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No-Core FCI Calculations in Nuclear Physics: Exact + MCSM

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This is a summary of the discussions at U. of Tokyo, Hongo on July 17th, and 18th, 2008 and of the discussions that continued during the meetings in Onuma Park, July 21-25, 2008 and the discussions that continued during the meetings in Oak Ridge National Laboratory, February 23-25, 2009. The plans for a collaboration are summarized in these notes.

I. JISP16

$$\hat{V} = \sum_{S,J,T} \mathcal{P}_{S,\mathcal{J},T} \sum_{\substack{n,\ell \\ n',\ell'}} |n,l\rangle \; A^{S,\mathcal{J},T}_{n\ell,n'\ell'} \; \langle n'\ell'| \; ; \qquad \hbar\Omega = 40\text{MeV}; \qquad \vec{\mathcal{J}} = \vec{\ell} + \vec{s} \tag{1}$$

$$\langle r|n\ell\rangle = \mathcal{R}_{n\ell}(r) \qquad \text{H.O. relative wfn} \tag{2}$$

nuclear.physics.iastate.edu has subroutines for $\{A^{S,\mathcal{J},T}_{n\ell,n'\ell'}\}$.

Sample of NN channels

TABLE I: Sample of NN channels

	S	ℓ (ℓ')	$\mathcal{J}$	T
$^1S_0$	0	0	0	1
$^3S_1$-$^3D_1$	1	0 (2)	1	0
$^1P_1$	0	1	1	1

Selections of ingredients for the initial project

- $H = T_{rel} + V_{NN} + V_{Coulomb}$, with bare JISP16 for V_{NN} and $V_{Coulomb}$ treated perturbatively
- Definitions of cutoffs
  A) N_{max} is the many-body cut off: maximum number of harmonic oscillator quanta above lowest possible number of quanta for a given nucleus = 0, 1, 2, 3, $\cdots$
  B) $Max(a)$ = single particle cut off ($1 \le a, b, c, d \le Max(a)$) - 4 lowest oscillator shells (hope to expand to 5 shells)
- Set of $\hbar\Omega$ values (= 10, 15, 20, 25, 30, 35, 40)

format

Need sets of $\langle abJT||V||cdJT\rangle$ doubly-reduced antisymmetric TBME's in convenient format. These will be developed at Iowa State and made available for downloading from nuclear.physics.iastate.edu

TABLE II: single-particle h.o. states "a" = $n_a \ell_a j_a$

a	n_a	ℓ_a	j_a
1	0	S	1/2
2	0	P	1/2
3	0	P	3/2
4	1	S	1/2
5	0	D	3/2
6	0	D	5/2

TABLE III: format in MCSM: free format (same as the OXBASH)

a	b	c	d	J	T	$\langle \|\|H\|\| \rangle_{JT}$
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.

II. NO-CORE FCI CALCULATIONS IN NUCLEAR PHYSICS: EXACT + MCSM

Comparison/Test/Advantages/Disadvantages

1. E_{gs}, r_{rms}, $Q_{n,p}$, μ (g-factor), occ. prob. for ^{4}He, ^{6}He, ^{6}Li, ^{7}Li, ^{7}Be; ^{10}B? [natural/unnatural parity - lowest only (w/o Lowson's method of the spurious C.M. motion)]
2. JISP16 bare, Coulomb (perturbative)
3. Basis space - F.C.I. {2, 3, 4, 5?; 6?, $\cdots$ } : for 2, 3, 4, 5, 6: $\sum_a (2j_a + 1) = 20$, 28, 40, 70, 112, respectively, for each n, p
   : $\hbar\Omega = 10$, 15, 20, 25, 30, 35, 40
4. snap shot comparison

