Ground-state shape transition in pairing model

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Liaoning Normal University Dalian

12/1/2020

Outline

- ***Introduction to pairing,   BCS VS Exact pairing***
- ***The new Iterative approach to the exact pairing model***
- ***Shape (Quantum) phase transitions***
- ***Summary***

Cooper Pair

PHYSICAL REVIEW VOLUME 104, NUMBER 4 NOVEMBER 15, 1956

Letters to the Editor

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Bound Electron Pairs in a Degenerate Fermi Gas*

LEON N. COOPER
Physics Department, University of Illinois, Urbana, Illinois
(Received September 21, 1956)

IT has been proposed that a metal would display superconducting properties at low temperatures if

$=(1/V)\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2)]$ which satisfy periodic boundary conditions in a box of volume V, and where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of electron one and electron two. (One can use antisymmetric functions and obtain essentially the same results, but alternatively we can choose the electrons of opposite spin.) Defining relative and center-of-mass coordinates, $\mathbf{R}=\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$, $\mathbf{r}=(\mathbf{r}_2-\mathbf{r}_1)$, $\mathbf{K}=(\mathbf{k}_1+\mathbf{k}_2)$ and $\mathbf{k}=\frac{1}{2}(\mathbf{k}_2-\mathbf{k}_1)$, and letting $\mathcal{E}_K+\epsilon_k=(\hbar^2/m)(\frac{1}{4}K^2+k^2)$, the Schrödinger equation can be written

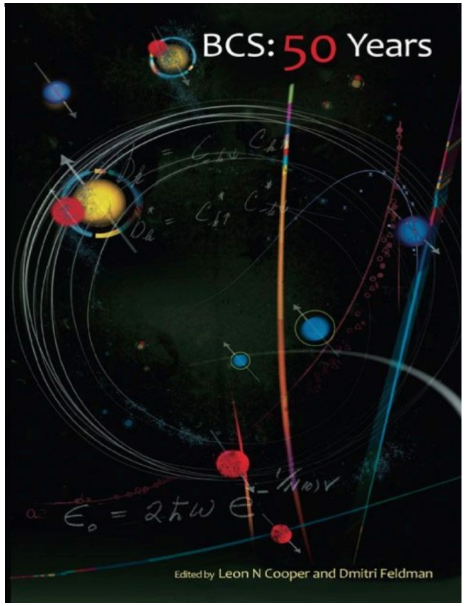
$$(\mathcal{E}_K+\epsilon_k-E)a_{\mathbf{k}}+\sum_{\mathbf{k}'}a_{\mathbf{k}'}(\mathbf{k}|H_1|\mathbf{k}')\times\delta(\mathbf{K}-\mathbf{K}')/\delta(0)=0 \qquad (1)$$

where

$$\Psi(\mathbf{R},\mathbf{r})=(1/\sqrt{V})e^{i\mathbf{K}\cdot\mathbf{R}}\chi(\mathbf{r},K),\qquad \chi(\mathbf{r},K)=\sum_{\mathbf{k}}(a_{\mathbf{k}}/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad (2)$$

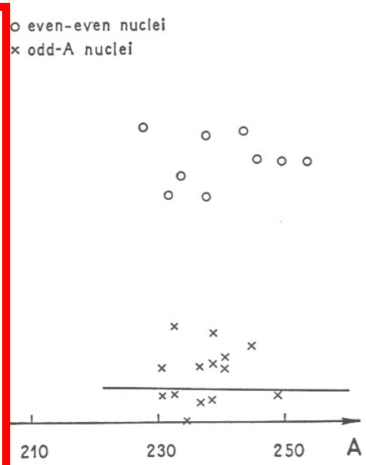
and

$$(\mathbf{k}|H_1|\mathbf{k}')=\left(\frac{1}{V}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}H_1e^{i\mathbf{k}'\cdot\mathbf{r}}\right)_{0\text{ phonons}}.$$



top of an inert

If the many-body system could be considered (at least to a lowest approximation) a collection of pairs of this kind above a Fermi sea, we would have (whether or not the pairs had significant Bose properties) a model similar to that proposed by Bardeen which would display many of the equilibrium properties of the superconducting state.



represent a collective odd-parity oscillation.

Limitations of BCS/HFB

PHYSICAL REVIEW C **78**, 064318 (2008)

Accuracy of BCS-based approximations for pairing in small Fermi systems

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[3]*Institute of Nuclear Theory and Department of Physics, University of Washington, Seattle, Washington 98105-6694, USA*
(Received 20 August 2008; published 31 December 2008)

We analyze the accuracy of BCS-based approximations for calculating correlation energies and odd-even energy differences in two-component fermionic systems with a small number of pairs. The analysis is focused on comparing BCS and projected BCS treatments with the exact solution of the pairing Hamiltonian, considering parameter ranges appropriate for nuclear pairing energies. We find that the projected BCS is quite accurate over the entire range of coupling strengths in spaces of up to about ~20 doubly degenerate orbitals. It is also quite accurate for two cases we considered with a more realistic Hamiltonian, representing the nuclei around ^{117}Sn and ^{207}Pb. However, the projected BCS significantly underestimates the energies for much larger spaces when the pairing is weak.

$$|BCS\rangle \propto e^{S_i^+} = \sum_N \frac{(S_i^+)^N}{N!}|0\rangle, \quad S_i^+($$

$$|PBCS\rangle \propto (S_i^+)^{N_{pair}}|0\rangle, \qquad S_i^+(Ex$$

$$|Exact\rangle = \prod_i^{N_{pair}} S^+(x_i)|0\rangle, \qquad S^+(x_i$$

Phys. Lett. 3 (1963) 277;   5 (1963) 82; Nucl. Pl
J. Dukelsky and G. Sierra, PRL 83, 172 (1999)

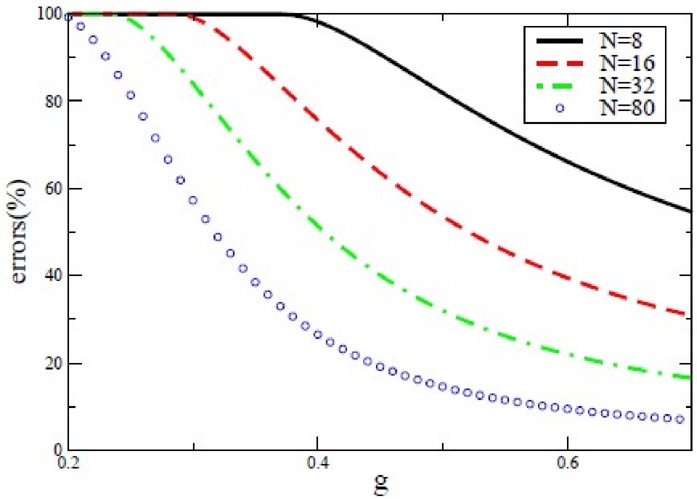


FIG. 2: Errors of the BCS approximation for correlatioı energies.

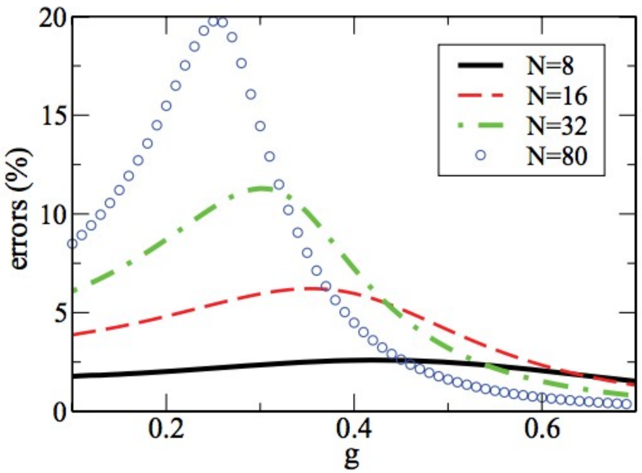
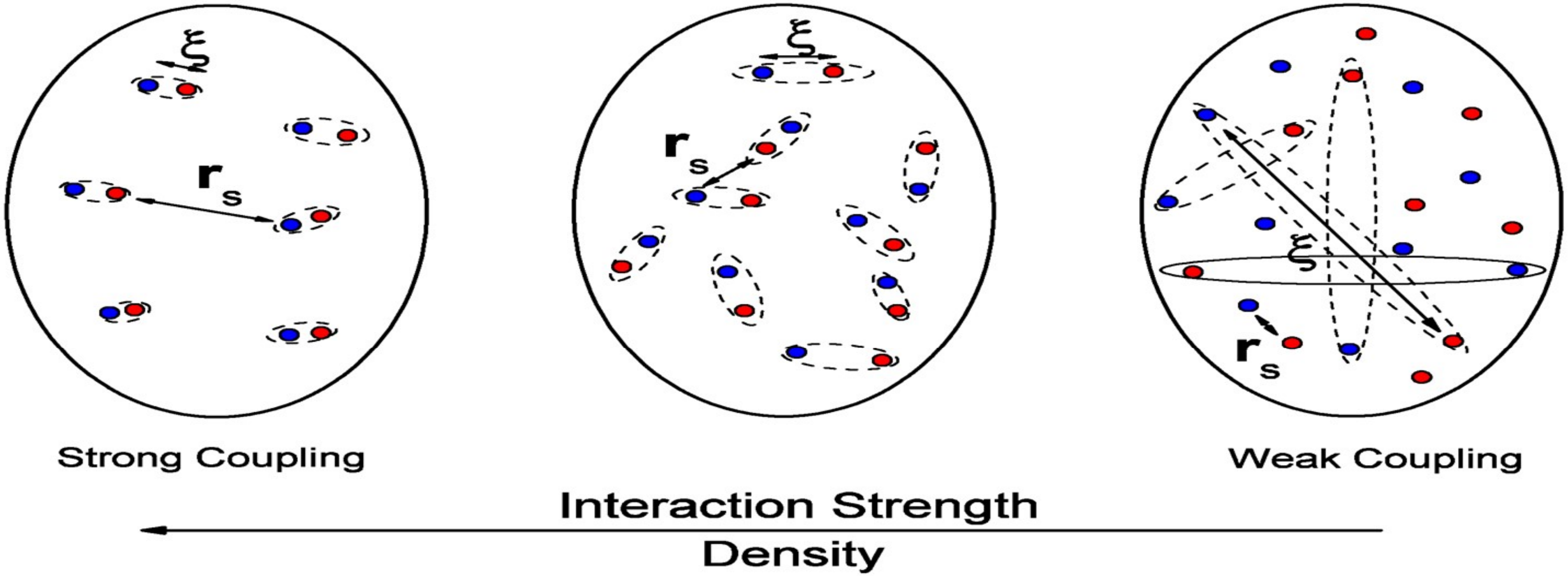


FIG. 3. (Color online) Errors for the correlation energies calculated in the PBCS approximation.

Limitations of BCS/HFB

Superconductors, High T_c	Ultracold Fermi gases	Finite Nuclei, metallic grain, Neutron Stars



BCS : a) The macroscopic limit system

b) The finite systems with "strong " pairing

Exact pairing : More appropriate for the description of loosely bound systems such as nuclei.

M. Schechter, Y. Imry, Y. Levinson, J. von Deft, Phys. Rev. B63 (2001) 214518

Exactly solvable model

Richardson's Exact Solution

(Phys. Lett. 3 (1963) 277;   5 (1963) 82; Nucl. Phys. 52 (1964) 221； 52 (1964)253)

ıme 3, number 6 PHYSICS LETTERS 1 February 1963

A RESTRICTED CLASS OF EXACT EIGENSTATES OF THE PAIRING-FORCE HAMILTONIAN *

R. W. RICHARDSON
H. M. Randall Laboratory of Physics,
University of Michigan, Ann Arbor, Michigan

Why are exactly solvable model important?

Received 23 November 1962

- The exponential complexity of the many body problem is reduced to a polynomial complexity.

- They can unveil physical properties that cannot described with existing many-body theories.

- They could constitute stringent test for many-body theories.

The standard pairing model

The Hamiltonian of the standard pairing model (BCS)

$$\hat{H} = \sum_{j=1}^{n} \epsilon_j \hat{n}_j - G \sum_{jj'} S_j^+ S_{j'}^-$$

According to the Richardson-Gaudin method, k-
written as

The pairing vacuum state

$$S_j^- |0\rangle = 0$$

$$|k;x\rangle = S^+(x_1) S^+(x_2) \cdots S^+(x_k) |0\rangle,$$

$$S^+(x_i) = \sum_{j=1}^{n} \frac{1}{x_i - 2\epsilon_j} S_j^+.$$

x_i satisfy the following set of Bethe ansatz equations (BAEs):

$$1 - 2G \sum_{j}^{n} \frac{\rho_j}{x_i - 2\epsilon_j} - 2G \sum_{i(\neq i')}^{k} \frac{1}{x_i - x_{i'}} = 0$$

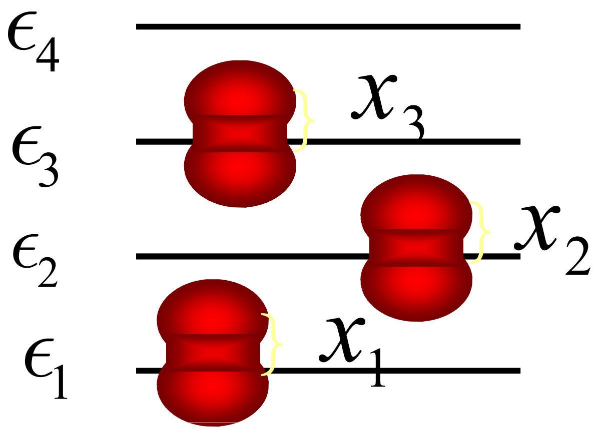
$$E_{n,k} = \sum_{i=1}^{k} x_i \qquad \rho_j = -(j + 1/2)/2$$

The question is how to solve BAEs

The standard pairing model

Here is the Bethe ansatz (BAEs) :

$k = 1, n = 4$



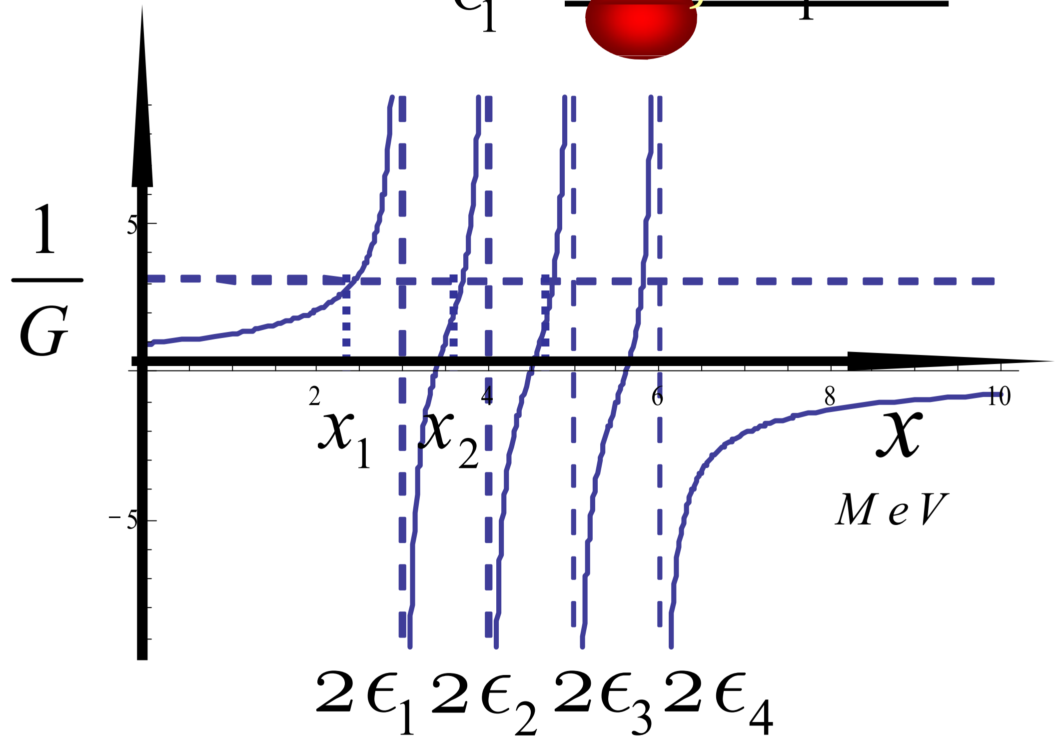
$$1 - 2G\sum_{j}^{n} \frac{\rho_j}{x_i - 2\epsilon_j} - 2G\sum_{i'=1(\neq i)}^{k} \frac{1}{x_i - x_{i'}} = 0,$$

$$E_{n,k} = \sum_{i=1}^{k} x_i$$

$$\rho_j = -1/2$$

$$1 + G\sum_{i} \frac{1}{x_i - 2\epsilon_j} = 0$$

$$E_{4,1} = x_1$$



Heine-Stieltjes correspondence

Through the Heine-Stieltjes correspondence, one can find solutions of BAEs by solving the second-order Fuchsian equation:

$$A(x)y''(x)+B(x)y'(x)-V(x)y(x)=0$$

Where $A(x)=\prod_{j=1}^{n}(x-2\epsilon_j)$ ***is a polynomial of degree n***

$$y(x)=\prod_{i=1}^{k}(x-x_i)$$

$$B(x)/A(x)=\sum_{j=1}^{n}\frac{2\rho_j}{x-2\epsilon_j}-\frac{1}{G}$$

Bethe ansatz equations

$$1-2G\sum_j\frac{\rho_j}{x_i-2\epsilon_j}-2G\sum_{i'=1(\neq i)}^{k}\frac{1}{x_i-x_{i'}}=0,$$

G. Szego, Amer. Math. Soc. Colloq. Publ. vol. 23, AMS,1975
T J Stieltjes, C. R. Acad Sci Paris 100 (1885) 439;620
E B Van Vleck, Bull. Amer. Math. Soc. 4 (1898) 426.

