Tsukuba-CCS workshop on "microscopic theories of nuclear structure and dynamics"
December 10-12, 2018, Center for Computational Sciences, University of Tsukuba

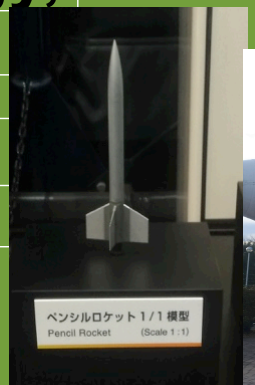
KTH ROYAL INSTITUTE OF TECHNOLOGY

Exact solution(s) of the pairing Hamiltonian

within numerical error

Chong Qi
KTH Royal Institute of Technology, Stockholm

- **Exact/Lanczos diagonalization**
- **Richardson approach: An iterative solver**
  CQ, T Chen Phys. Rev. C 92, 051304(R) (2015);
  X. Guan, X. Ai, CQ, to be submitted
  - ***Quasi-exact solutions can be derived***
  - ***Both methods can be generalized to T=1 pairing***



Does finite size effect matter?

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

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

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[2]*DPTA/Service de Physique nucléaire, F-91680 Bruyères-le-Châtel, France*
[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.

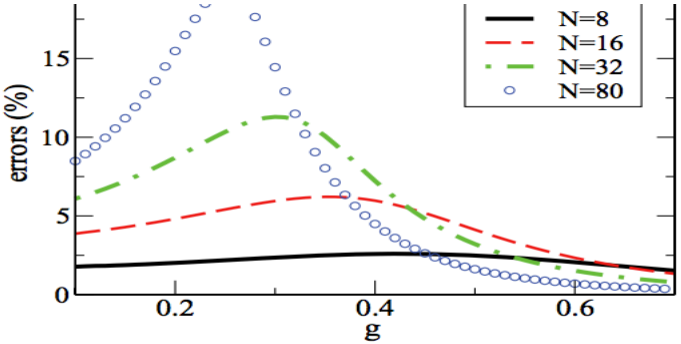


FIG. 3. (Color online) Errors for the correlation energies calculated in the PBCS approximation.

Half-filled degenerate systems

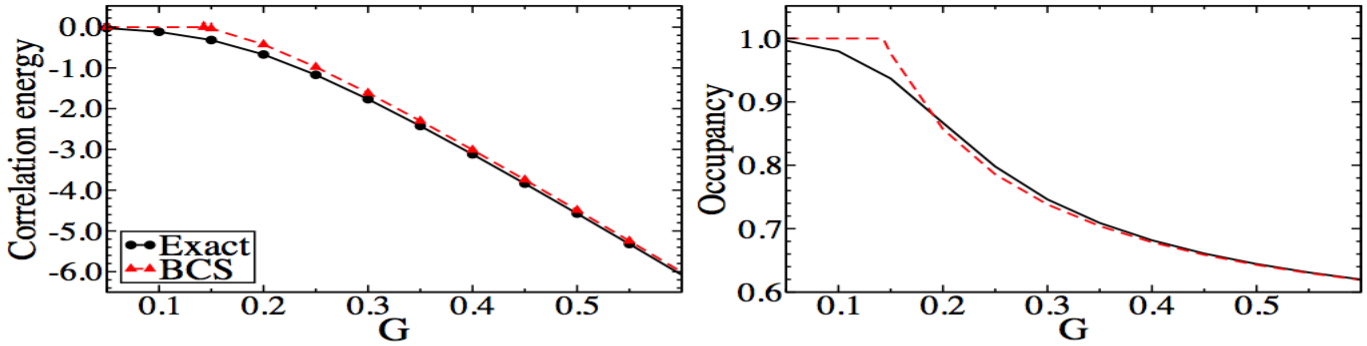
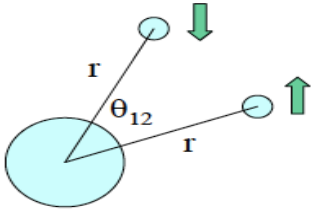


FIG. 1. Left: Comparison between the correlation energies from the BCS model and exact solution for a half-occupied system with $N = 4$ pairs and two $\Omega = 4$ orbitals separated by one unit. Right: The corresponding occupancy of the lower level from the two calculations.

Two-body clustering and alpha clustering

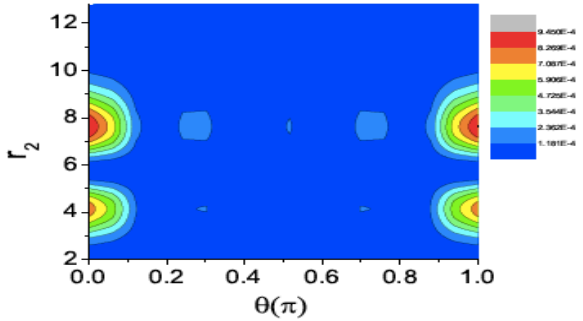


Configuration mixing from higher lying orbits is important for clustering at the surface

