

Whither HF and HFB theory?

G.F. Bertsch
University of Washington

Darmstadt
May 7, 2012

1. Goals
2. Some successes
3. Some problems
4. Designing an effective Hamiltonian

From model to theory

Characteristics of good theories

- need only a small set of parameters
- have wide predictive power
- have intrinsic criteria for limits of validity

Goals for HFB theory

- global applicability (but with cuts generated by internal criteria)
- quantitative assessment of performance

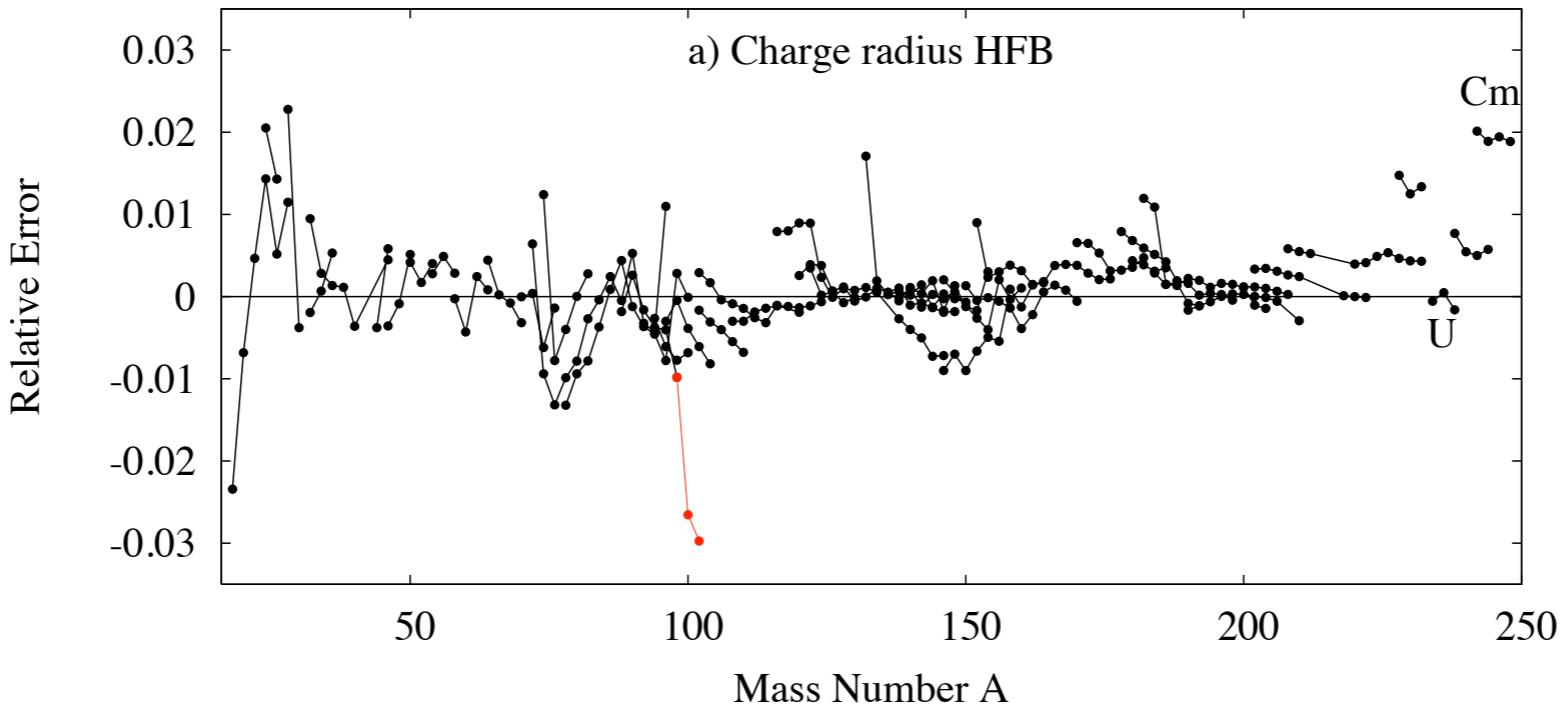
Two examples of successes

