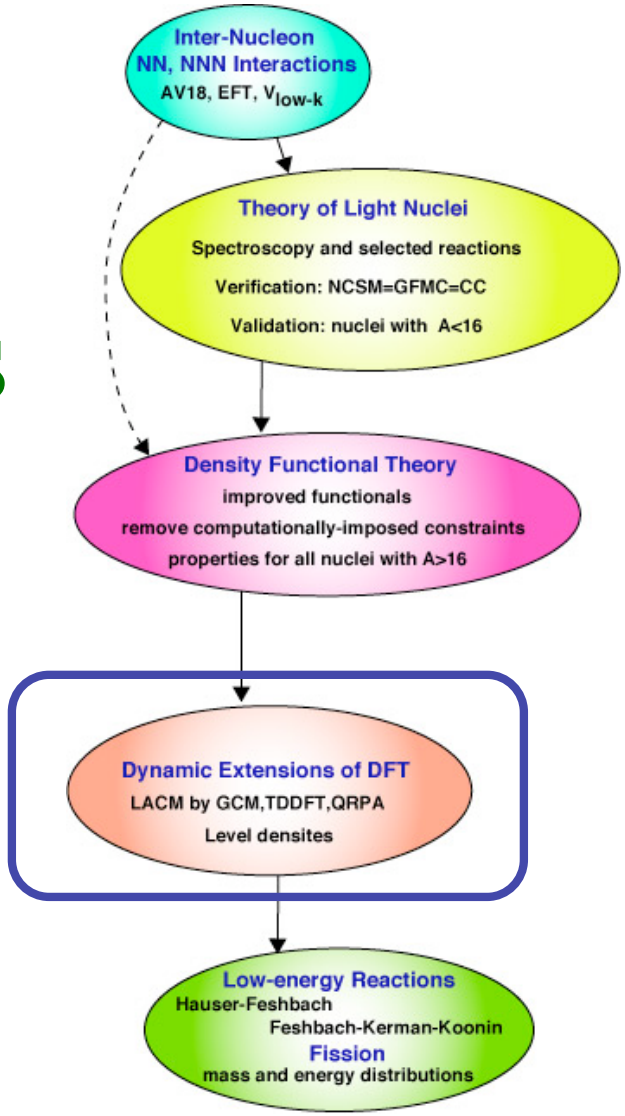
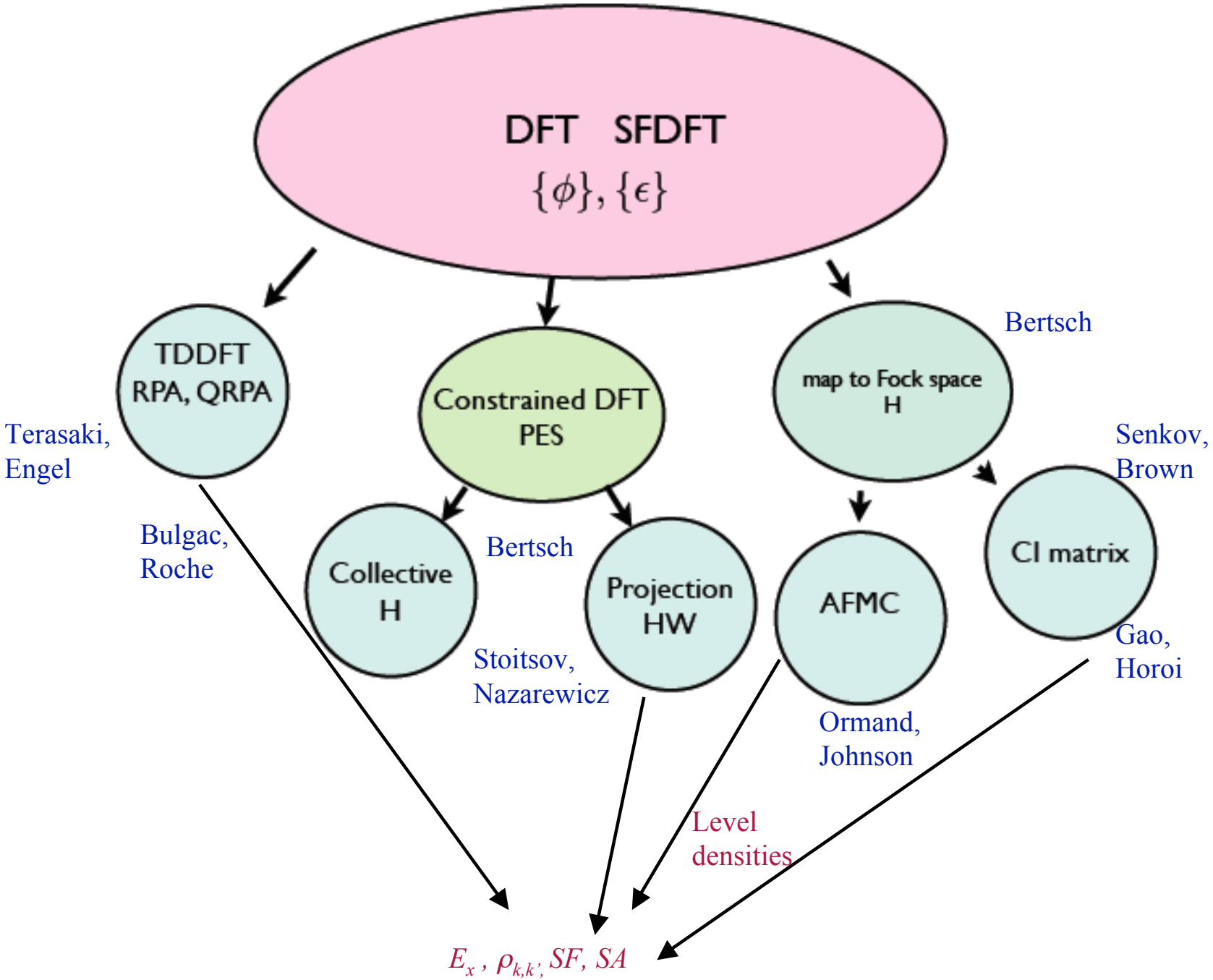
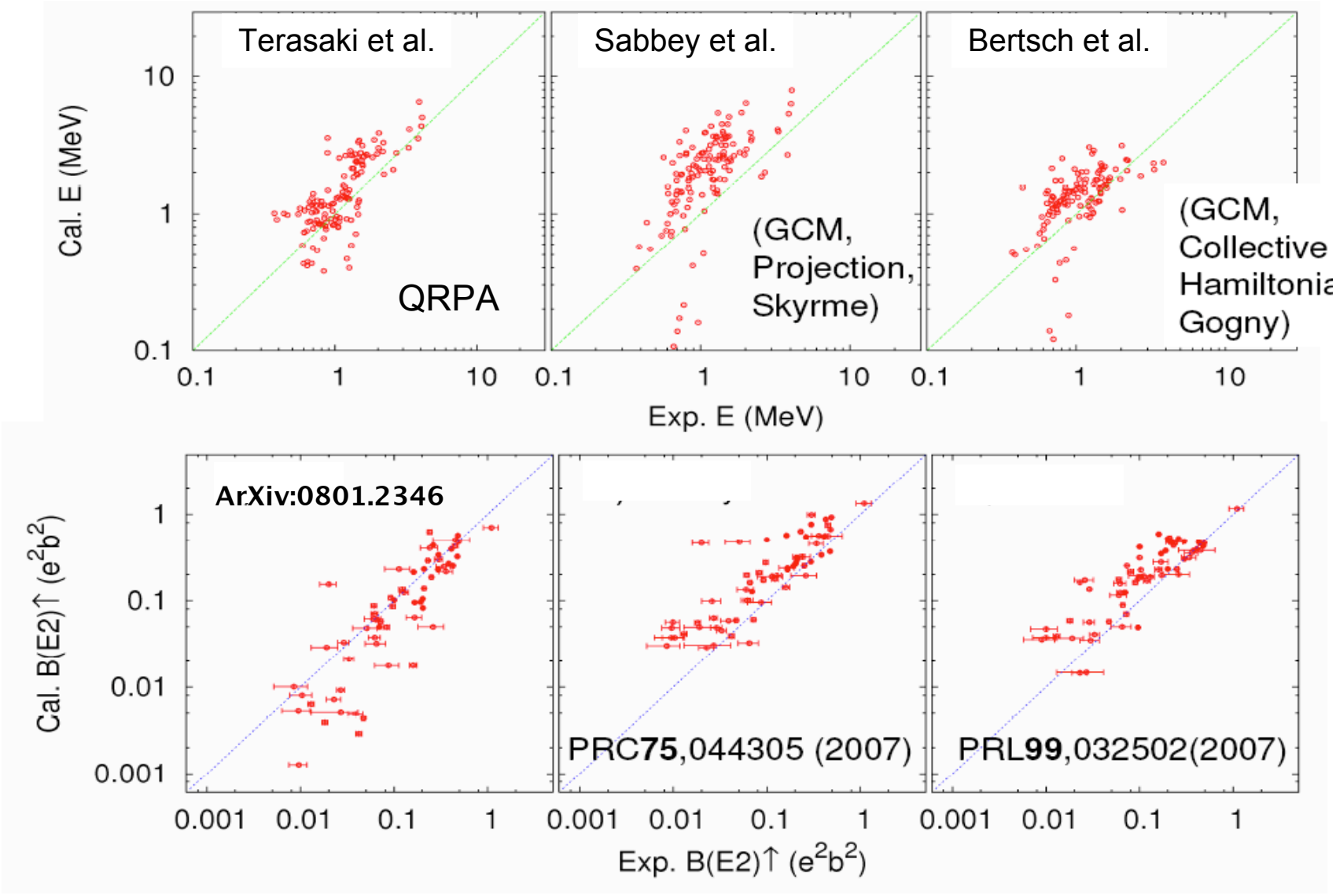
DFT Extensions for Dynamics, Excited States



