Microscopic approach to shell model

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What should we consider as fully microscopic shell-model calculations?

- The starting point is a realistic potential V_{NN}
- An effective shell-model hamiltonian H_{eff} is then derived by way of the many-body theory of the effective hamiltonian
- The shell model calculation is performed using only quantities obtained from the shell-model hamiltonian, both single-particle energies and residual two-body interaction are derived from the theory

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Why to perform fully microscopic shell-model calculations?

- To understand if it is possible to perform a shell-model calculations without parameters
- To test the many-body theory that underlies the derivation of a theoretical shell-model hamiltonian
- Without phenomenological parameters, the predictive power is enhanced
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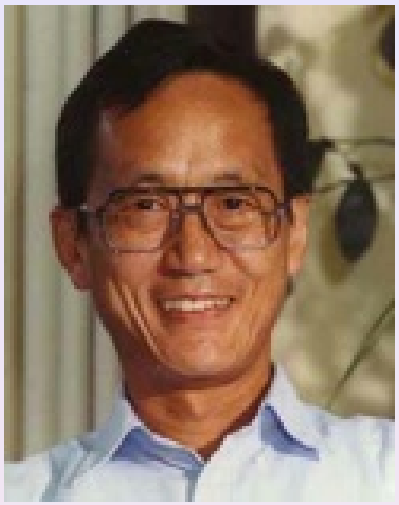

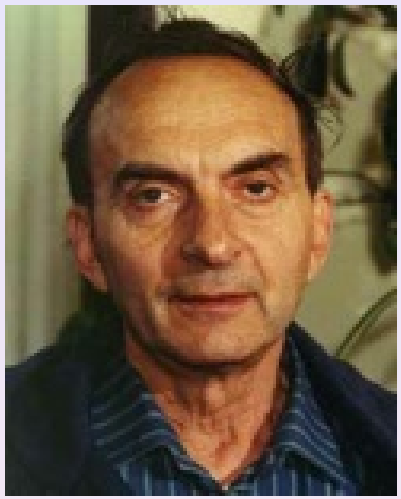

T. T. S. Kuo and G. E. Brown

T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85** *(1966) 40*

Phase 1: the realistic nucleon-nucleon potential

There are a plenty of V_{NN}s on the market: most of the modern ones reproduce quite well the physics of the two-nucleon system

- CD-Bonn
- Nijmegen I,II,93
- Argonne V18
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The trouble with realistic V_{NN}s is the strong short-range repulsion

This is a notable shortcoming since we will derive the shell-model effective hamiltonian from such potentials using the time-dependent degenerate linked-diagram perturbation theory

It is necessary to manage the short-range repulsion

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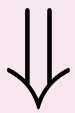


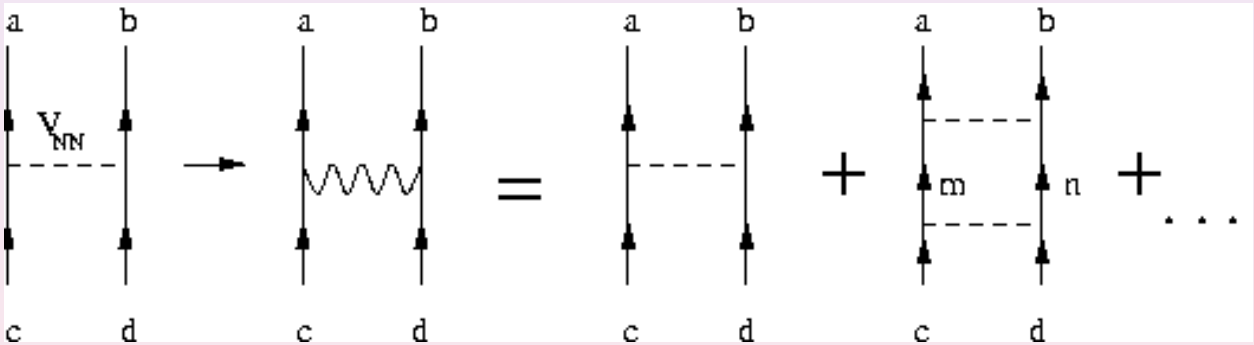
It is necessary to manage the short-range repulsion

Phase 1: the realistic nucleon-nucleon potential

As we said before, the short-range component of the free nucleon-nucleon potential V_{NN} has to be renormalized in order to fit with a perturbative scheme

The reaction matrix G

The standard way to renormalize the short-range repulsion is to resort to the theory of the Brueckner reaction matrix G



It can be written by way of an integral equation:

$$G(ab,cd) = V_{NN}(ab,cd) + \frac{1}{2}\sum_{\alpha\beta}\frac{V_{NN}(ab,\alpha\beta)G(\alpha\beta,cd)}{\epsilon_c+\epsilon_d-\epsilon_\alpha-\epsilon_\beta} \quad ,$$

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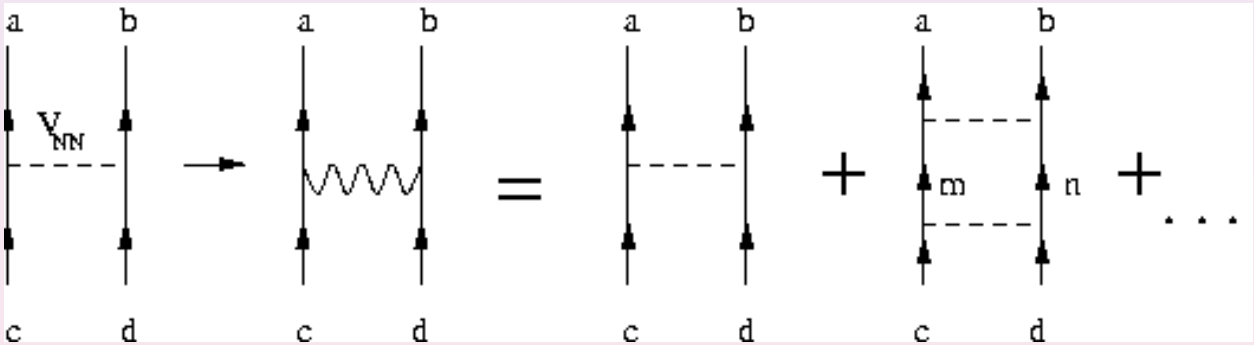

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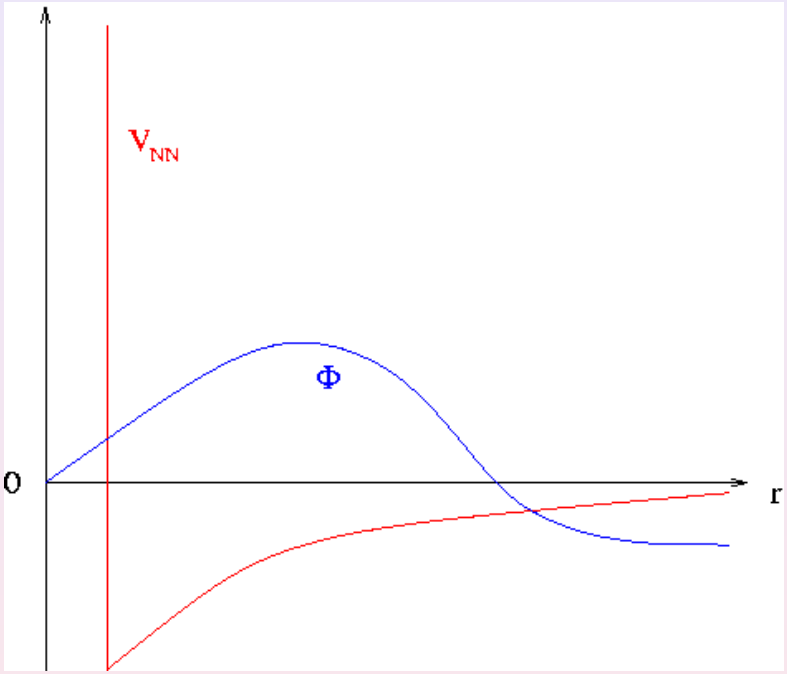