1. Charge Radii
2. 2+ excitations

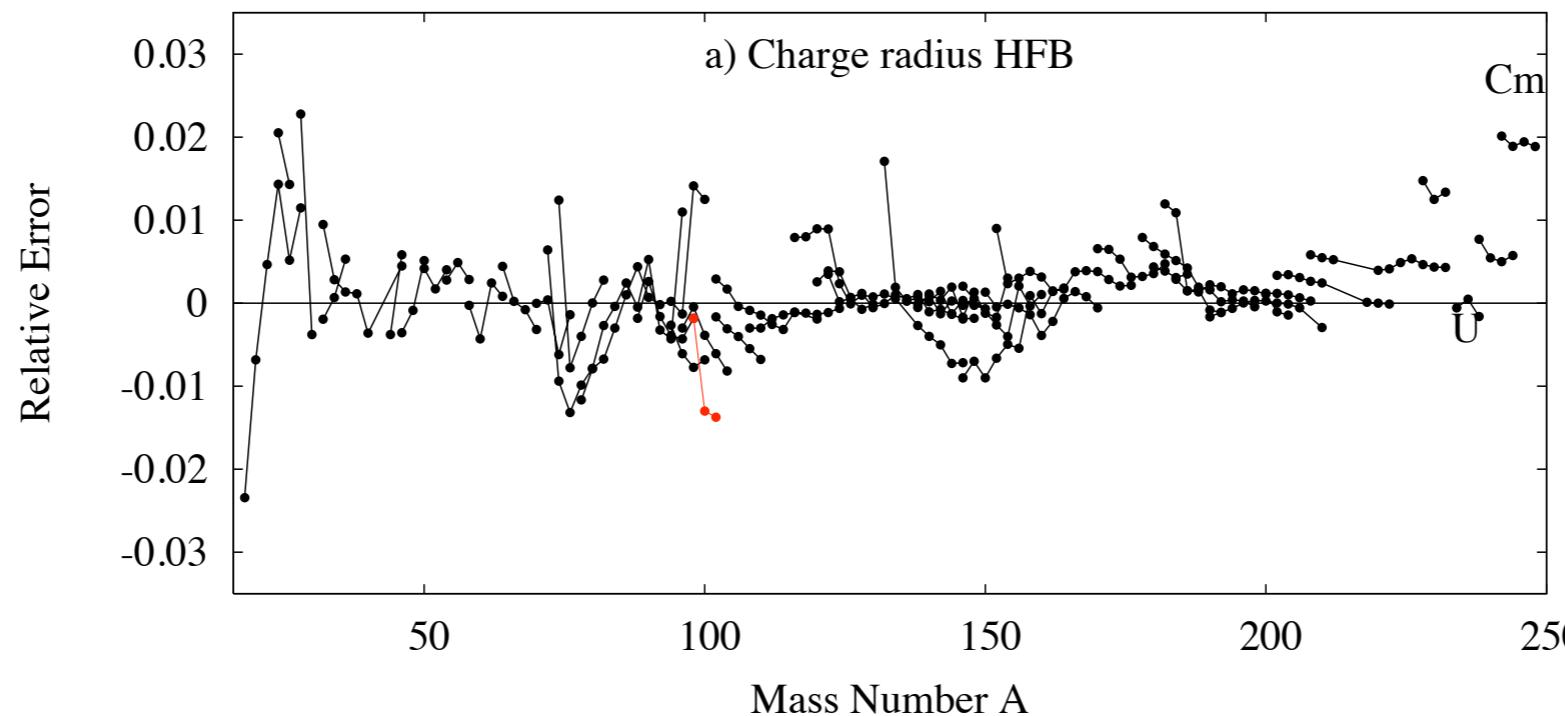
Charge radii

Experimental data from Angeli, ADNDT 87 (2004)

HFB



Relative Error



Performance on charge radius

TABLE II. Comparison of calculated charge radii with experiment: $\bar{\epsilon}$ is the mean of ϵ [see Eq. (18)]; σ is its rms dispersion about the average. Three hundred thirteen nuclear radii were included in the comparison as in Fig. 6. In the column “HFB (new)” we use the modern value $r_p = 0.875$ fm for the proton charge radius [48].