G. Bertsch, University of Washington,
A. Bulgac, University of Washington,
Z. Gao and M. Horoi, Central Michigan University,
C. Johnson, San Diego State University,
E. Ormand, Lawrence Livermore National Laboratory,
K. Roche, Oak Ridge National Laboratory,
R. Senkov and B.A. Brown, Michigan State Unversity,
M.V. Stoitsov and W. Nazarewicz, University of Tennessee and ORNL,
J. Terasaki and J. Engel, University of North Carolina at Chapel Hill


DFT SFDFT
$\{\phi\}, \{\epsilon\}$
TDDFT
RPA, QRPA
Constrained DFT
PES
map to Fock space
H
Bertsch
Terasaki,
Engel
Senkov,
Brown
Bulgac,
Roche
Collective
H
Bertsch
Projection
HW
AFMC
CI matrix
Stoitsov,
Nazarewicz
Gao,
Horoi
Ormand,
Johnson
Level
densities
E_x , $\rho_{k,k'}$, SF, SA

Global calculations of the lowest 2^+ states



Deformed QRPA code including general Skyrme functional in progress (Terasaki, Engel)

Time-Dependent Superfluid Local Density Approximation (TD-SLDA)

(generalization of Kohn-Sham LDA to superfluid systems, Bulgac, 2002)

Bulgac (UW), Roche (ORNL), Yu (Lund → Wuhan)

Space-time lattice, use of FFTW for spatial derivative

No matrix operations (unlike (Q)RPA)

$$N_x^3 \times N_t, \qquad N_x \approx 50...100, \qquad N_t \approx 10^4...10^5$$

$$\text{number of } \psi_n(\vec{r},\sigma,t) \approx O(N_x^3 \times N_t)$$

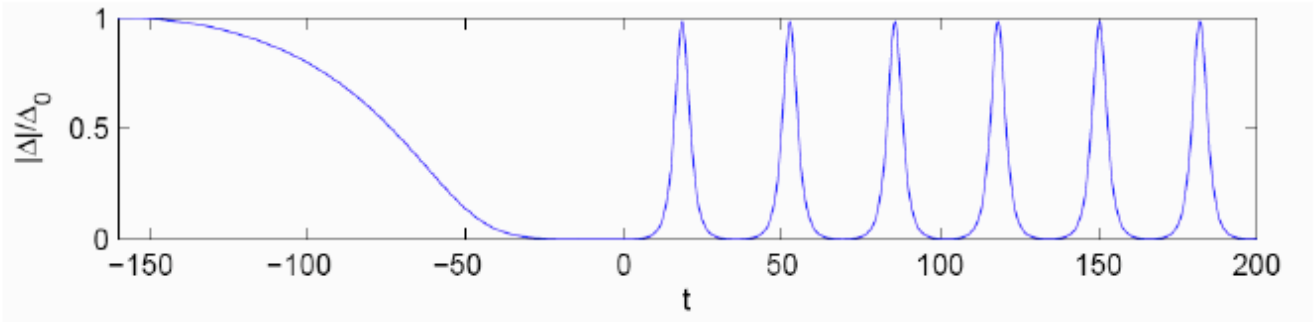
Observables and spectrum →

$$Q(\omega) = \sum_\sigma \int d^3r dt Q(\vec{r},\sigma,t)\rho(\vec{r},\sigma,t)\exp(i\omega t)$$

All nuclei (odd, even, spherical, deformed)

