New Quantum Monte Carlo Approaches for the Structure of the Atomic Nucleus

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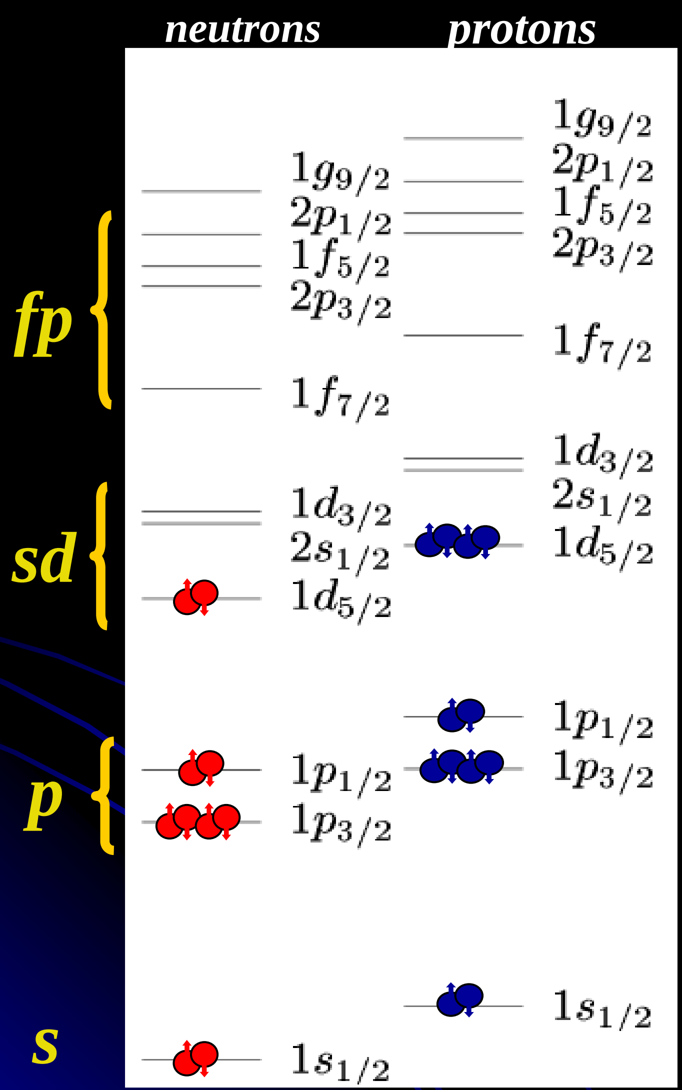
Laboratoire de Physique Corpusculaire de Caen

supervised by

Olivier Juillet

The Nuclear Shell Model

Mean field approximation



ex **: ^{22}Mg**

Goeppert-Mayer & Jensen (1948)

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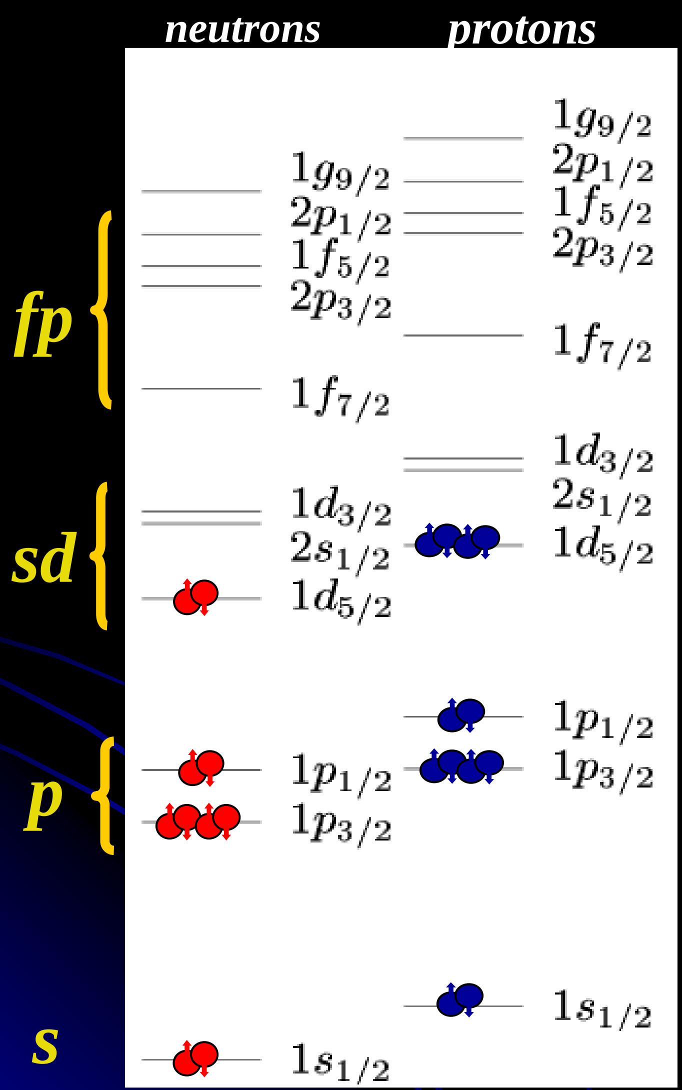

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↓

Diagonalization in the configuration space

↓

Spectroscopy, Transition probabilities…

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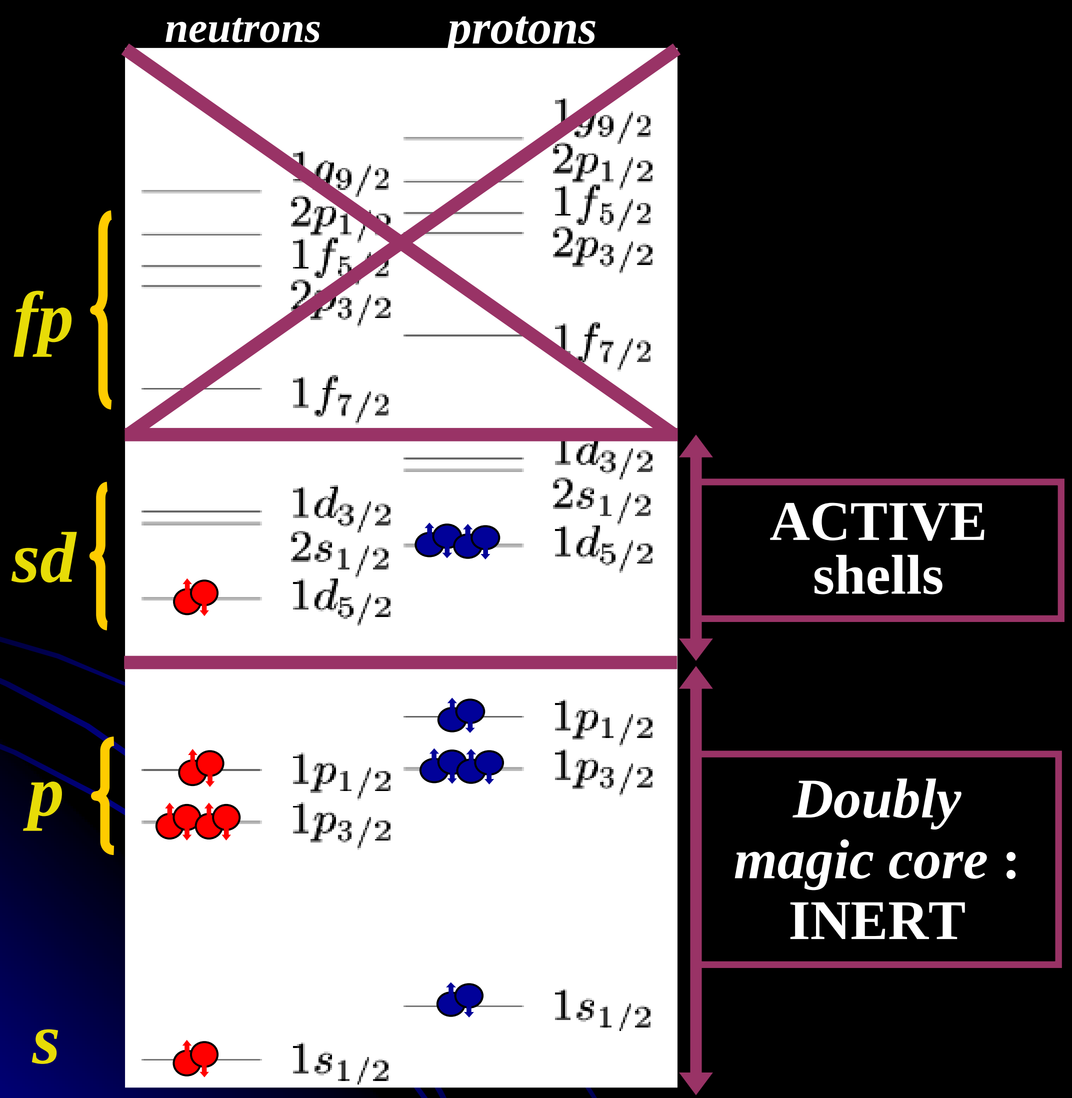

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effective

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Spectroscopy, Transition probabilities…