The action of G on the non-correlated wave function Φ_{ab}, which is eigenfunction of the unperturbed hamiltonian H_0, is equal to the action of V_{NN} on the correlated wave function Ψ_{ab} ($\Psi_{ab} \rightarrow 0$ when $r \rightarrow r_c$)

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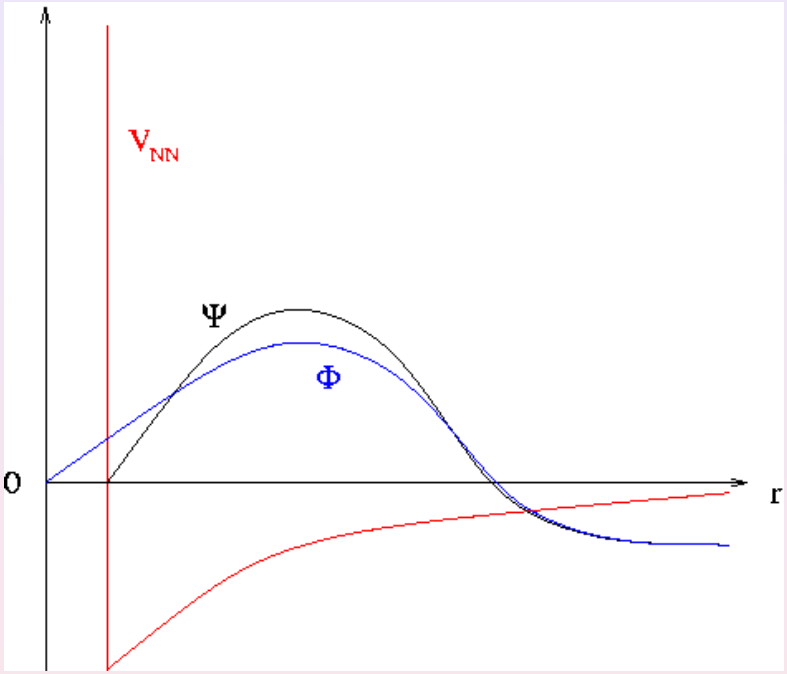

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Low-momentum nucleon-nucleon potentials: the $V_{\mathrm{low-k}}$

Inspiration to renormalize V_{NN}:

- Effective field theory (EFT)
- Renormalization group (RG)

from EFT: we restrict the configurations of $V_{NN}(k, k')$ to those with $k, k' < k_{\mathrm{cutoff}} = \Lambda$

S. Bogner, T. T. S. Kuo, L. Coraggio, A. Covello, and N. Itaco, Phys. Rev. C **65**, *051301(R) (2002)*

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The two-nucleon hamiltonian:

In the full momentum space

$$\int_0^\infty [H_0(k,k') + V_{NN}(k,k')]\langle k|\Psi_\nu\rangle k^2 dk = E_\nu \langle k'|\Psi_\nu\rangle$$

In a reduced model space $P = \int_0^\Lambda |k\rangle\langle k| k^2 dk$

$$\int_0^\Lambda [H_0(k,k') + V_{\mathrm{low-k}}(k,k')]\langle k|\Phi_\mu\rangle k^2 dk = \tilde{E}_\mu \langle k'|\Phi_\mu\rangle$$

Fundamental constraint: $\tilde{E}_\mu \in \{E_\nu\}$

How to construct $\langle k|H_{\mathrm{eff}}|k'\rangle$?

$\Downarrow$

Unitary transformation: Lee-Suzuki approach

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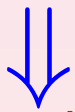

Unitary transformation: Lee-Suzuki approach

Phase 1: the realistic nucleon-nucleon potential

It is necessary to construct a new hamiltonian $\mathcal{H}$ by way of a similarity transformation

$$\mathcal{H} = \Omega^{-1} H \Omega$$

It is also necessary that the operator Ω satisfies the decoupling condition between the model space P and its coplementary space $Q = 1 - P$:

$$Q\mathcal{H}P = Q\Omega^{-1} H \Omega P = 0$$

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Lee and Suzuki suggested that, without loss of generality, the wave operator could have the following form

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Using this form for Ω, then $\mathcal{H}$ will satisfy the following identities in the P and Q subspaces

$$
\begin{aligned}
P\mathcal{H}P &= PHP + PHQ\omega \ , \\
P\mathcal{H}Q &= PHQ \ , \\
Q\mathcal{H}Q &= QHQ - \omega PHQ \ , \\
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Finally we rewrite decoupling equation for the operator ω

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0 \quad .$$

The latter is a non-linear matrix equation in ω that can be solved with iterative techniques, and whose solution allows to construct the wave operator Ω, and consequently any effective operator in the model space P

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A numerical test: deuteron binding energy with the CD-Bonn potential

Λ (in fm^{-1})	$PV_{\mathrm{eff}}P$ (in MeV)	V_{NN} (in MeV)
1.6	-2.225	-2.225
1.8	-2.225	
2.0	-2.225	
2.2	-2.225	

Phase 1: the realistic nucleon-nucleon potential

A numerical test: phase shifts in the $^1S_0$ channel (in degrees)

$E_{\rm lab}$ (MeV)	CD-Bonn	$V_{\rm low-k}$	Expt.
1	62.1	62.1	62.1
10	60.0	60.0	60.0
25	50.9	50.9	50.9
50	40.5	40.5	40.5
100	26.4	26.4	26.8
150	16.3	16.3	16.9
200	8.3	8.3	8.9
250	1.6	1.6	2.0
300	-4.3	-4.3	-4.5

G matrix *vs* V_{low-k}

G matrix

- Energy dependent
- Model space dependent - it depends on the Pauli operator Q_{2p}
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Phase 2: the shell-model effective hamiltonian

Schrödinger equation for A-nucleon system:

$$H|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle$$

Rewrite the above equation in terms of the wave operator Ω

$$\Omega^{-1}H\Omega\Omega^{-1}|\Psi_\nu\rangle = \mathcal{H}\Omega^{-1}|\Psi_\nu\rangle = E_\nu\Omega^{-1}|\Psi_\nu\rangle$$

We want Ω so that

$$\mathcal{H}|\Psi_i^P\rangle = E_i|\Psi_i^P\rangle$$

$|\Psi_i^P\rangle$ eigenfunctions of the model space P $\quad E_i \in \{E_\nu\}$

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Let us consider again the Lee-Suzuki approach to the derivation of the effective hamiltonian in terms of the operator ω

First of all we consider that our hamiltonian H can be written as a sum of an unperturbed term H_0 and an interaction one H_1

$$H = H_0 + H_1$$

A basic assumption we make is that H_0 is degenerate in the model space

$$PH_0P = \epsilon P$$

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Under the above conditions, and taking into account of the decoupling equation, we can write H_1^{eff} in terms of ω

$$H_1^{\text{eff}} = H^{\text{eff}} - PH_0P = P\mathcal{H}P - PH_0P = PH_1P + PH_1Q\omega$$

We now use the above equation to write ω as a function of H_1^{eff}:

$$\omega = Q\frac{1}{\epsilon - QHQ}QH_1P - Q\frac{1}{\epsilon - QHQ}\omega H_1^{\text{eff}}$$

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We insert last relation for ω into the identity that defines H_1^{eff}, in order to obtain a recursive equation

$$H_1^{\text{eff}}(\omega) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P -$$
$$-PH_1Q\frac{1}{\epsilon - QHQ}\omega H_1^{\text{eff}}(\omega)$$

The blue term in the above equation is the so-called $\hat{Q}$-box:

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The blue term in the above equation is the so-called $\hat{Q}$-box:

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P$$

Phase 2: the shell-model effective hamiltonian

The $\hat{Q}$-box is calculated by way of a perturbative expansion and can be expressed as a sum of Goldstone diagrams

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The diagrams belonging to the perturbative expansion have to satisfy the following requirements:

- they need to be "valence linked", i.e. the incoming and outcoming lines should belong to the model space P
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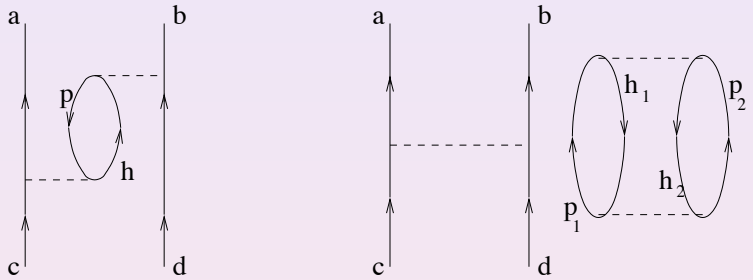
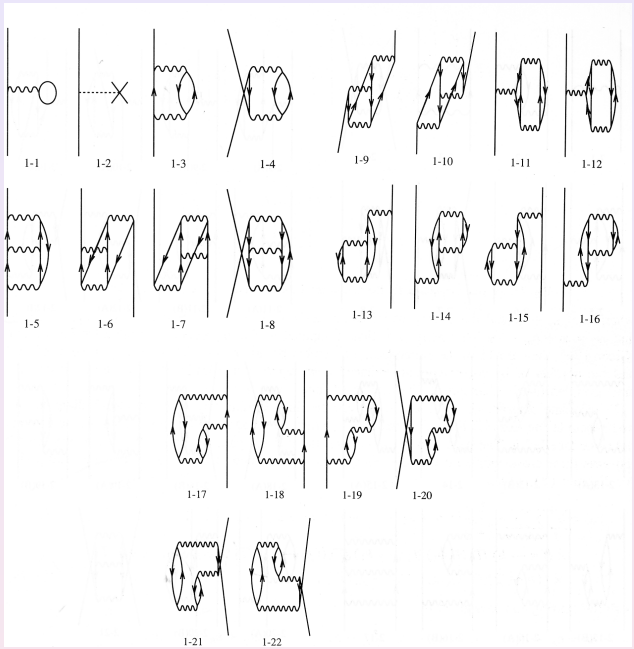
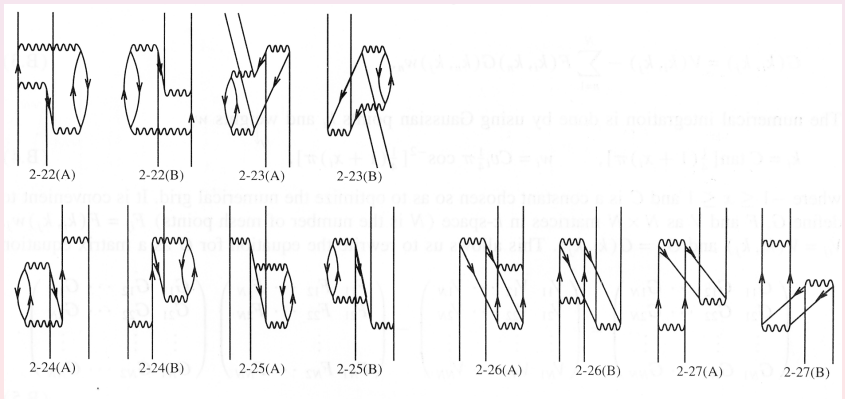


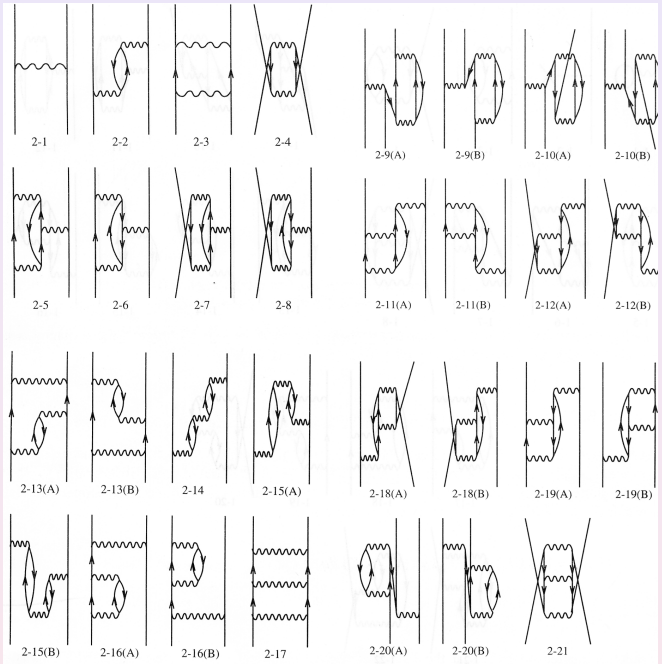
The states a, b, c, d belong to the model space P

The configurations $p\ h$, $p_1\ h_1\ p_2\ h_2$ belong to the space Q

Phase 2: the shell-model effective hamiltonian







M. Hjorth-Jensen, E. Osnes, and T. T. S. Kuo, Phys. Rep. **261** *(1995) 125*

Phase 2: the shell-model effective hamiltonian

Since our single-particle energies are calculated theoretically, we need to include a certain class of diagrams that are usually neglected: the so-called self-consistency corrections

The sum at all orders of this class of diagrams makes results independent from the choice of the unperturbed hamiltonian $H_0 = T + U = \sum_i (p_i^2/2M + M\omega^2 r_i^2/2)$ and is equivalent to employ a Hartree-Fock basis

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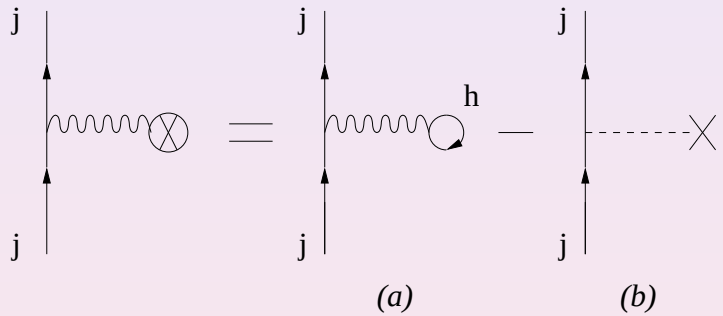

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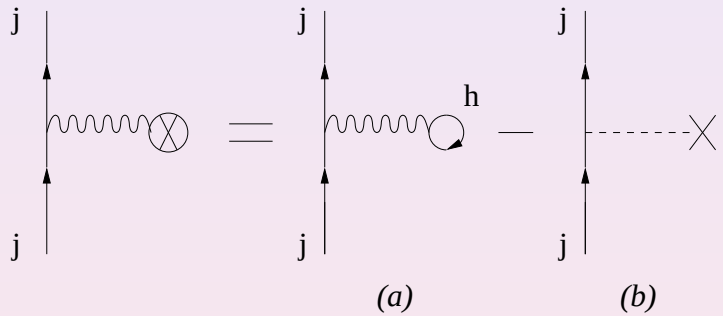

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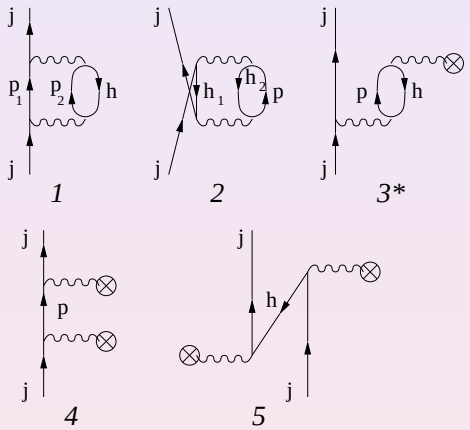