Any quantum numbers of QRPA modes

Fully selfconsistent, no self-consistent symmetries imposed



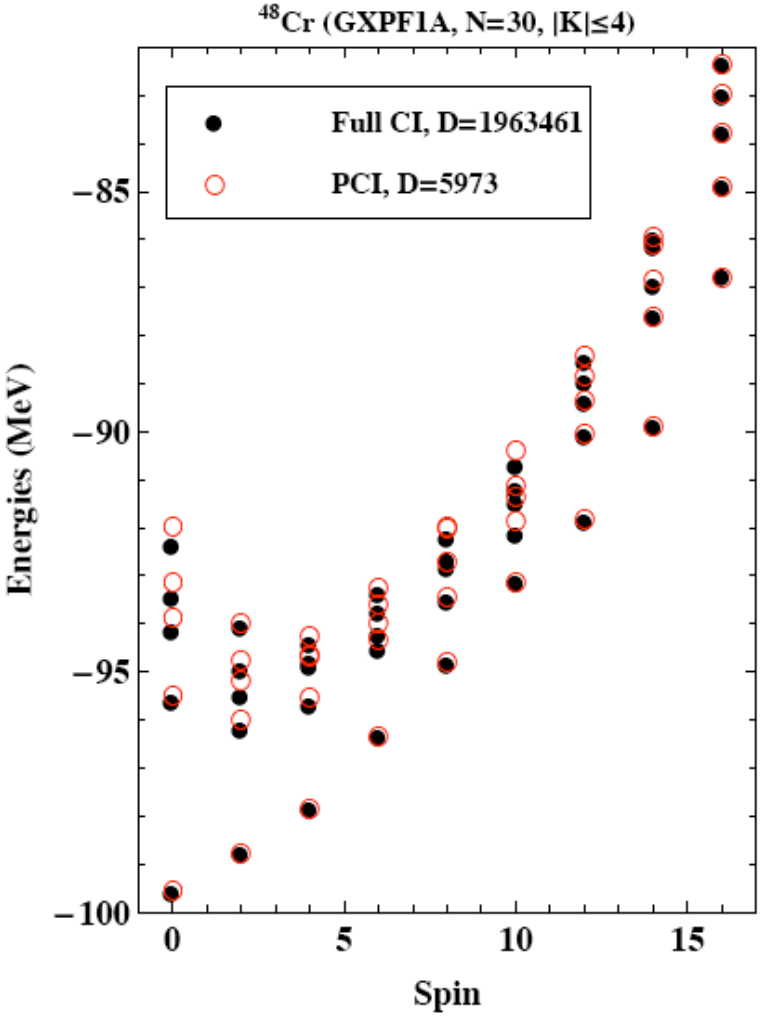
Higgs mode of the pairing field in a homogeneous unitary Fermi gas - Bulgac, Yoon

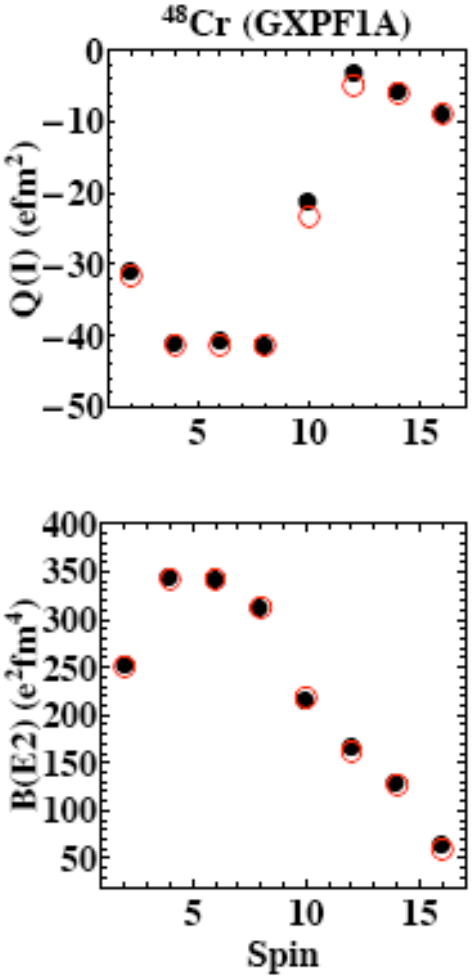
Projected Configuration Interaction (PCI)

$$\phi_i(sph) \xrightarrow{DFT} \phi_j(def) \sim \phi_j(\varepsilon_2,\varepsilon_4,\ldots)$$

$$DFT \xrightarrow{MAP\ to\ Fock} H_{CI} \xrightarrow{\phi_j(\varepsilon_2,\varepsilon_4,\ldots)} H(\varepsilon_2,\varepsilon_4,\ldots)$$

R. Rodriguez-Guzman, Y. Alhassid, **G. Bertsch**, arXiv:0709.0508, (2007)





$$\left|\Psi_{JM}\right\rangle = \sum_{K\kappa} f^J_{K\kappa} P^J_{MK} \left|\Phi_{K\kappa}(\varepsilon_2,\ldots)\right\rangle$$

Basis $\Phi_{K\kappa}$ includes particle-hole excitations corresponding to many shapes

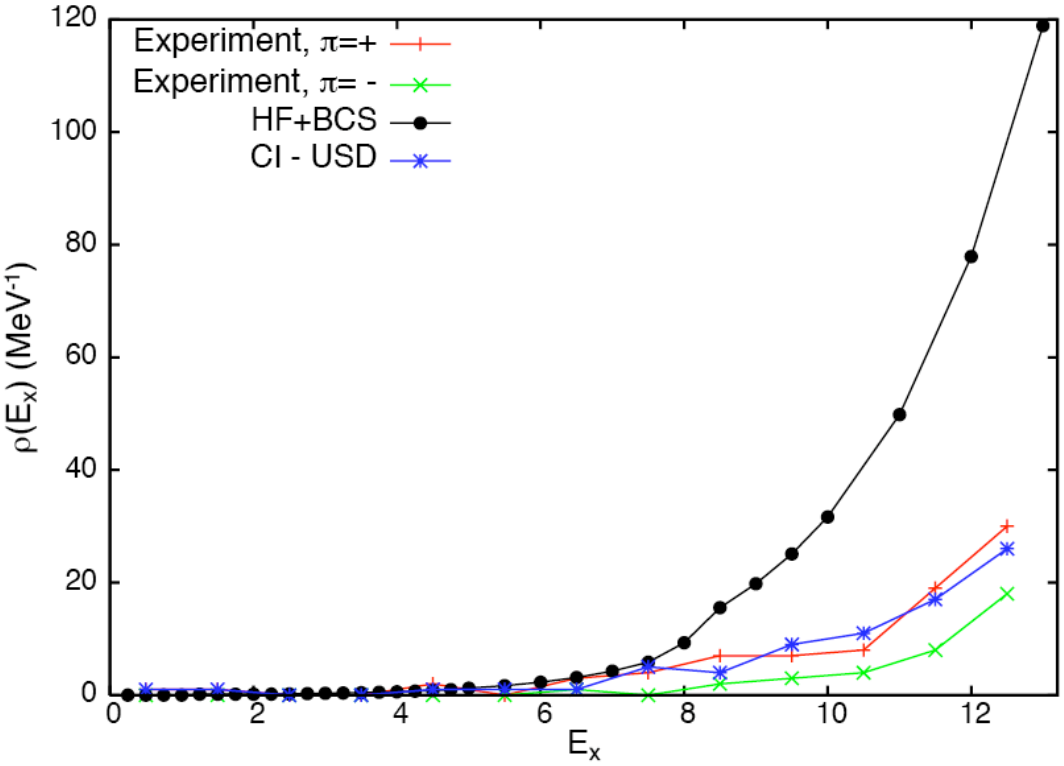
Advantages:

- used DFT-generated orbitals and effective Hamiltonians
- DFT identifies relevant configurations on the Potential Energy Surface (PES)
- Significantly lower dimensions than the full CI

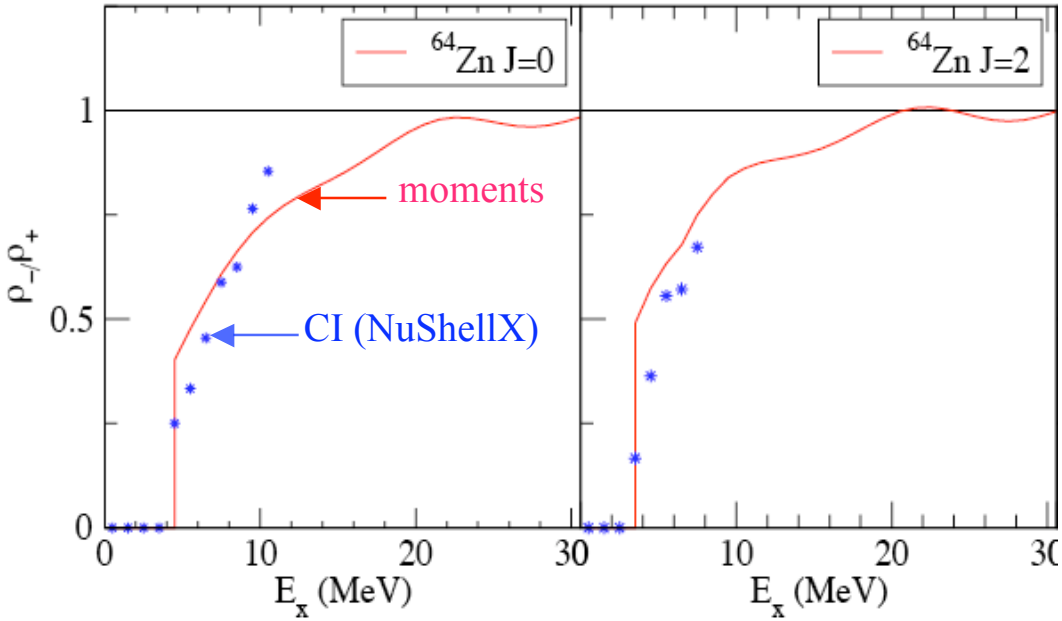
Gao and Horoi, in preparation

Accurate Nuclear Level Densities

Comparison of CI (Horoi) with HF+BCS (Goriely), and experiment



Ratio of unnatural to natural level density using moments method (Horoi - Phys. Rev. Lett. **98**, 262503 (2007) + refs), compared with recent CI (NuShellX) calculations



Will be used in reaction modeling (see Thompson's talk)

NLD and Statistical Spectroscopy

M. Horoi et al, PRC **67**, 054309 (2003), PRC **69**, 041307(R) (2004), NPA **785**, 142 (2005).

$$\rho(E_x,J,\pi) = \sum_{p\in conf} D_p(J,\pi)(FRG)\Big(E,E_p(J),\sigma_p(J)\Big)$$

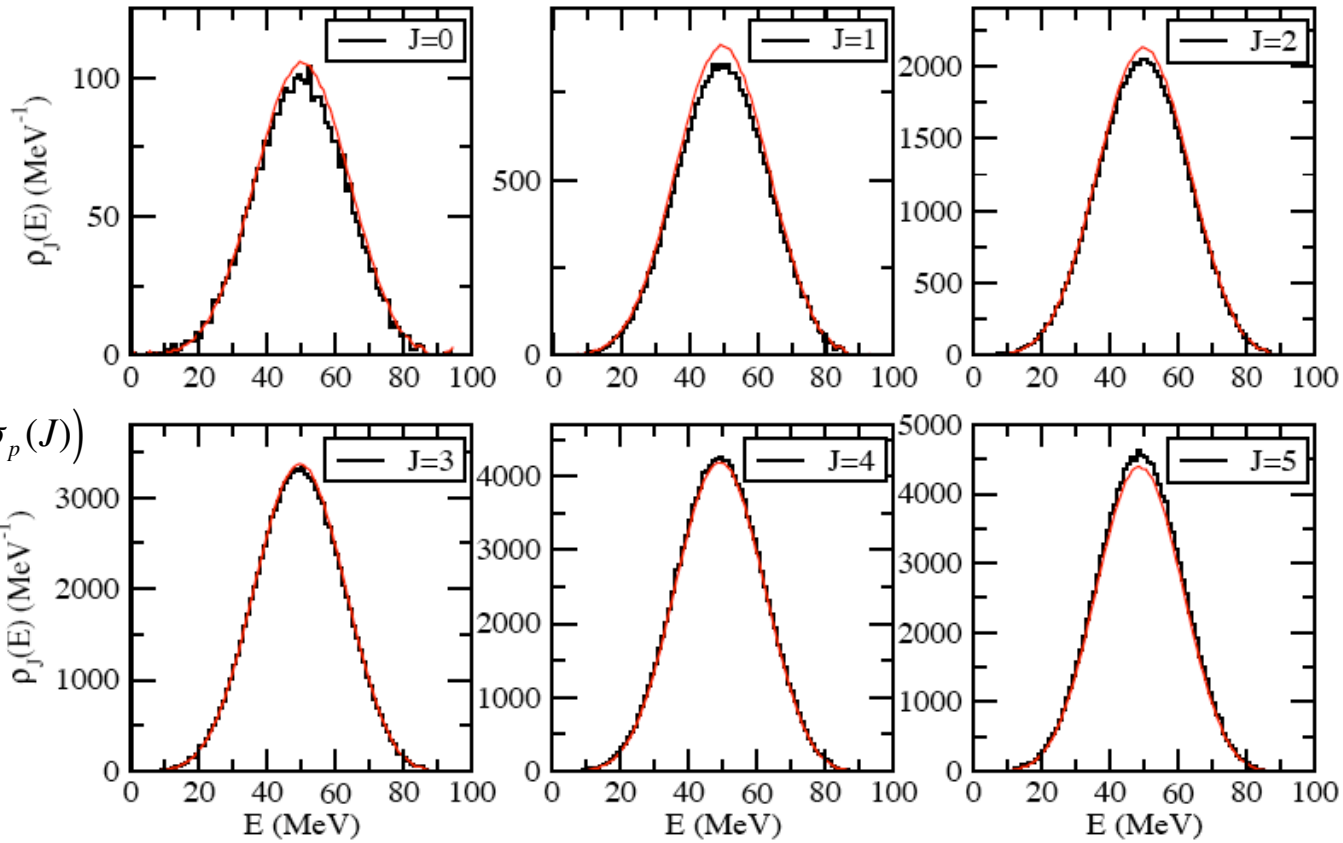
$$E_p(J),\sigma_p(J) \leftarrow Tr_{SD} < M \mid H^q \mid M >_{SD}$$