TABLE IV: snap shot comparison

snap shot comparison	FCI	MCSM	NCSM
C.M.	approx.	approx.	exact
Coulomb	perturbative	perturbative	exact
Spectra	OK	some	OK
wfns $\rightarrow$ occ.probs.	$\surd$	$\surd$	$\surd$
(diagonals of OBDM)			
Dimension	$\lesssim 10^{10}$	$\lesssim 10^{30}$	$\lesssim 10^{10}$

figures

1. s.p. state range: N_{max} and $Max(a)$
2. E_{gs}, r_{rms}, $\cdots$ as a function of N_{shell} in ^{4}He, ^{6}He, ^{6}Li, ^{7}Li, ^{7}Be, (^{10}B,) $\cdots$
3. E_{gs}, r_{rms}, $\cdots$ as a function of $\hbar\Omega$ in ^{4}He, ^{6}He, ^{6}Li, ^{7}Li, ^{7}Be, (^{10}B,) $\cdots$

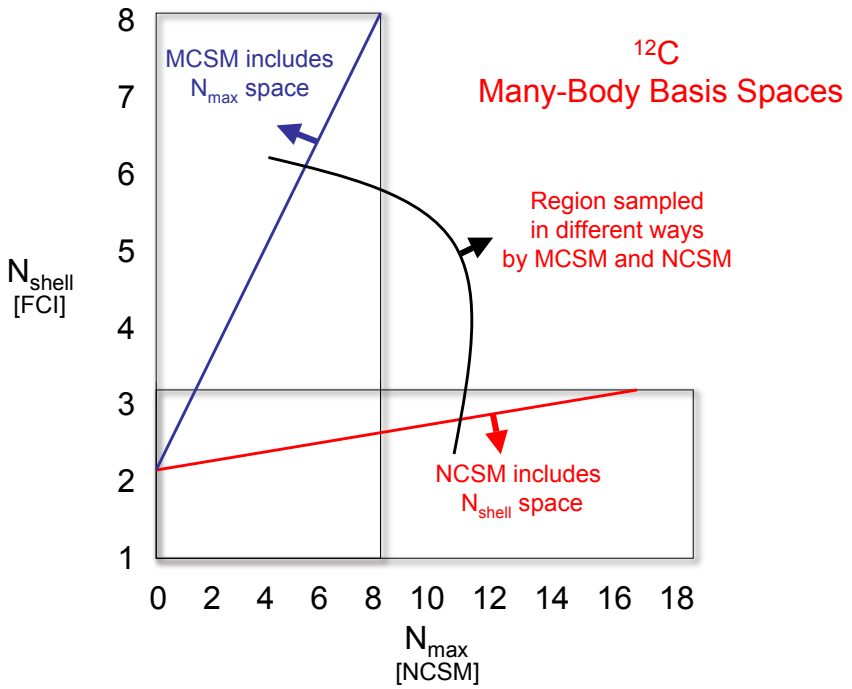

FIG. 1: Overview of the basis spaces covered with the many-body methods discussed here for the case of ^{12}C. N_{max} is defined as the number of oscillator quanta above lowest possible number of quanta. N_{shell} is the number of oscillator shells counting the $0S$ shell as the first shell. The MCSM incorporates a Full Configuration Interaction (FCI) space. That is, all single-particle states in the included shells are available to all particles without additional restrictions except for symmetry constraints.

III. INITIAL ESTIMATED SCHEDULE OF ACTIVITIES

1. $\surd$ Calculate Hamiltonian matrix element files with $Max(a) = 4$ shell truncation for JISP16 and store on nuclear.physics.iastate.edu along with documentation: (J.P. Vary - now completed)
2. MCSM code updated to accept input from Hamiltonian matrix element files with $Max(a) = 4$ truncation (T. Abe, others?, schedule?)
3. $\surd$ MFDn updated and tested to accept Hamiltonian matrix element files with $Max(a) = 4$ truncation (P. Maris, J. P. Vary, - now completed)
4. Production runs of MCSM (T. Abe, others?, schedule?) and $\surd$ MFDn (P. Maris, Sept.-Oct. 2008) for the cases listed above
5. Draft of first paper presenting these results (who?, schedule?).

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[3] J. P. Vary, "The Many Fermion Dynamics Shell Model Code," Iowa State University, 1992 (unpublished); J. P. Vary and D. C. Zheng, *ibid* 1994 (unpublished).
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