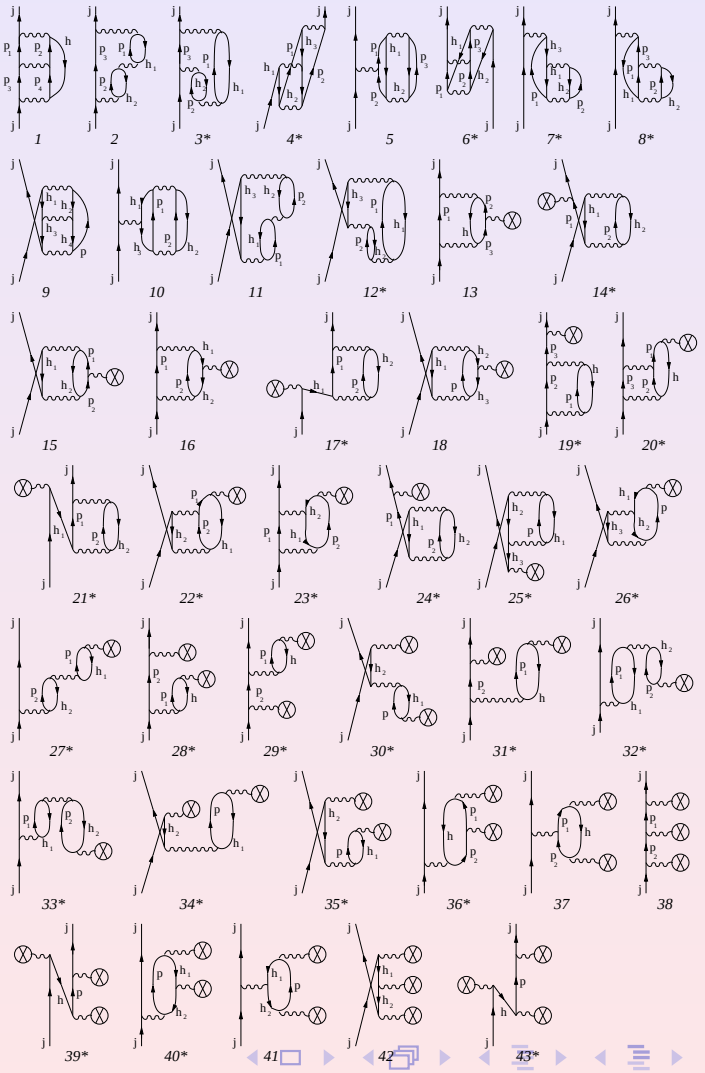

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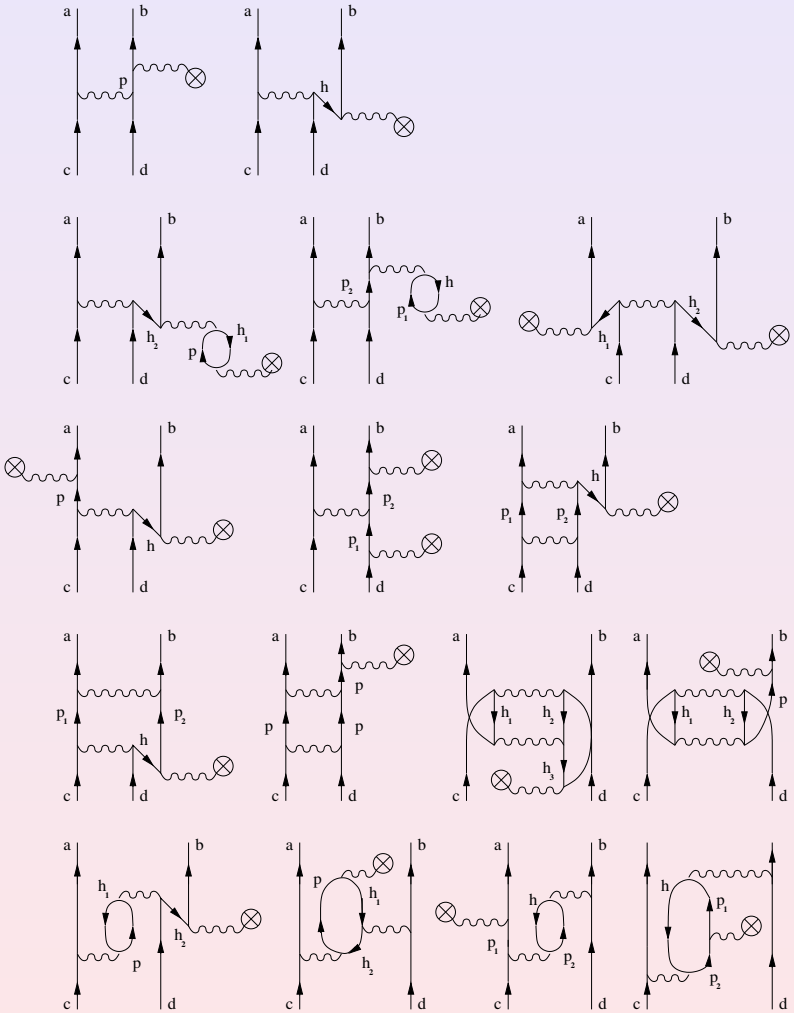

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$\hat{Q}$-box diagrams and all effective operators (electric quadrupole transitions, magnitic dipole transitions, ...) up to third order in perturbation theory.

We calculate the Padè approximant [2|1] of the $\hat{Q}$-box, in order to obtain a better estimate of the value to which the perturbation series should converge

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We have chosen to test our calculations with those of NCSM for ^{6}Li with N^{3}LO potential: its structure should be made up by the ^{4}He core plus one valence proton and one valence neutron

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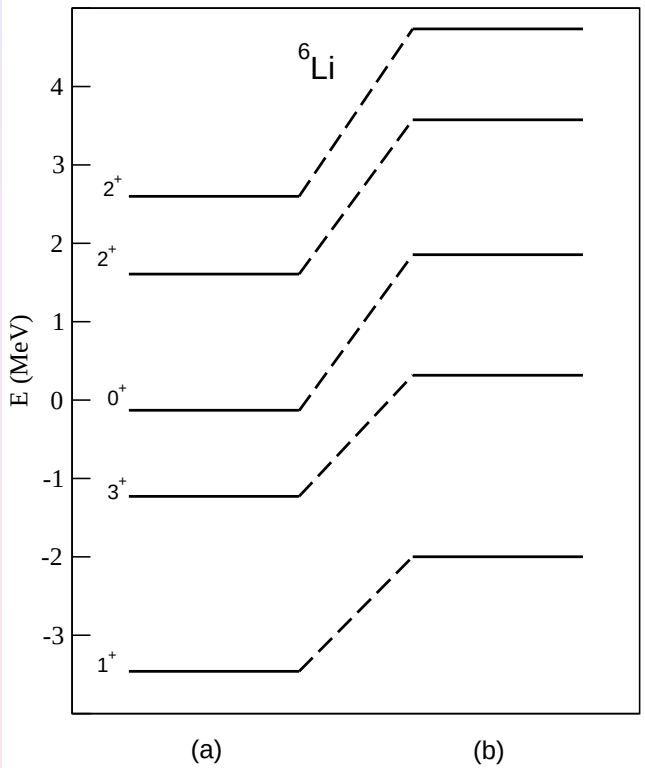
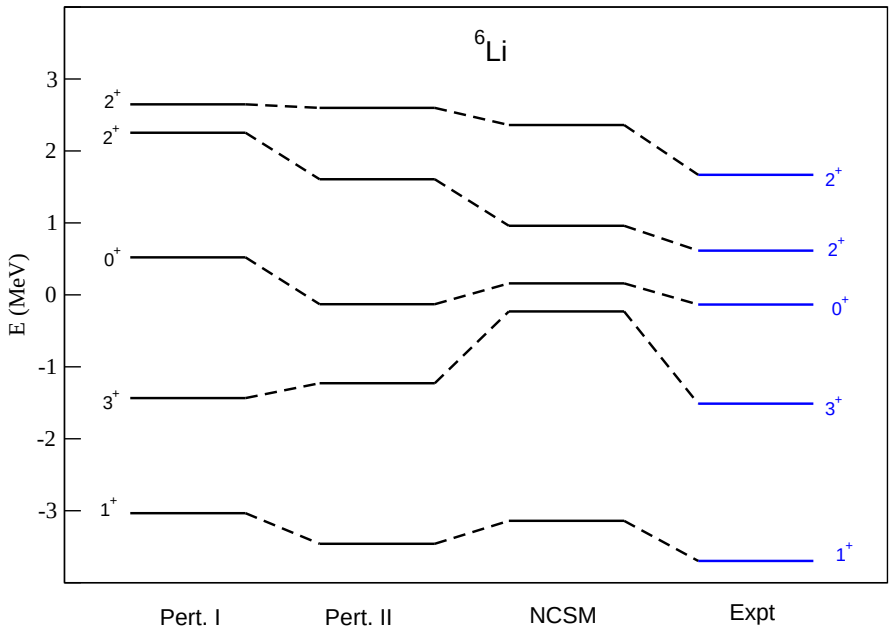