Heine-Stieltjes correspondence

$$A(x)y''(x)+B(x)y'(x)-V(x)y(x)=0$$

In search for polynomial solutions, we write

the expansion coefficients

$$y(x)=\sum_{\mu=0}^{k}a_{\mu}x^{\mu} \qquad V(x)=\sum_{\mu=0}^{n-1}b_{\mu}x^{\mu}$$

Substitution of $y(x)$, $V(x)$ into *Fuchsian equation* yields two matrix equations. By solving these two matrix equations, we can obtain the solutions $\{a_{\mu}\}$, $\{b_{\mu}\}$

If we set $a_k=1$, the coefficient a_{k-1} becomes equal to the negative sum of the $y(x)$ zeros

$$E_{n,k}=-a_{k-1}=\sum_{i=1}^{k}x_i$$

(Xin Guan, Kristina D. Launey, Mingxia Xie, Lina Bao, Feng Pan, and Jerry P. Draayer, <u>*Phys. Rev. C 86* (2012) 024313)</u>

(Xin Guan, Kristina D. Launey, Mingxia Xie, Lina Bao, Feng Pan, and Jerry P. Draayer, Comp. Phys. Comm. <u>185 (2014) 2714)</u>

Heine-Stieltjes correspondence

Furthermore, for giving the value of x approaches twice the single-particle energy, we have a simple one

For spherical systems

$$\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)^2 + (1-2\rho_j)\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)' - \frac{1}{G}\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) + \sum_{j'\neq j}^{n} \frac{2\rho_j}{2\epsilon_{j'} - 2\epsilon_j}\left[\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) - \left(\frac{y'(2\epsilon_j)}{y(2\epsilon_j)}\right)\right] = 0$$

For doubly degenerate case, the above equation set reduces to a much simpler one as

For deformed systems

$$\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)^2 - \frac{1}{G}\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) + \sum_{j'=j}^{n} \frac{1}{2\epsilon_{j'} - 2\epsilon_j}\left[\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) - \left(\frac{y'(2\epsilon_j)}{y(2\epsilon_j)}\right)\right] = 0$$

Much easier way which can be applied in more general cases

(Chong Qi and Tao Chen , Phys. Rev. C 92 (2015) 051304(R))

Iterative approach

$$\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)^2 - \frac{1}{G}\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) + \sum_{j'=j}^{n}\frac{1}{2\epsilon_{j'}-2\epsilon_j}\left[\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)-\left(\frac{y'(2\epsilon_j)}{y(2\epsilon_j)}\right)\right]=0$$

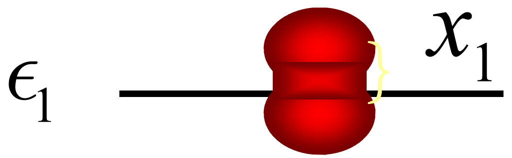
Initial value

$y_2(x)$

$$y_1(x) = (a_0 + a_1 x)$$

$$y^a{}_2(x) = (a_0 + a_1 x)\times(x - 2\epsilon_2 + Random\_value)$$

$$k = 1, n = 1$$

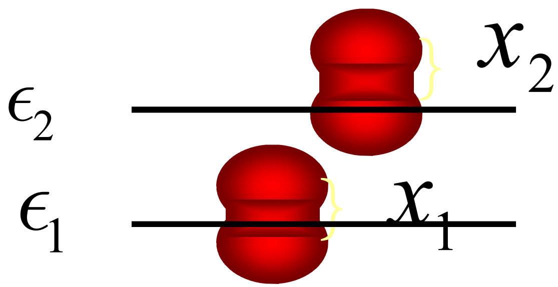


x_i is the energy of pair

$$1 - 2G\sum_j \frac{\rho_j}{x_i - 2\epsilon_j} = 0$$

$$E = x_1$$

$$k = 2, n = 2$$



x_i is the energy of pair

Iterative approach

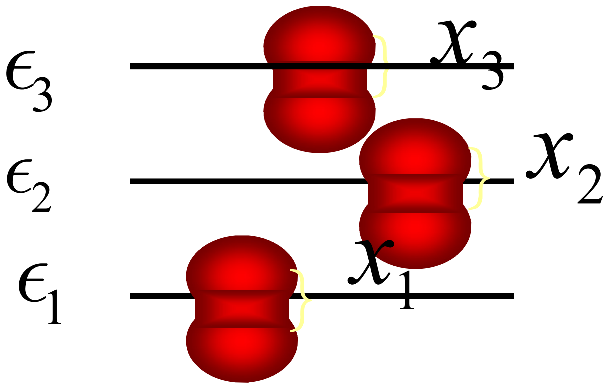
$$\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right)^2 - \frac{1}{G}\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) + \sum_{j'=j}^{n}\frac{1}{2\epsilon_{j'}-2\epsilon_j}\left[\left(\frac{y'(2\epsilon_{j'})}{y(2\epsilon_{j'})}\right) - \left(\frac{y'(2\epsilon_j)}{y(2\epsilon_j)}\right)\right] = 0$$

New Initial value

$y_3(x)$ New Initial value

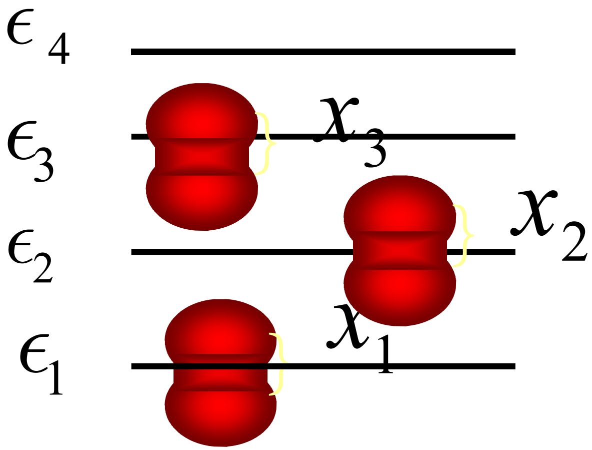
$$y^a{}_3(x) = y_2(x) \times (x - 2\epsilon_3 + Random\_value)$$