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Limitation : the dimension

sd

Noyau	*Dim*
^{18}O	14
^{19}O	37
^{20}O	81
^{21}O	119
^{22}O	142

fp

Noyau	*Dim*
^{42}Ca	30
^{43}Ca	145
^{44}Ca	565
^{45}Ca	1 651
^{46}Ca	3 952
^{47}Ca	7 531
^{48}Ca	12 022
^{49}Ca	15 666
^{50}Ca	17 276

$2d_{5/2}$-$1g_{7/2}$-$2d_{3/2}$-$3s_{1/2}$-$1h_{11/2}$

Noyau	*Dim*
^{102}Sn	36
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^{106}Sn	31 124
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^{108}Sn	323 682
^{109}Sn	828 422
^{110}Sn	1 853 256
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^{114}Sn	12 655 280
^{115}Sn	15 064 787
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Number of valence neutrons

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^{112}Sn	6 210 638	^{112}Sb	$\approx 1{,}1.10^{8}$
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^{115}Sn	15 064 787		
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+ *1* proton

Number of valence neutrons

Motivation

The size of the N-body basis grows exponentially with the number of valence nucleons and / or the number of valence levels

Quantum Monte Carlo methods could be an alternative to the direct diagonalization of the Hamiltonian

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Shell Model Monte Carlo

S.E. Koonin, D.J. Dean, K. Langanke

***Phys. Rept.*, 278 (1997)**

Provides the ground state or the thermodynamical properties

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→ ***Provides the ground state or the thermodynamical properties***

Objective

An alternative to diagonalization to obtain the « yrast spectroscopy »

QMC : *the fundamentals*

- ***Correlated state*** $|\Psi\rangle$
- ***Slater determinant*** $|\Phi\rangle$

Diagonalization of the Hamiltonian

$$|\Psi\rangle = \sum_{\Phi} C_{\Phi} |\Phi\rangle \quad \textbf{\textit{with}} \quad |\phi_i\rangle = |n_i l_i j_i m_i \tau_i\rangle \quad \textbf{\textit{ONB}}$$

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Quantum Monte Carlo (QMC)

$$|\Psi\rangle = \int_{\Phi} \mathfrak{D}\Phi P(\Phi)|\Phi\rangle$$ ***with any*** $|\phi_i\rangle$

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$P(\Phi)$: *Real & positive*

The exact state is reformulated in terms of an average of independent particle states

$$|\Psi\rangle \propto \mathbb{E}\big[|\Phi\rangle\big]$$

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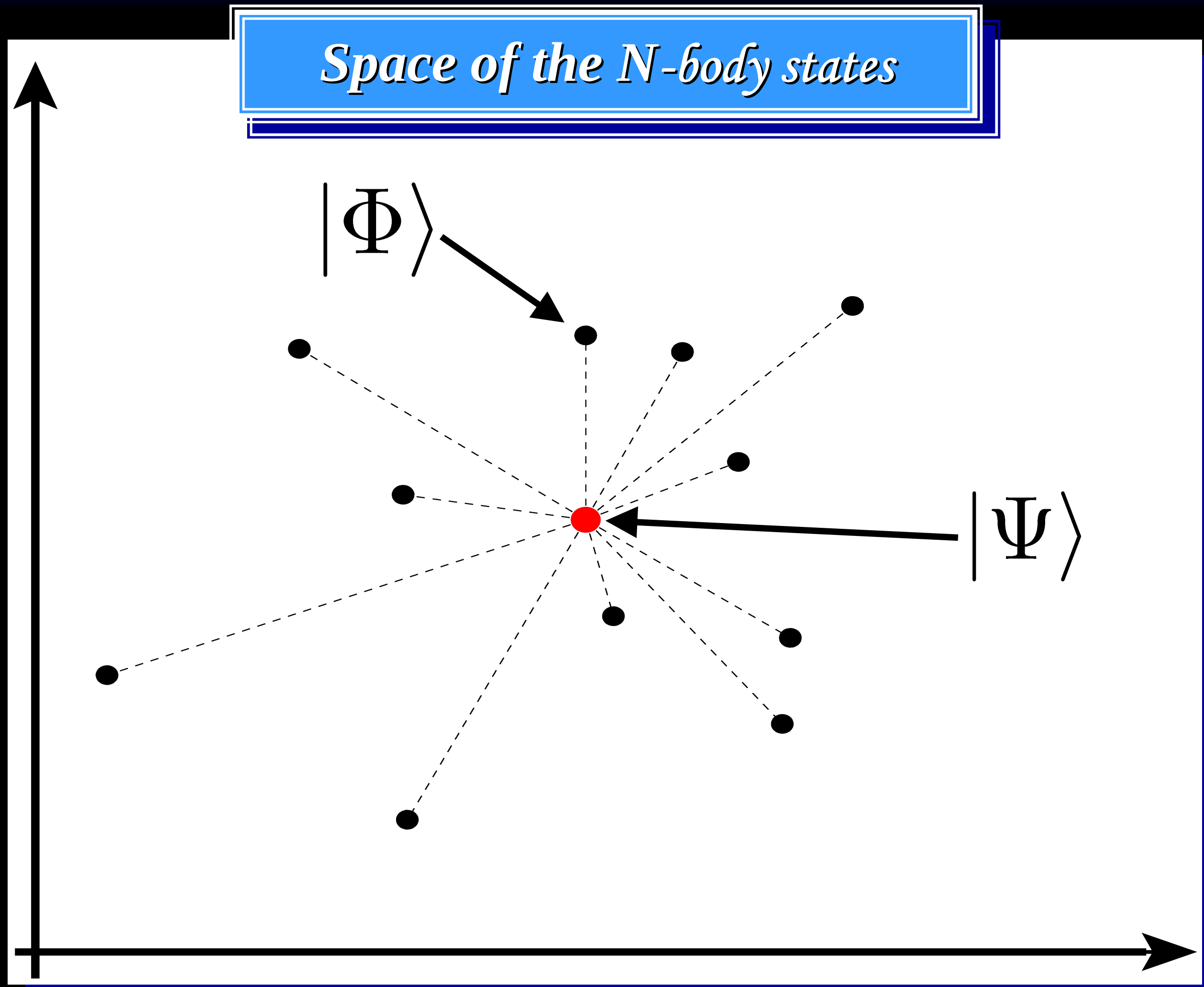