$$\Psi_2(\mathbf{r_1},\mathbf{r_2}) = (\chi_1\chi_2)_0\Phi_2(r_1,r_2,\theta_{12}) = (\chi_1\chi_2)_0\frac{1}{4\pi}\sum_p\sqrt{\frac{2j_p+1}{2}}X_p\phi_p(r_1)\phi_p(r_2)P_{l_p}(\cos\theta_{12}),$$

r_1=9fm

^{210}Pb



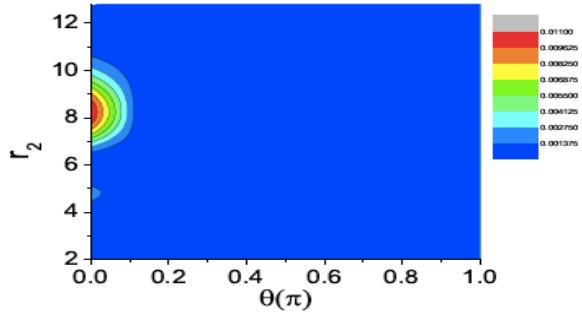
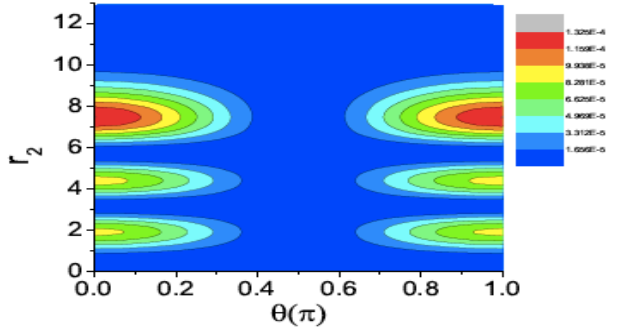
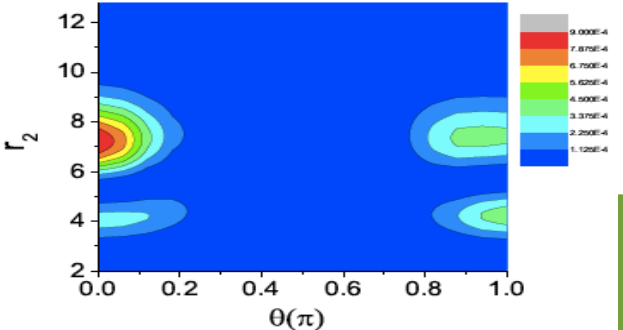


FIG. 10: (color online). The square of the two-neutron wave function $|\Psi_{2\nu}(r_1,r_2,\theta)|^2$ with $r_1 = 9$ fm as a function of r_2 and θ. Left: the leading configuration; Right: 4 major shells

^{206}Pb





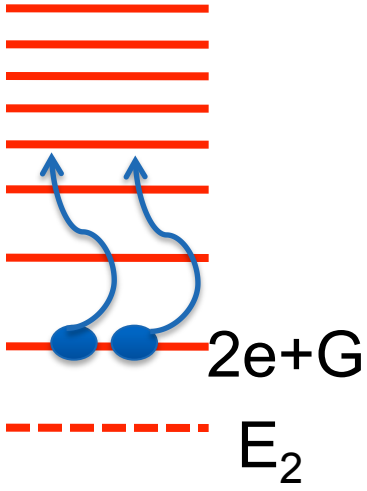
For two particles in a non-degenerate system with a constant pairing, the energy can be evaluated through the dispersion relation

$$G\sum_i \frac{2j_i+1}{2\varepsilon_i - E_2} = 2. \qquad (10)$$

The corresponding wave function amplitudes are given by

$$X_i = N_n \frac{2j+1}{2\varepsilon_i - E_2} \qquad (11)$$

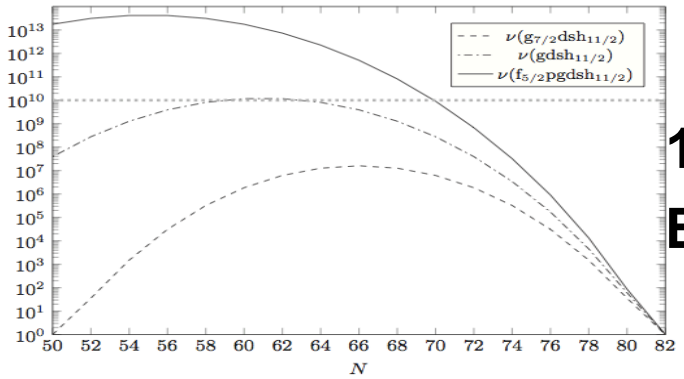
The correlation energy induced by the monopole pairing corresponds to the difference



$$\Delta = \varepsilon_\delta - \frac{1}{2}E_2$$

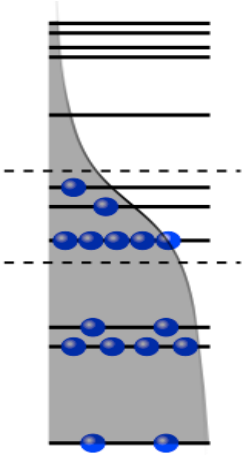
where δ denotes the lowest orbital. As the gap Δ increases the amplitude X_i becomes more dispersed, resulting in stronger two-particle correlation. This difference, or more