Theory	$\bar{\epsilon}$	σ
HFB	0.001	0.006
HFB (new)	0.005	0.007
CHFB+5DCH	0.006	0.007
Finite surface	0.0000	0.012

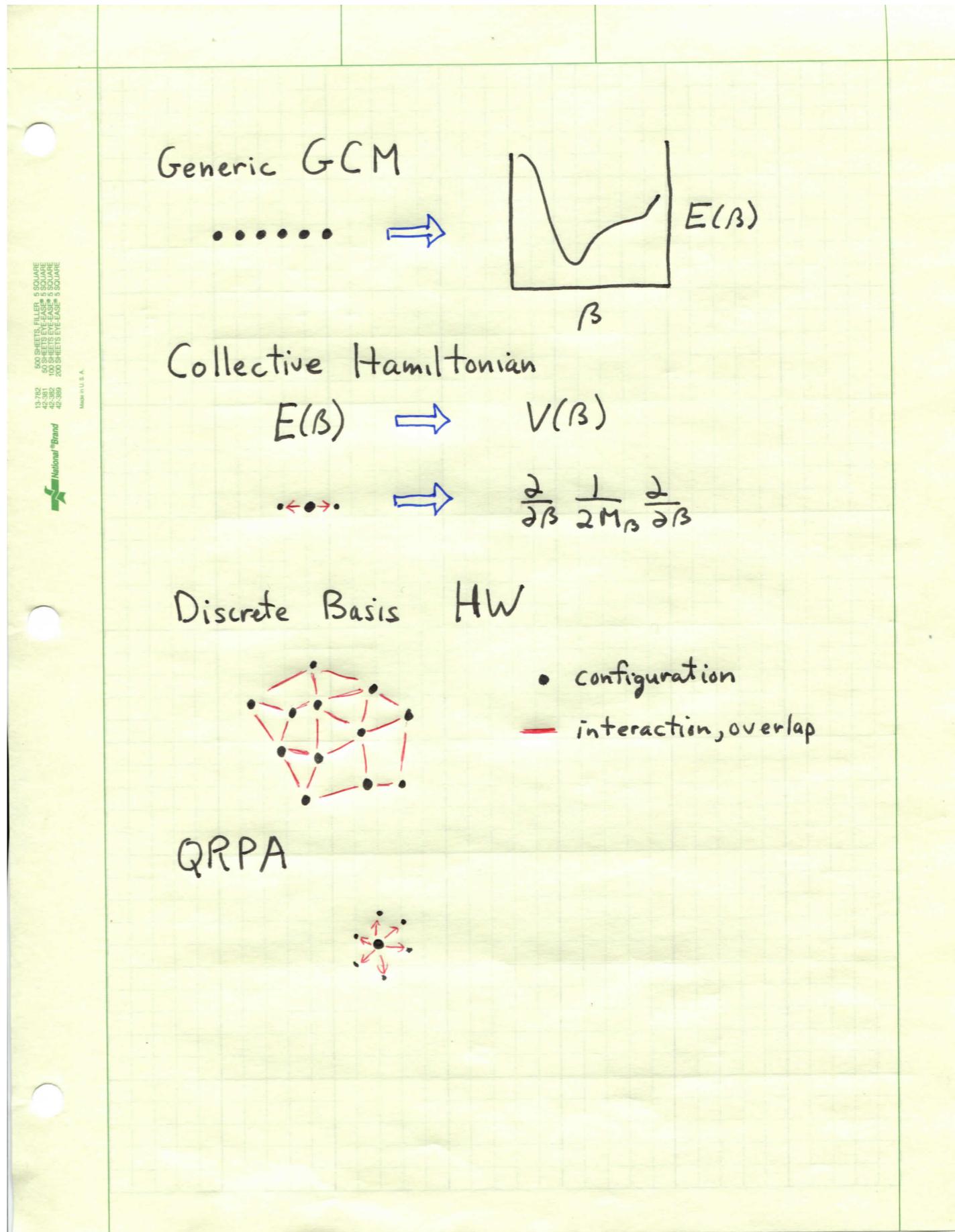
Extensions of self-consistent mean-field theory for spectroscopy

Generator Coordinate Methods

Collective Hamiltonian
GOA

Discrete-basis Hill-Wheeler

Quasiparticle RPA



Phys. Rev. C 81, 014303 (2010) [23 pages]

Structure of even-even nuclei using a mapped collective Hamiltonian and the D1S Gogny interaction

Abstract

References

Citing Articles (17)

Supplemental Material

Download: PDF (2,889 kB) Export: BibTeX or EndNote (RIS)