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Imaginary Time Propagation

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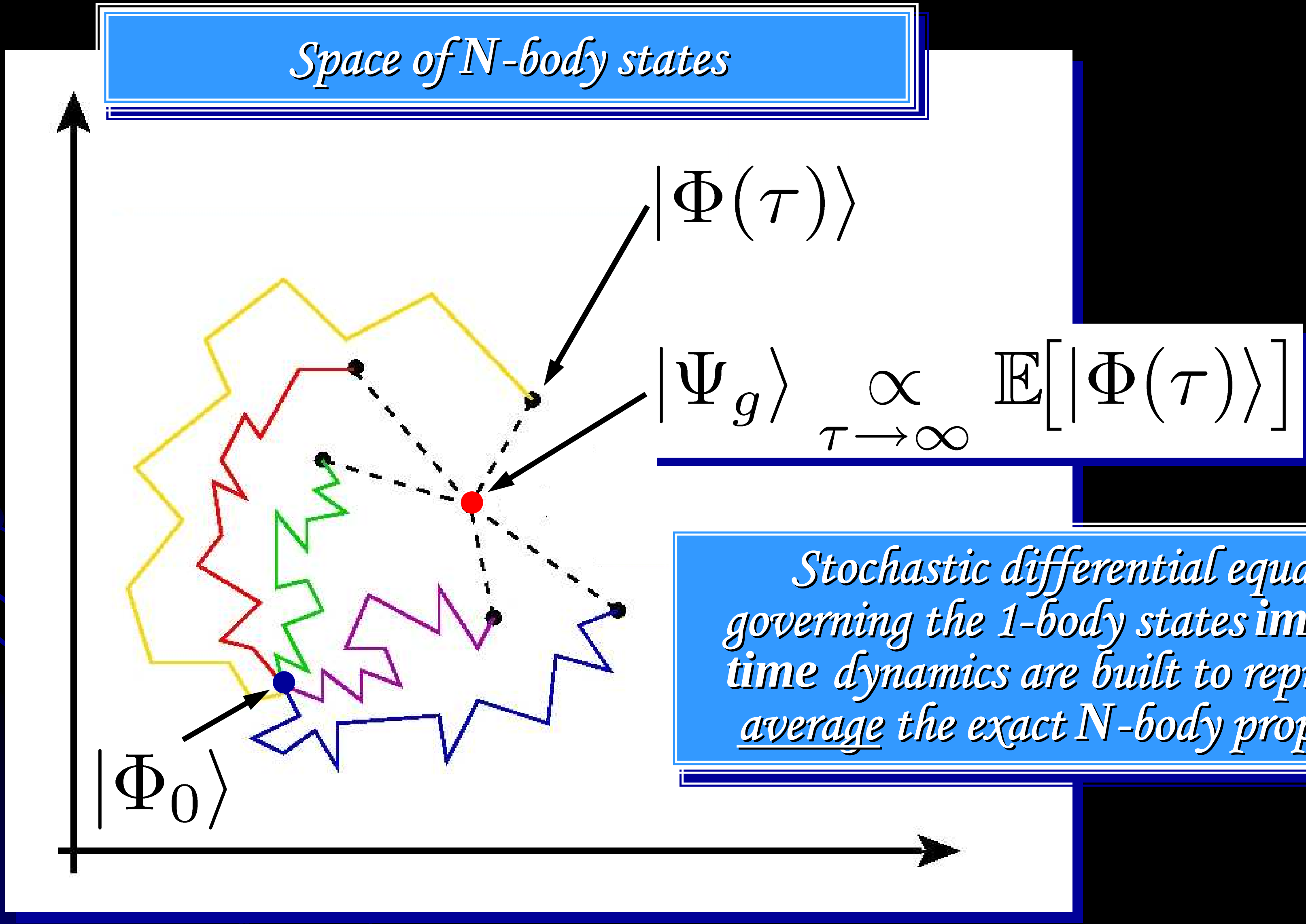
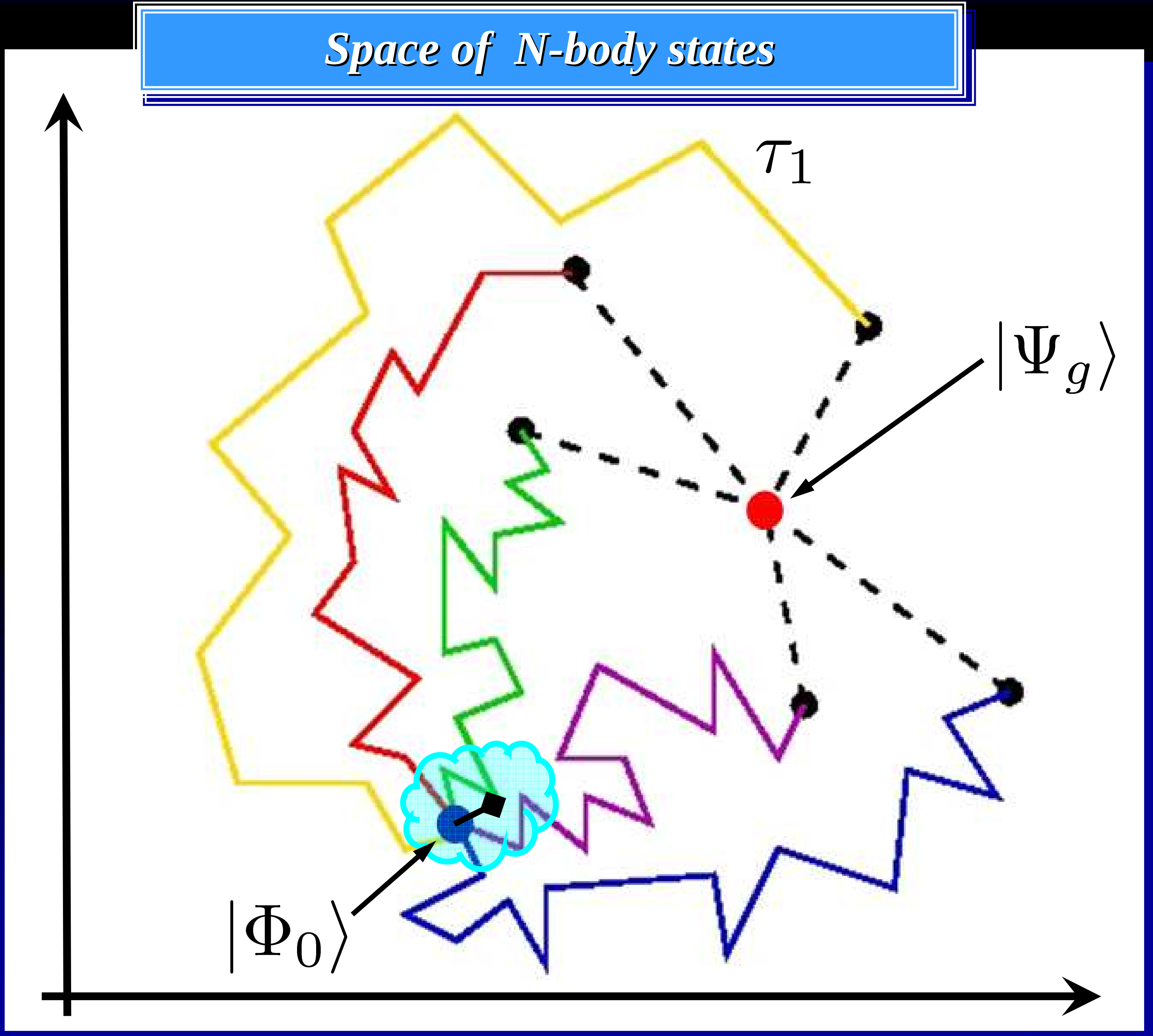


Stochastic differential equations governing the 1-body states imaginary time *dynamics are built to reproduce* <u>*in average*</u> *the exact N-body propagation*

QMC : *Importance of the initial state*



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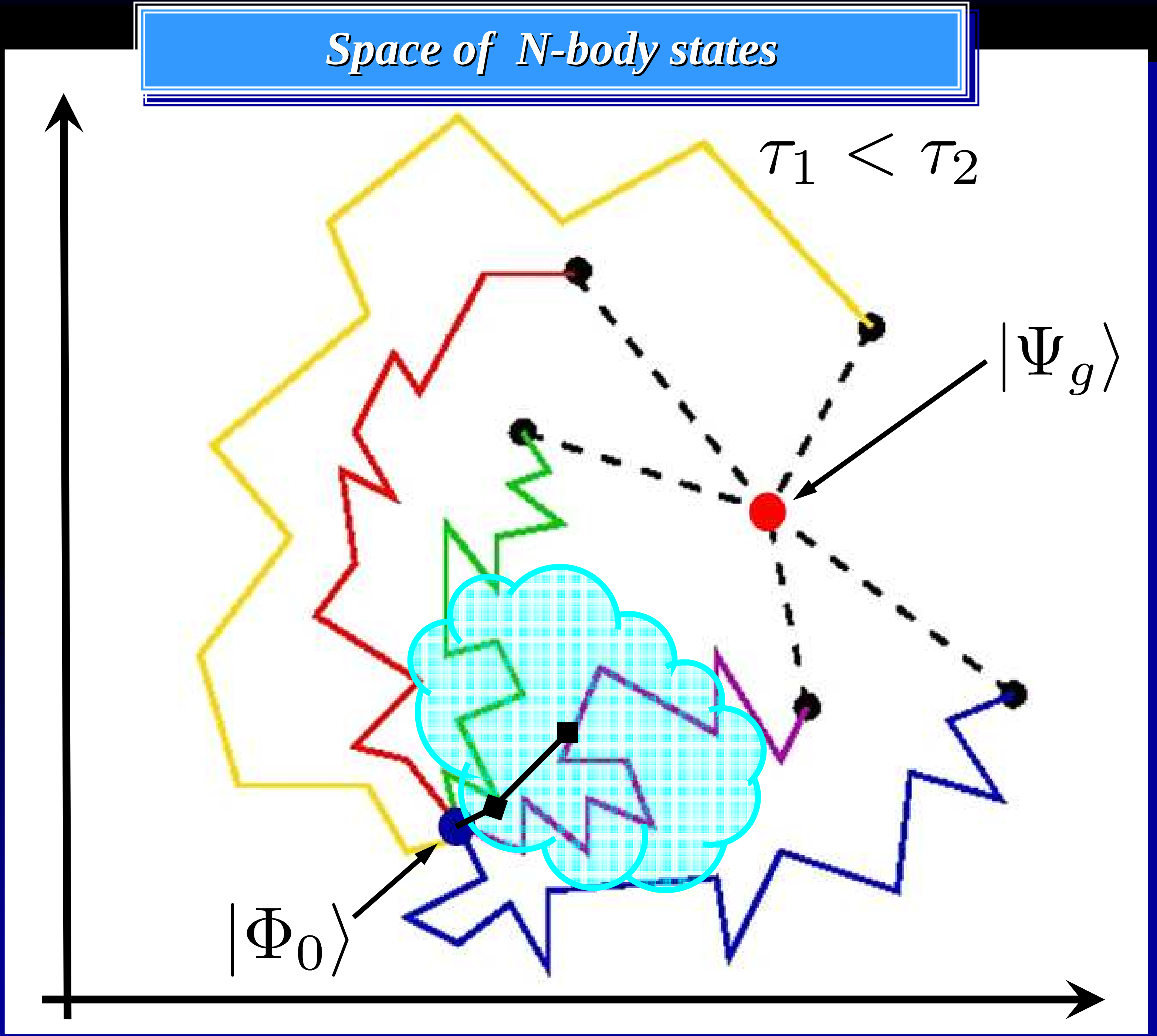

