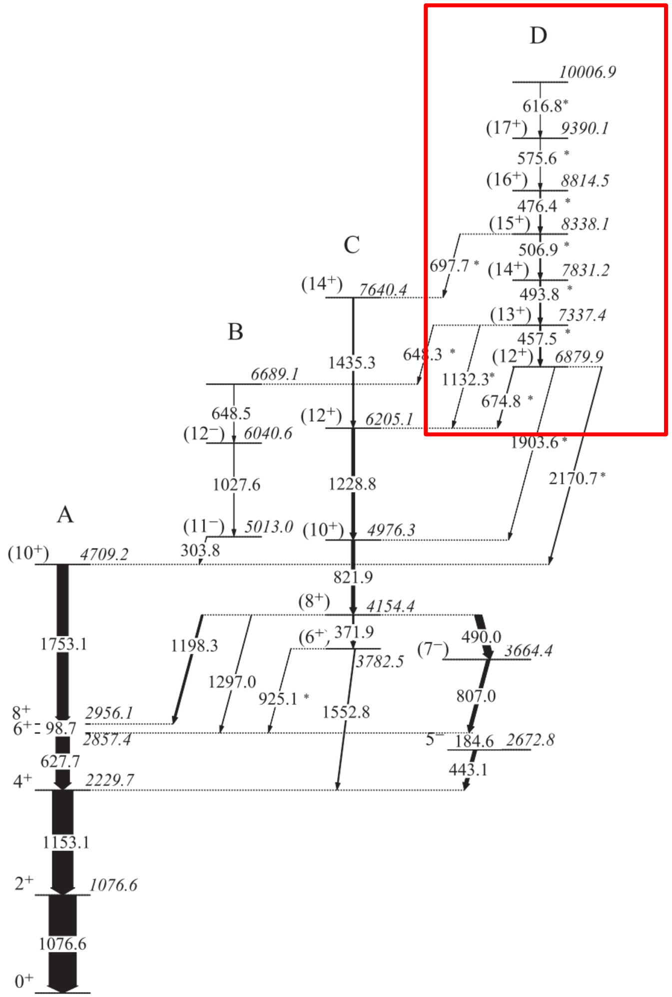
Quadrupole moments and magnetic moments

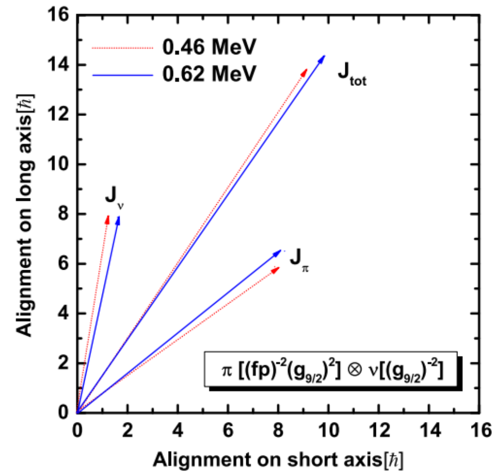
B(M1) and B(E2) transition probabilites

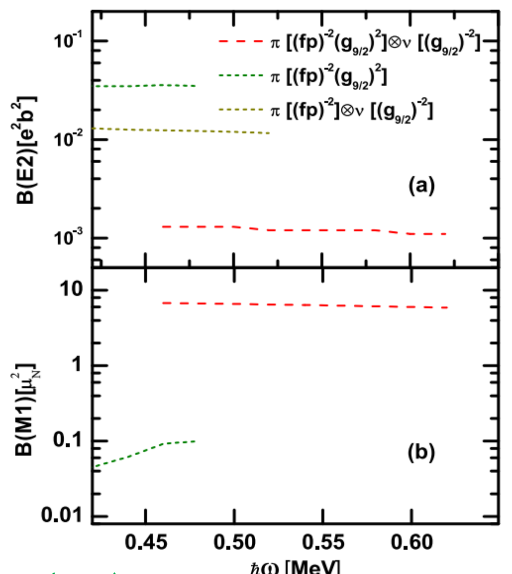
$$B(M1) = \frac{3}{8\pi}\mu_{\perp}^2 = \frac{3}{8\pi}(\mu_x \sin\theta_J - \mu_z\cos\theta_J)^2,$$

$$B(E2) = \frac{3}{8}\left[Q_{20}^{p}\cos^2\theta_J + \sqrt{\frac{2}{3}}Q_{22}^{p}(1+\sin^2\theta_J)\right]^2$$

Candidate magnetic rotation sequence in ^{86}Sr







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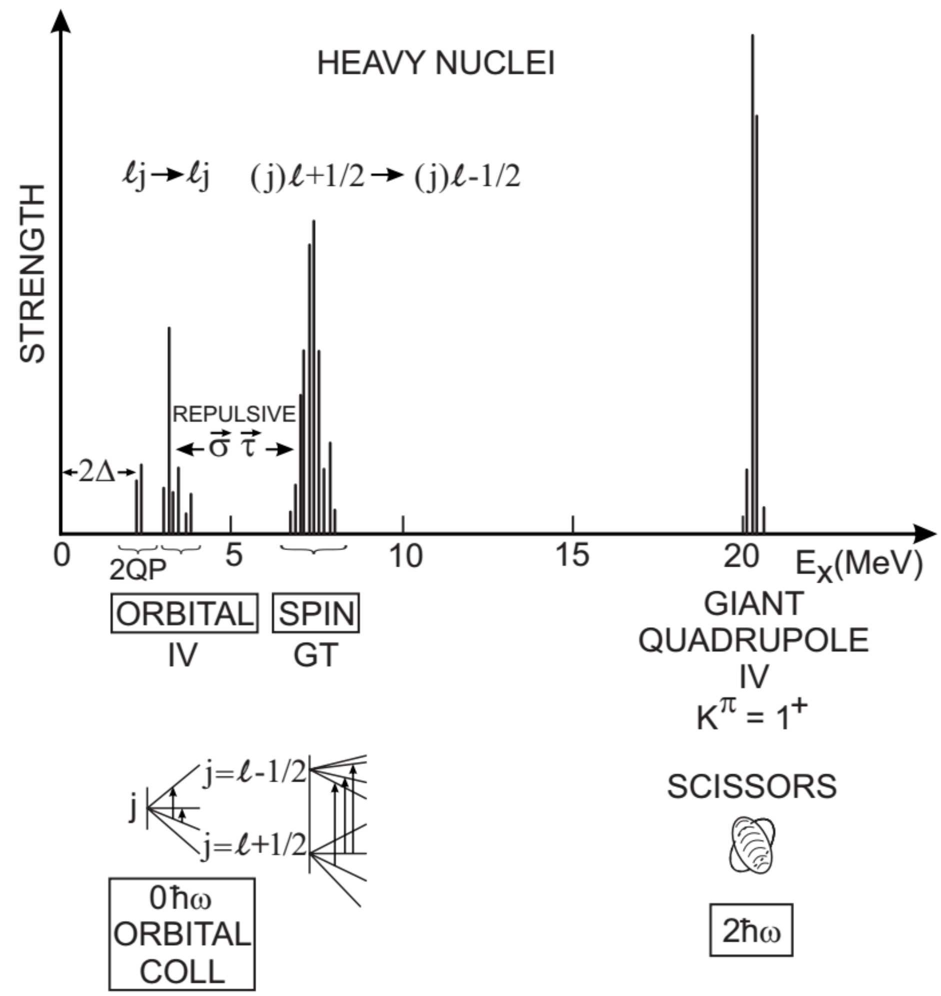
COLLEGE OF PHYSICS JILIN UNIVERSITY