(a) intrinsic many-body hamiltonian
(b) non-intrinsic many-body hamiltonian

Calculation of ^{6}Li energy spectrum with N^{3}LO



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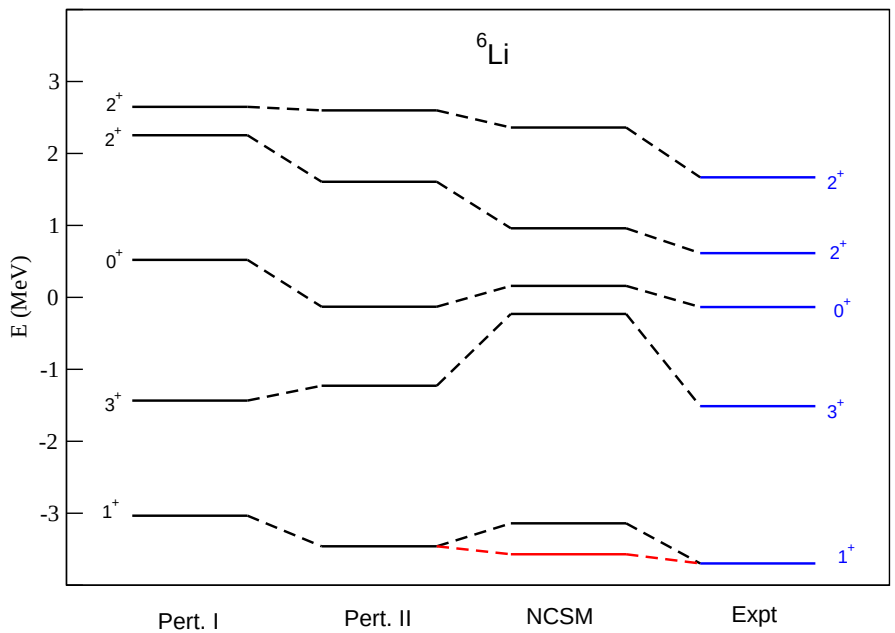

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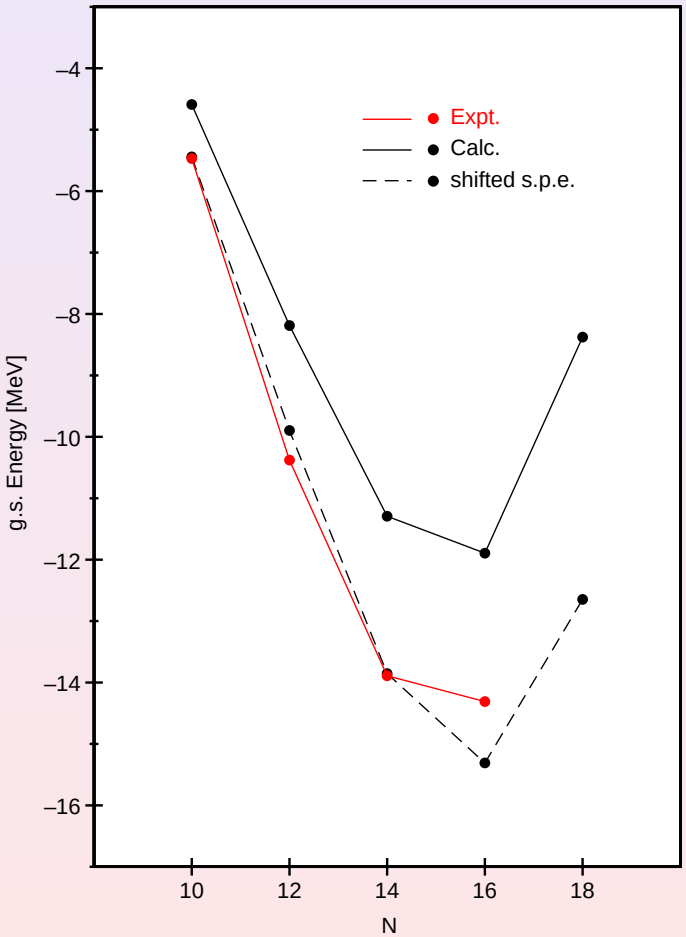
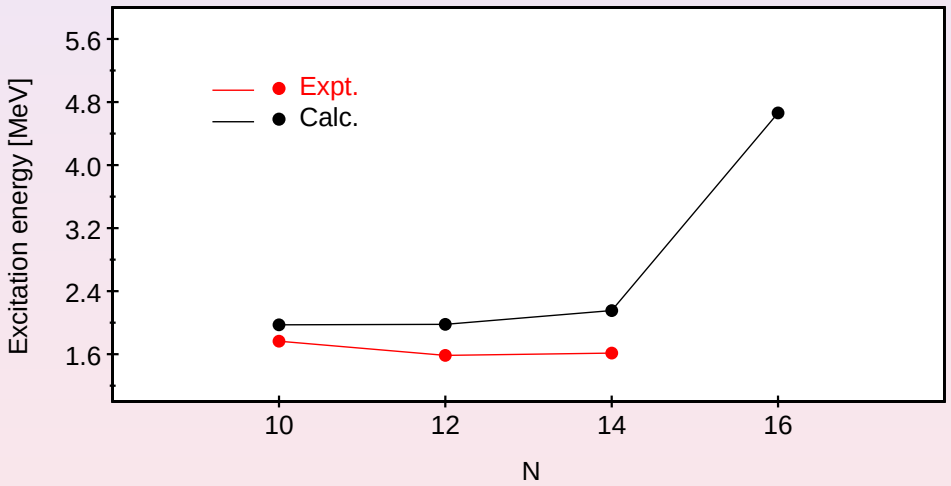
Results: the carbon isotopic chain

g.s. energies of even-mass isotopes



Excitation energies of 2^+ yrast states



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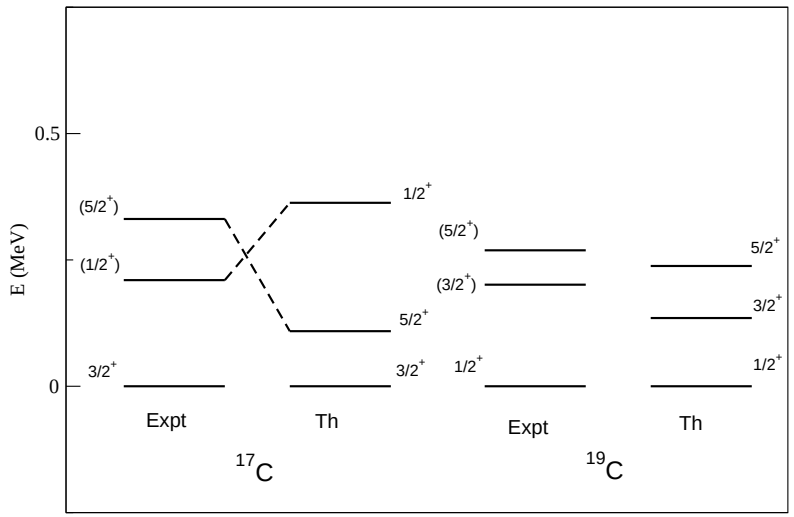

$B(E2; 2_1^+ \rightarrow 0_1^+)$ transiton rates

Nucleus	Calc.	Expt.
^{16}C	1.8	$2.6 \pm 0.2 \pm 0.7$ [a] 4.15 ± 0.73 [b]
^{18}C	3.0	$4.3 \pm 0.2 \pm 1.0$
^{20}C	3.7	< 3.7