J.-P. Delaroche^{1,*}, M. Girod¹, J. Libert², H. Goutte¹, S. Hilaire¹, S. Péru¹, N. Pillet¹, and G. F. Bertsch^{3,*}

¹CEA, DAM, DIF, F-91297 Arpajon, France

²Institut de Physique Nucléaire IN2P3-CNRS/Université Paris-Sud, 91406 Orsay Cedex, France

³Department of Physics and Institute of Nuclear Theory, Box 351560, University of Washington Seattle, Washington 98915, USA

DOI: 10.1103/PhysRevC.81.014303 | Published: 14 March 2010

Phys. Rev. C 81, 014303 (2010) [23 pages]

Structure of even-even nuclei using a mapped collective Hamiltonian and the D1S Gogny interaction

Abstract

References

Citing Articles (17)

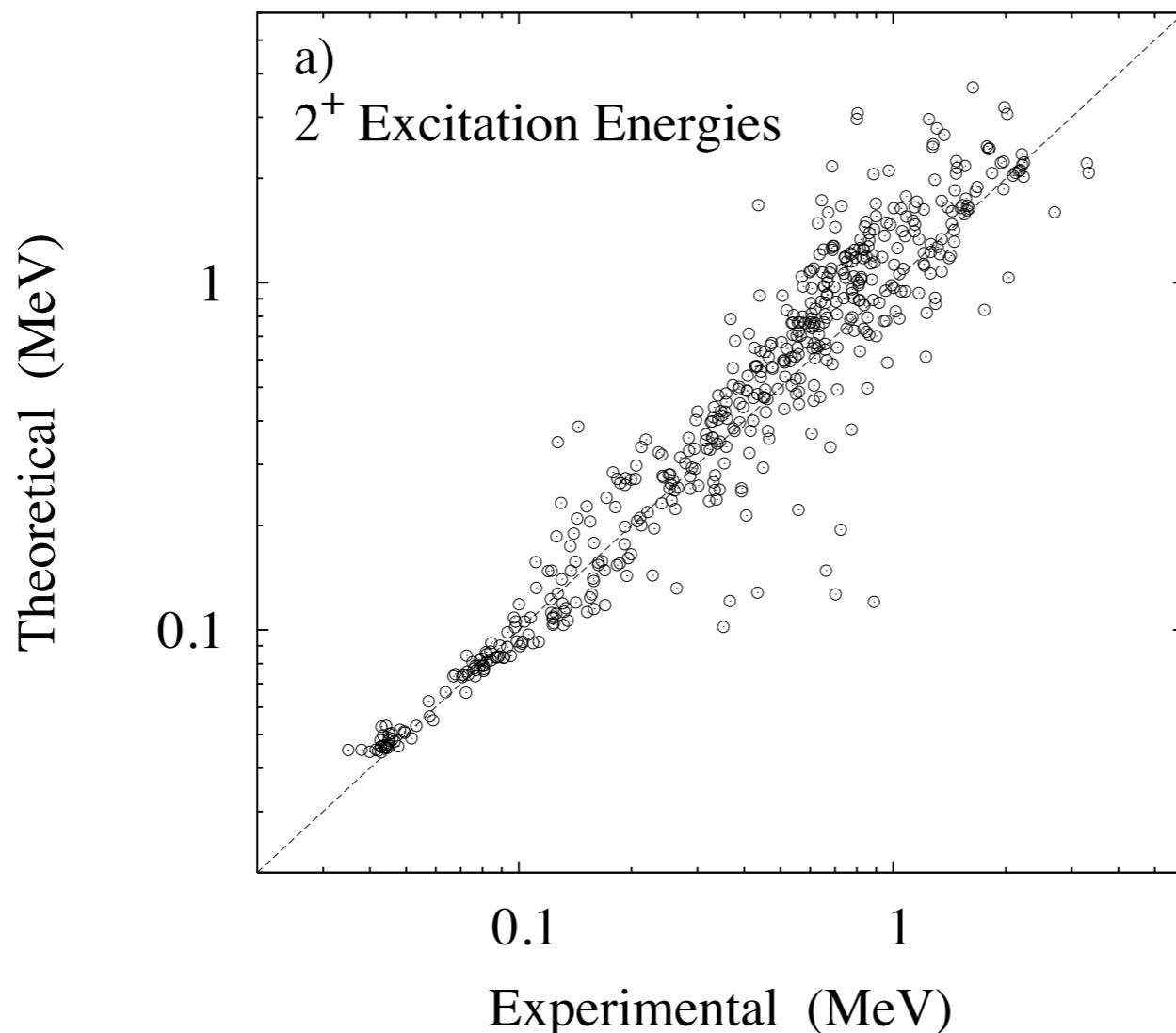
Supplemental Material

Download: PDF (2,889 kB) Export: BibTeX or EndNote (RIS)