Y. Zhen, J. Li, et. al., J. Phys. G: Nucl. Part. Phys. 42 (2015) 085108

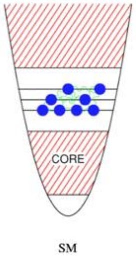
原子核磁偶极跃迁

集体振动激发中的磁偶极跃迁



理论方法

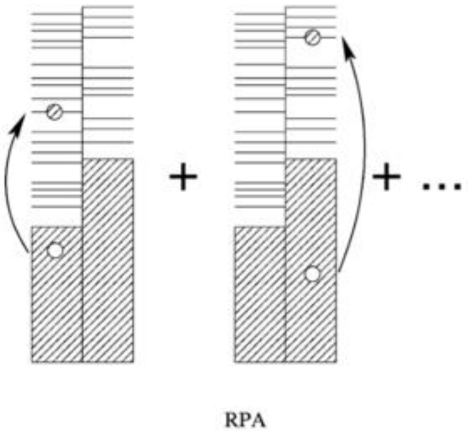
❑壳模型(np-nh)



❑Random Phase Approximation (RPA) 无规位相近似：

✓非相对论密度泛函

✓相对论密度泛函

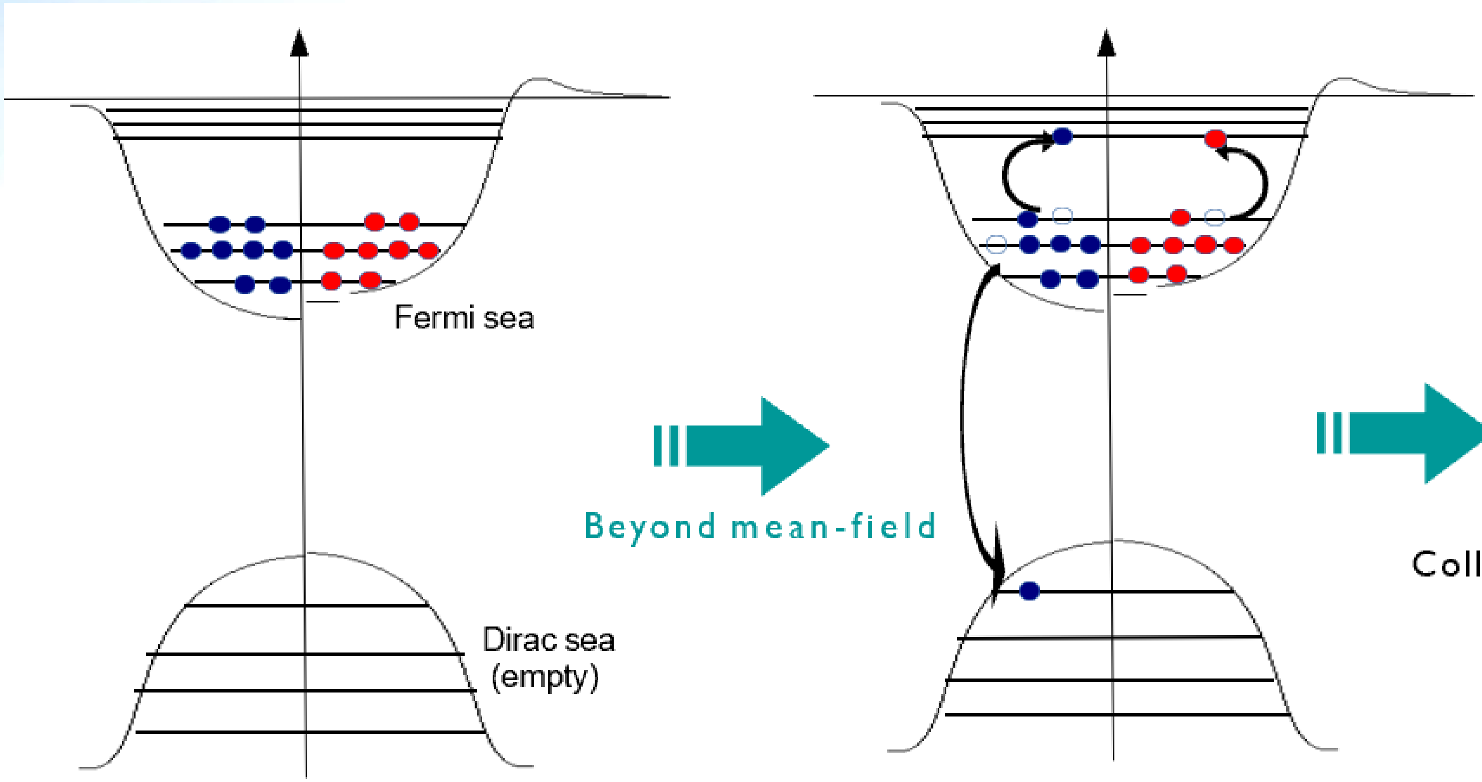


1p-1h

多粒子多空穴：

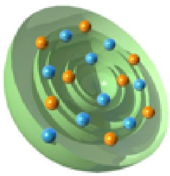
- 2ndRPA(2p-2h)
- RPA+PVC

Collective vibration (phonon)

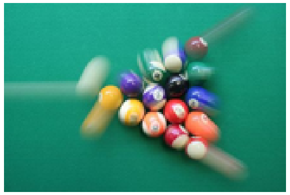


Collective vibration
(phonon)