$$E_x = E - E_{g.s.}$$

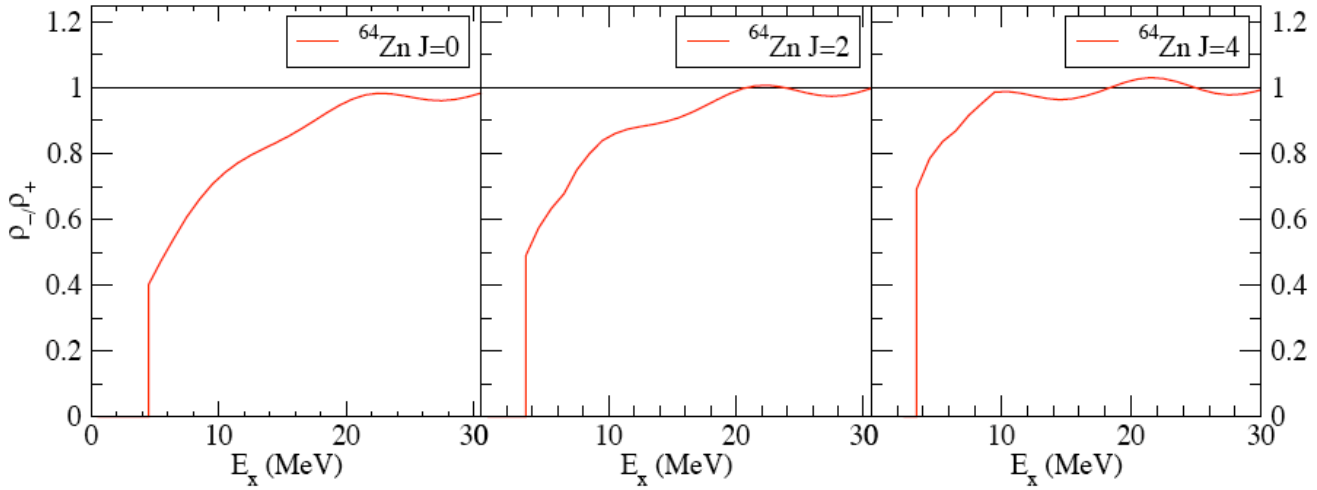
$E_{g.s.}$ from Exponential Convergence Method (ECM), PRL **82**, 2064 (1999).

Other methods:
- Ormand, PRC **56**, R1678 (1997): SMMC.
- Nakada and Alhassid, PRL **79**, 2939 (1997): SMMC
- Langanke, Phys. Lett. B **438**, 235 (1998): SMMC
- Teran and Johnson, PRC **74**, 067302 (2006): use higher moments.

^{28}Si $\pi = +$ staircase: exact shell model



$f_{5/2}$, $p_{3/2}$, $p_{1/2}$, $g_{9/2}$ model space



Coupled Cluster (CC) vs CI for Heavy Nuclei ^{56}Ni, ^{55}Ni, ^{57}Ni

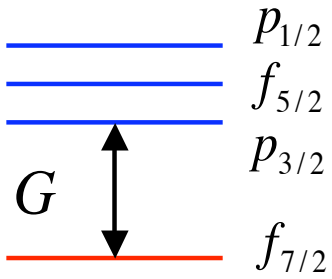
GXPF1A effective interaction

CI calculations: M. Horoi, B.A. Brown

Coupled-cluster (CC, CR-CC) calculations: J. Gour, M. Włoch, M. Lodriguito, P. Piecuch

^{56}Ni: Phys.Rev.Lett. 98, 112051 (2007)

^{55}Ni, ^{57}Ni: submitted to Phy.Rev.Lett

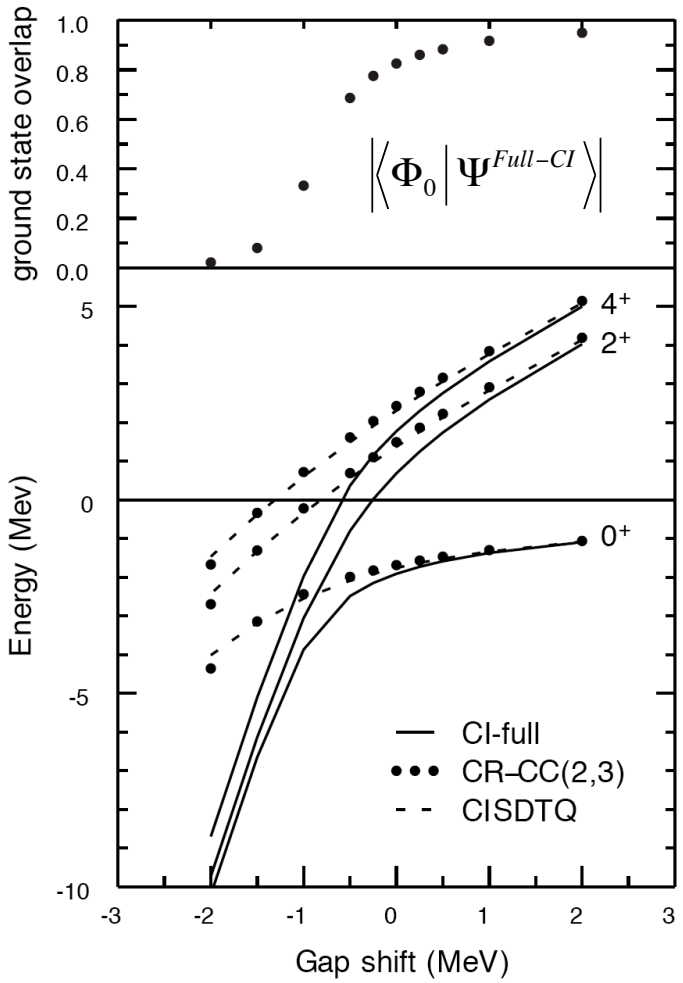


$$\Delta G = \left[\varepsilon_{pf_{5/2}} - \varepsilon_{f_{7/2}}\right] - \left[\varepsilon_{pf_{5/2}} - \varepsilon_{f_{7/2}}\right]_0$$