EPAPS

- README.TXT
- 5dch.txt
- heading_5dch-table-eng.doc

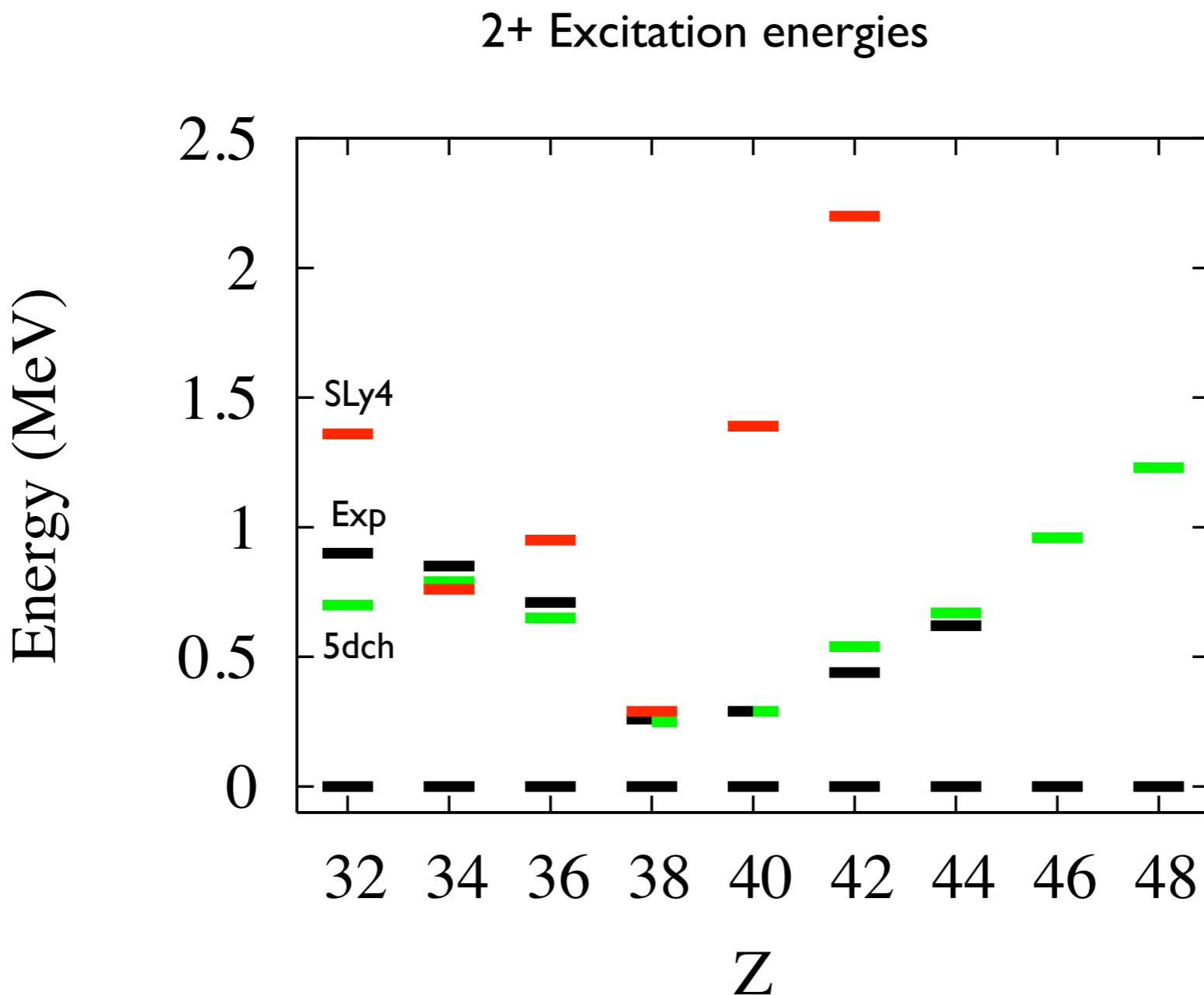
The first excited 2+ state



$$E_{theory} = (1.12 \pm 40\%) \times E_{exp} \quad \text{over 2 orders of magnitudes}$$