$k = 3, n = 3$



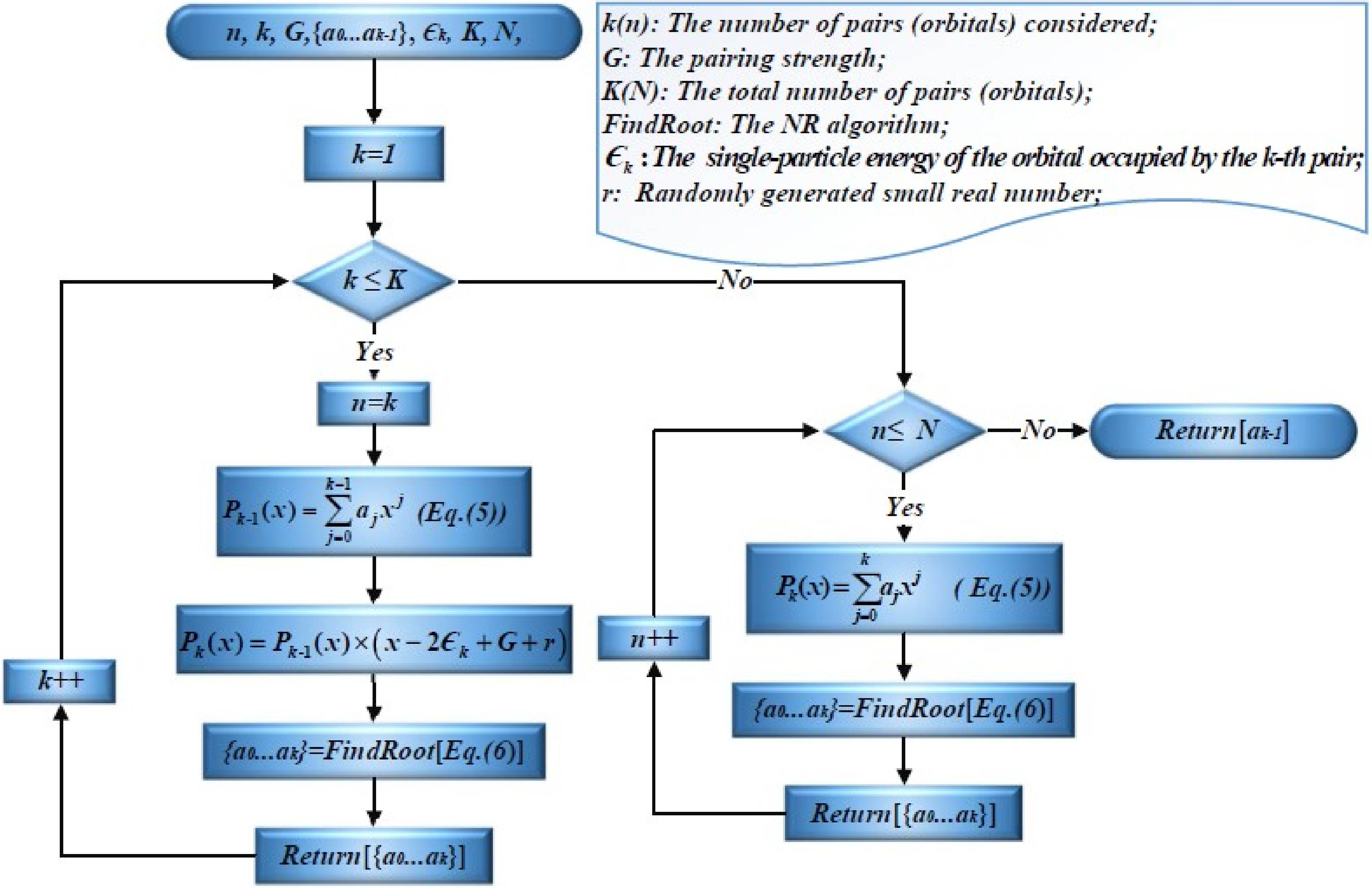
x_i is the energy of pair

$k = 3, n = 4$



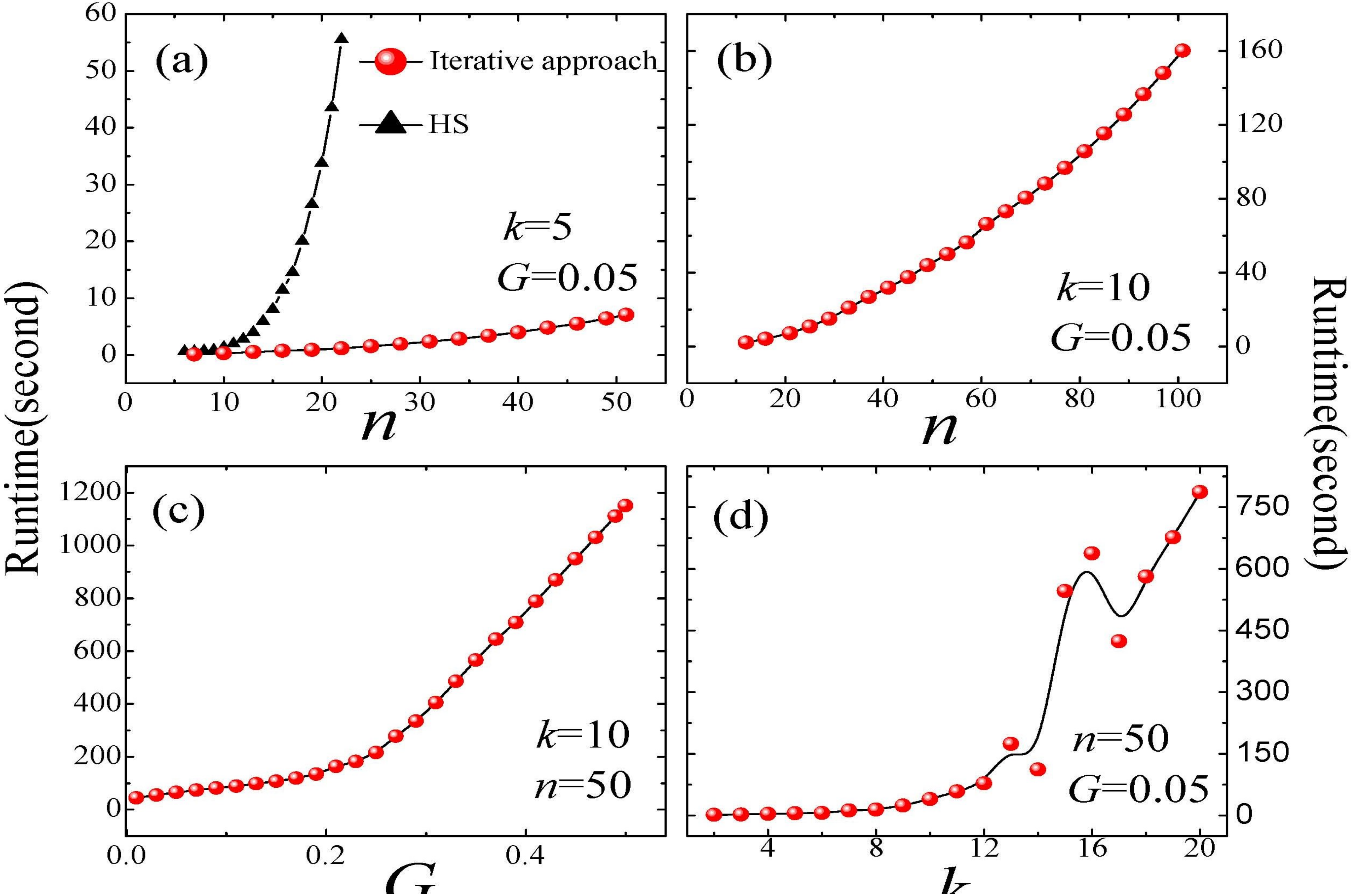
x_i is the energy of pair

Iterative approach

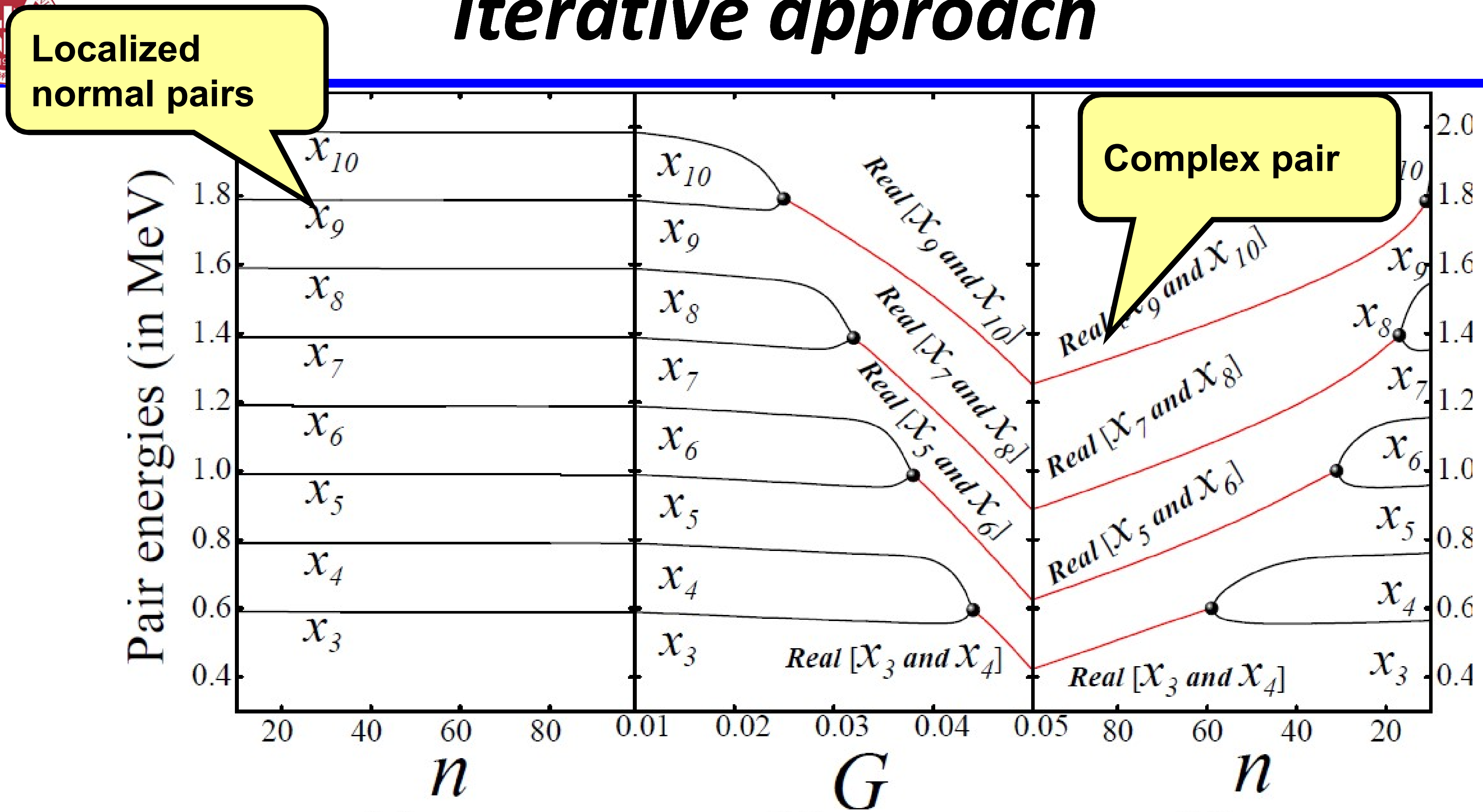


(Xin Guan, Xin Ai and Chong Qi, Phys. Rev. C under review)

Iterative approach



Iterative approach



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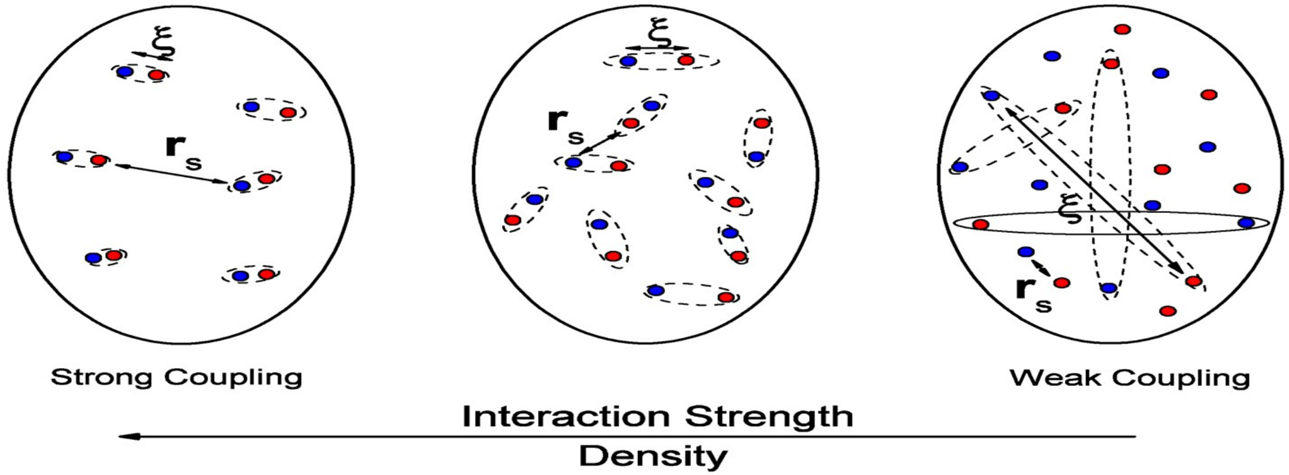


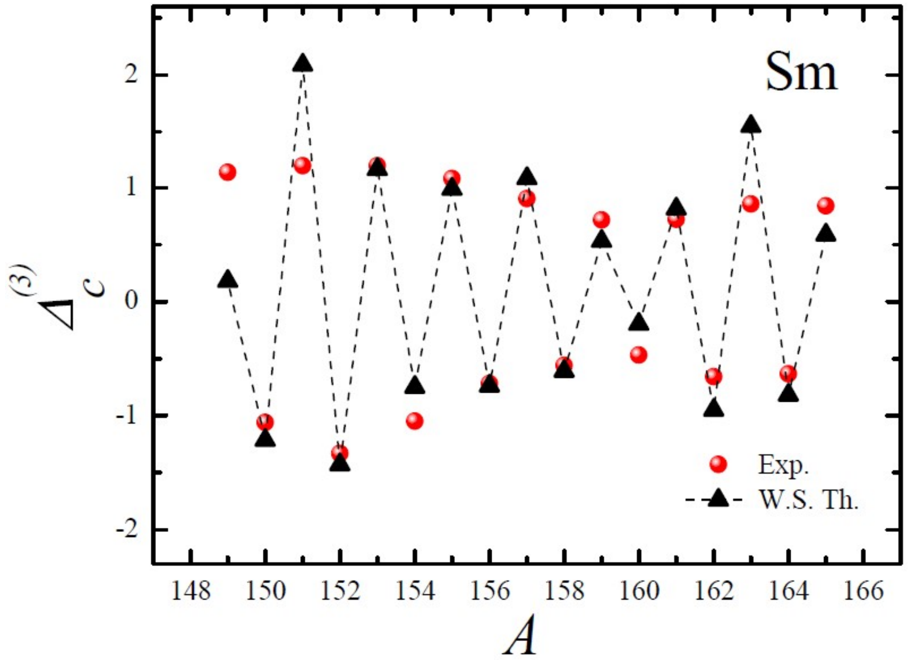
Numerical results

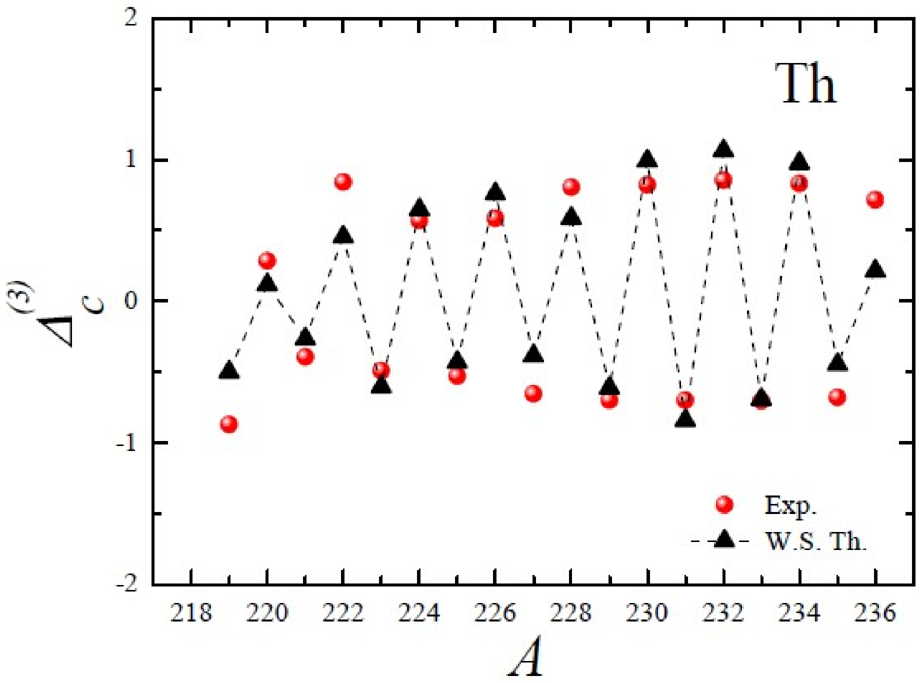
The single-particles are taken from Woods-Saxon potential

Two valence shell from 82 to 184 G=0.06 MeV

The odd-even mass difference

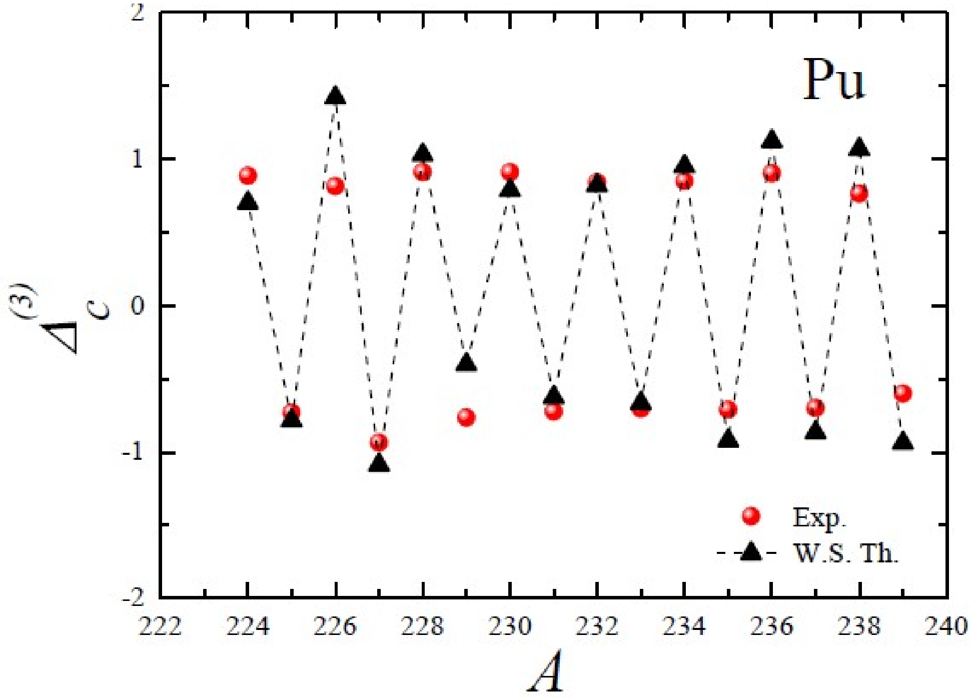
$$\Delta_c^{(3)}(Z,N-1) \equiv \frac{1}{2}(BE(Z,N) - 2BE(Z,N-1) + BE(Z,N+2))$$