Mean-field ground-state
= independent (quasi)particles
= 0-th order approximation

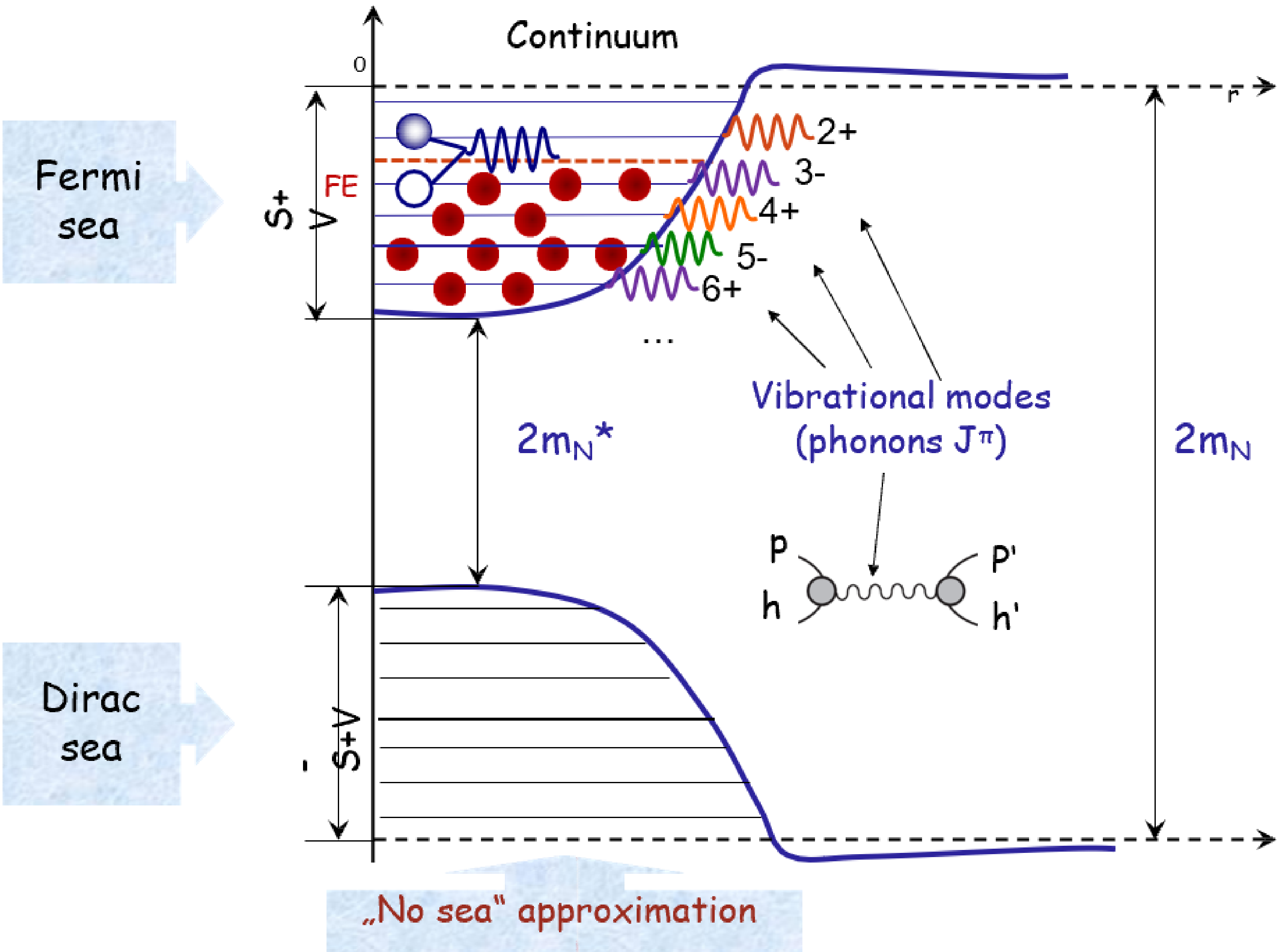


correlations



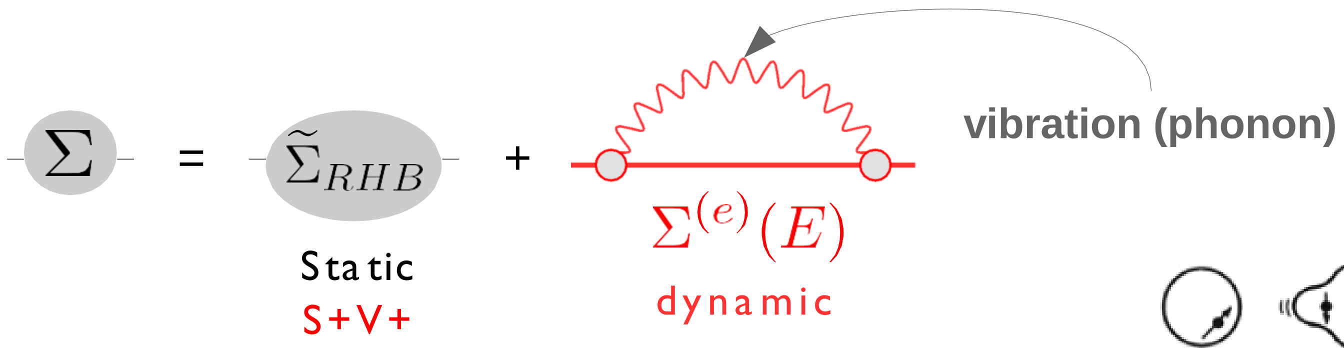
Random phase
Approximation (RPA)

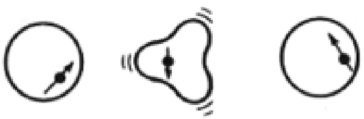
Particles vibration coupling(PVC)

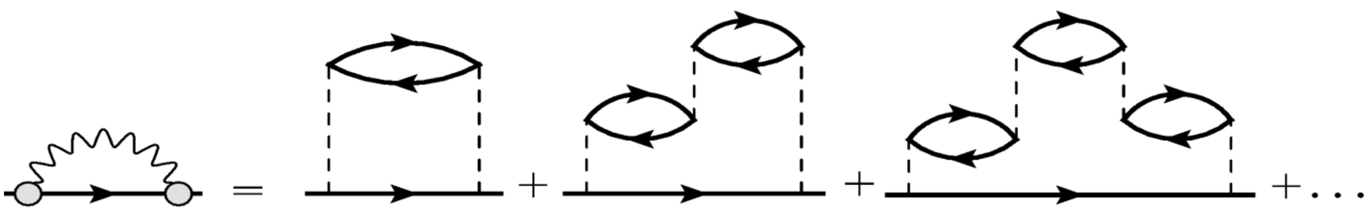


Particles vibration coupling(PVC)