Exact diagonalization:
Seniority-zero coupling for many shells



10^2 in seniority space

Extension to more shells



Exact diagonalization

- Shell model calculations restricted to the v=0 subspace
- There are as many independent solutions as states in the v=0 space.
- **Valid for any forms of pairing.**
- **A bridge between DFT and CI**
- **Starting point for local CI calculations.**

$$|v'_{k+1}\rangle = H|v_k\rangle$$

Efficient ED algorithm

> Avoid zero matrix element; OpenMP (Xiaoyu Liu, KTH), OpenAcc (bachelor project KTH)

•>One can readily solve a half-filled system with upto 36-38 doubly-degenerate orbitals and 18-19 pairs (Dim: $9*10^9$-$3.5*10^{10}$, shell-model dimension: $4*10^{20}$-$7*10^{21}$).

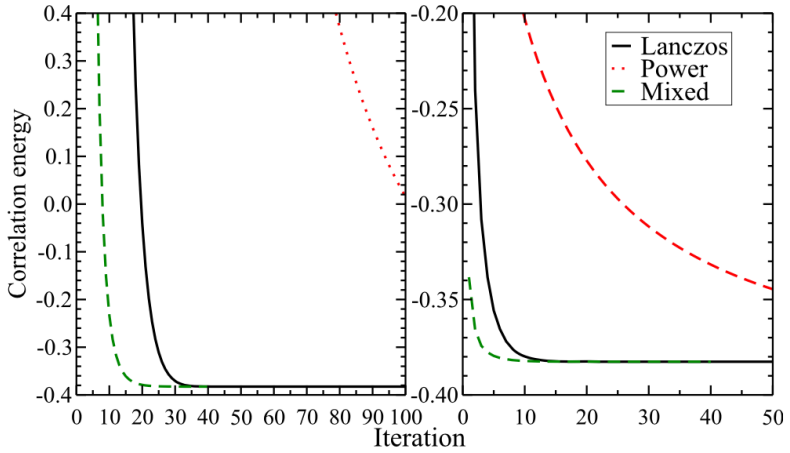


Figure 7. Correlation energies calculated by using the Lanczos approach, power iteration and the mixed approach as a function of iteration for a half-occupied system with $n = 10$ pairs and 20 doubly degenerate orbitals separated by one unit. For the pairing Hamiltonian we take the coupling constant as $G = 0.2$. The left and right panels correspond to calculations starting with a random vector and the Hartree–Fock vector, respectively. Four trial vectors are kept for the mixed calculation at each iteration.

C Qi, Journal of Physics G: Nuclear and Particle Physics 44 (4), 045107 (2017)


PDC's supercomputer Beskow

Richardson's approach

ume 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

Received 23 November 1962

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

$$H_P = \sum_k \varepsilon_k n_k + g \sum_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$|\Psi\rangle = \prod_{\alpha=1}^{M} \Gamma^\dagger_\alpha |0\rangle, \quad \Gamma^\dagger_\alpha = \sum_k \frac{1}{2\varepsilon_k - E_\alpha} c^+_{k\uparrow} c^+_{-k\downarrow}$$

Richardson equation

$$1 + g \sum_{k=0} \frac{1}{2\varepsilon_k - E_\alpha} + 2g \sum_{\beta(\neq\alpha)=1}^{M} \frac{1}{E_\alpha - E_\beta} = 0, \quad E = \sum_{\alpha=1}^{M} E_\alpha$$

Richardson equation

- A set of *M* nonlinear coupled equations with *M* unknowns (E_α) and it is very difficult to solve.
- The pair energies are either real or complex conjugated pairs (but do not have clear physical meaning)
- The wave function is not given directly but can be constructed

$$1 + g\sum_{k=0}\frac{1}{2\varepsilon_k - E_\alpha} + 2g\sum_{\beta(\neq\alpha)=1}^{M}\frac{1}{E_\alpha - E_\beta} = 0, \qquad E = \sum_{\alpha=1}^{M} E_\alpha$$

For two pairs in a single-j shell

$$E_\alpha = -(\Omega - 1)g \pm i\sqrt{\Omega - 1}g$$

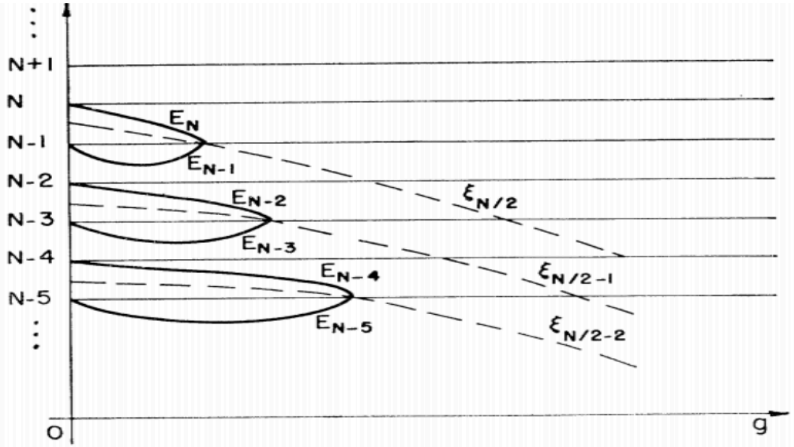


FIG. 1. Qualitative behavior of the pair energies in the ground state. The single-particle levels ϵ_n are labeled by the value of n on the left. The points where two pair energies come together are the singular points. The two corresponding pair energies are real or complex as the interaction strength is less than or greater than its value at this point.