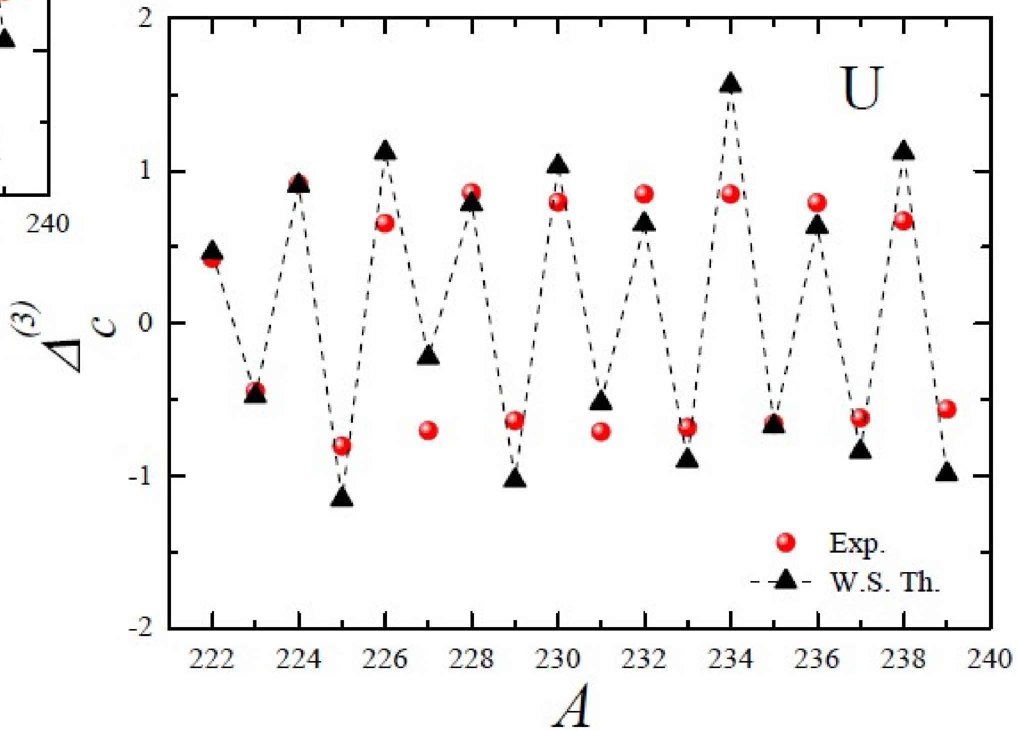




(Xin Guan, Xin Ai and Chong Qi, Phys

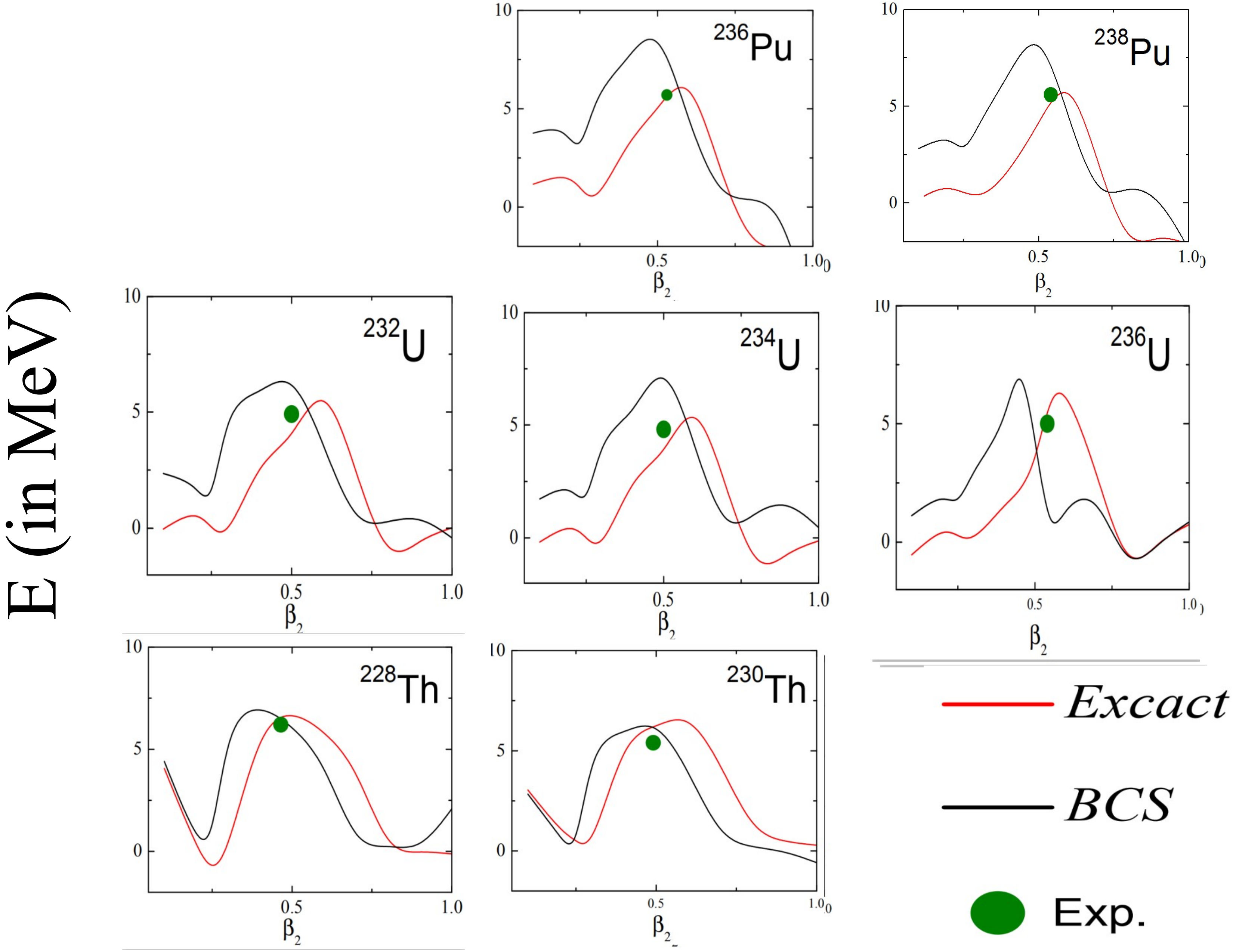
Numerical results





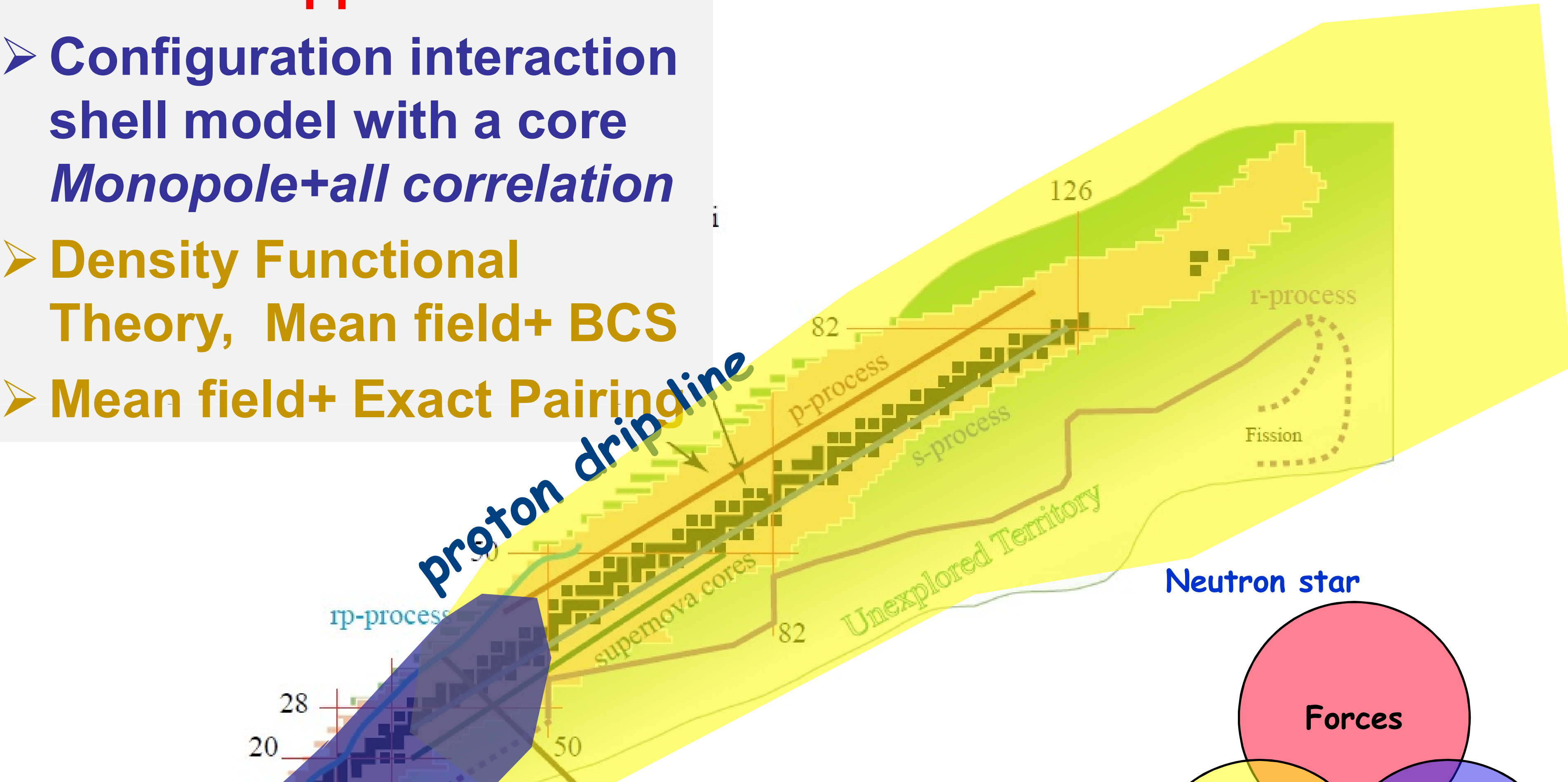
The exact solution of pairing model can be applied for heavy nuclear systems such as actinide nuclei.

Energy surface

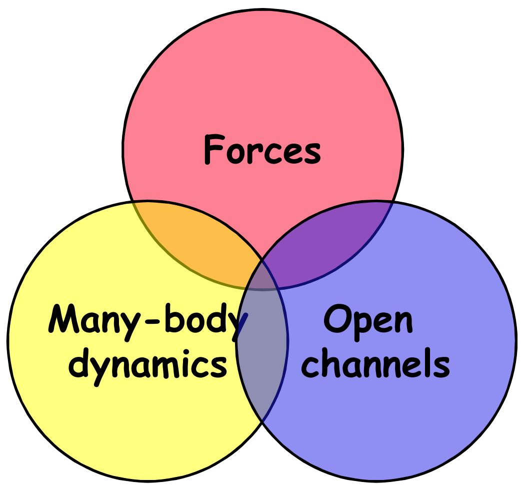


Objective

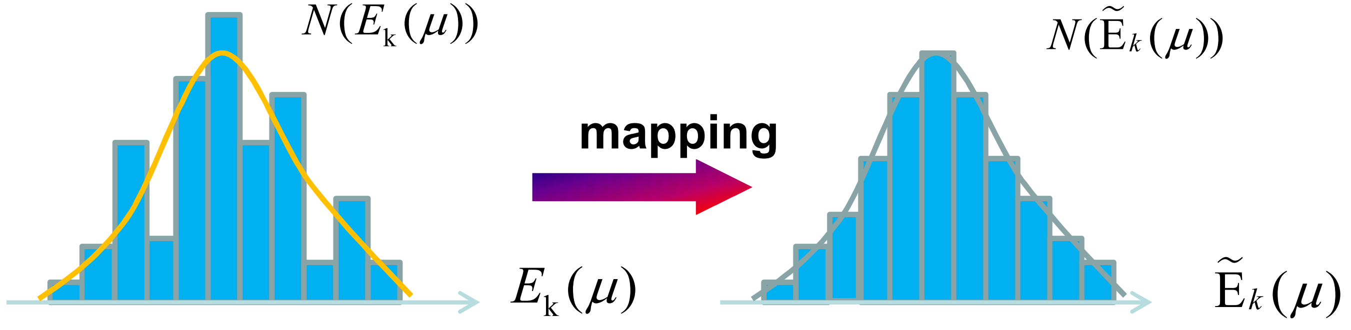
- **Ab initio approaches**
- **Configuration interaction shell model with a core**
  Monopole+all correlation
- **Density Functional Theory, Mean field+ BCS**
- **Mean field+ Exact Pairing**



PDC's supercomputer Beskow



Statistical measures



$P(S)$: **The distribution of the nearest-neighbor level spacing**

S **is calculated from the unfolded spectrum with**

$$S_\mu = \widetilde{E}_k(\mu+1) - \widetilde{E}_k(\mu).$$

a. Poisson statistics with

$$P(S) = e^{-S}$$

b. GOE prediction for the chaotic system

$$P(S) = (\pi/2) S e^{-\pi S^2/4}$$

$\Delta_3(L)$: The spectral rigidity

(Dyson, J. Math. Phys. 3, 140 (1962); J. Math. Phys. 3, 157 (1962))

$$\Delta_3(\alpha, L) = \frac{1}{L}\min_{A,B}\int_{\alpha}^{\alpha+L}\left[N(\widetilde{\mathrm{E}})(A\widetilde{E}+B)\right]^2 d\widetilde{E}$$

which is the average of the least-square deviations between the number staircase function $N(\widetilde{\mathrm{E}})$ obtained from fitting the unfolded spectrum and its best linear fitting over the energy interval [α, α+L]. A smoother

$$\overline{\Delta}_3(L) = \frac{1}{n_\alpha}\sum_{\alpha}\Delta_3(\alpha, L)$$

a. **For a regular spectrum,**

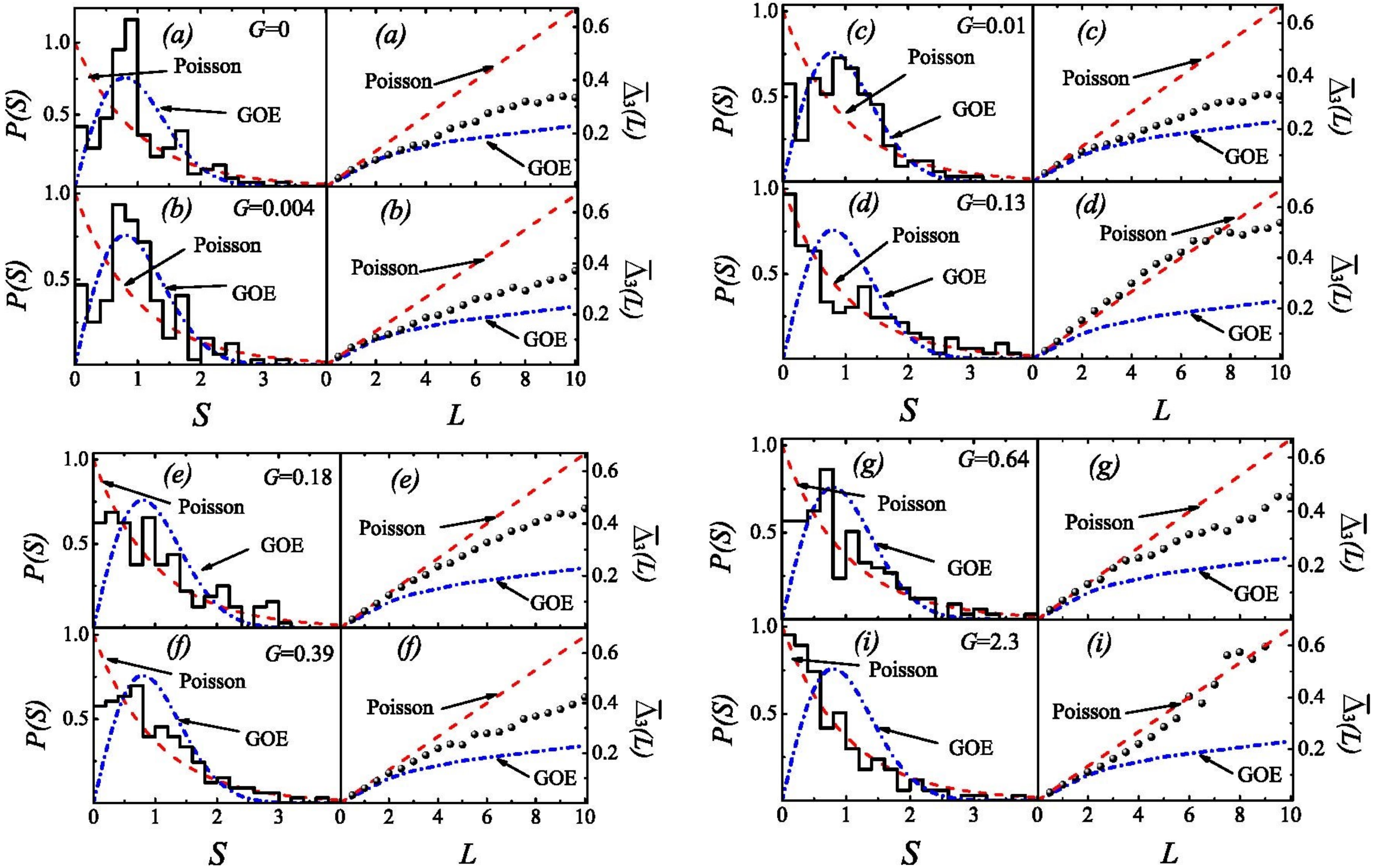
$$\overline{\Delta}_3(L) = L/15$$

b. **In the large-*L* limit, for a chaotic system with the GOE statistics**

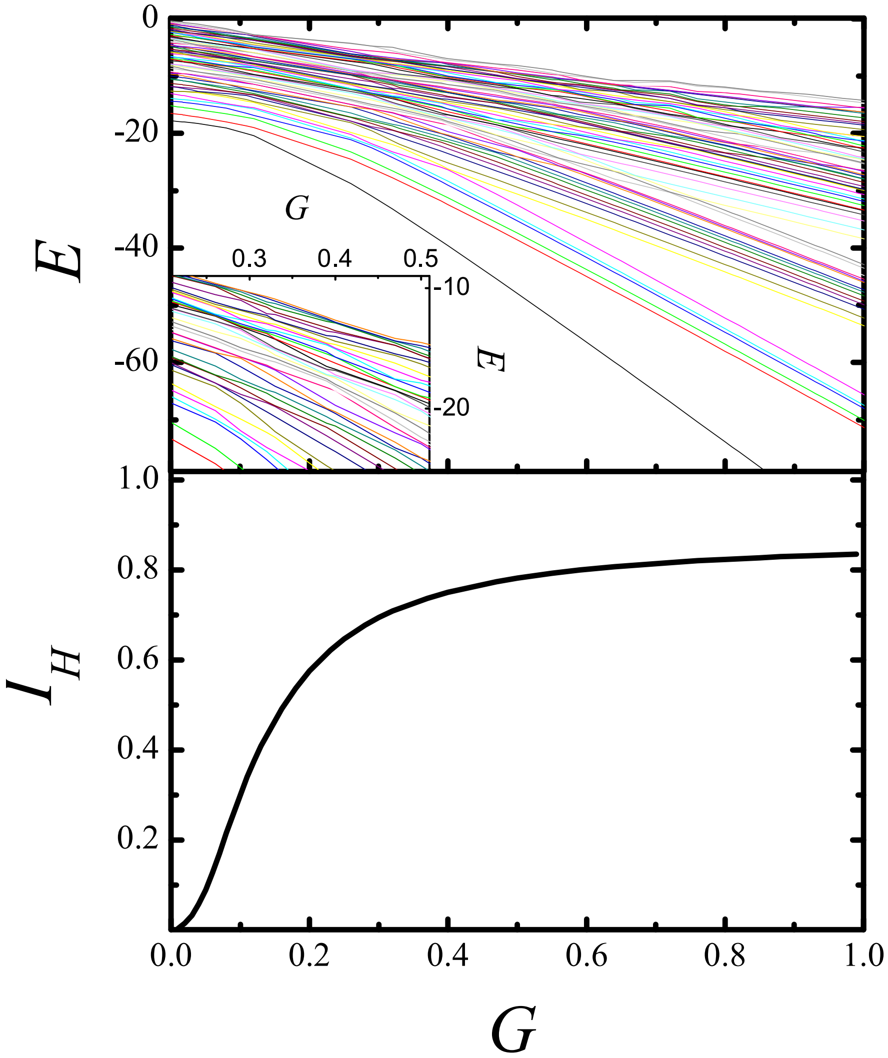
$$\overline{\Delta}_3(L) \approx \frac{1}{\pi^2}(\ln L - 0.0687)$$

we consider 6 j-levels and an even system with k=5 pairs.