- (Quasi-)Particle-Vibration Coupling (PVC) in the nucleonic self-energy:



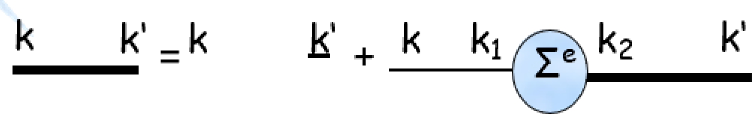




One-body propagator G:
Dyson's equation

$$\left(\varepsilon - \hat{\mathcal{H}}_{RHB} - \hat{\Sigma}^{(e)}(\varepsilon)\right)\hat{G}(\varepsilon) = 1$$

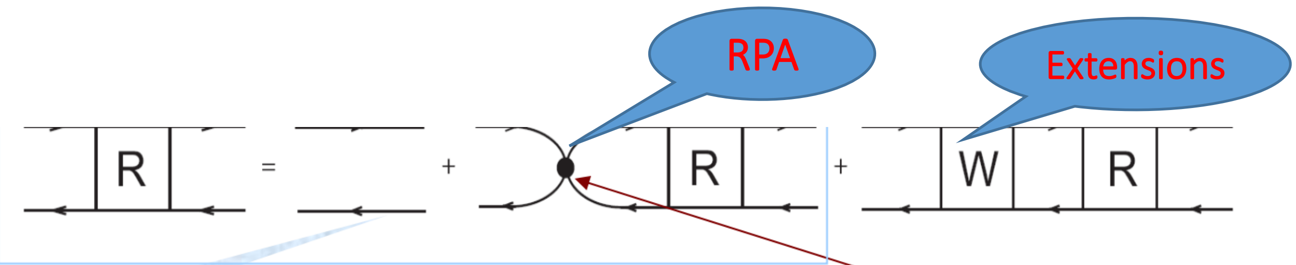
Energy dependence



G = G₀ + G₀ Σᵉ G

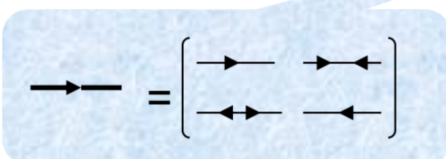
RPA+PVC: linear response theory

Bethe-Salpeter Equation (BSE):



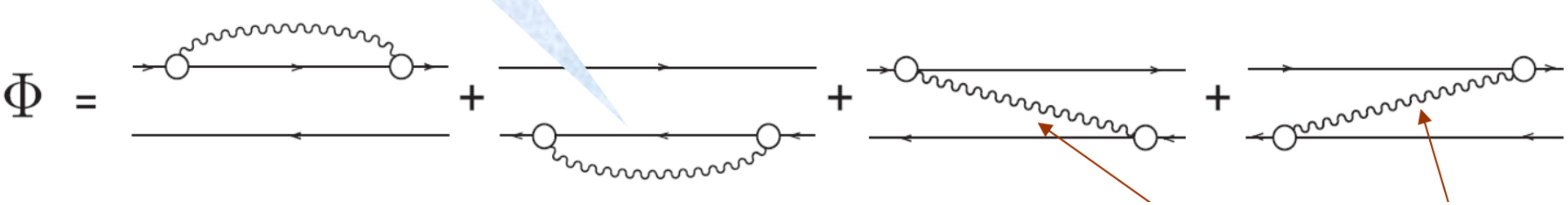
$$V = \frac{\delta \Sigma^{RMF}}{\delta \rho}$$

Self-consistency



$$R(\omega) = A(\omega) + A(\omega)\left[V + W(\omega)\right] R(\omega)$$

$$W(\omega) = \Phi(\omega) - \Phi(0)$$



Response to external field: strength function

Strength function:

$$S(E) = -\frac{1}{\pi} \lim_{\Delta \to +0} Im\, \Pi_{PP}(E + i\Delta)$$

Polarizability:

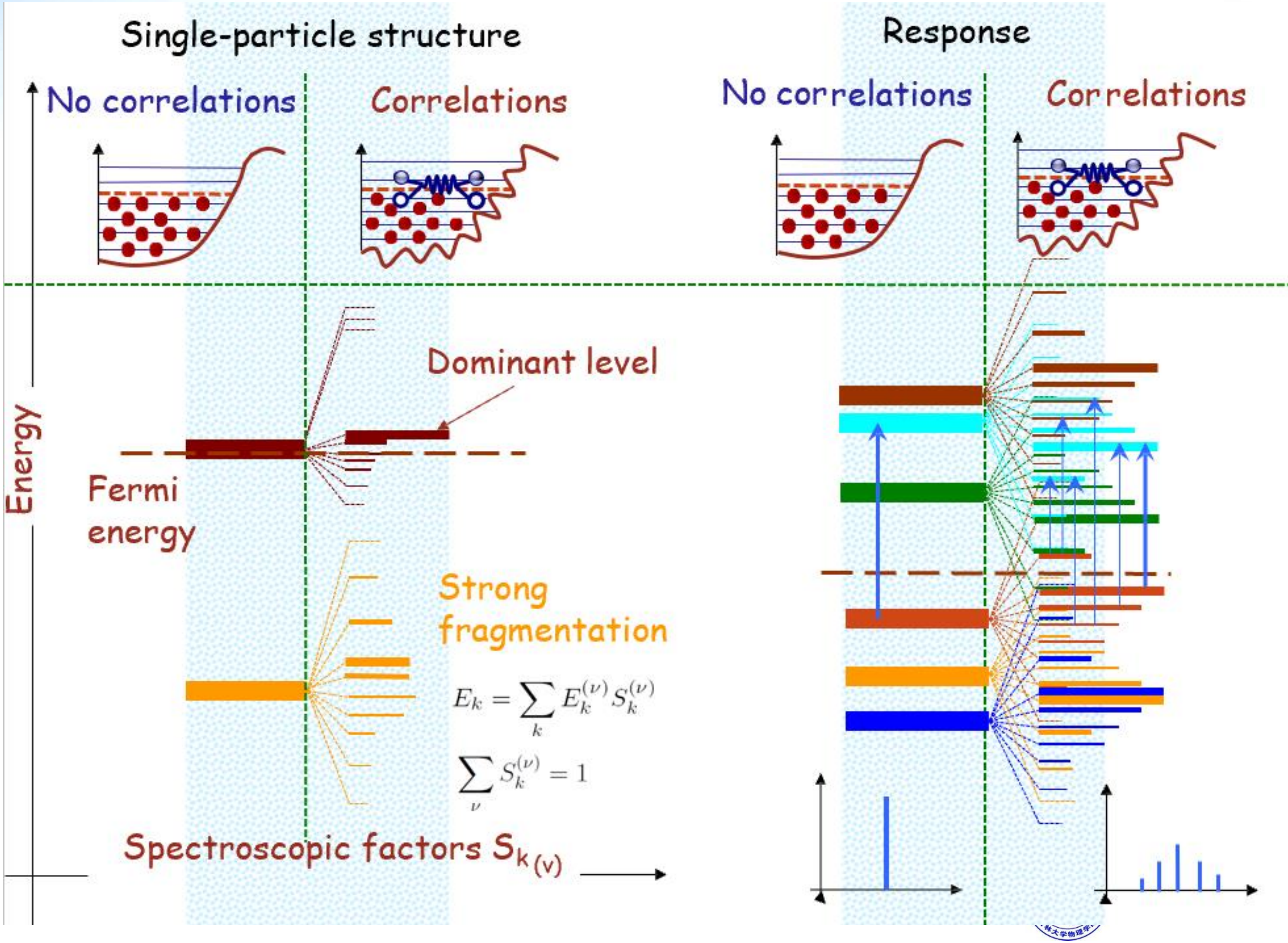
$$\Pi_{PP}(\omega) = P^{\dagger} R(\omega) P := \sum_{k_1 k_2 k_3 k_4} P^*_{k_1 k_2} R_{k_1 k_4, k_2 k_3}(\omega) P_{k_3 k_4}$$