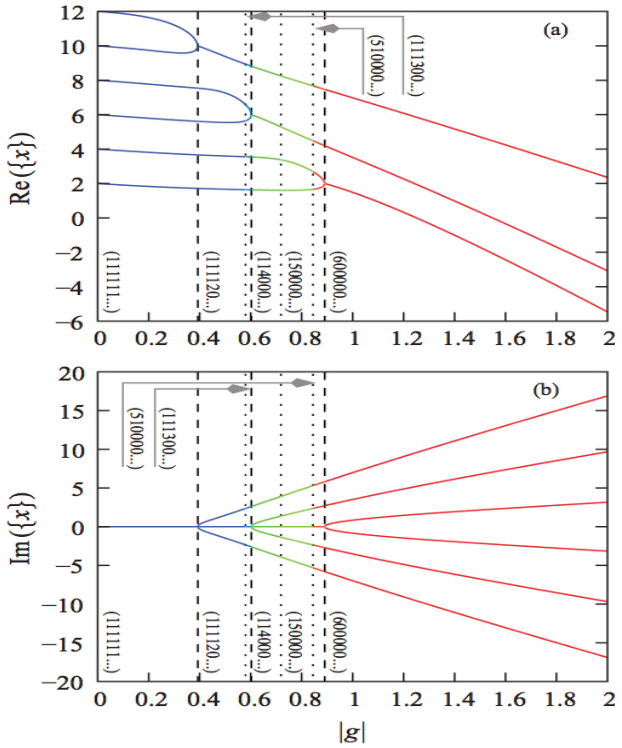


FIG. 1. (Color online) The real (a) and imaginary (b) parts of the RG variables of the "picket-fence" model, employed in Ref. [20], as a function of the interaction strength $|g|$. The critical interaction strengths are highlighted by means of dashed lines.

J. Dukelsky, S. Pittel, and G. Sierra
Rev. Mod. Phys. 76, 643 (2004)

S. De Baerdemacker, PRC 86, 044332 (2012)

PHYSICAL REVIEW B **83**, 235124 (2011)

Gaudin models solver based on the correspondence between Bethe ansatz and ordinary differential equations

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[1]*Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, D-80333 München, Germany*
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(Received 7 March 2011; revised manuscript received 28 April 2011; published 13 June 2011)

We present a numerical approach which allows the solving of Bethe equations whose solutions define the eigenstates of Gaudin models. By focusing on a different set of variables, the canceling divergences which occur for certain values of the coupling strength no longer appear explicitly. The problem is thus reduced to a set of quadratic algebraic equations. The required inverse transformation can then be realized using only linear operations and a standard polynomial root-finding algorithm. The method is applied to Richardson's fermionic pairing model, the central spin model, and the generalized Dicke model.

DOI: 10.1103/PhysRevB.83.235124 PACS number(s): 02.60.Cb, 02.30.Ik, 71.10.Li

$$\Lambda(z) \equiv \sum_{k=1}^{M} \frac{1}{z-\lambda_k} = \frac{P'(z)}{P(z)}, \qquad \frac{\partial \Lambda(z)}{\partial z} + \Lambda^2(z) = -\sum_{\alpha} \frac{1}{(z-\lambda_\alpha)^2} + \sum_{\alpha,\beta} \frac{1}{(z-\lambda_\alpha)(z-\lambda_\beta)}$$

$$= \sum_{\alpha \neq \beta} \frac{2}{(z-\lambda_\alpha)(\lambda_\alpha - \lambda_\beta)}, \qquad (9)$$

$$P(z) = \prod_{k=1}^{M} (z-\lambda_k)$$

- **Number of non-linear equations = number of shells**
- **Only works for doubly-degenerate systems**

Heine-Stieltjes correspondence

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

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

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

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

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

- **Number of non-linear equations = number of shells + number of pairs + 1**
- **works for both spherical and deformed systems**
- **Non-solution exists; Very time consuming and only applicable to small systems**

PHYSICAL REVIEW C **92**, 051304(R) (2015)

Exact solution of the pairing problem for spherical and deformed systems

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[2]*Department of Physics, Stockholm University, Stockholm, SE-106 91, Sweden*

(Received 30 September 2015; published 12 November 2015)

There has been increas
solution for certain pairi
equations involved. In th
The method is found to b
important and convenient
the method to study the sl

$$\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)^2 - \frac{1}{G}\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right) - \sum_{j\neq\delta}\frac{\left[\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right) - \left(\frac{P'(2\varepsilon_j)}{P(2\varepsilon_j)}\right)\right]}{2\varepsilon_\delta - 2\varepsilon_j} = 0.$$

ne can derive the exact
to solve the nonlinear
d polynomial approach.
nuclei. It also provides
s an example, we apply