Results: the *sd*-shell region

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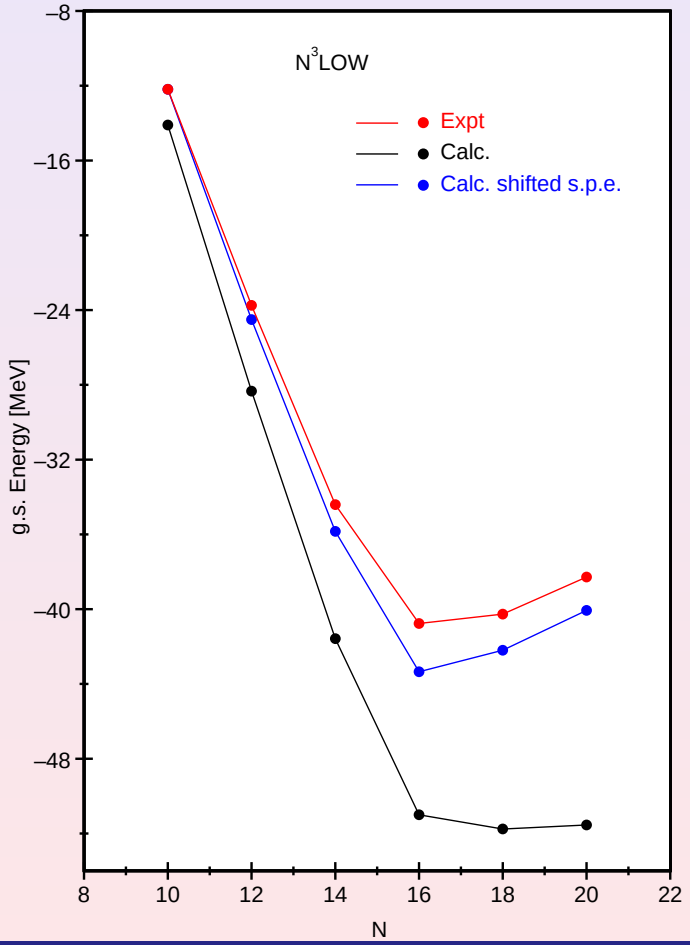

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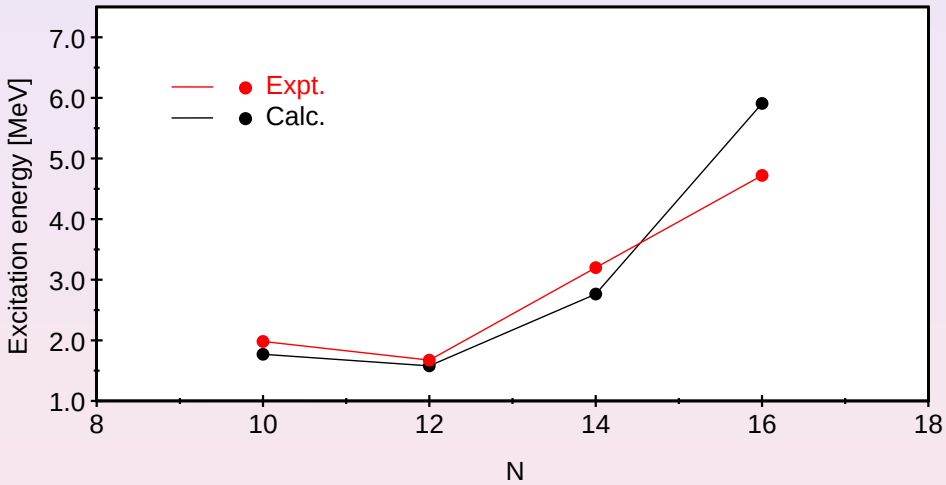
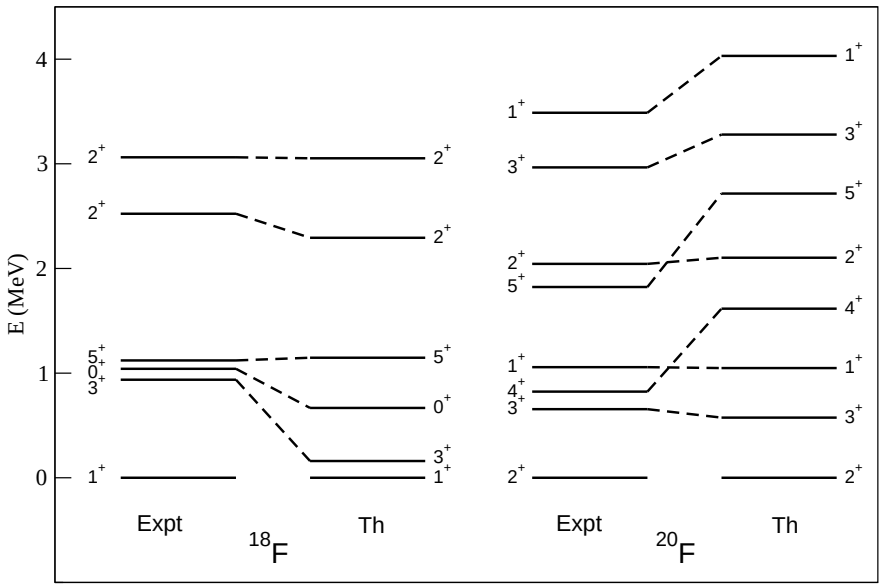
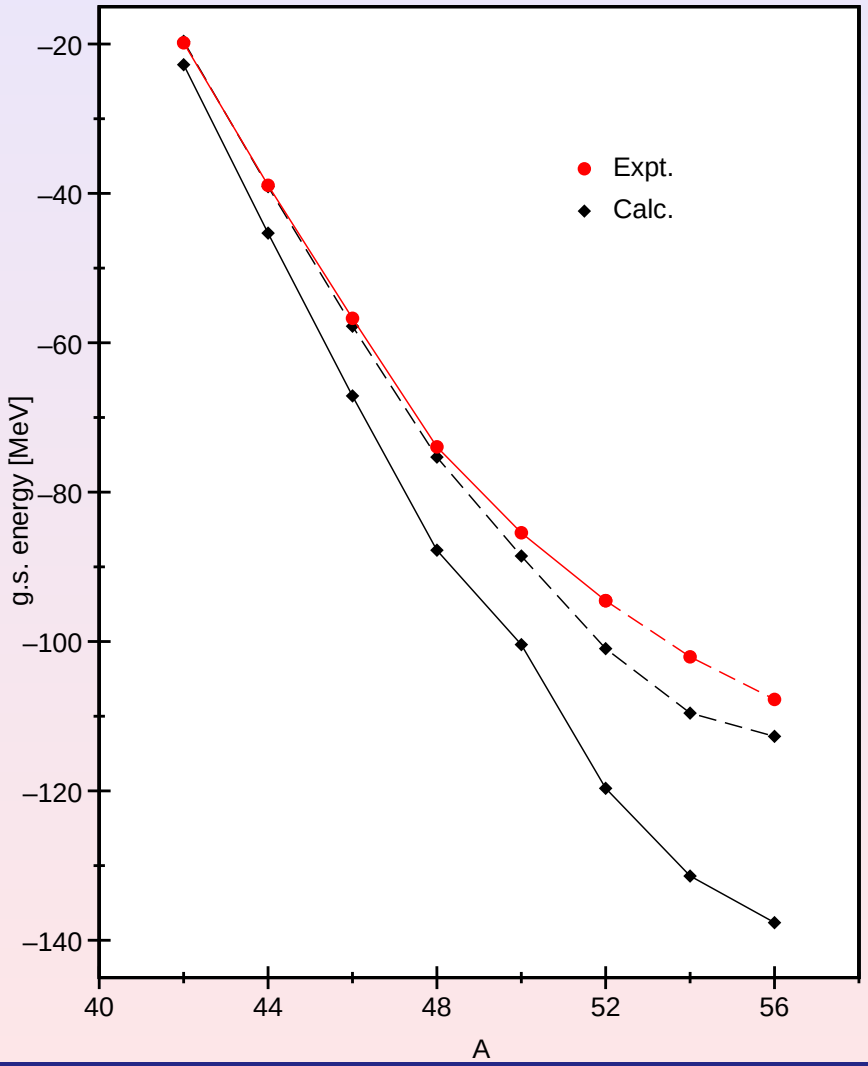