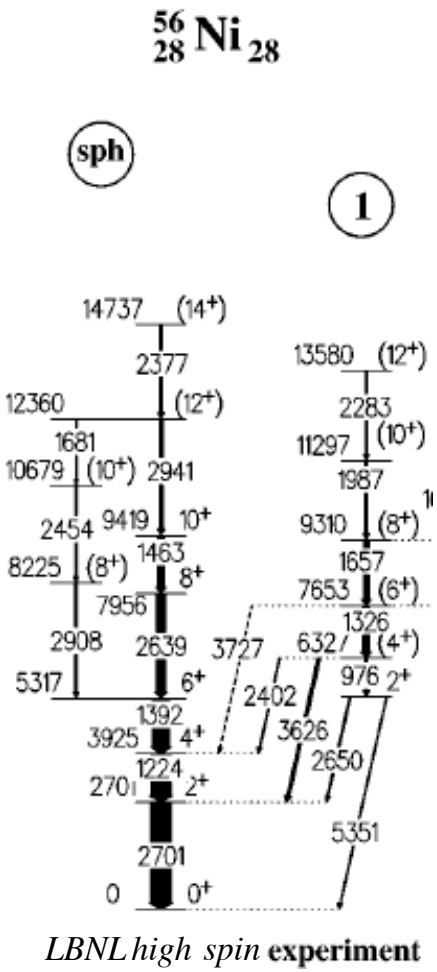
Generic Scaling:

$$CR-CC(2,3) \sim n_o^3 n_u^4 \qquad CISDTQ \sim n_o^4 n_u^6$$

^{56}Ni

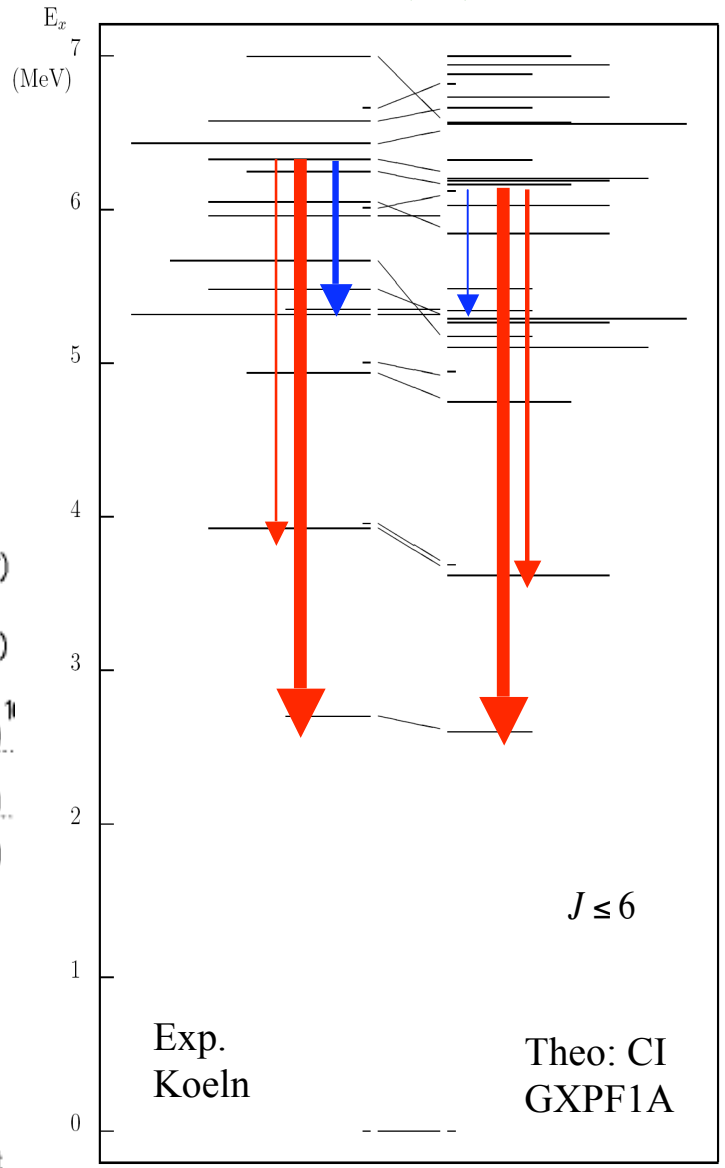


Succes story:
Low Spin States in ^{56}Ni - complete spectroscopy



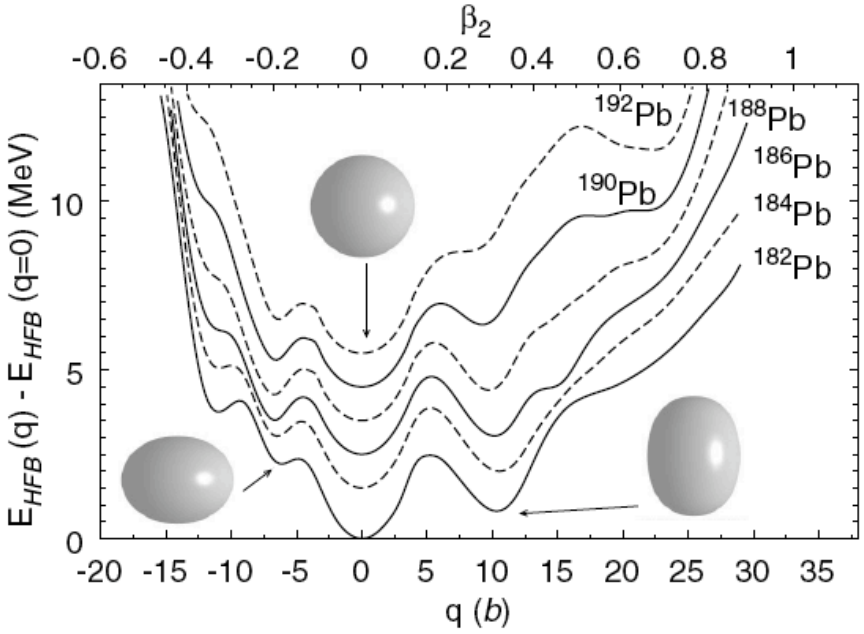
LBNL high spin **experiment**

Configuration Interaction (CI)