External field

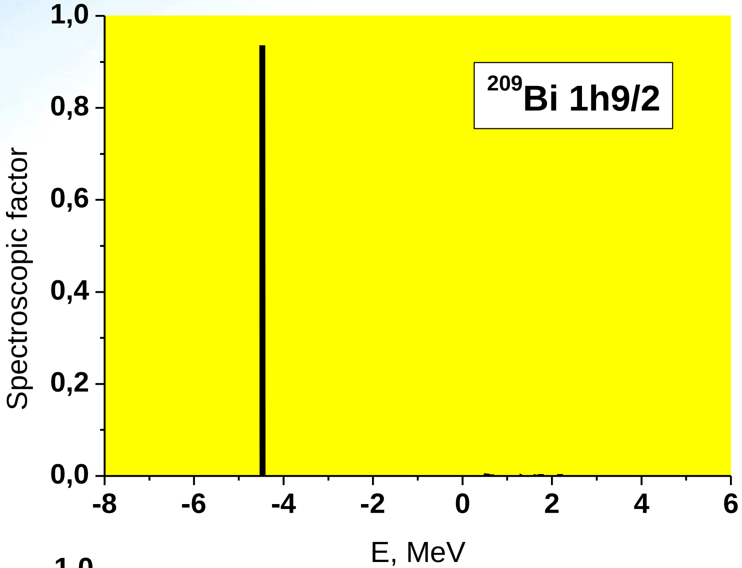
Density matrix variation $$\delta\rho_{k_1 k_2}(\omega) = \sum_{k_3 k_4} R_{k_1 k_4, k_2 k_3}(\omega) P_{k_3 k_4}$$

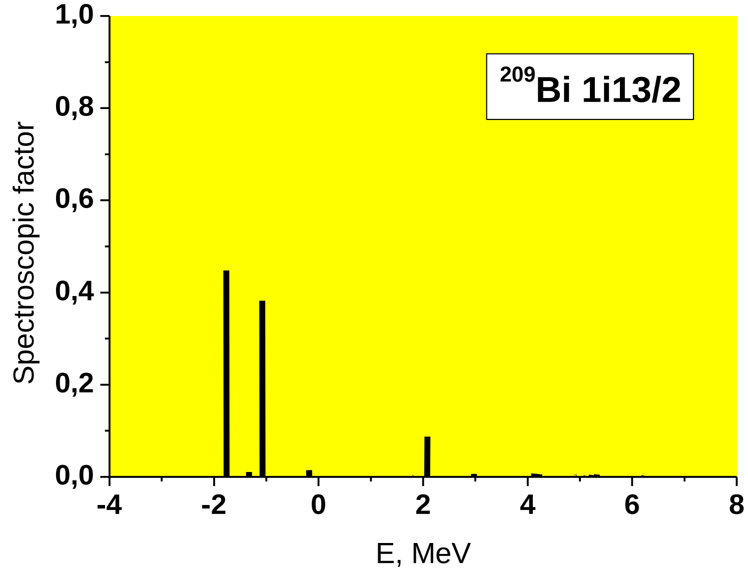
transition density $$\rho^{\nu}_{k_1 k_2} = \lim_{\Delta \to +0} \sqrt{\frac{\Delta}{\pi S(\Omega^{\nu})}}\, Im\, \delta\rho_{k_1 k_2}(\Omega^{\nu} + i\Delta)$$

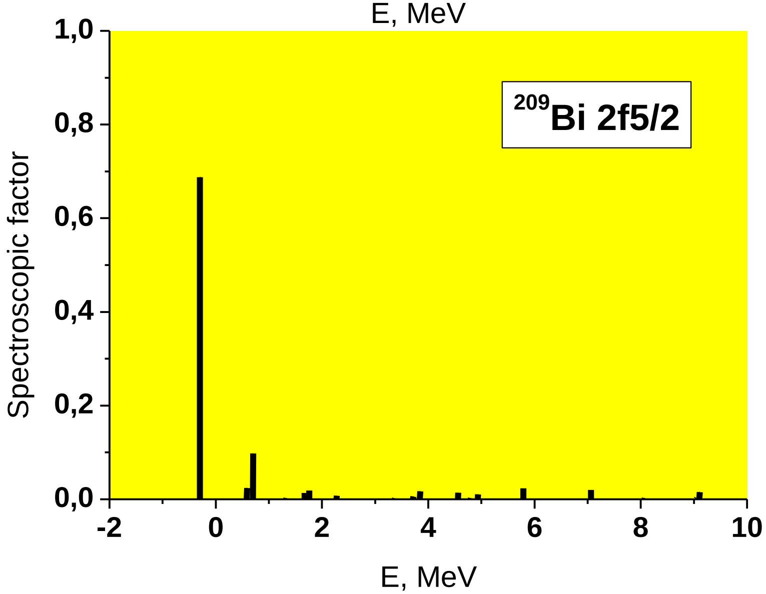
Fragmentation of states in odd and even systems (schematic)