- **Number of non-linear equations = number of pairs**
- **works for both deformed and nearly spherical systems; Extendable to spherical**
- **Very efficient! But limited by the stability of the NLE solver for very large systems**

Our (ultimate) iterative solver

$$P(x) = \prod_{i=1}^{k}(x - x_i) = \sum_{j}^{k} a_j x^j,$$

$$\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)^2 + (1-\Omega_\delta)\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)' - \frac{1}{G}\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right)$$

$$= \sum_{j\neq\delta} \frac{\Omega_j}{2\varepsilon_\delta - 2\varepsilon_j}\left[\left(\frac{P'(2\varepsilon_\delta)}{P(2\varepsilon_\delta)}\right) - \left(\frac{P'(2\varepsilon_j)}{P(2\varepsilon_j)}\right)\right]$$

- Number of non-linear equations = number of pairs
- works for both deformed and spherical systems (N of shells>= N of pairs)
- Super efficient and stable!; Initial guess, Monte Carlo + Newton- Raphson

Pair structure tractable

- Start with 1 pair in 1 orbital and small G, $x_1=2\varepsilon_1-G+r$, derive P_1
- Add the second pair $x_2=2\varepsilon_2-G+r$, derive $P_2-\langle P_1 * x_2$
- ..., N pair in N (doubly degenerate) shells
- Add remaining shells; Increase G to desired value

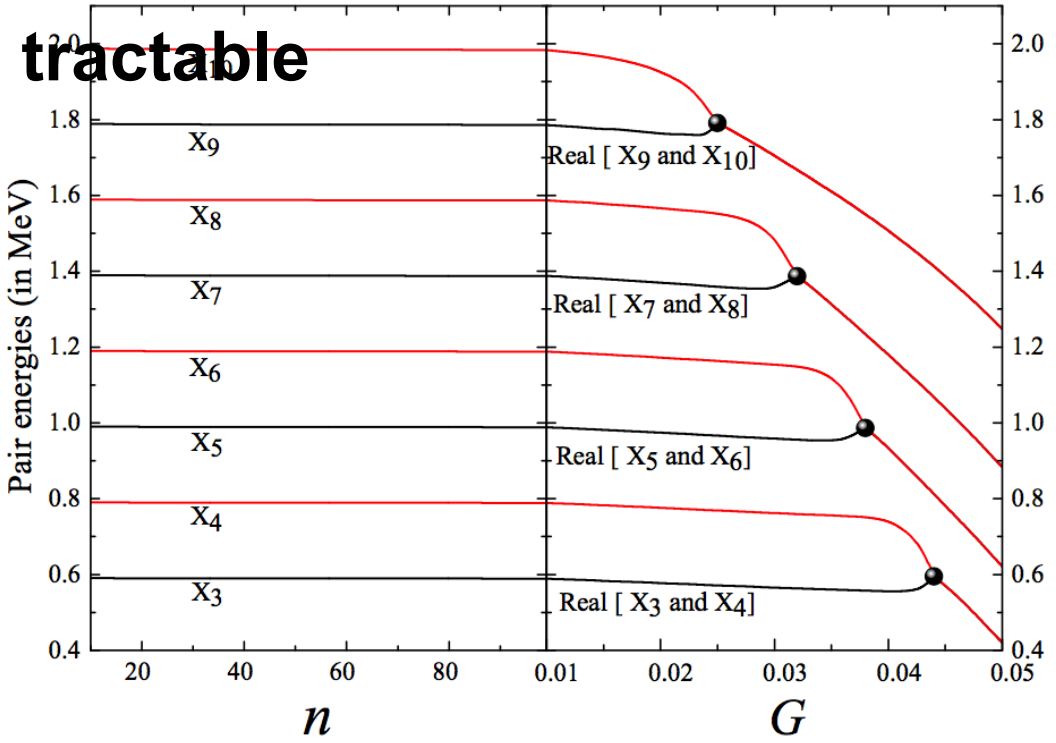


FIG. 5: (Color online) The real part of the two surface pair energies x_9 and x_{10} (in MeV), for a doubly-degenerate equally spaced model with the number of pairs $k = 10$, as a function of the orbital number n as well as the pairing interaction strength G.

Pair structure tractable

$$E^{(1)}_{\rm corr} = \sum_i^N x_i - (2\varepsilon_i - G),$$

those of the HF configuration at small G values. For two pairs in a single-j shell, x' are complex numbers

$$x'_{1,2} = (2 - \Omega_j)G \pm \sqrt{\Omega_j - 1}Gi. \quad (12)$$

For two pairs in two doubly-degenerate orbitals separated by one unit, one has

$$x'_{1,2} = \pm[1 - \sqrt{1 - G^2}], \quad (13)$$

which become complex with $G \geq 1$.