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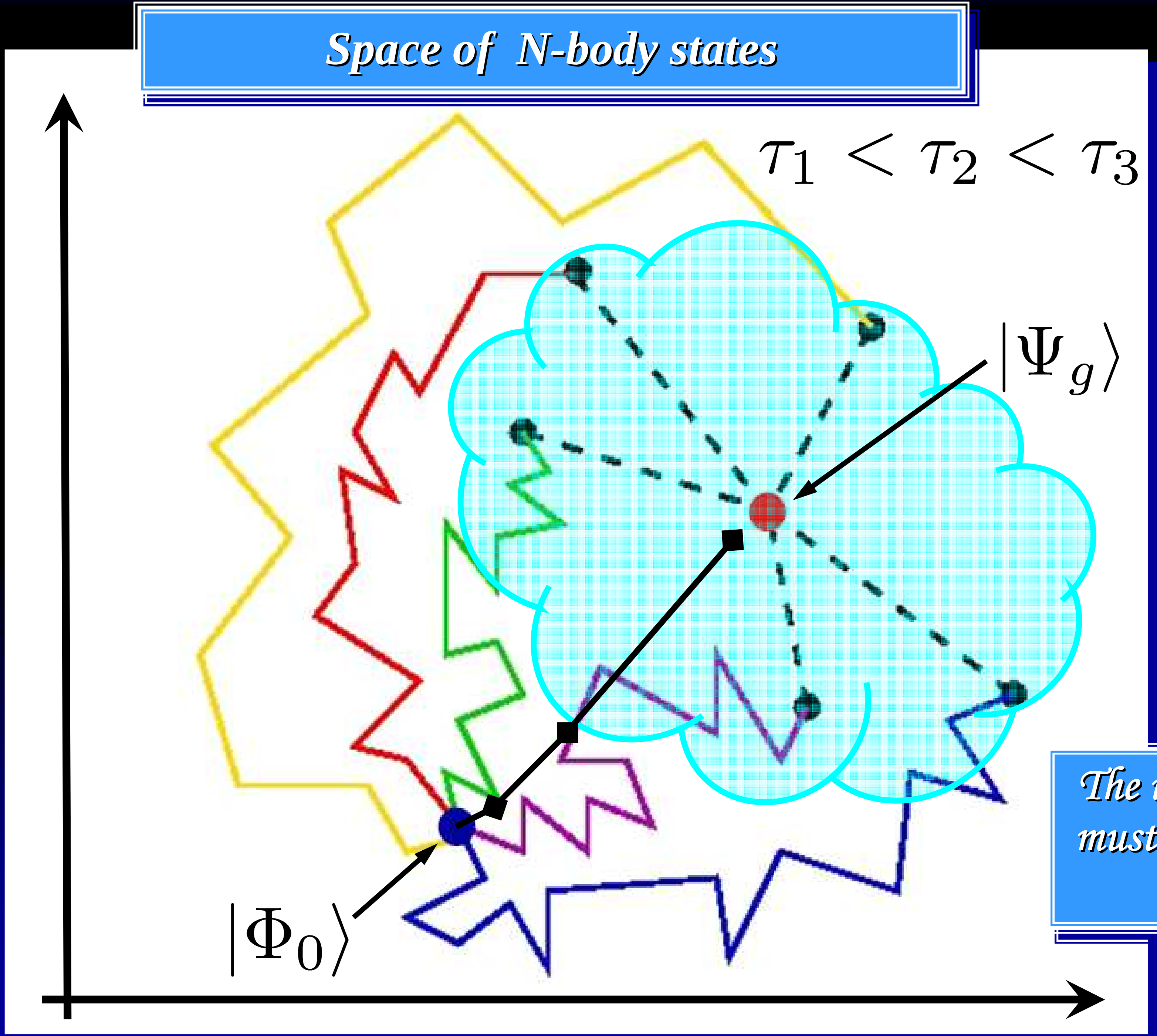
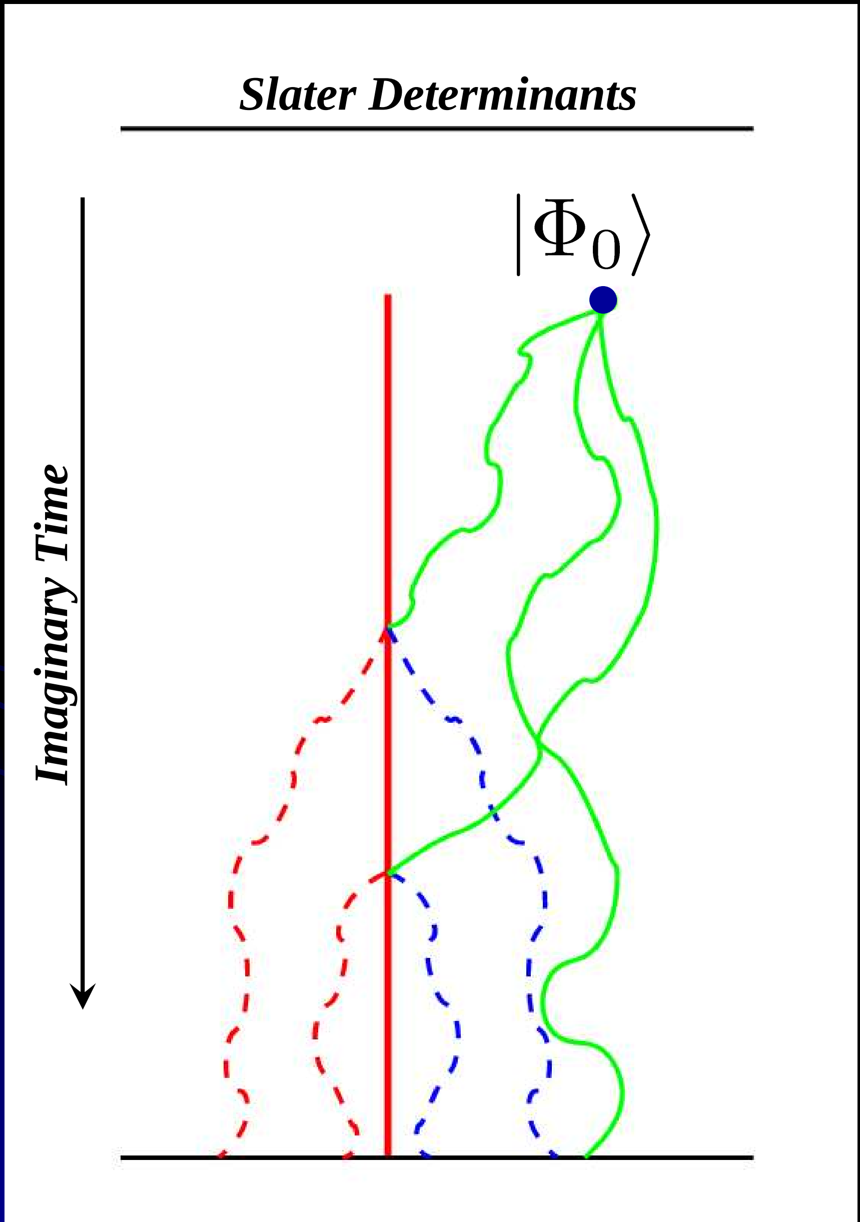