$$\varepsilon_{f7/2}=2.532MeV,\quad \varepsilon_{h9/2}=3.184MeV,\quad \varepsilon_{i13/2}=4.905MeV,$$
$$\varepsilon_{f5/2}=6.152MeV,\quad \varepsilon_{p1/2}=7.341MeV.\quad \varepsilon_{p3/2}=5.790MeV,$$



Applications and discussions



All excited J = 0 levels including ground level in the model (in MeV) for even system with k = 5 pairs as functions of G (in MeV), in which the single-particle energies are obtained from the spherical shell model and the corresponding information entropy of the ground state as a function of G.

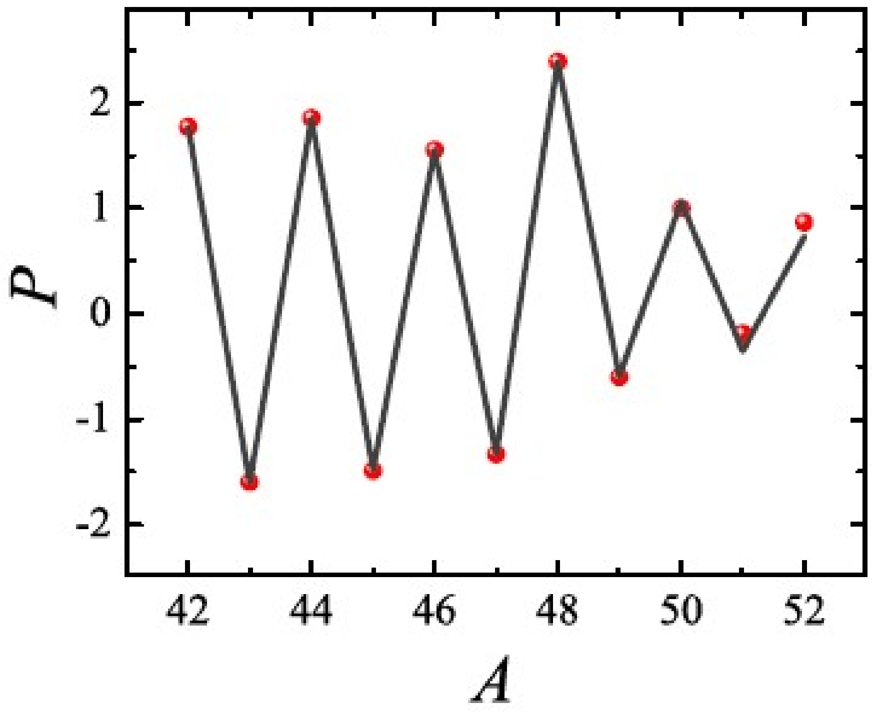
$$I_H(|g\rangle) = -\sum_{i=1}^{d} |\omega_i|^2 \log_d(|\omega_i|^2)$$

Y. Alhassid, A. Novoselsky, and N. Whelan, PRL 65, 2971 (1990); W. D. Heiss and M. Muller, PRE66,016217(2002).

A realistic example: The single-particle energies of the valence neutrons are obtained from 40Ca and 41Ca binding energies and the single-particle excitation energies in the 41Ca spectrum.

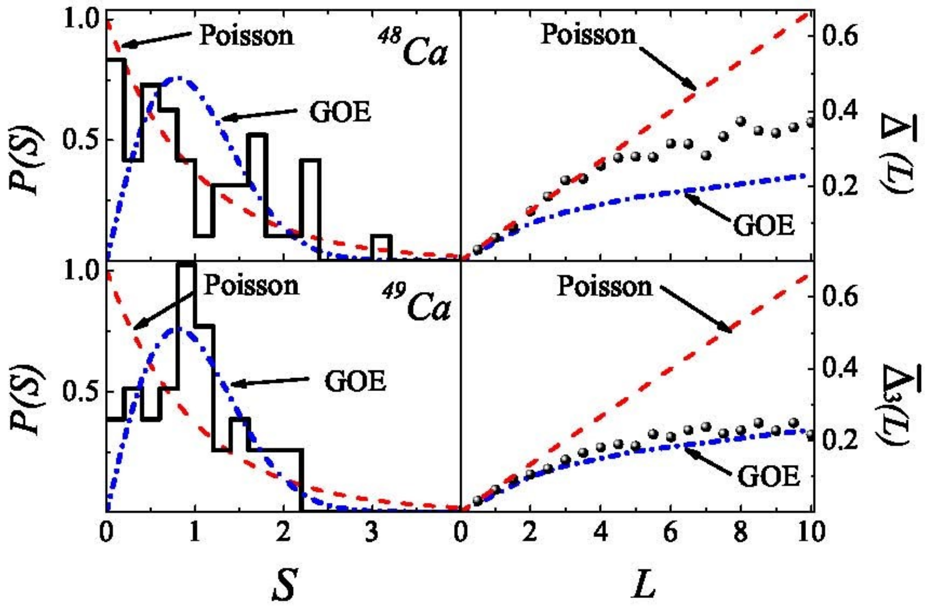
$\varepsilon_{f7/2} = -2.50 MeV,\quad \varepsilon_{p3/2} = -0.56 MeV,\quad \varepsilon_{g9/2} = 1.95 MeV.$

$\varepsilon_{f5/2} = 0.08 MeV,\quad \varepsilon_{p1/2} = 1.11 MeV,$

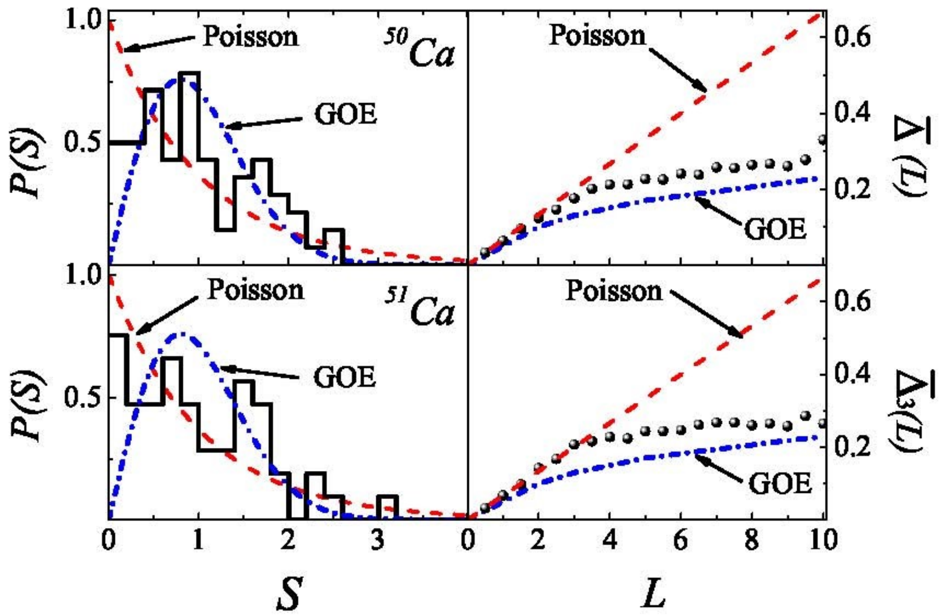


The theoretical values and the corresponding experimental values of the pairing gaps P (in units of MeV) of 42-52Ca as functions of the mass number A.

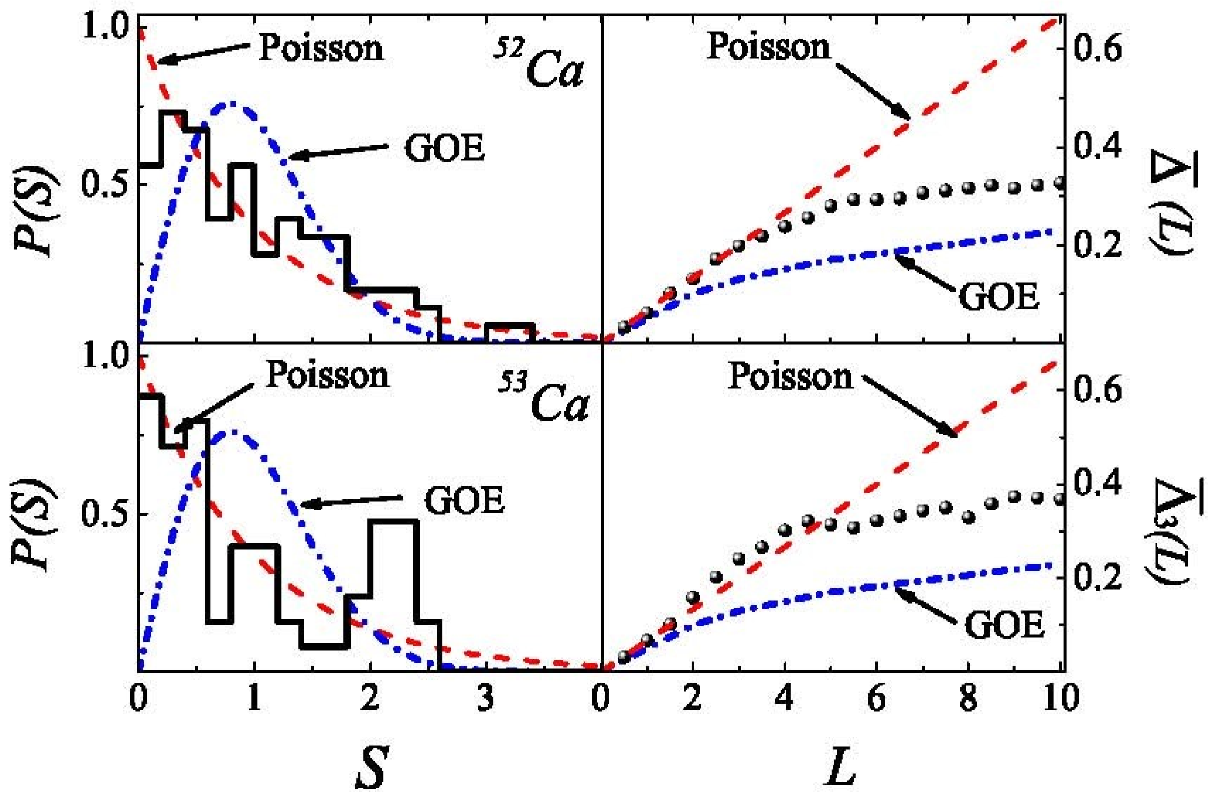
Applications and discussions



The statistical results of the J = 0 levels in 48Ca with G = 0.4385MeV, and the J = 3/2 levels in 49Ca with G = 0.44MeV.



The statistical results of the J = 0 levels in 50Ca with G = 0.331MeV and the J = 3/2 levels in 51Ca with G = 0.291MeV.



The statistical results of the J = 0 levels in 52Ca with G = 0.175MeV and the J = 3/2 levels in 53Ca with G = 0.03MeV.

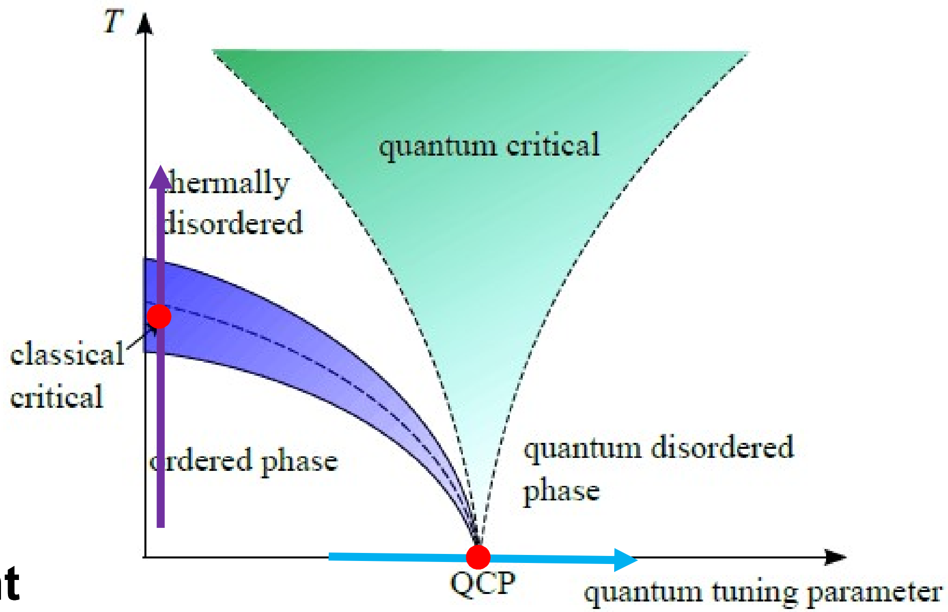
Xin Guan, K.D. Launey, Jianzhong Gu, Feng Pan, and J. P. Draayer, ***Phys. Rev. C*** **88 (2013) 044325.**

A chaotic behavior indeed exists in realistic nuclear systems.