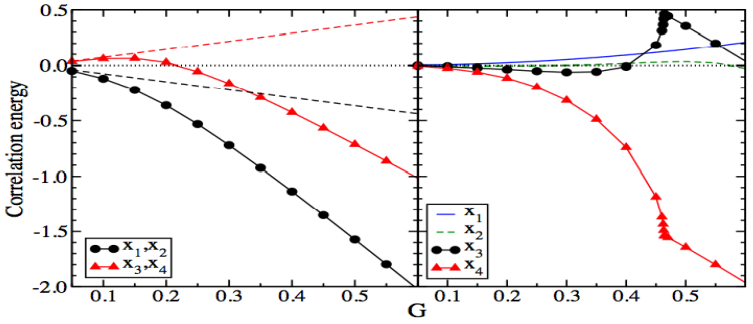


FIG. 2. Left: Correlation energies for each pair, $x'_i = x_i - 2\varepsilon_i + G$, as a function of the pairing strenghth, G, within the Richardson model for a half-occupied system with $N = 4$ pairs and two $\Omega = 4$ orbitals separated by one unit. The dashed lines correspond to the solutions when only one $\Omega = 4$ orbital is considered (i.e., fully occupied) where x' cancel each other. Right: Same as left panel but for a system with $N = 4$ pairs in eight equally-spaced doubly-degenerate orbitals separated by one unit.

Total energy ‘predictable’

$$
\begin{aligned}
E(n) &= \frac{n(n-1)}{4}G - \left[\frac{n}{2}\right](j+1)G, \qquad (9)\\
&= \left[\frac{n}{2}\right]\left(\left[\frac{n}{2}\right]-1\right)G + \delta_{v,1}\left[\frac{n}{2}\right]G + \left[\frac{n}{2}\right]E_2
\end{aligned}
$$

$$
\begin{aligned}
E(n) \simeq\ & \left[\frac{n}{2}\right]\left(\left[\frac{n}{2}\right]-1\right)\mathcal{G} + \delta_{v,1}(\varepsilon_b+\delta)\\
& + \left[\frac{n}{2}\right]E_2,
\end{aligned}
$$

S.A. Changizi, C. Qi, R. Wyss, Nucl. Phys. A (2015)

10 pairs in deformed system

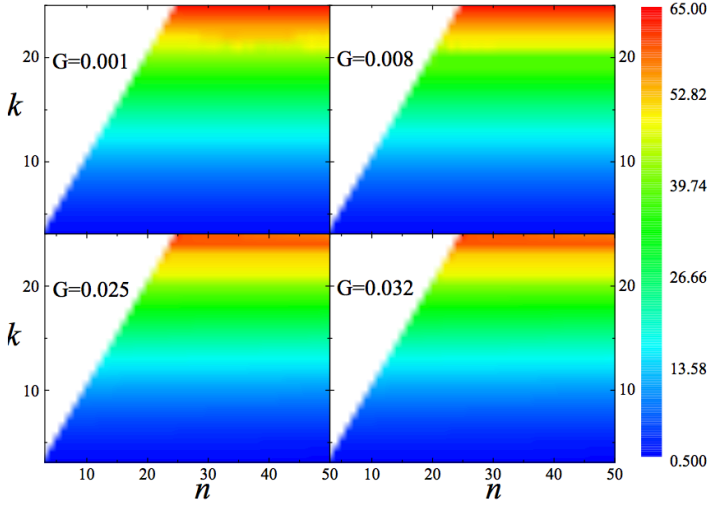


FIG. 1: (Color online) The ground-state energy (in MeV) as a function of the orbital number n as well as the number of pairs $k = 10$ for a doubly-degenerate system with $\Omega_i = 1$ ($j = 1/2$) and the pairing strength $G = 0.001$, 0.008, 0.025 and 0.032 MeV under the present model.

ε_i=i/10

10 pairs in spherical system

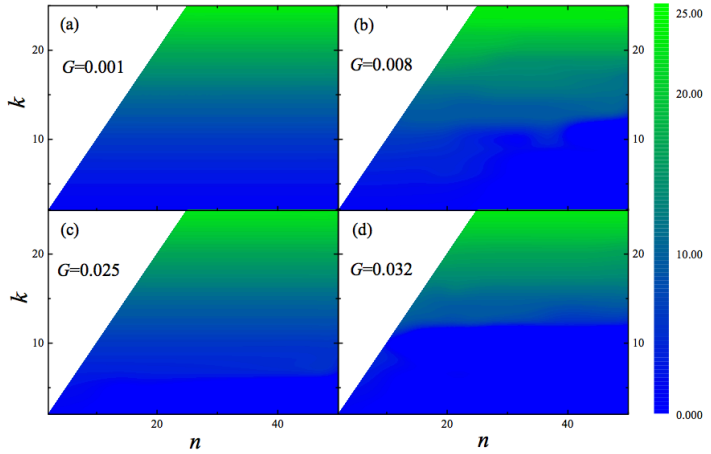


FIG. 2: (Color online) The ground-state energy (in MeV) as a function of the orbital number n as well as the number of pairs $k = 10$ for a high degenerate system with $\Omega_i = 1, \ldots, k$ ($j = 1/2, \ldots, k/2$) and the pairing strength $G = 0.001$, 0.008, 0.025 and 0.032 MeV under the present model.