M. Horoi et al., in preparation

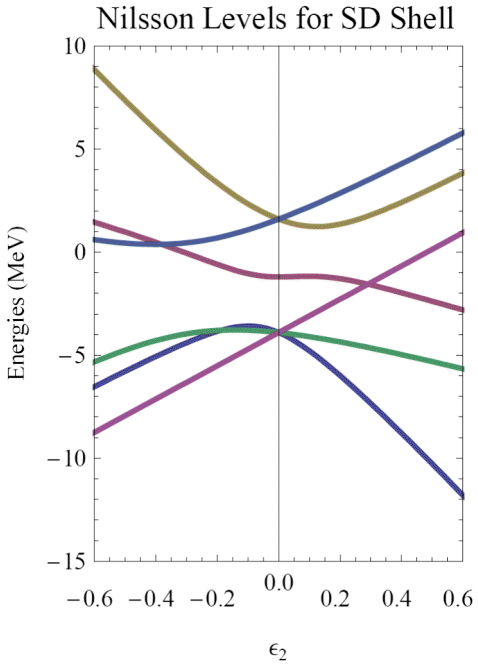
Challenge: Can we accurately describe shape coexistence using the DFT extensions (QRPA, time-dependent, CI, CC, …)?



Egido et al, PRL **93**, 082502 (2004)

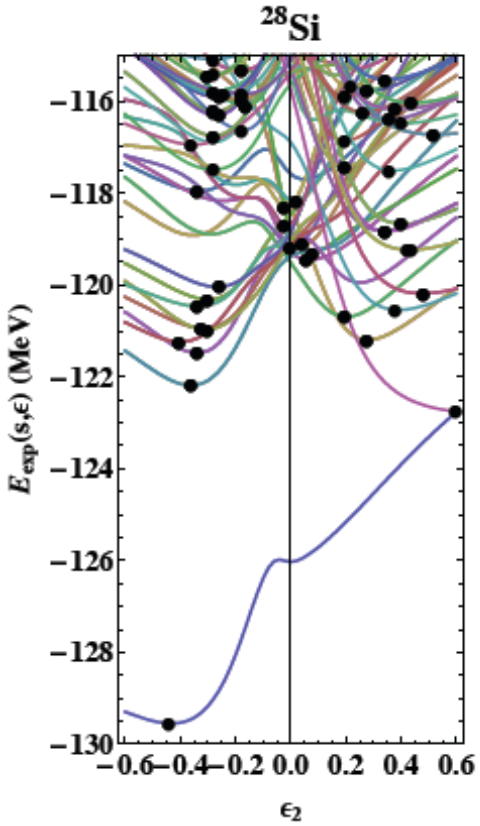
Full CI investigation of the shape coexistence region around ^{76}Sr in the $f_{5/2}pg_{9/2}$-shell: 2008 - 2009 (Horoi, Gao)

Choices of the PCI basis



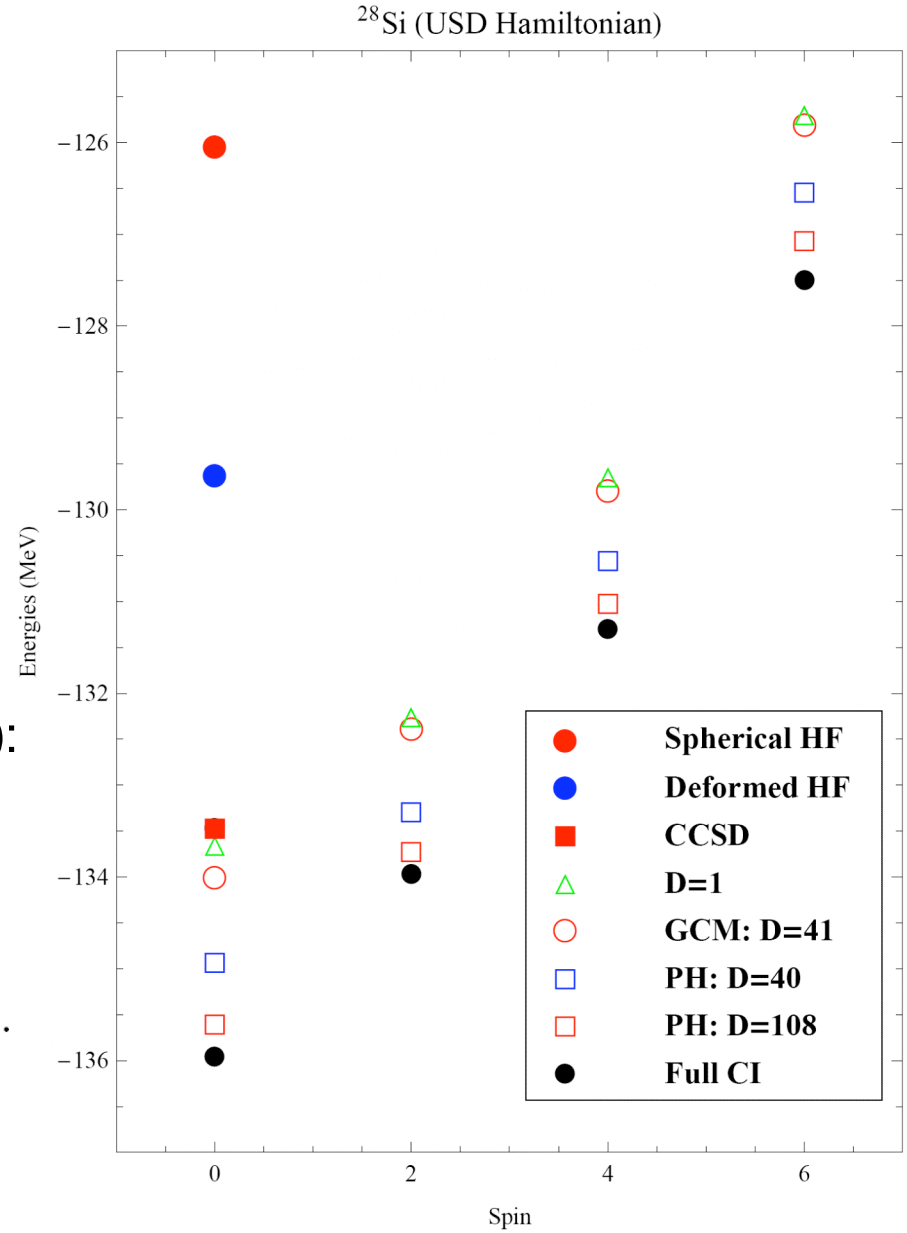
The GCM Method:
Only the G.S SDs
41 shapes
with -0.6< ϵ_2 <0.6
by 0.03