The initial Slater determinant must be a good approximation of the exact state

The Sign Problem



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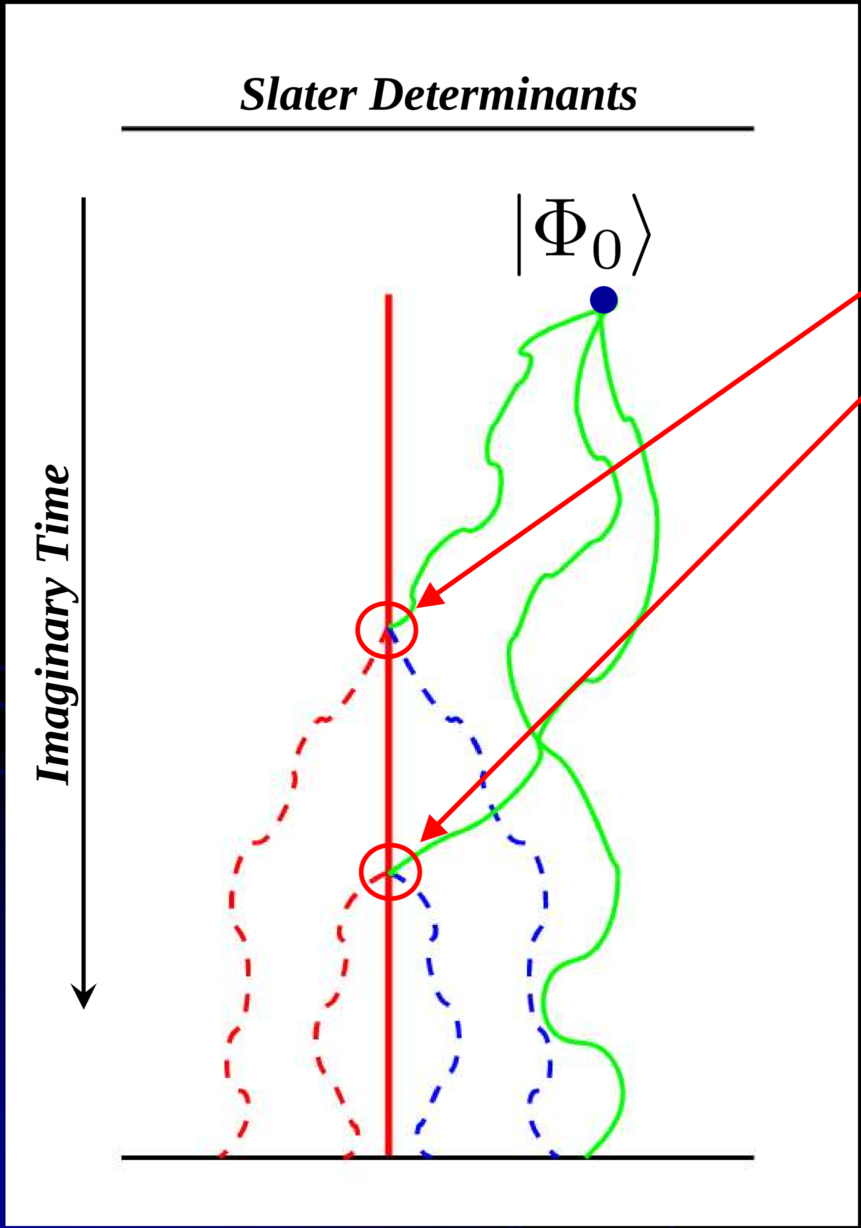
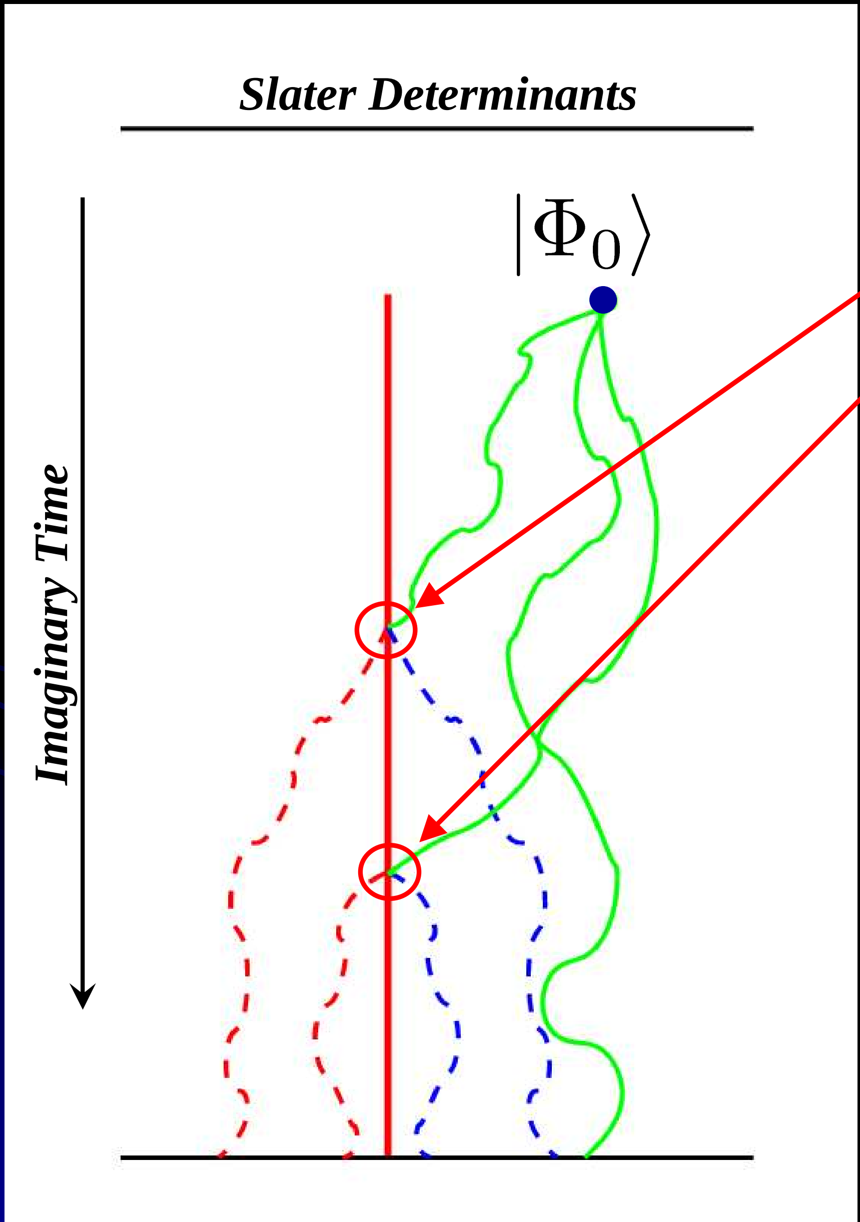


Nodal Surface

$$\langle \Psi_g | \Phi(\tau_0) \rangle = 0$$

The Sign Problem



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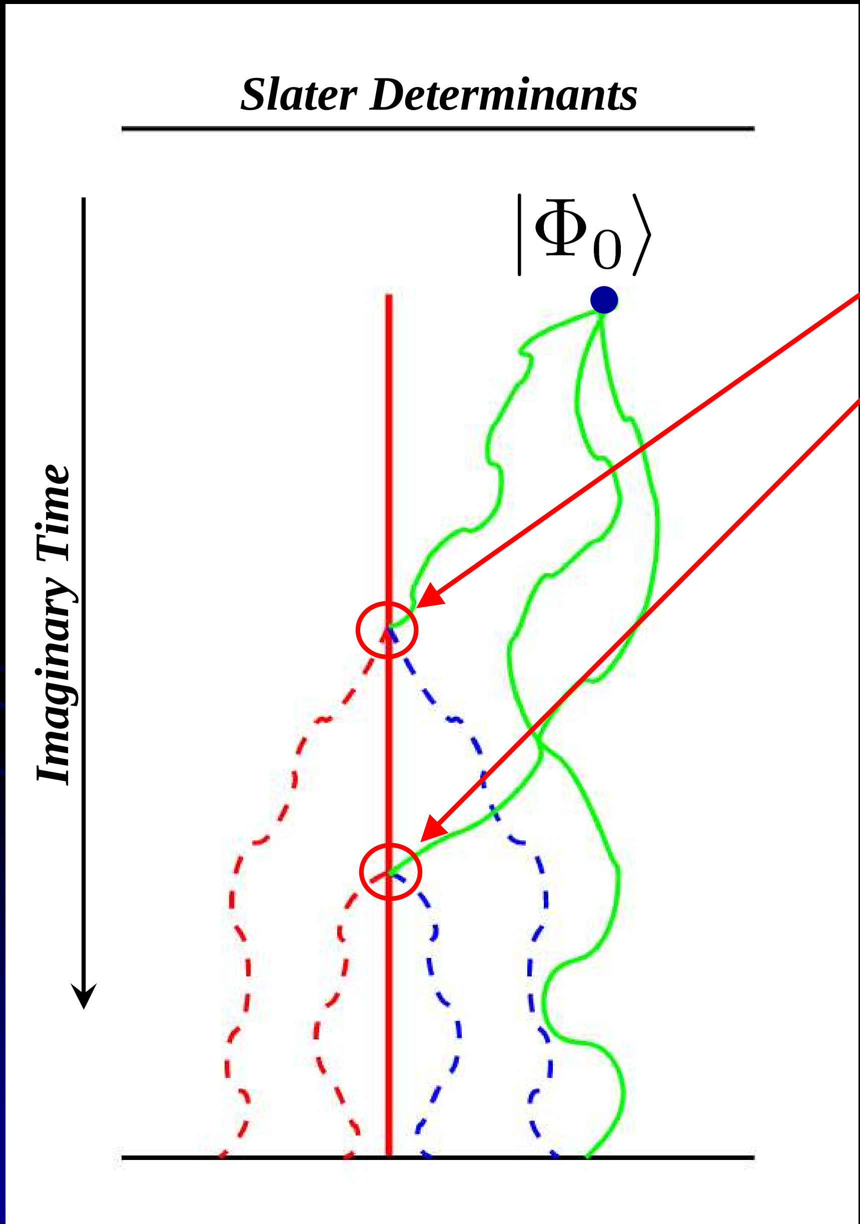