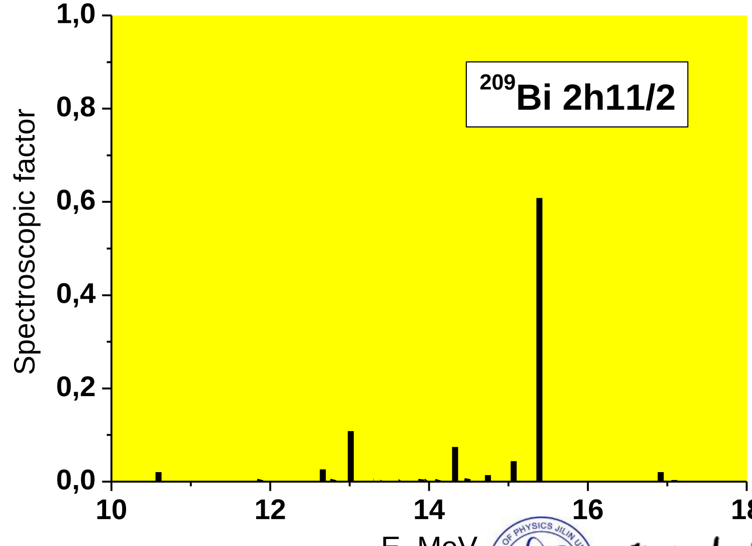


^{209}Pb单粒子强度分布









M1 transitions in RPA + PVC

$$B(0 \to \nu; M1) = |\sum_{M_O M_\nu} \langle \nu | \hat{O} | 0 \rangle|^2$$

$$= |\sum_{ph} \underbrace{(-1)^{j_p+1/2} \langle p \| \sqrt{\frac{3}{4\pi}} \hat{\boldsymbol{\mu}} \| h \rangle} \times [\tilde{\rho}_{ph}(1^+_\nu) + \tilde{\rho}_{hp}(1^+_\nu)]|^2$$

总结展望

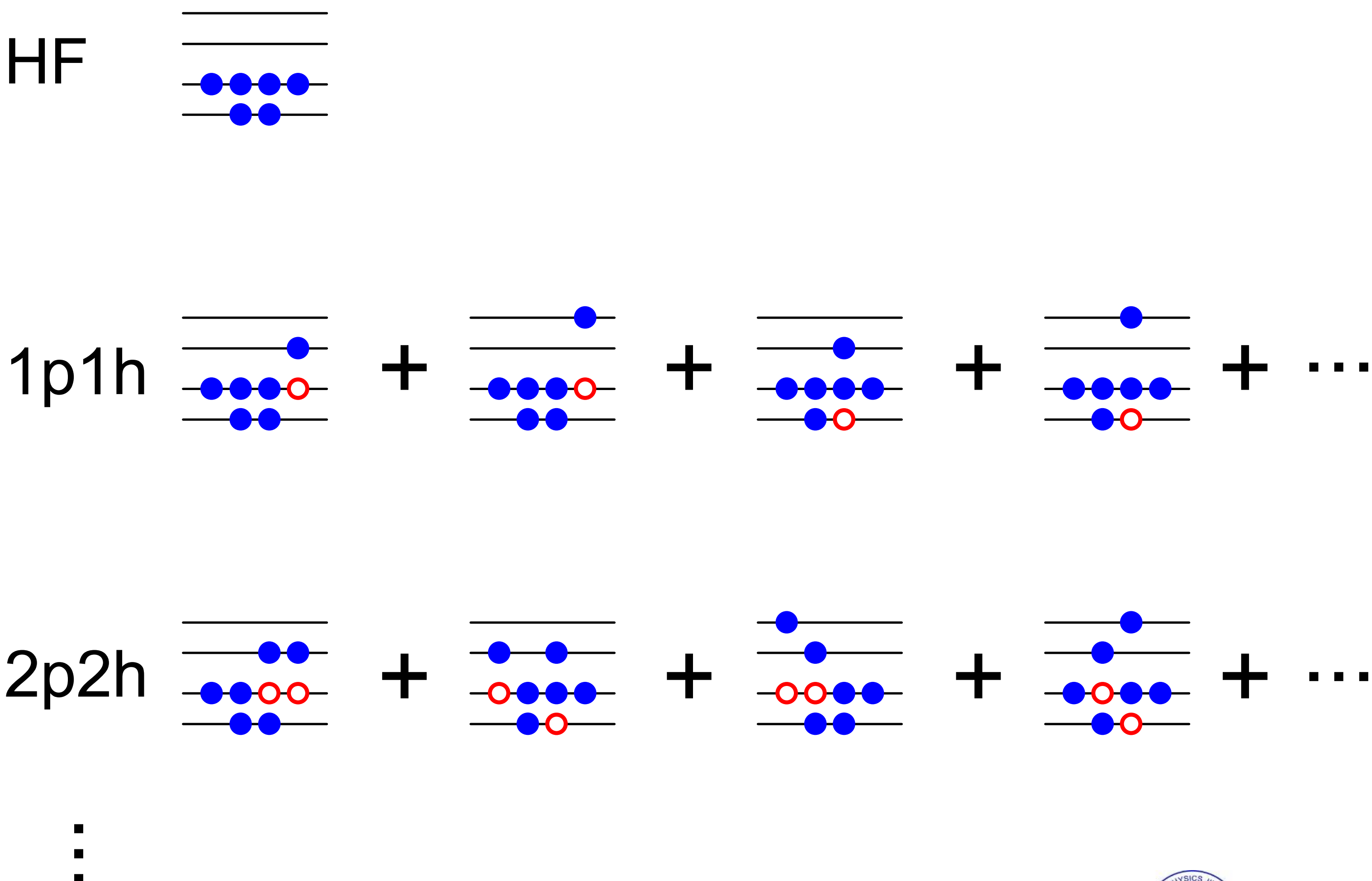
- 协变密度泛函理论

- 核磁矩
  - 球形奇A核：满壳(微扰理论)⟹开壳(粒子和声子耦合)
  - 形变奇A核：轴对称形变⟹三轴形变

- 磁偶极跃迁
  - 集体转动
  - 集体振动：满壳(PVC)⟹开壳(准粒子振动耦合QVC)