ε_i=i/10

Total energy vs space and G

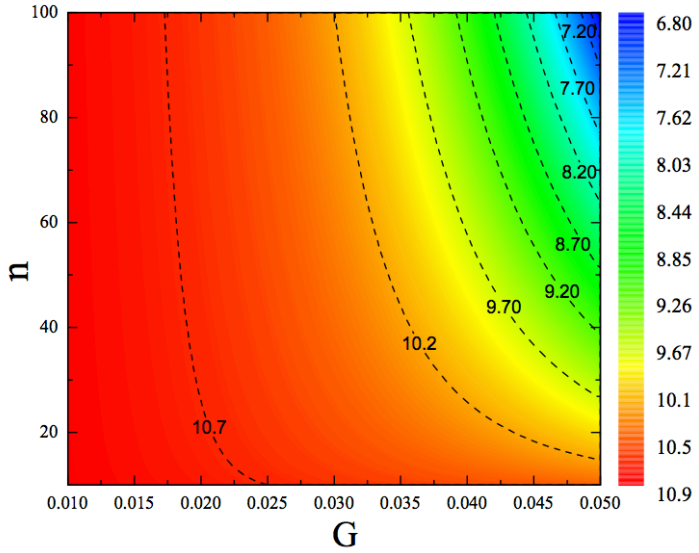


FIG. 3: (Color online) The ground-state energy (in MeV) for a doubly-degenerate equally spaced model with the number of pairs $k = 10$, as a function of the orbital number n as well as the pairing interaction strength G.

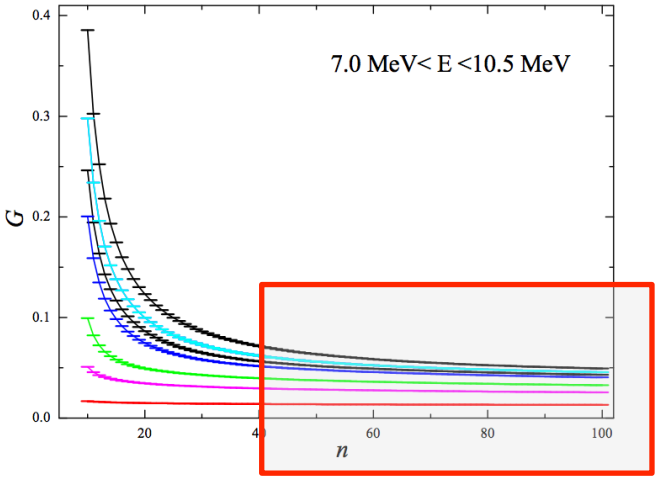
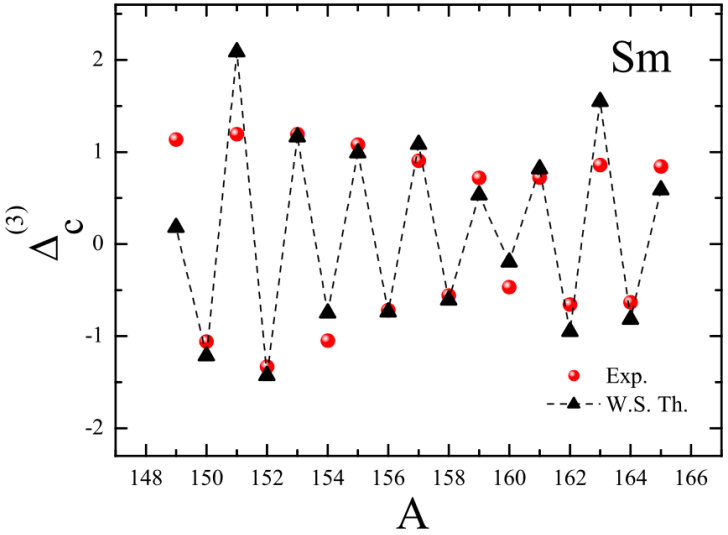


FIG. 4: (Color online) The iso-energy curve of the ground-state energy $7.0 < E < 10.5$ MeV for a doubly-degenerate equally spaced model with the number of pairs $k = 10$, as function of the orbital number n as well as the pairing interaction strength G.