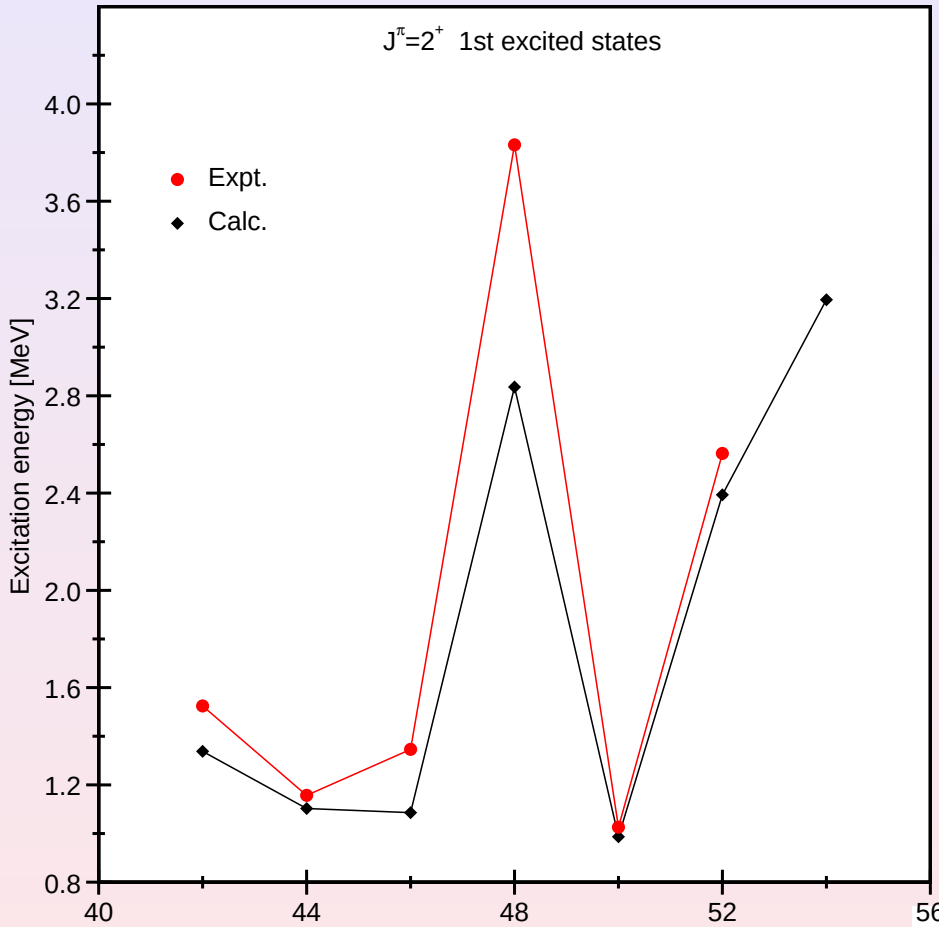
Results: the *sd*-shell region

Energy spectra of even-mass fluorine isotopes



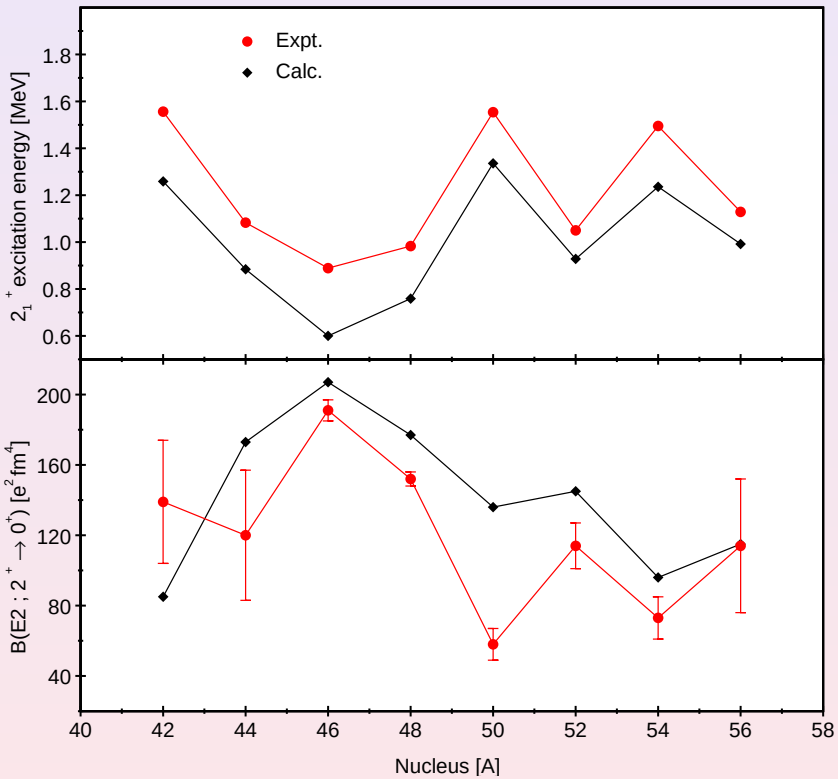
Results: the calcium isotopes





Results: the titanium isotopes

Excitation energies of 2^+ yrast states and their $B(E2; 2^+ \rightarrow 0^+)$



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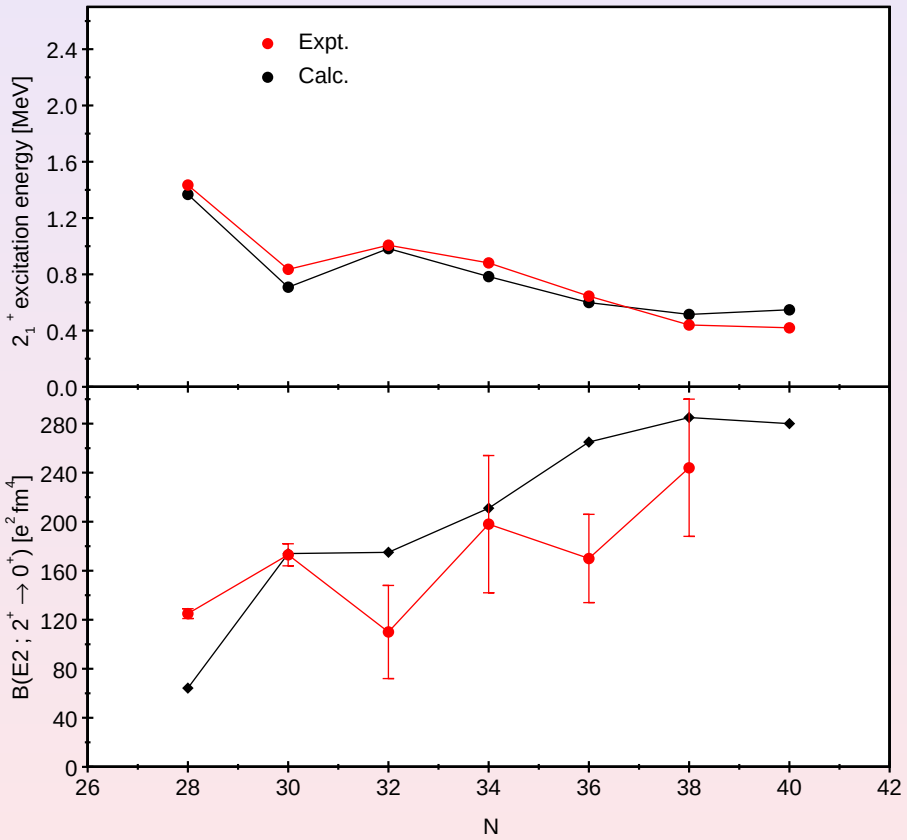
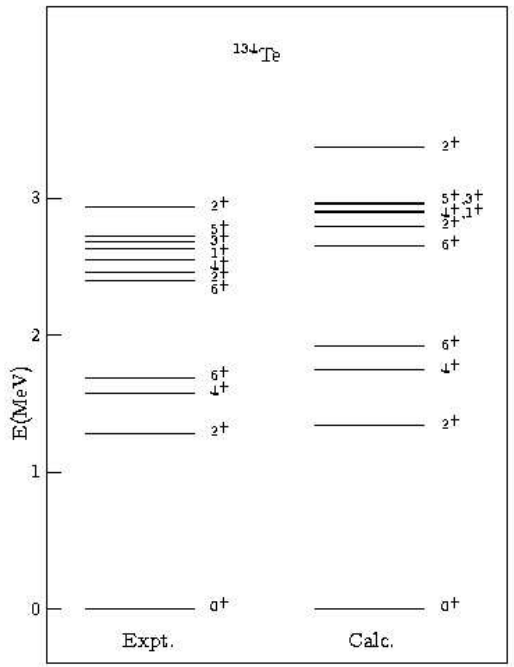
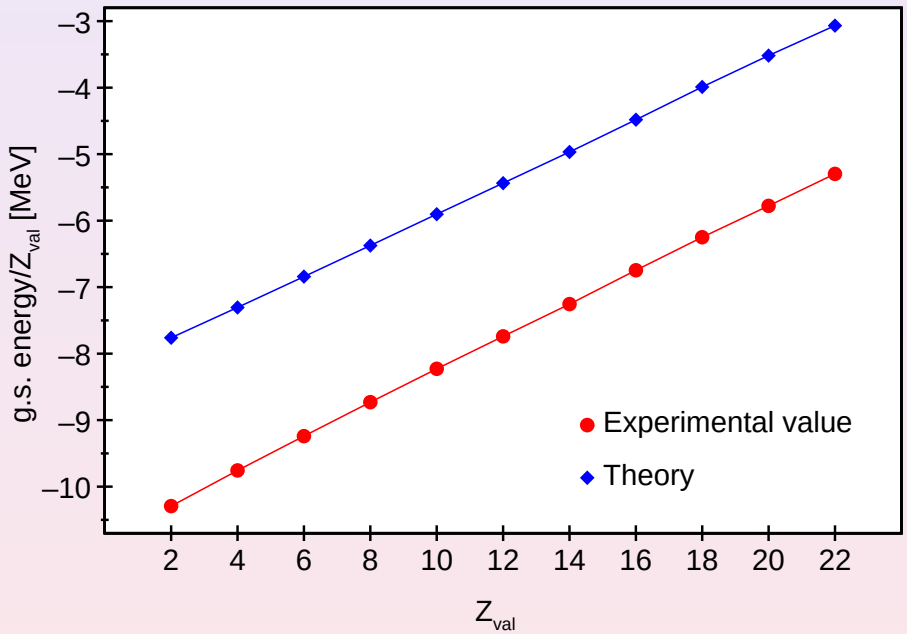