物理楼
谢谢大家！

Schematic picture for collective excitations



微观理论

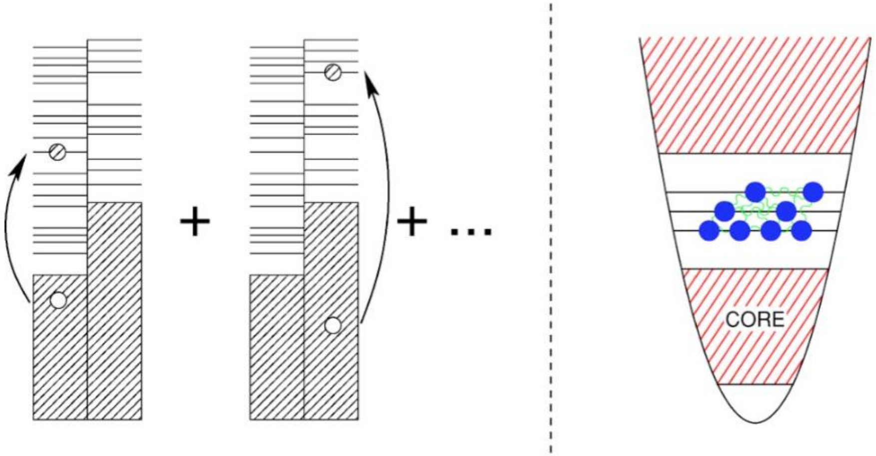
◇ Shell Model

pf-shell nuclei

Koonin: PR 1997; Caurier: RMP 2005

◇ Random Phase Approximation (RPA) based on density functionals

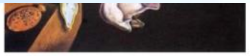
- Non-relativistic density functional
- Relativistic density functional



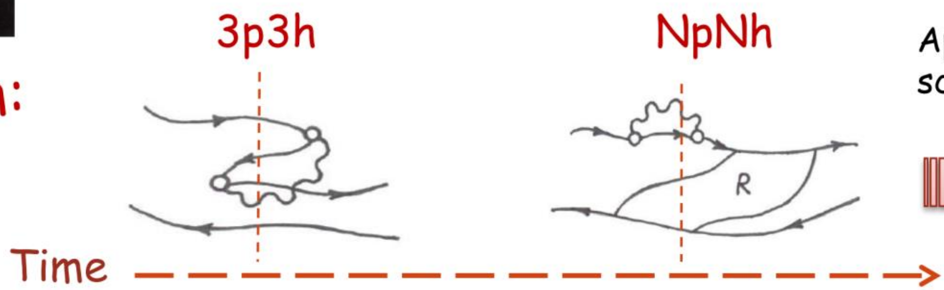
RPA SM

from K. Langanke, Rev. Mod. Phys. 75, 819, 2003

Time blocking



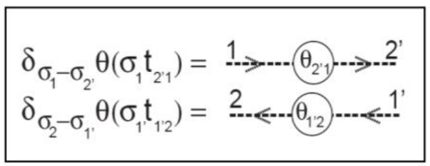
Problem:
'Melting' diagrams



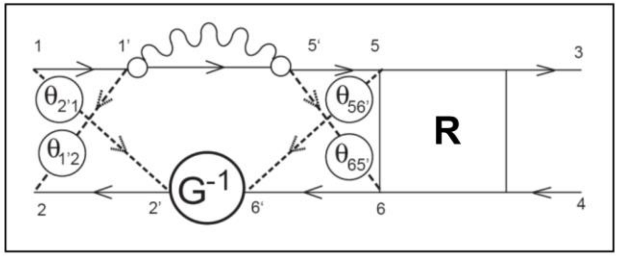
Approx. schemes

Unphysical result: negative cross sections

Solution:
Time-projection operator:

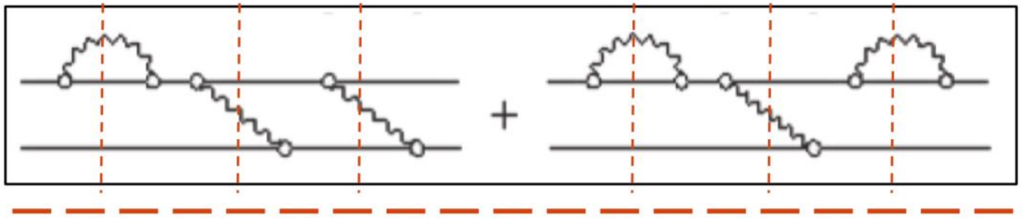


V.I. Tselyaev, Yad. Fiz. 50,1252 (1989)