Classical vs Quantum phase transitions

- **Classical phase transition**
  is the transformation of a thermodynamic system from one phase or state of matter to another one by heat transfer

Combined phase transition diagram



- **Quantum phase transition**
  is a phase transition between different quantum phases at zero temperature by varying a physical parameter—such as magnetic field or pressure (in condensed matter)

Cejnar Jolie Casten Rev Mod Phys 82,2155 2010

Quantum phase transition **is a ground-state phase transition due to collective quantum fluctuations trigged by varying a physical parameter**

Phase transitions: order

➢ 1st-order vs. 2nd-order transition:

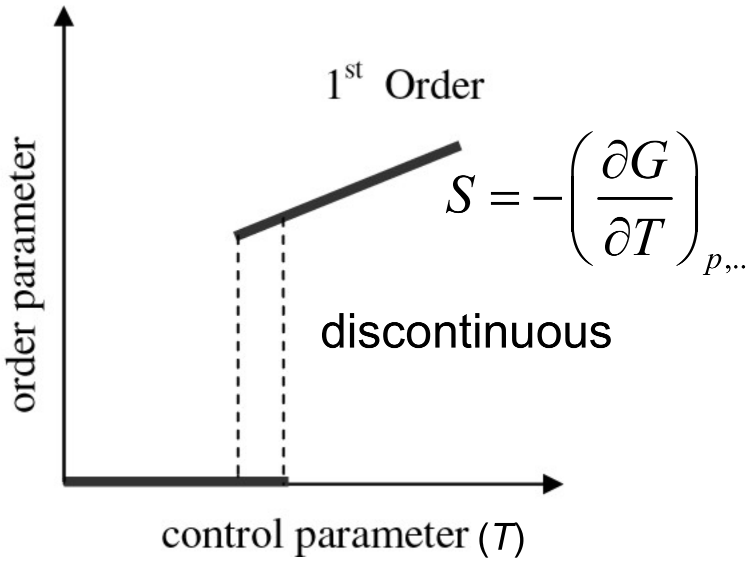
Ehrenfest classification:

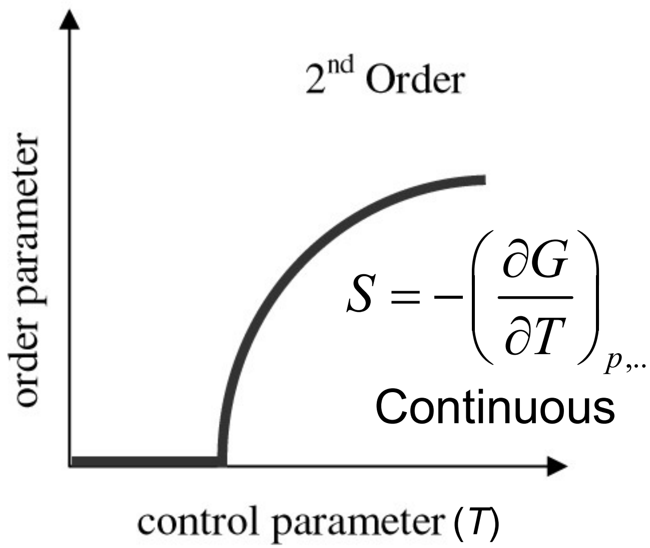
The order of a phase transition is defined to be the order of the lowest-order derivative, which changes discontinuously at the phase boundary

$$G = H - ST$$ Gibbs free energy

➢ Order parameter

(entropy *S*, volume, Magnetization)



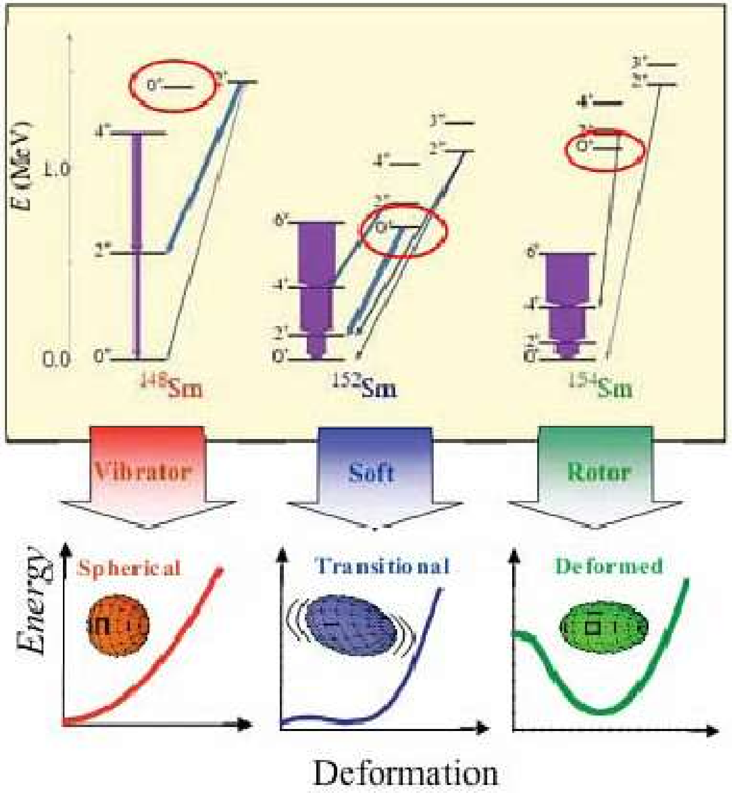


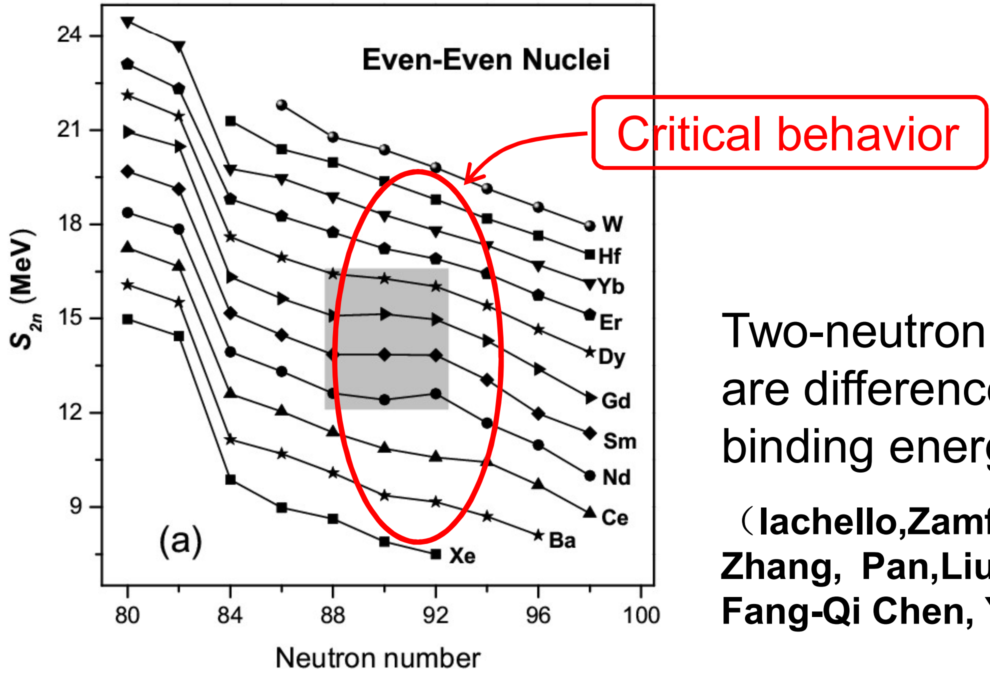
***Quantum phase transition* is normally 2nd-order**

Quantum phase transitions in nuclei

Quantum phase transitions in nuclei are reflected by rapid structural transformation with varying *N* or *Z*.

In practice, this refers to the deformation of nuclei, and the control parameter is *N* or *Z*.



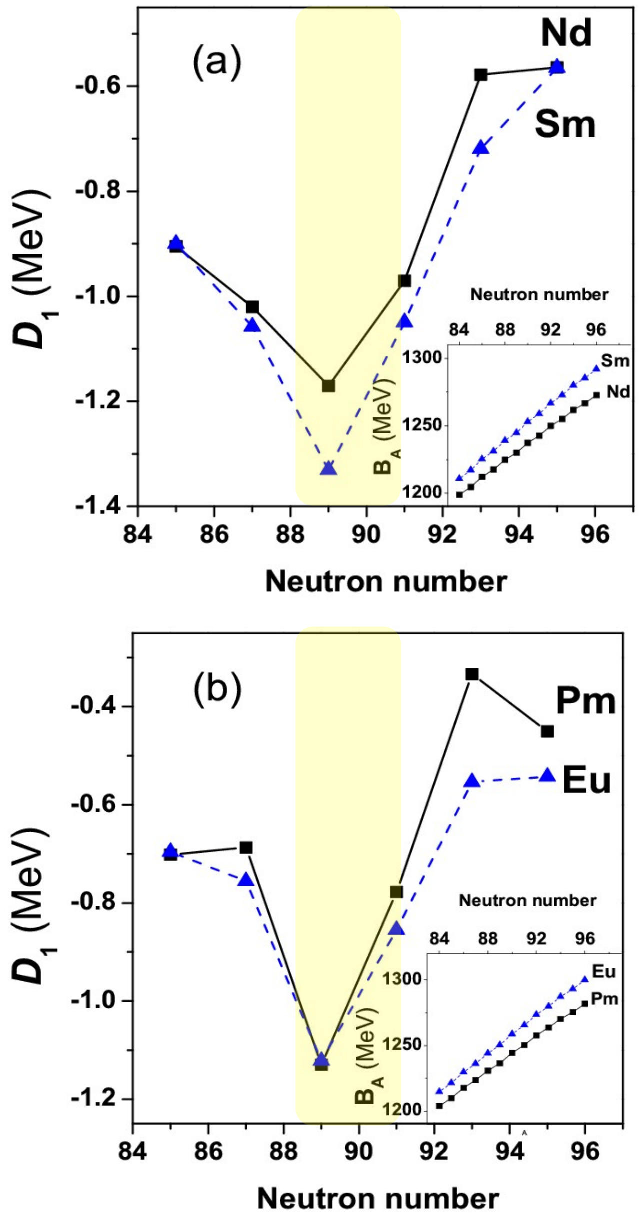


Two-neutron separation energies (S_{2n}), which are differences (proxies for derivatives) of binding energies,

（Iachello,Zamfir,Casten PRL 81, 1191 (1998)
Zhang, Pan,Liu,Luo,Draayer, PRC 85, 064312 (2012)
Fang-Qi Chen, Yang Sun,and Peter Ring, PRC 88, 014315 (2013)）

Quantum phase transitions in nuclei

- **The experimental data reveals that the odd-even mass difference reaches a minimum value, showing the signature of critical behavior at the neutron number N~90**
- **The odd-even effect provides the most important evidence of pairing interactions, *but how these interactions relate to the phase transition is yet to be resolved***
- **it is crucial to explore possible microscopic mechanism with an appropriate pairing model that can account for the ground state phase transitions**



Zhang, Bao,Guan,Pan,Draayer, *Phys. Rev. C* 88, 064305 (2013)

Numerical results

Model calculations for Nd, Sm, and Gd isotopes are performed for valence neutrons in the sixth HO shell with 22 Nilsson levels (orbits) for valence neutrons.

The odd-even mass difference

$$\mathrm{P(Z,N)} = E_B(Z,N+1) + E_B(Z,N-1) - 2E_B(Z,N)$$

The two-neutron separation energy

$$S_{2n}(Z,N) = E_B(Z,N) - E_B(Z,N-2)$$

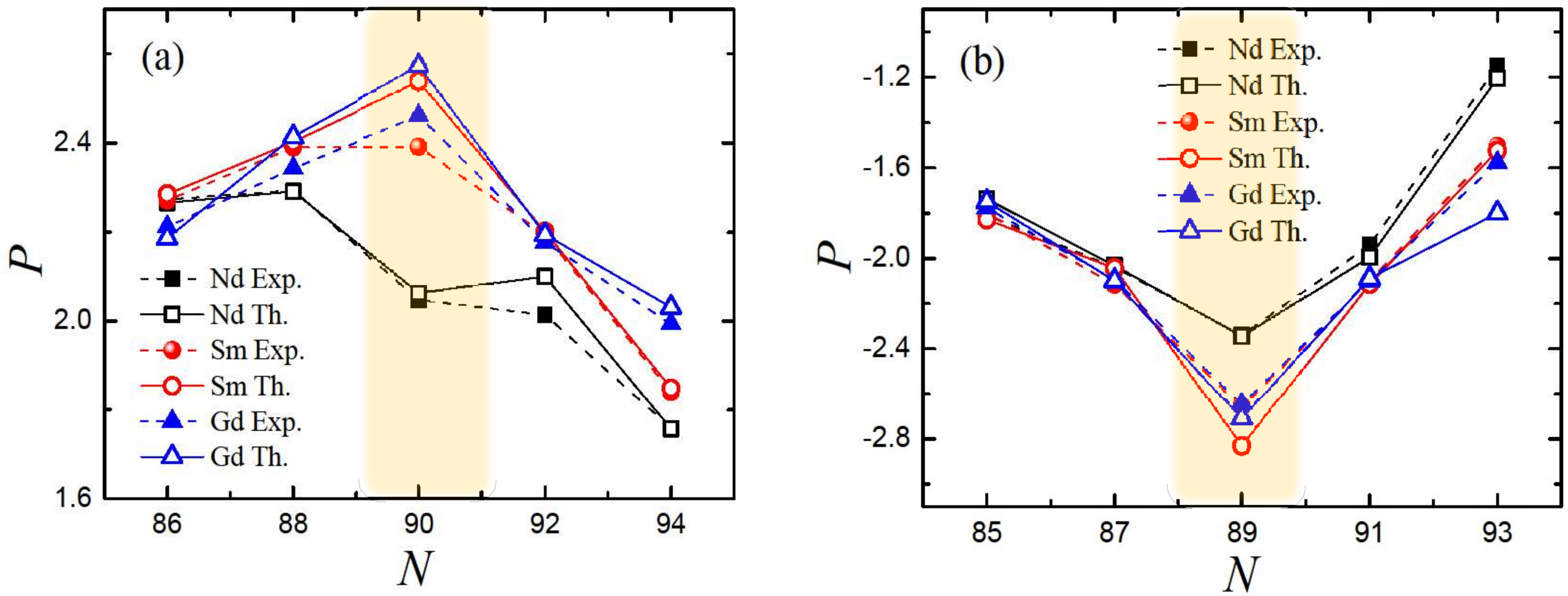
The α -decay energy Q_α

$$Q_\alpha(Z,N) = E_B(Z-2,N-2) - E_B(Z,N) + E_B(2,2)$$

The double β^- -decay energy $Q_{2\beta^-}$

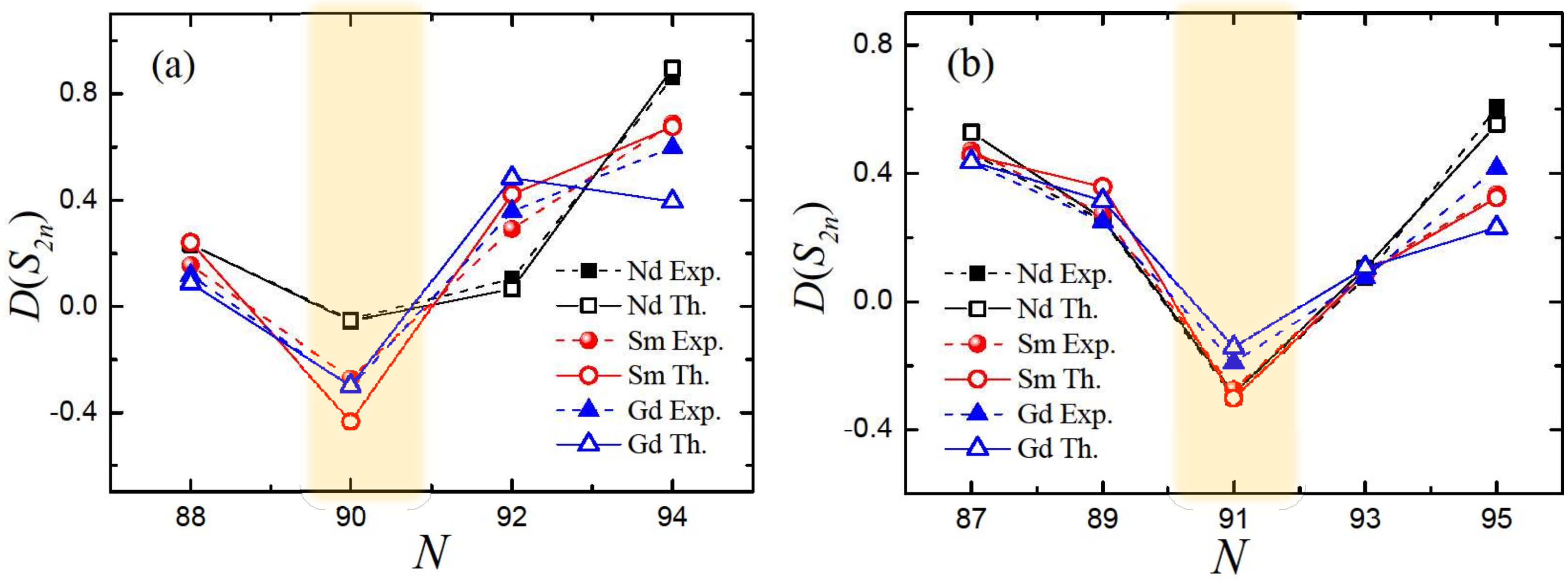
$$Q_{2\beta^-}(Z,N) = E_B(Z+2,N-2) - E_B(Z,N) + 2M_m - 2M_P$$

Odd-even mass differences



Both the theoretical values P(Z,N) as functions of N and the corresponding experimental values for even-even and odd-A, Nd，Sm, and Gd have a peak or a valley at N~90.