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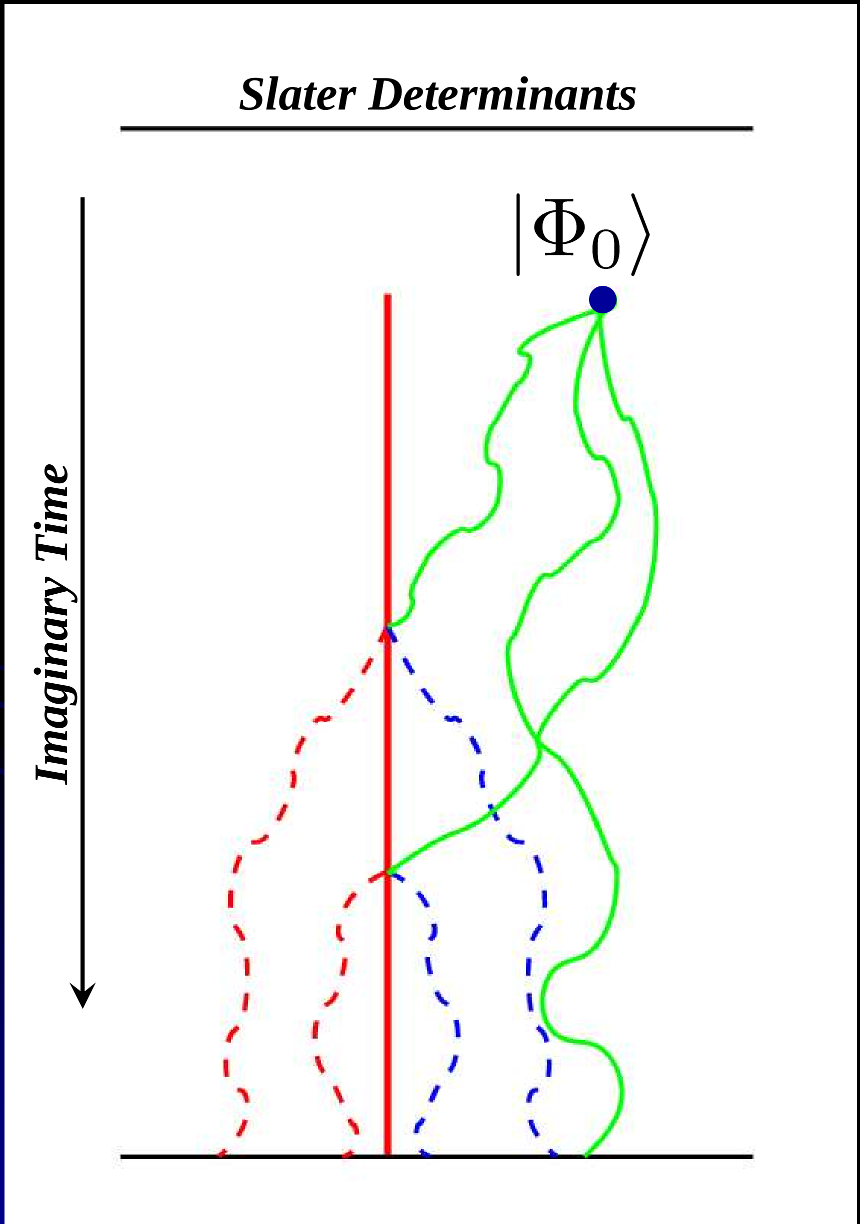
$$\langle \Psi_g | \mathrm{e}^{-(\tau - \tau_0)\hat{H}} | \Phi(\tau_0) \rangle = 0$$

$$\mathbb{E}[\langle \Psi_g | \Phi(\tau) \rangle] = 0$$

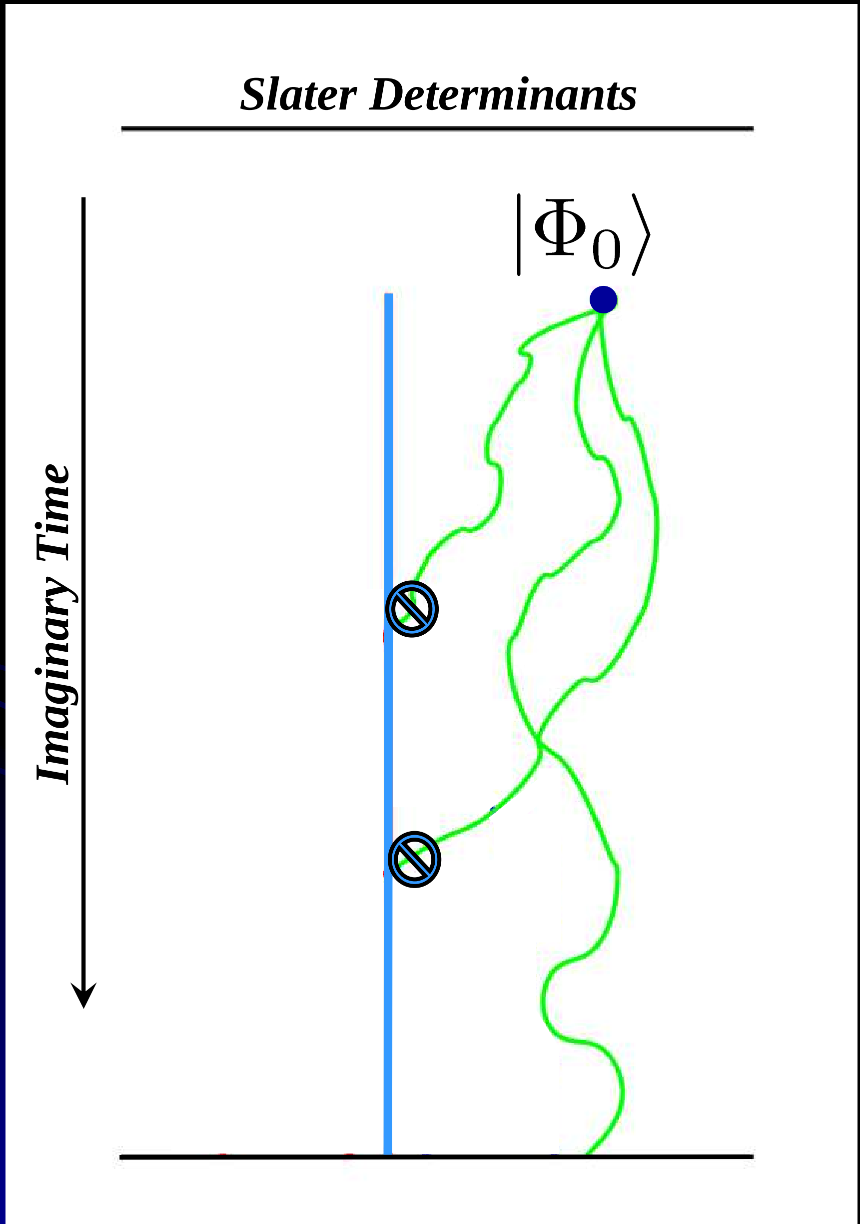
Useless trajectories which degrade the signal to noise ratio : this is the sign problem

The Sign Problem



How to avoid the sign problem ?

The Sign Problem



How to avoid the sign problem ?

Impose an approximate nodal surface using a test **N***-body state*

$$|\Psi_g\rangle \longrightarrow |\Psi_T\rangle$$

Finally, we avoid the sign problem if :

$$\forall\tau \; \langle\Psi_T|\Phi(\tau)\rangle > 0$$

Constrained Path AFQMC

S. Zhang, J. Carlson, J.E. Gubernatis

***Phys. Rev. Lett.*, 74, 3652 (1995)**

Fixed-Node DMC,GFMC

D.M. Ceperley, B. Alder

***Phys. Rev. Lett.*, 45, 566 (1980)**

Choice for the initial and test state

Variational method with *<u>projection</u>* *on the symmetries*

$$E = \frac{\langle \Phi_0 | \hat{P}^{J\,\dagger}_{M} \hat{H} \hat{P}^{J}_{M} | \Phi_0 \rangle}{\langle \Phi_0 | \hat{P}^{J\,\dagger}_{M} \hat{P}^{J}_{M} | \Phi_0 \rangle}$$

$$\hat{P}^{J}_{M} = \frac{2J+1}{16\pi^2} \int \mathrm{d}\Omega \, D^{J\,*}_{M\,M}(\Omega) \hat{R}(\Omega)$$

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<u>2 possibilities</u> :
- ***Variation BEFORE projection***
- ***Variation AFTER projection***

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« *Simplified* » VAMPIR *Method*

Variation After Mean-field Projection In realistic model space

K.W. Schmid, F. Grümmer, A. Faessler, *Phys. Rev. C*, 29,1 (1984)