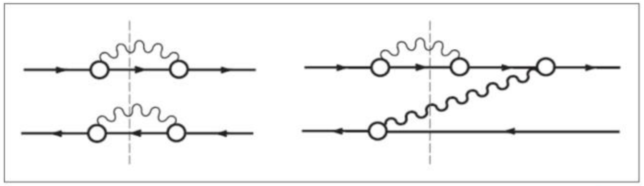


Partially fixed

Allowed terms: 1p1h, 2p2h



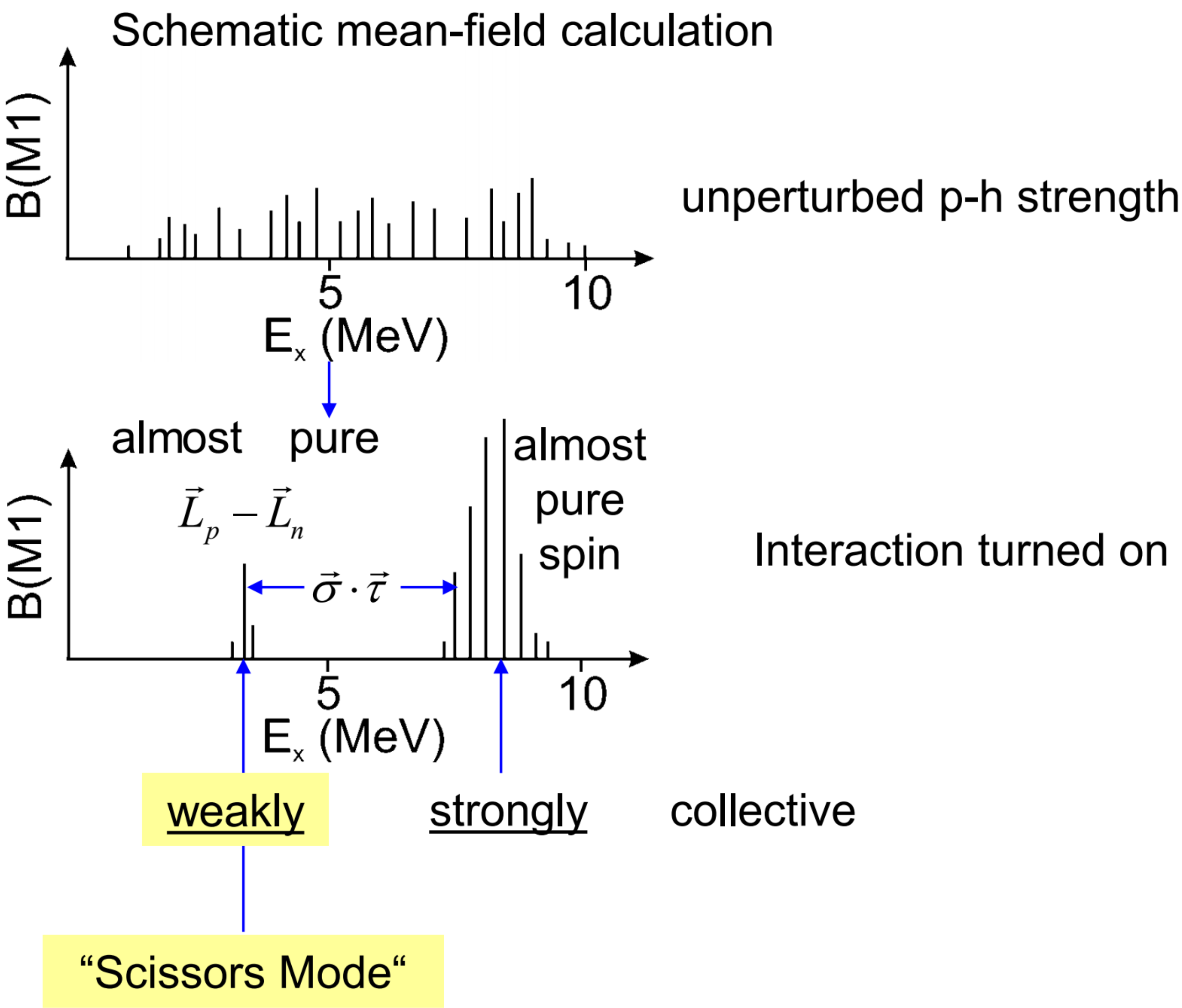
Blocked terms: 3p3h, 4p4h,...



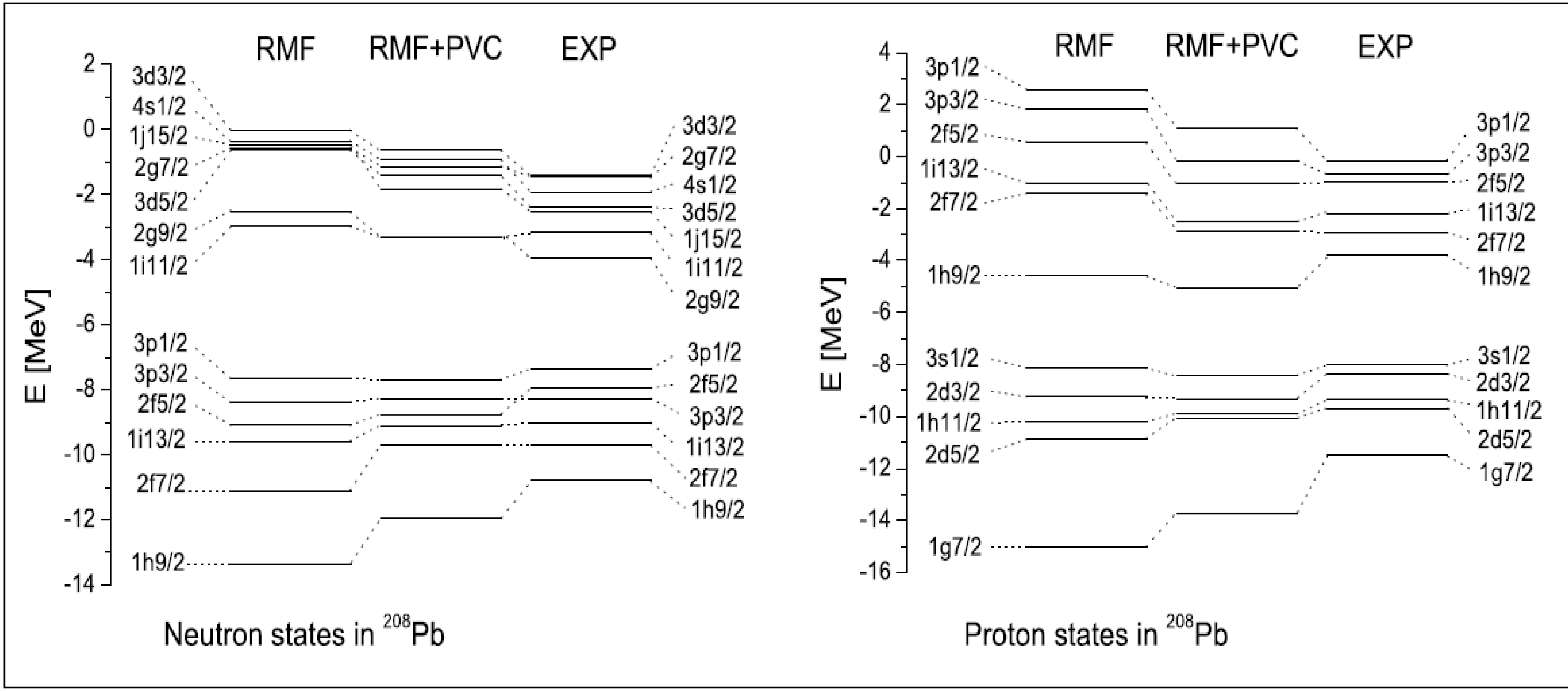
Time blocking approximation =
= „one-fish" approximation!

- Separation of the integrations in the BSE kernel
- R has a simple-pole structure (spectral representation)
  »» Strength function is positive definite!

M1 transitions



磁矩：考虑粒子振动(声子)耦合效应(PVC)



- **RMF+PVC: better single particle energy level/ wave function**

✓ **Coupling (particle + particle-hole excitations): closed shell ±1 nucleon**

➢ **Coupling (particle + collective phonons): all spherical odd A nuclei**

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