Results: the $N = 82$ isotones





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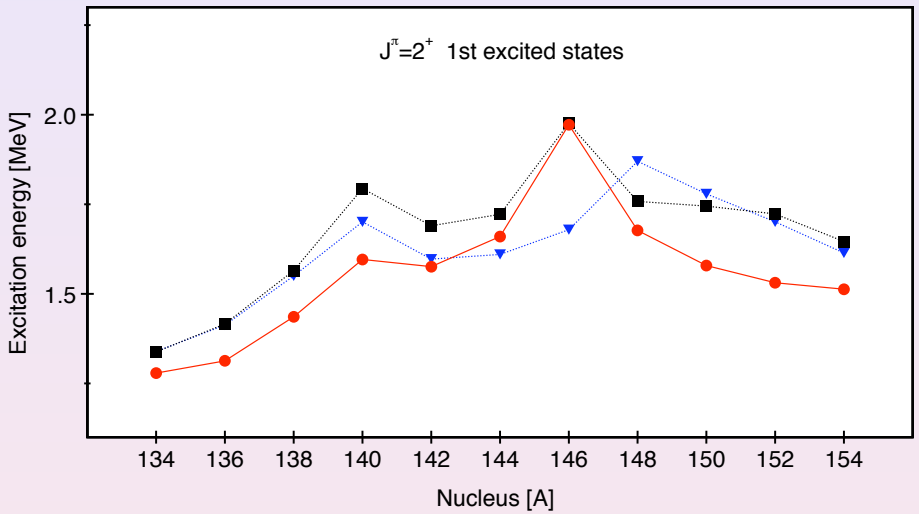

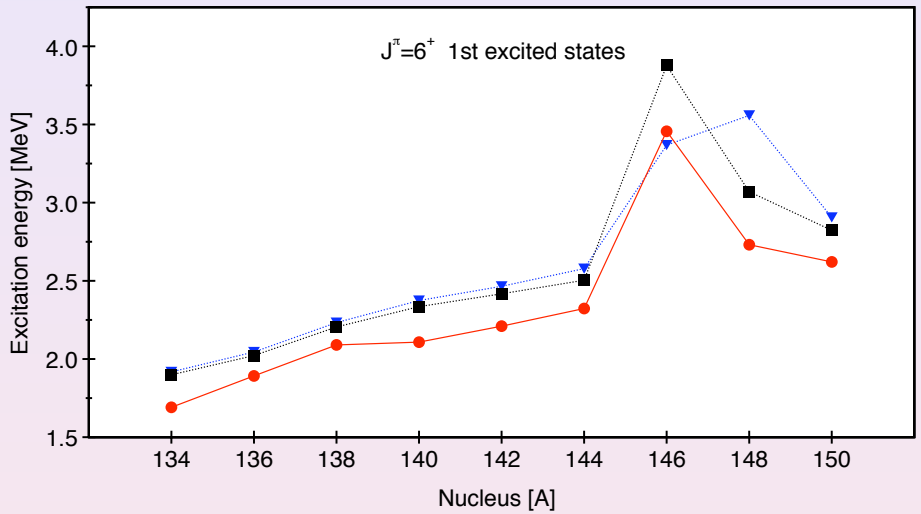

- Blue triangles: microscopic shell-model calculations
- Black squares: fitted $2s_{1/2}$ single-particle energy
- Red dots: experimental data

Concluding remarks

- The agreement of our results with the experimental data testifies the reliability of a fully microscopic shell-model calculation
- Pure three-body forces seem to contribute mainly to the ground-state energy relative to the closed core of single-particle spectra
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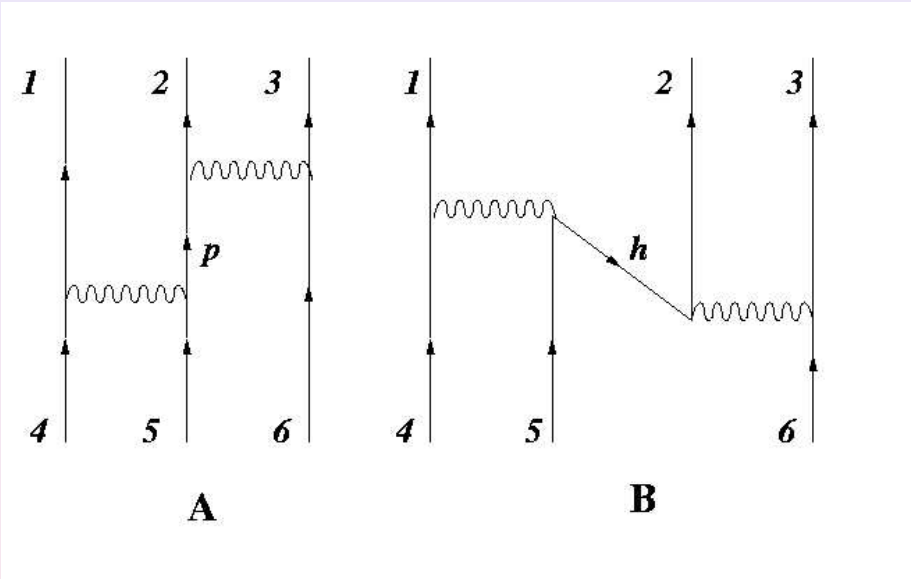

These terms introduce density dependence into the effective shell-model hamiltonian

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- Perspectives: benchmark calculations with other many-body approaches (*p*-shell nuclei)