Sm isotopes

Two valence shell from 82 to 184 G=0.06 MeV

The odd-even mass difference



Binding energies of Ca isotopes

WS + constant pairing

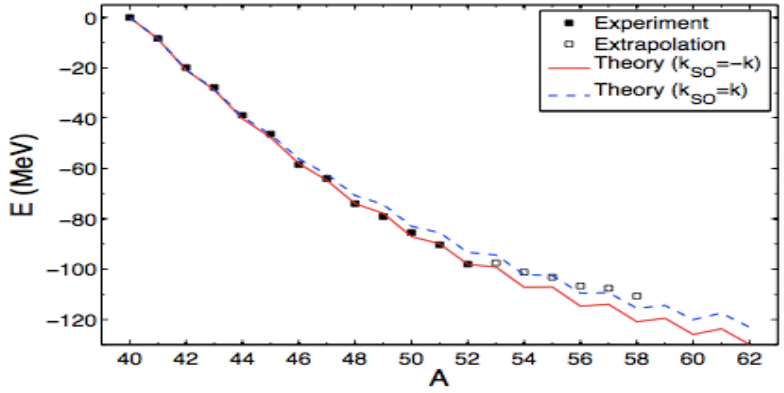
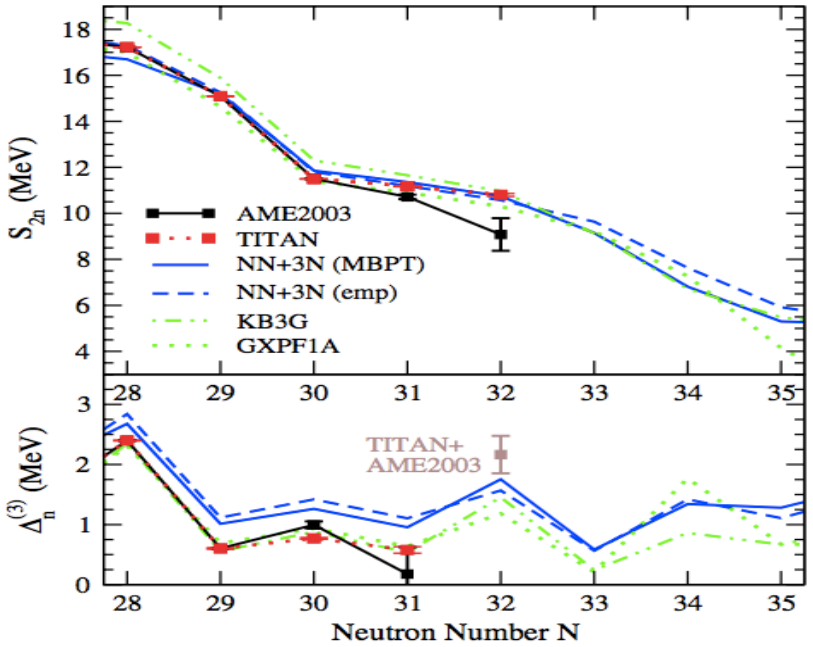


FIG. 6. (Color online) Experimental [34, 37] and calculated ground-state energies of Ca isotopes, relative to that of ^{40}Ca, as a function of mass number A.

Z.X. Xu and C. Qi, Phys. Lett. B 724, 247 (2013).



A. T. Gallant et al., PRL 109, 032506 (2012)

Calculations with three-body interaction

J.D. Holt, T. Otsuka, A. Schwenk, and T. Suzuki, J. Phys. G 39, 085111 (2012).

G. Hagen, M. Hjorth-Jensen, G.R. Jansen, R. Machleidt, T. Papenbrock, Phys.Rev.Lett. 109, 032502 (2012).

Summary and outlook

- Exact diagonalization vs Richardson approach
- Numerical challenges and polynomial approach for solving the Richardson equation
- Applications
- Future

*HF+Exact pairing for the whole nuclear chart (w/o self-consistence, done; w. self-consistence, code to be implemented, ev8/Sky3D)

*Applications in alpha decay, pair-transfer reaction *(and fission)*

*Benchmark MC/CC solutions of the pairing Hamiltonian

*Starting point for MC+CI calculations (with both pairing and full Hamiltonian)->MC(P)CI

Thank you!

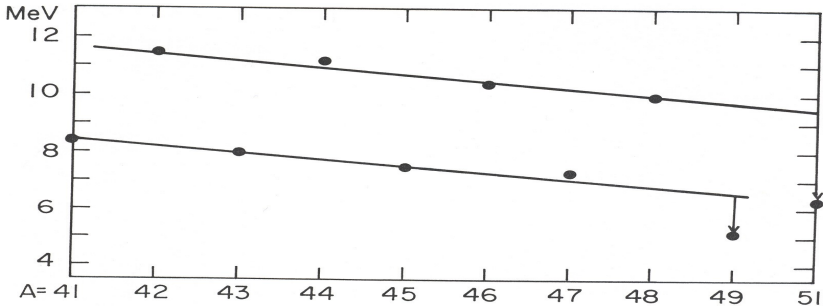
Seniority coupling and binding energy

Semi-magic nuclei

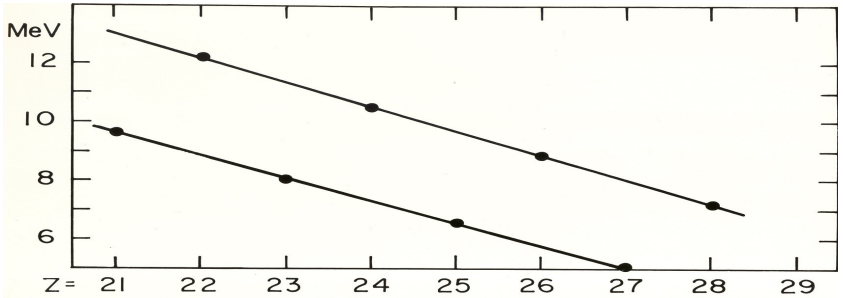
$$\hat{V} = a + b\mathbf{t}_1 \cdot \mathbf{t}_2 + GP_0,$$

Binding energies of ground states in j^n configuration

$$E\left(j^n\right) = Cn + \frac{1}{2}n(n-1)\alpha + \left[\frac{1}{2}n\right]\beta$$



Neutron separation energies from Ca isotopes



Proton separation energies from *N*=28 isotones

I. Talmi, Simple models of complex nuclei (Harwood, Chur, Switzerland, 1993)