VS

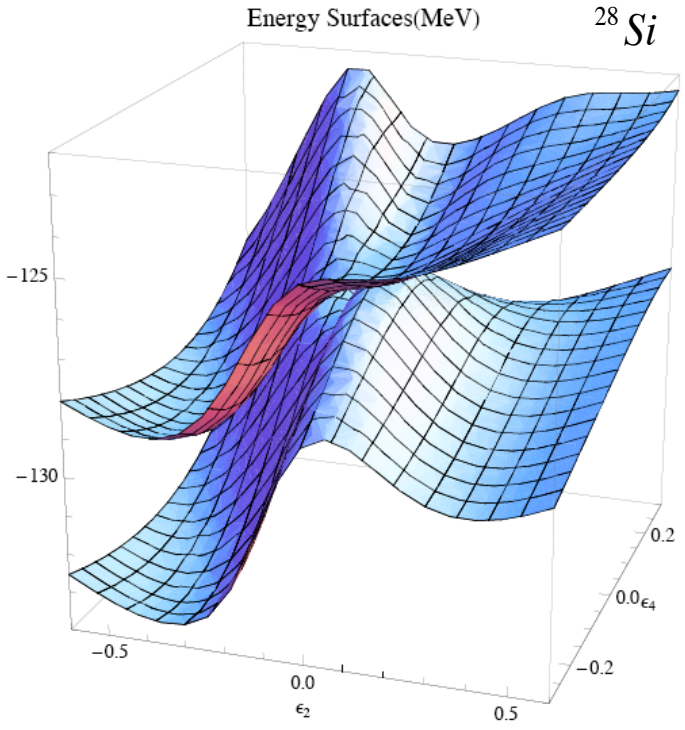


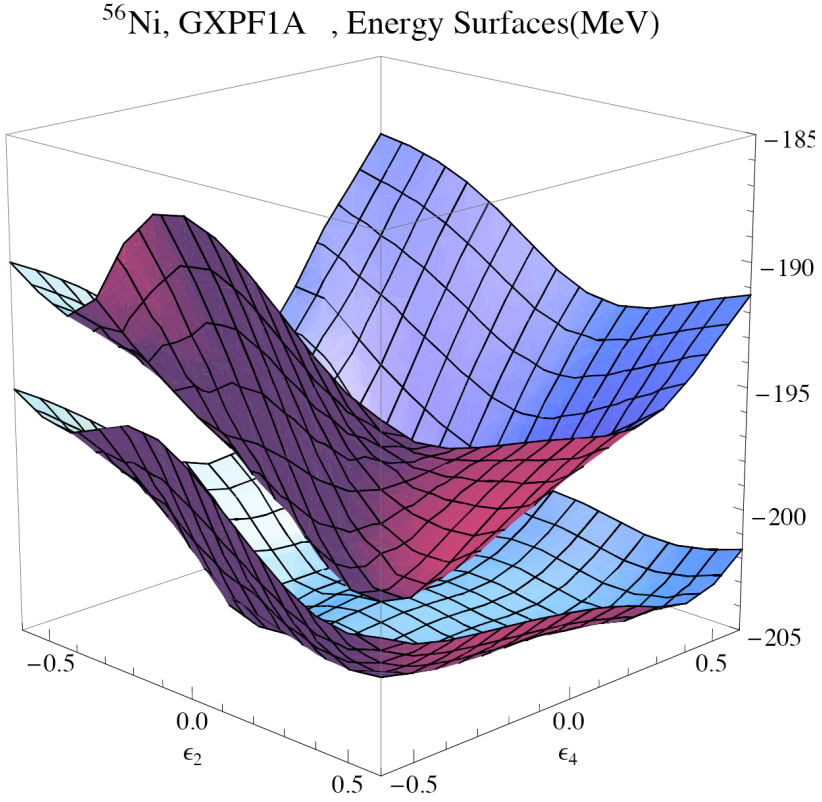
Particle-Hole states(PH):
40 total SD's
with the same shape
at minimum

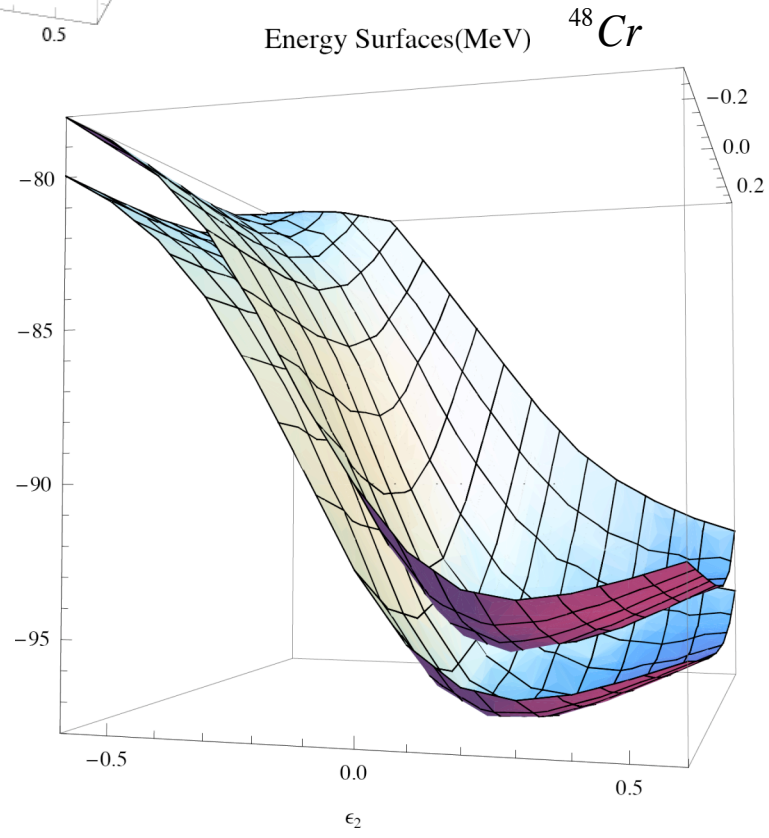
$$\epsilon_2 = -0.40, \epsilon_4 = -0.20.$$



Potential Energy Surfaces (PES)







Configuration Interaction (CI): Spherical basis vs Deformed basis

$$\phi_i(sph) \xrightarrow{DFT} \phi_j(def) \sim \phi_j(\varepsilon_2, \varepsilon_4, \ldots)$$

$$DFT \xrightarrow{MAP} H(sph) \sim H_{CI} \xrightarrow{\phi_j(def)} H(def)$$

Gao, Horoi, Bertsch