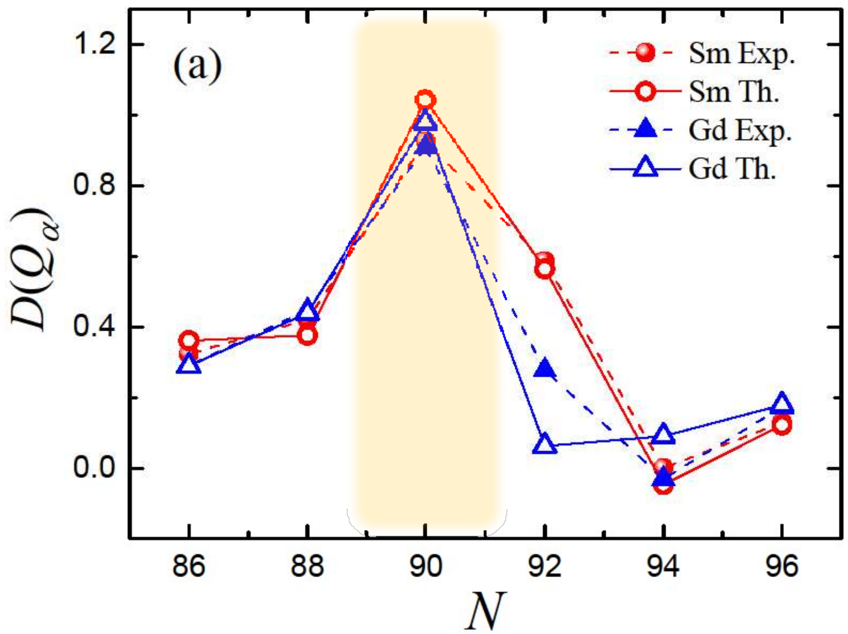
Odd-even differences of two-neutron separation energy

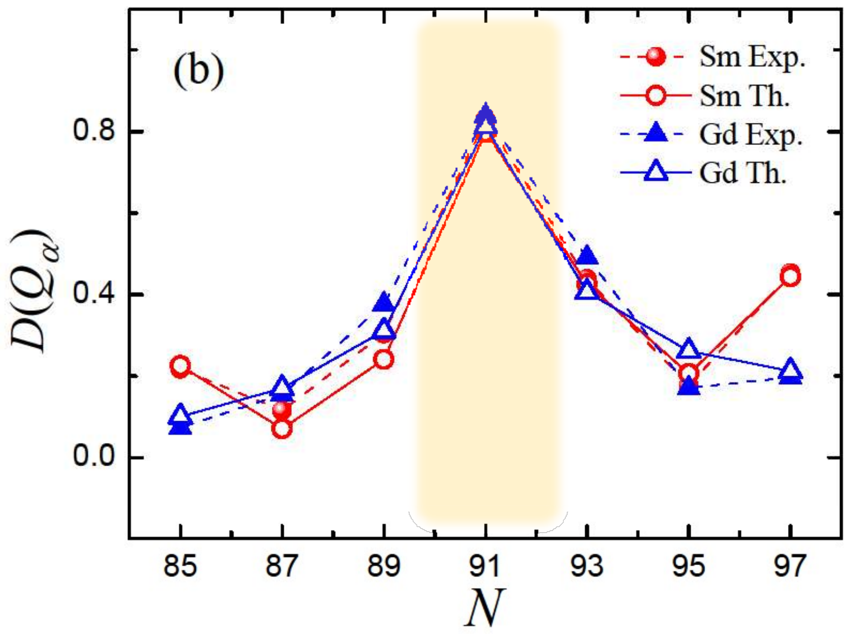


$$D(S_{2n}(Z,N)) = S_{2n}(Z,N-1) - S_{2n}(Z,N)$$

In comparison with the corresponding experimental data, the calculated results of the model for these isotopes, reproduce the critical phenomena reasonably well.

Odd-even differences of α-decay energy

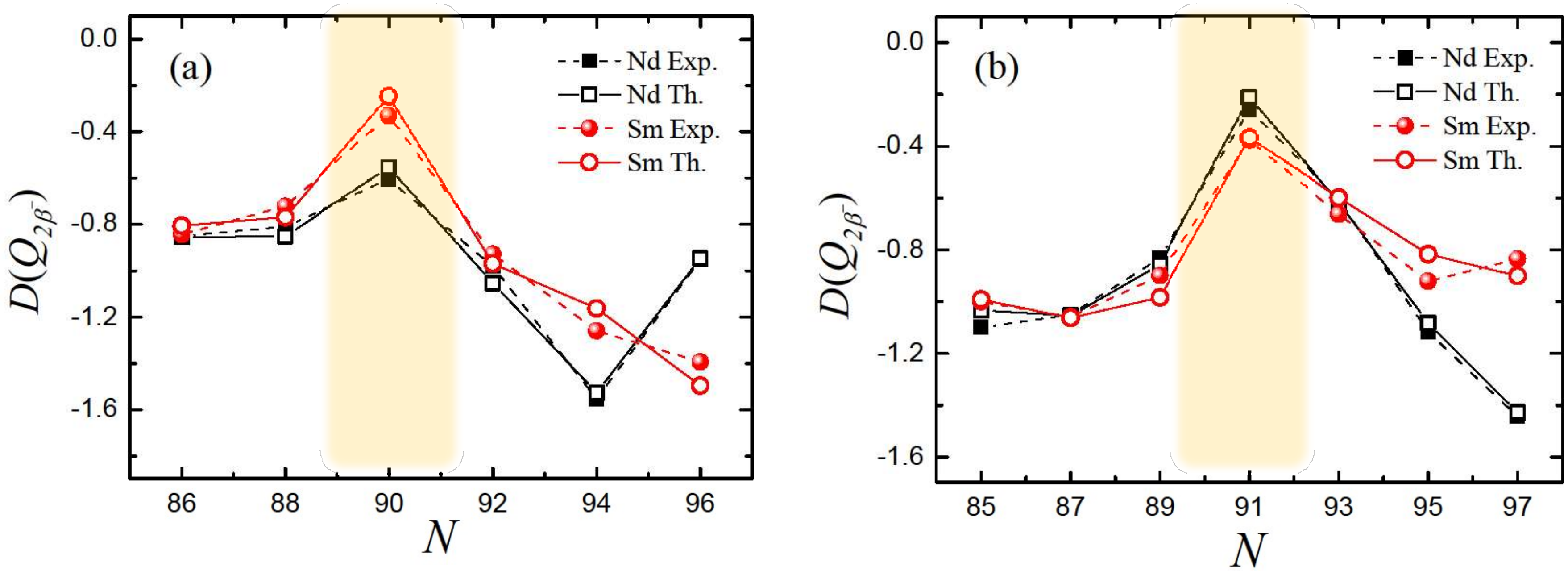




$$D(\mathrm{Q}_\alpha(Z,N)) = \mathrm{Q}_\alpha(Z,N-1) - \mathrm{Q}_\alpha(Z,N)$$

In comparison with the corresponding experimental data, the calculated results of the model for these isotopes, reproduce the critical phenomena reasonably well.

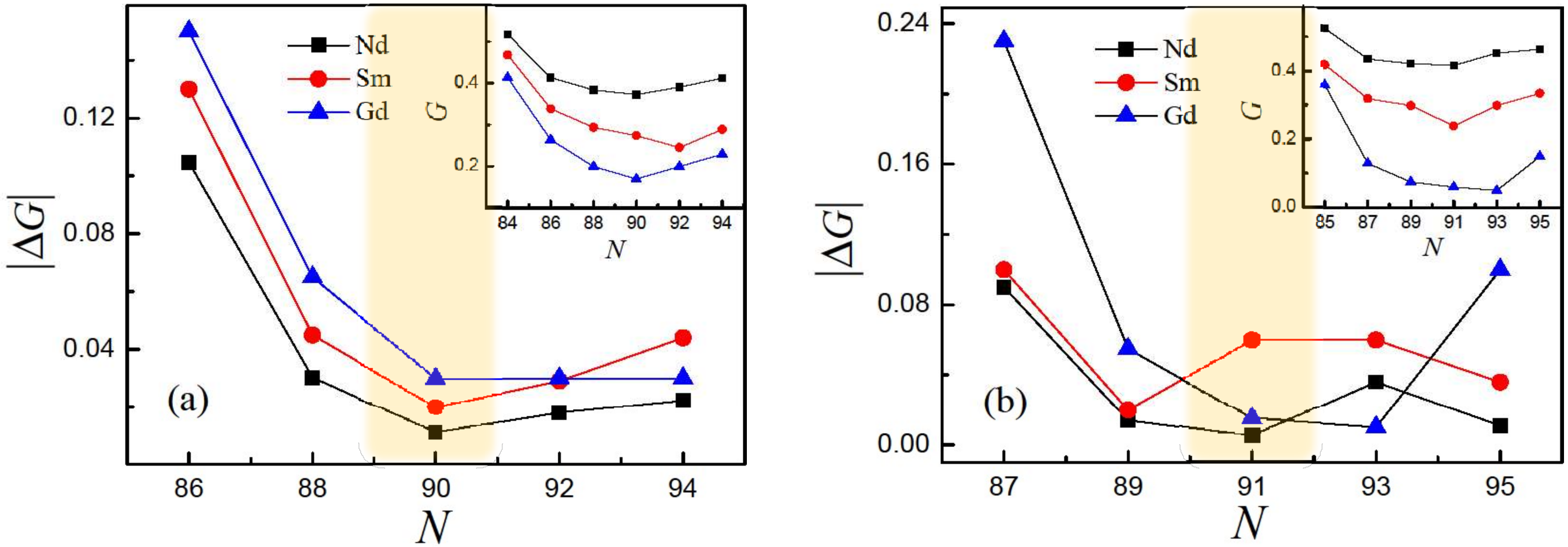
Odd-even differences of double β-decay energy



$$D(\mathrm{Q}_{2\beta^-}(Z,N)) = \mathrm{Q}_{2\beta^-}(Z,N-1) - \mathrm{Q}_{2\beta^-}(Z,N)$$

In comparison with the corresponding experimental data, the calculated results of the model for these isotopes, reproduce the critical phenomena reasonably well.

Pairing strength

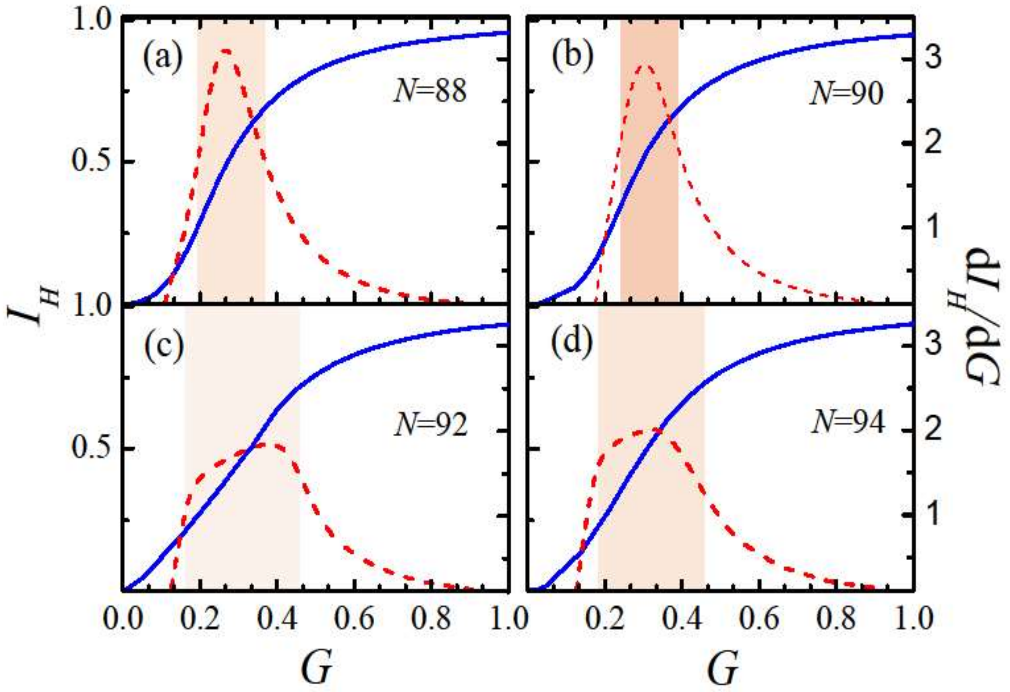


$$\left|\Delta G(Z,N)\right| = \left|G(Z,N+2) - G(Z,N)\right|$$

The pairing interaction strength G and its difference $|\Delta G|$ reaches its minimum value or becomes flattening at the critical point N values, where the odd-even differences all reach the extreme values

The information entropy measures the correlations among the mean-field single-pair product states with k pairs in the ground state in the model.

$$I_H(|g\rangle) = -\sum_{i=1}^{d} |\omega_i|^2 \log_d(|\omega_i|^2)$$



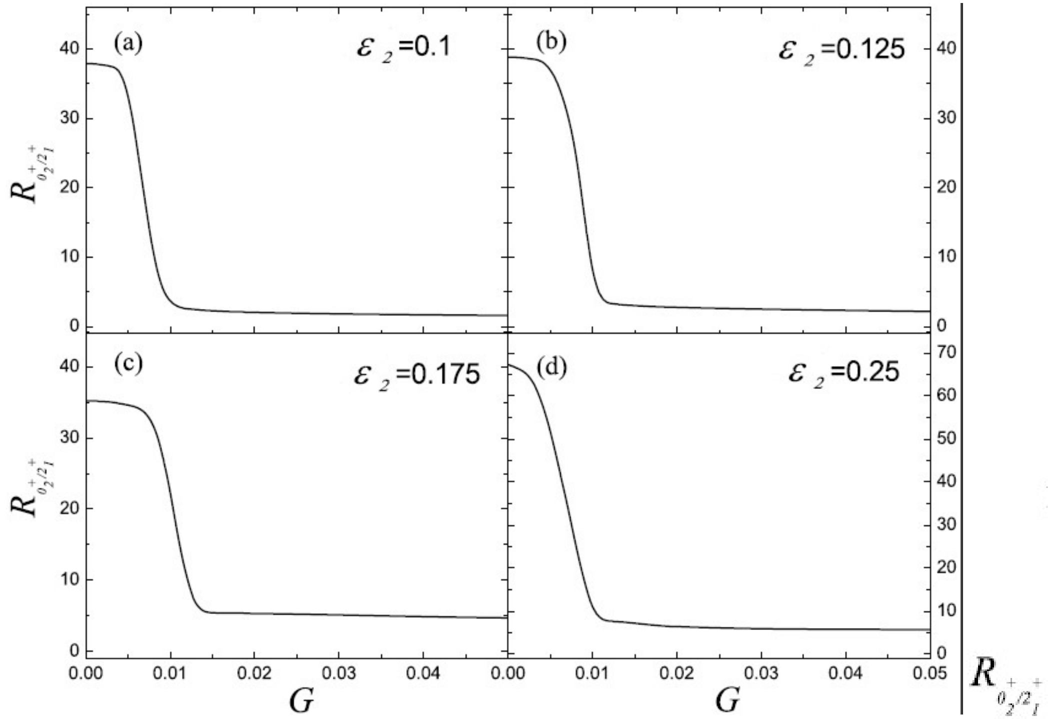
The results demonstrate that the ground state phase transition is indeed much more sensitive to the variation of the pairing interaction strength G around N~90, which thus naturally explains the critical behavior in the present model.