E. Bender, K.W. Schmid, A. Faessler, *Phys. Rev. C*, 52,6 (1995)

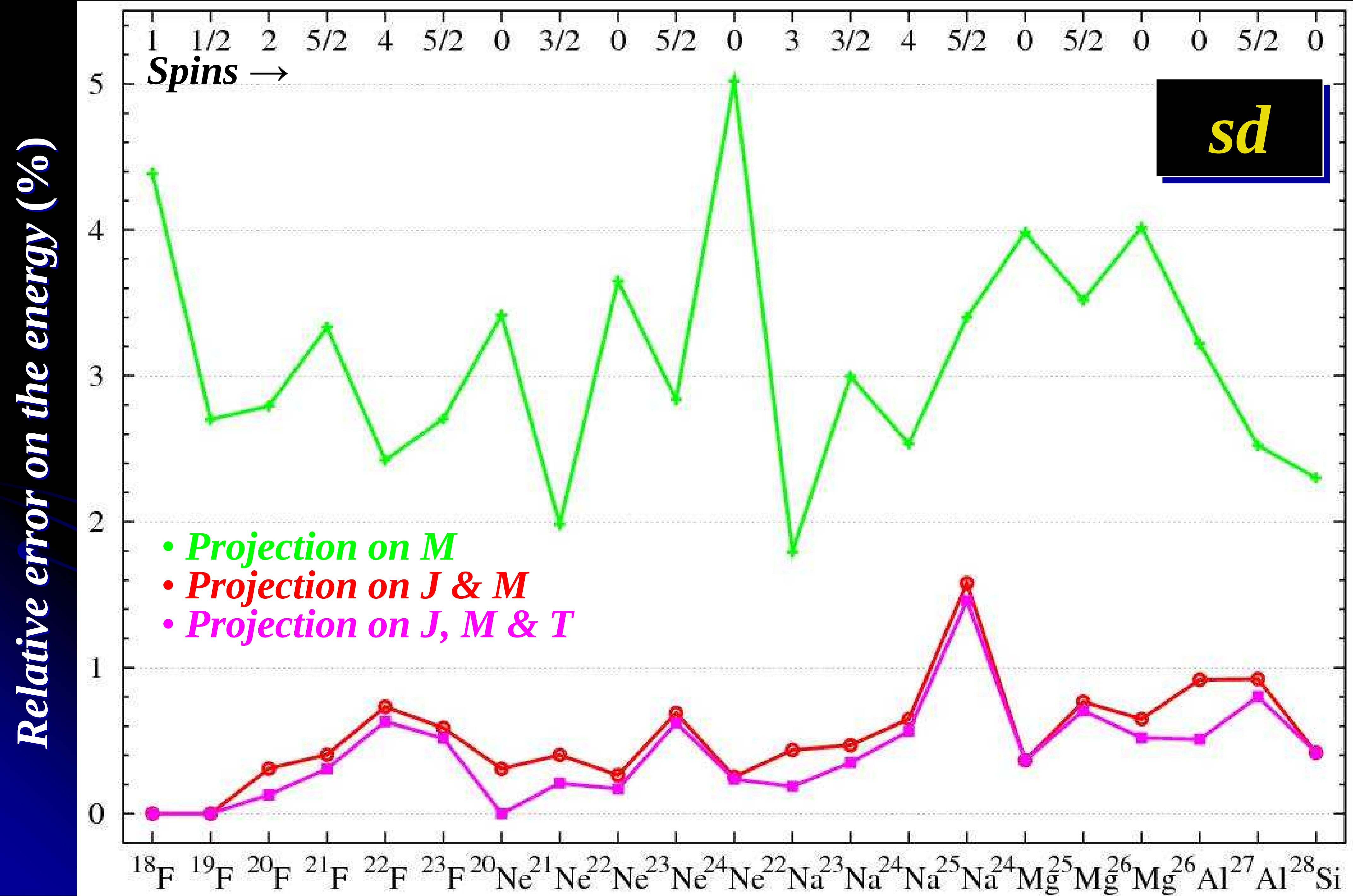
$$|\Psi_T\rangle = \hat{P}^{J}_{M} |\Phi_0\rangle$$

Test state — *Initial Déterminant*

Simplifications :

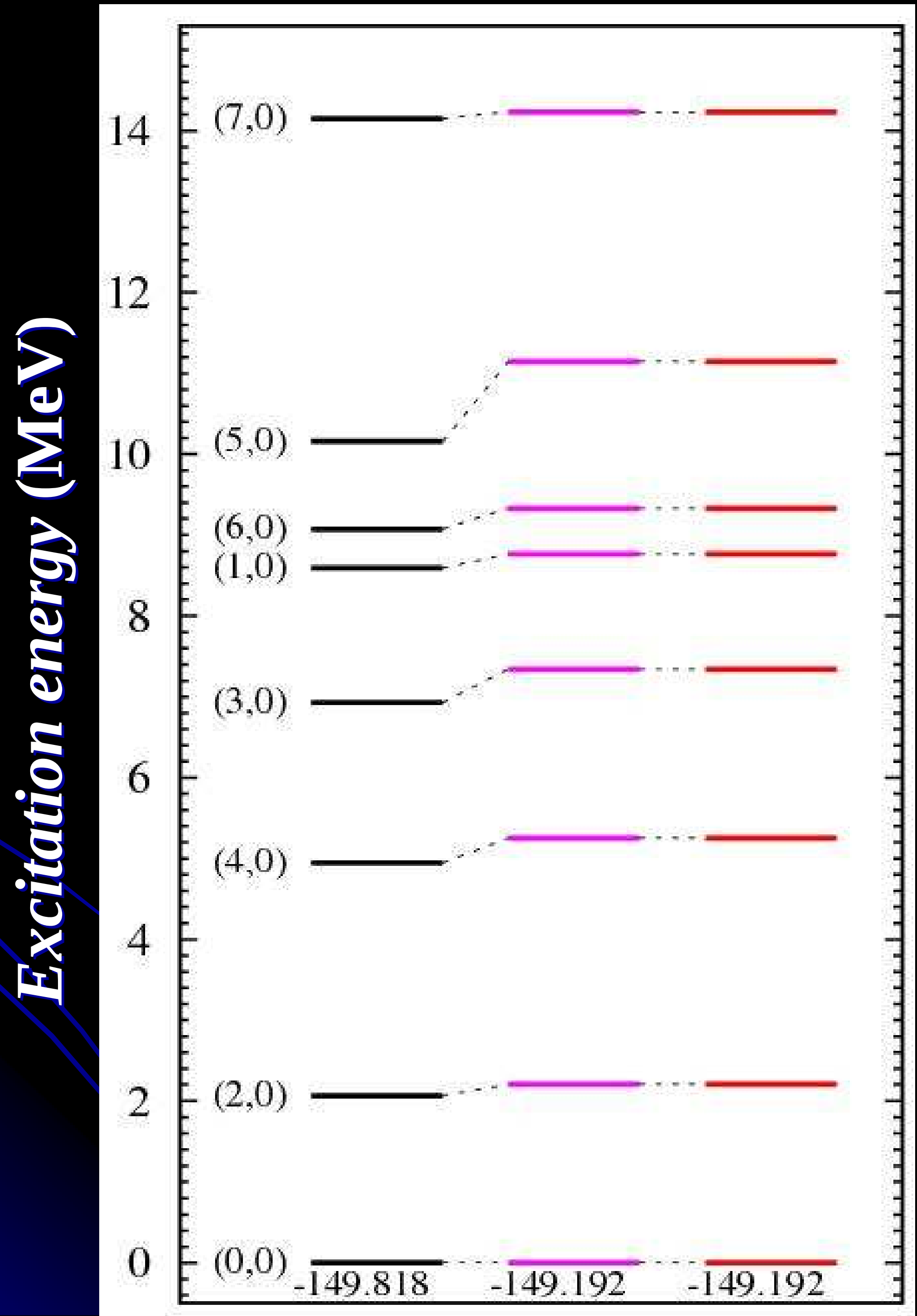
- ***A single déterminant instead of a superposition of HFB states with axial symmetry***
- $|\Phi_0\rangle = |\Phi_Z\rangle \otimes |\Phi_N\rangle$