Xin Guan, Haocheng Xu, Yu Zhang, Feng Pan,and Jerry P. Draayer
Phys. Rev. C 94, 024309 (2016)

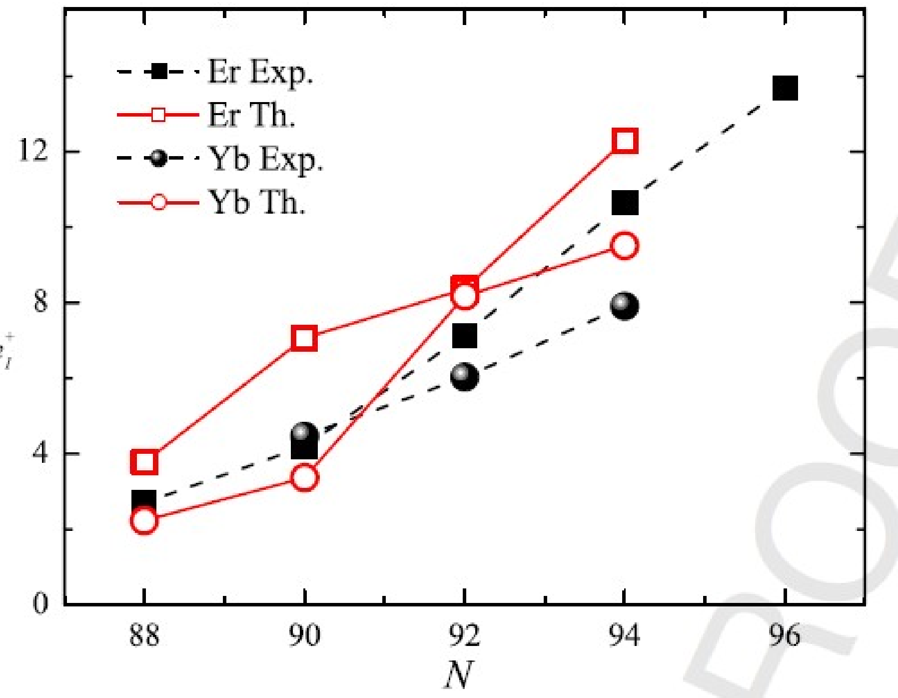
Motivation

Nuclear shapes

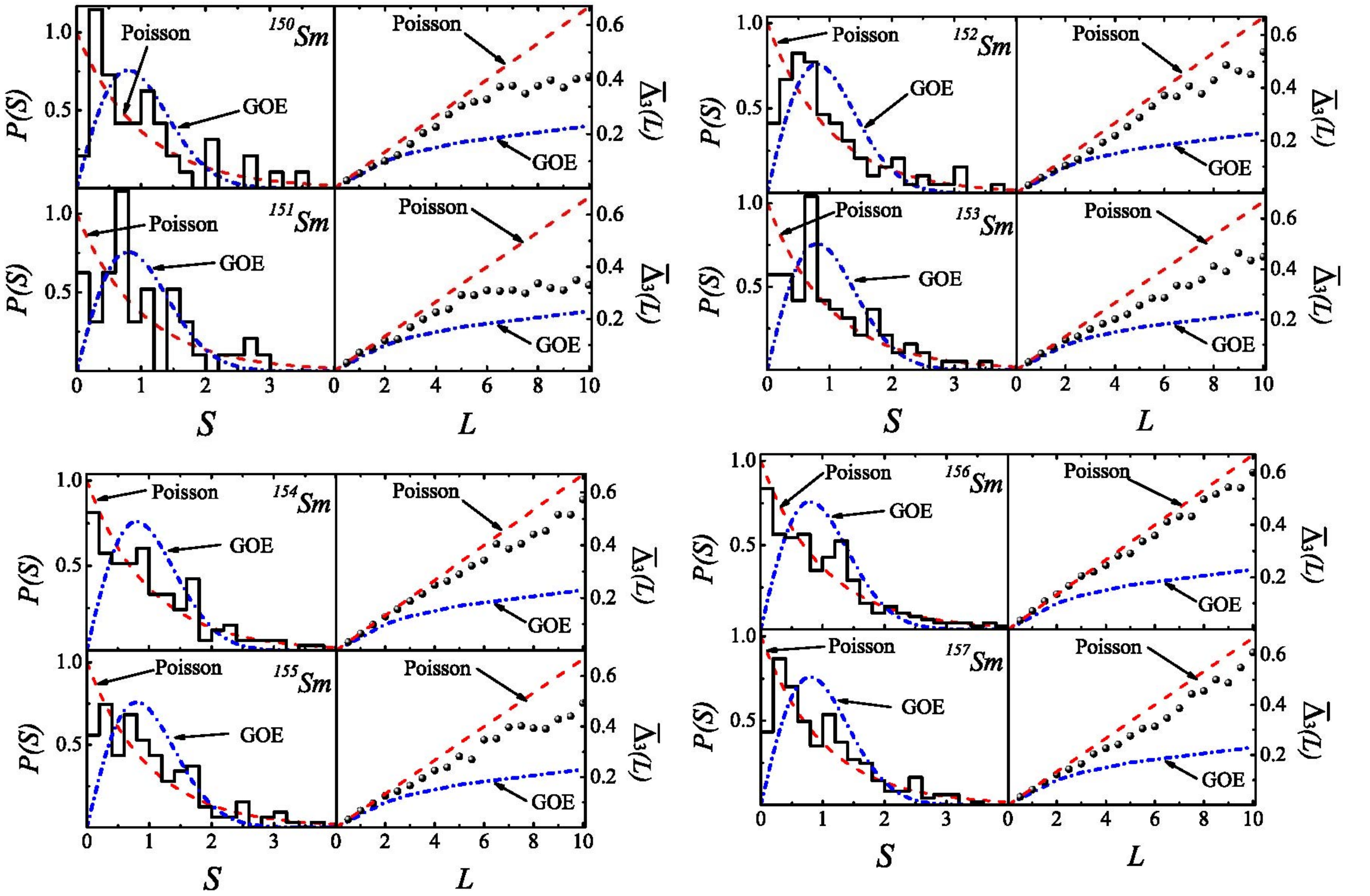
Shape phase transition   Shape coexistence   Super deformation   nuclear fission



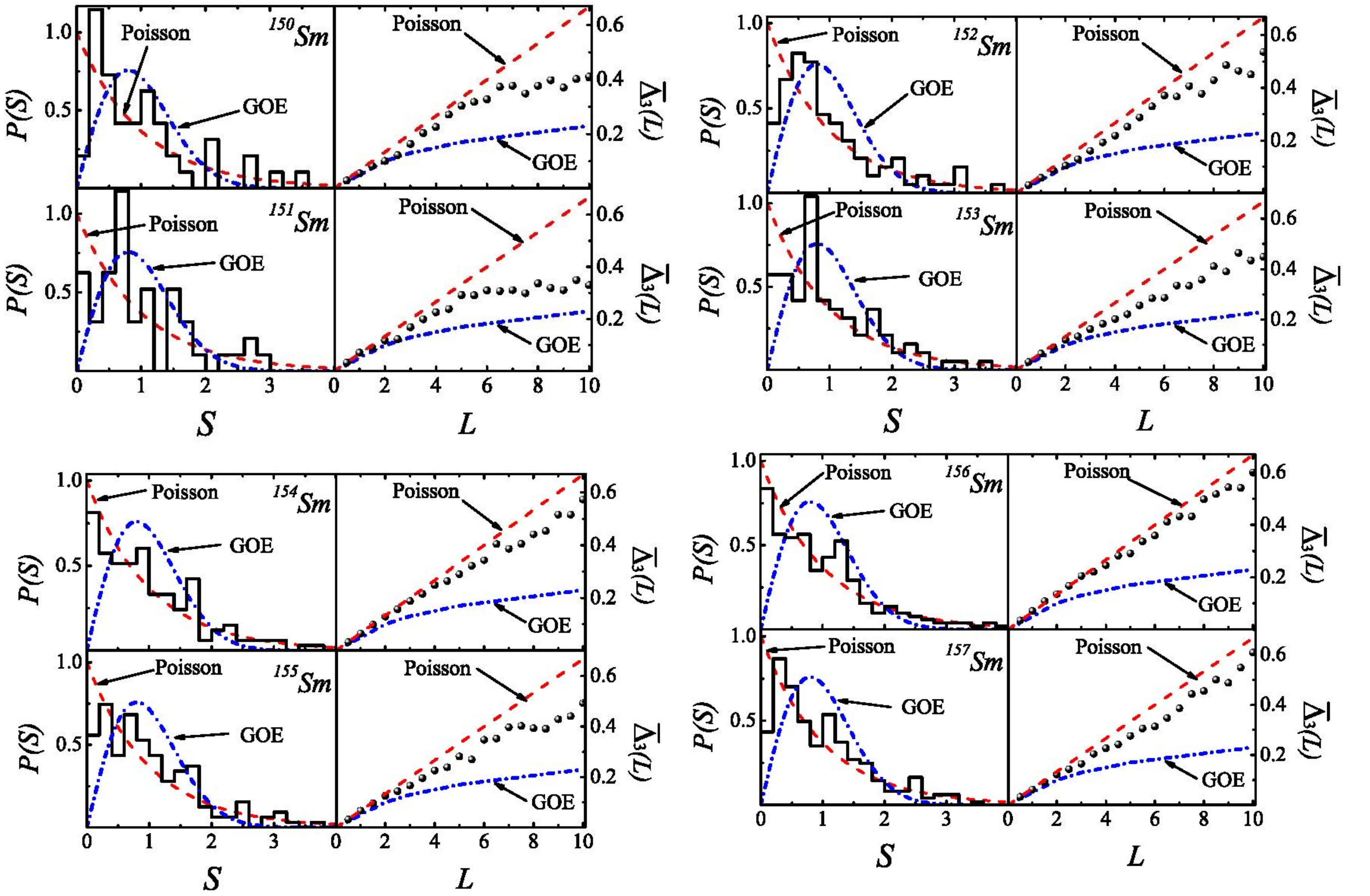
(Xin Guan, et al. *Nucl. Phys. A* (2019) 986)



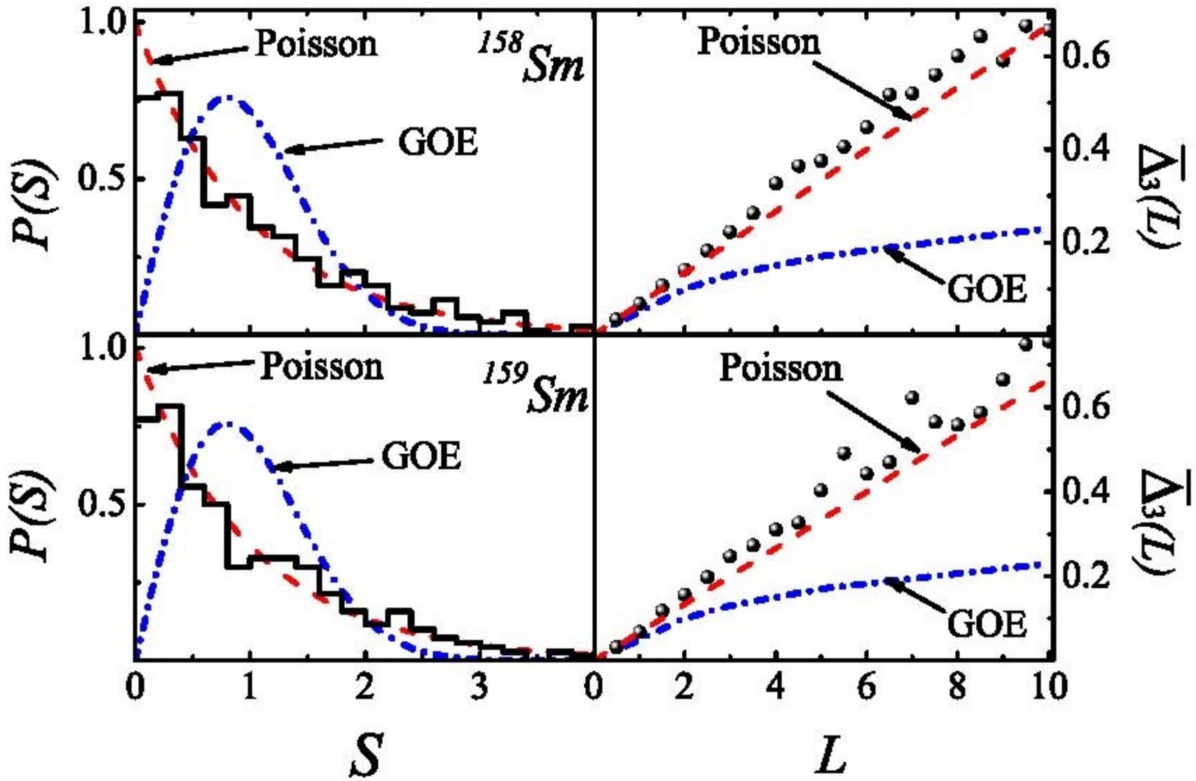
Applications and discussions



Applications and discussions



Applications and discussions



The statistical results of the J = 0 levels in Sm isotopic chains.

Yangon YueXin Guan, *EPJA* under review (2020).

The transitional region is the most sensitive region to perturbation, leading generically to the typical signature of quantum chaos .

Summary

- *For finite system, the exact pairing incorporates mesoscopic correlations absent in BCS and PBCS. Important in small grains, quantum dots, atomic nucleus, etc…*
- *The new Iterative approach to the exact pairing model could be appropriated for the whole nuclear chart .*
- *The critical behavior reflects the competition of different simultaneous interactions including the dominant pairing interaction.*
- *The exact pairing model could application for the nuclei in actinide regions through the analysis of the multi-dimensional potential energy surface, the fission path, the fission barrier ….*

The main collaborators:

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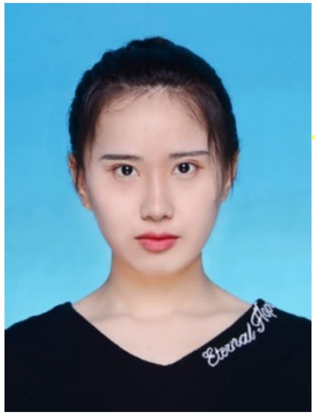
Graduate student

Xin Ai



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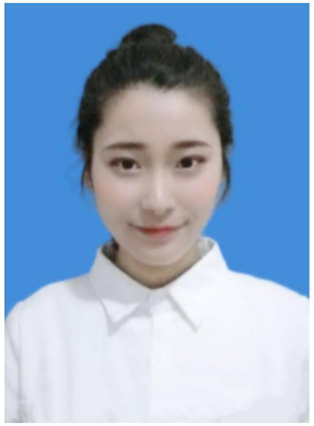

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