Application : Ground States



Application : an even-even nucleus

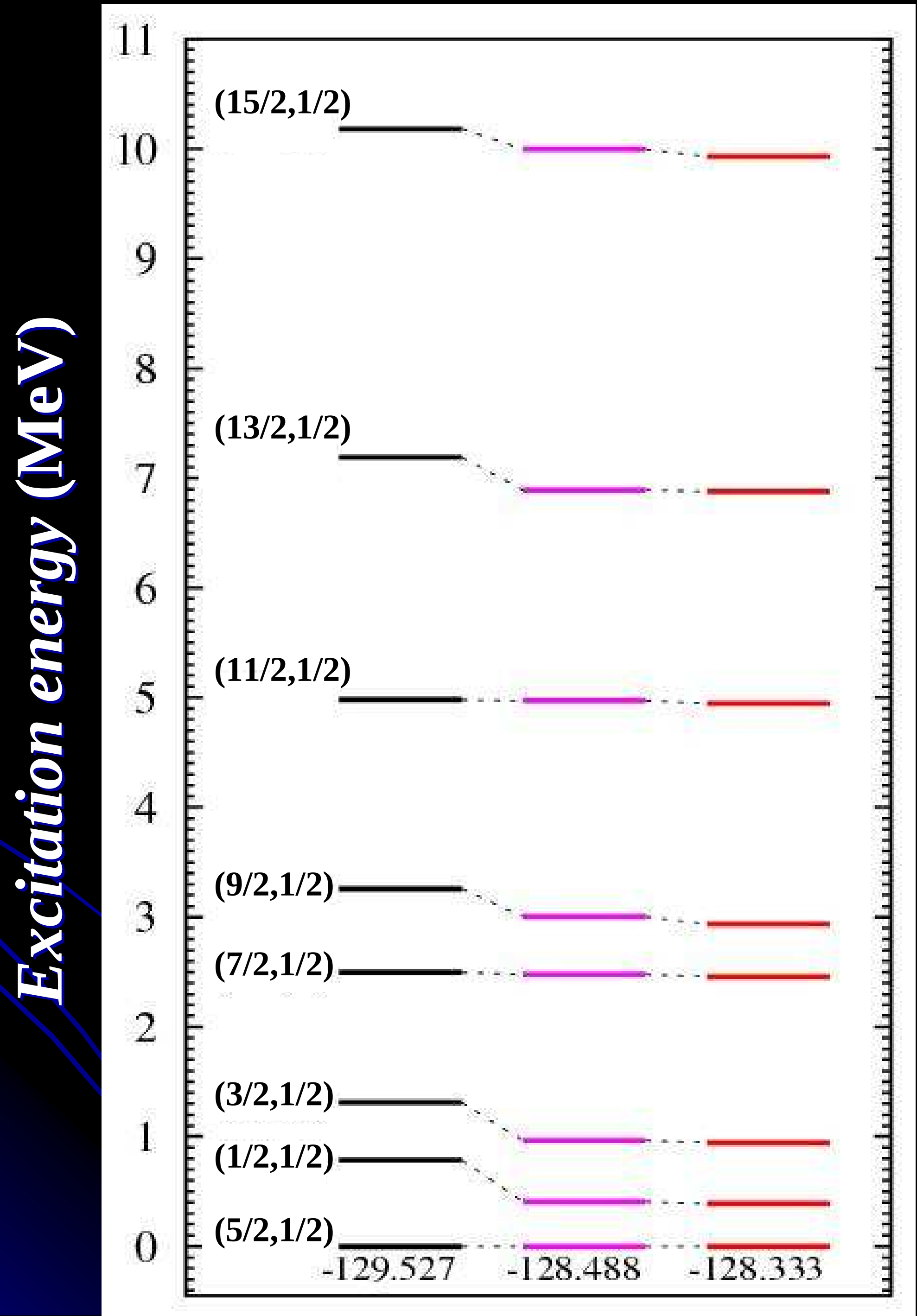
^{28}Si



- *Diagonalization* (J, T)
- *J & M projection*
- *J, M, T projection*

Application : an odd-even nucleus

^{27}Al



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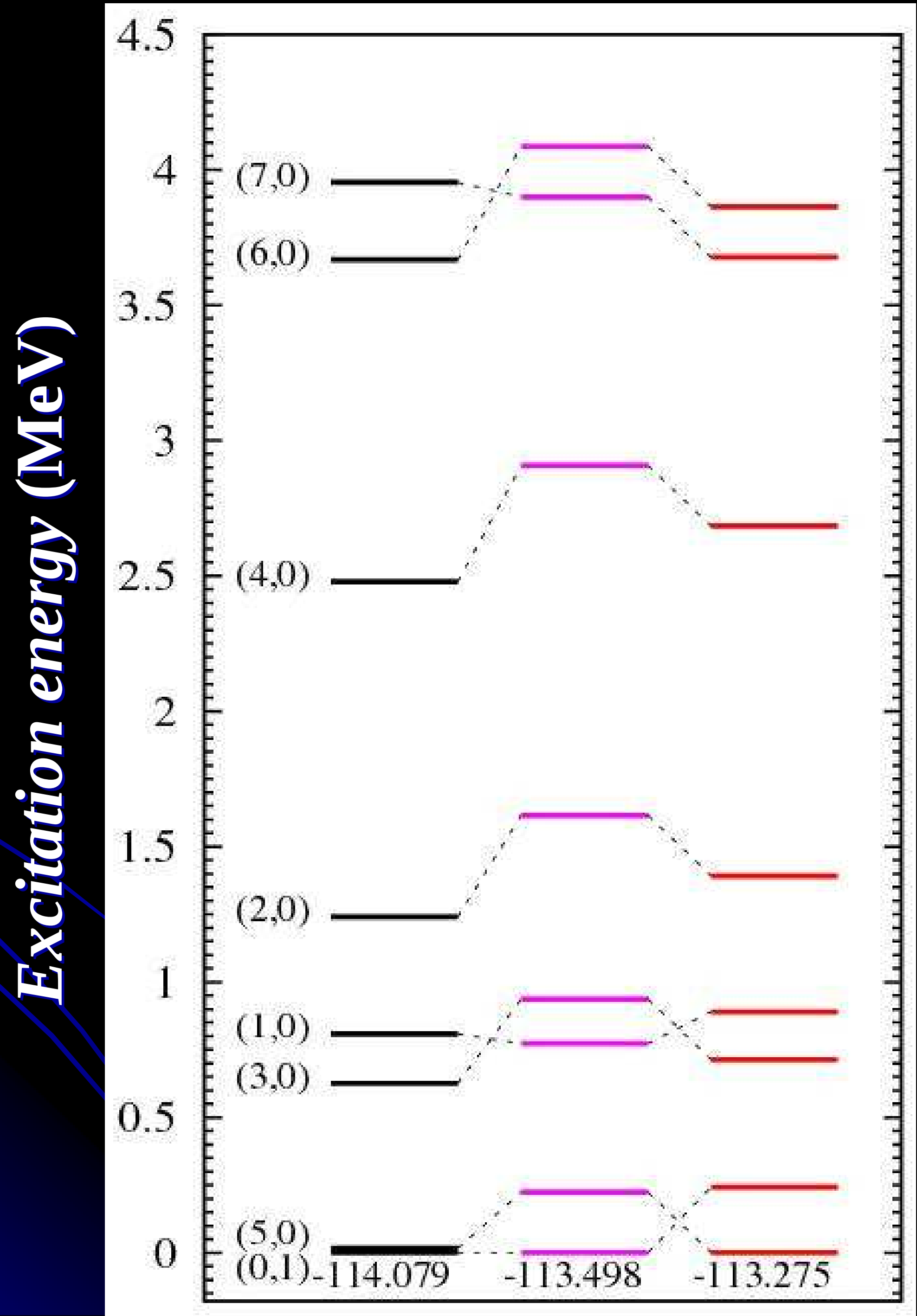
Application : an odd-odd nucleus

^{26}Al



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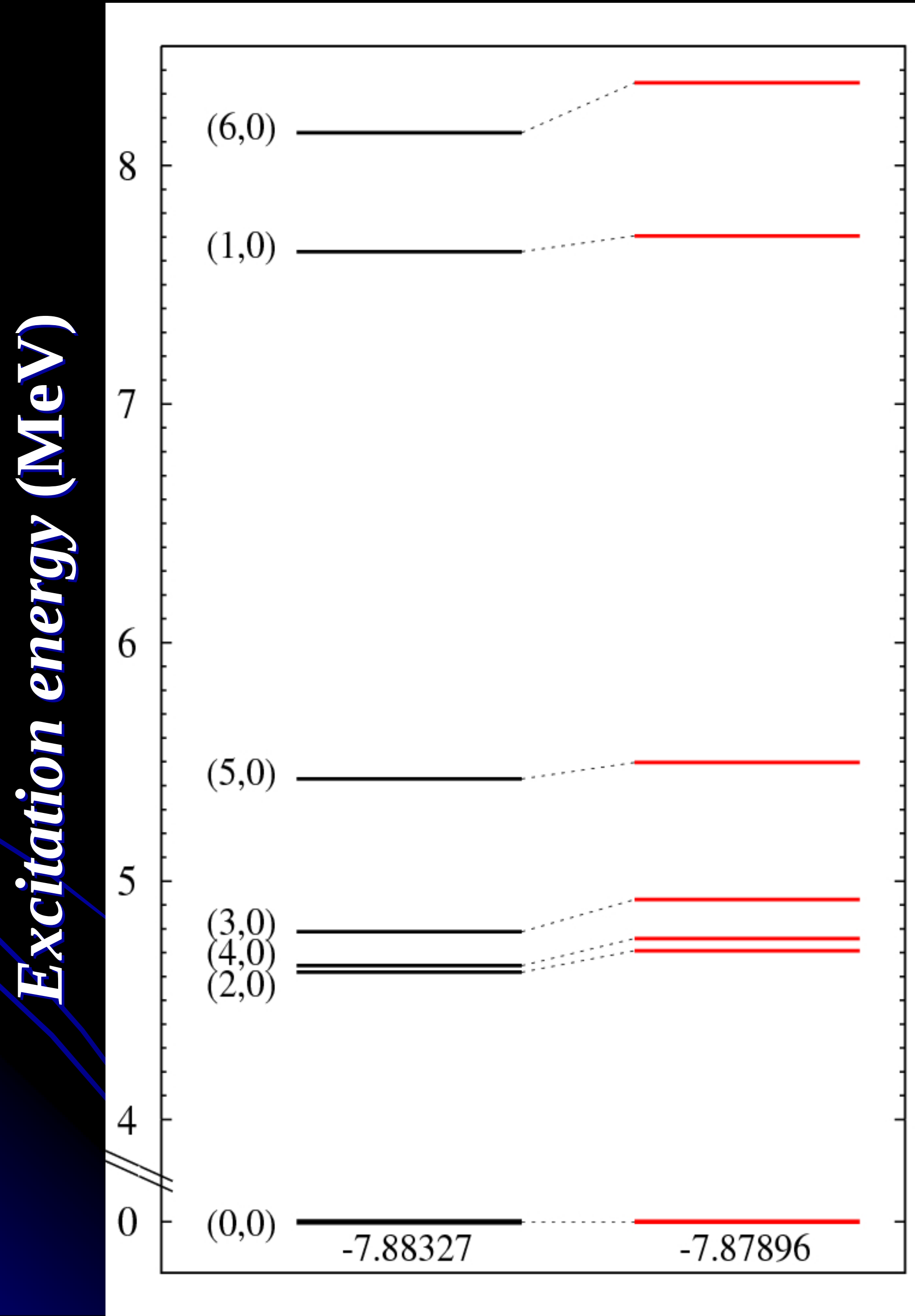
Application : a semi-magic nucleus

^{48}Ca



- ***Diagonalization*** (J,T)
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Conclusions

Objective : *An alternative to the diagonalization for the nuclear Shell Model to obtain the « yrast spectroscopy »*

Method :

Results :

Perspectives :

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Perspectives :

- *Quantum Monte Carlo calculations ;*
- *Can the approximation reproduce correctly other obervables ?*

MERCI DE VOTRE ATTENTION

Journées des Théoriciens Nucléaires

19-20 Oct. 2010

Institut de Physique Nucléaire de Lyon

Bonnard Jérémy