Dispersion from $\langle \log(E_t/E_x) \rangle$

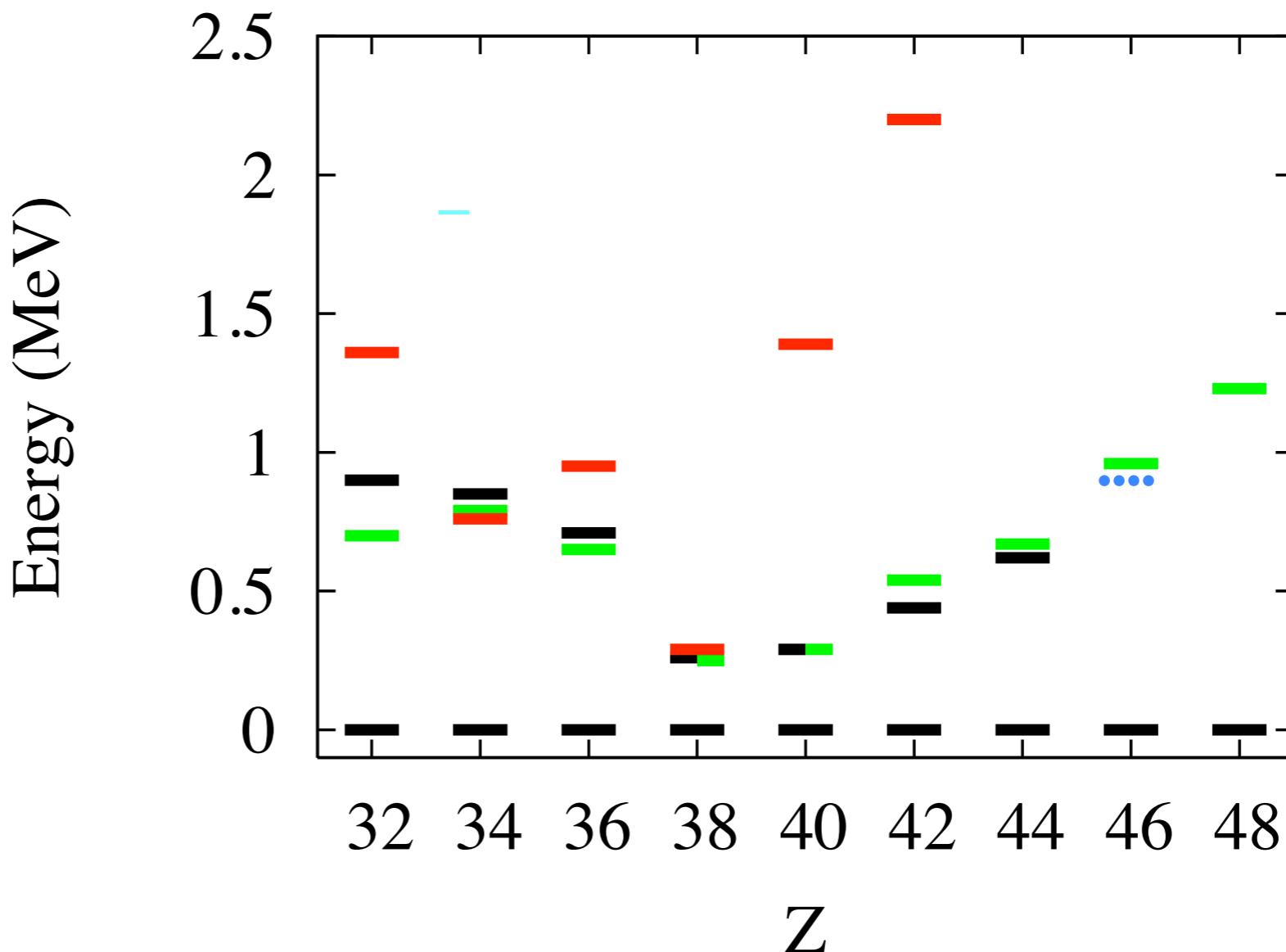
The CEA global survey, on the N=Z line

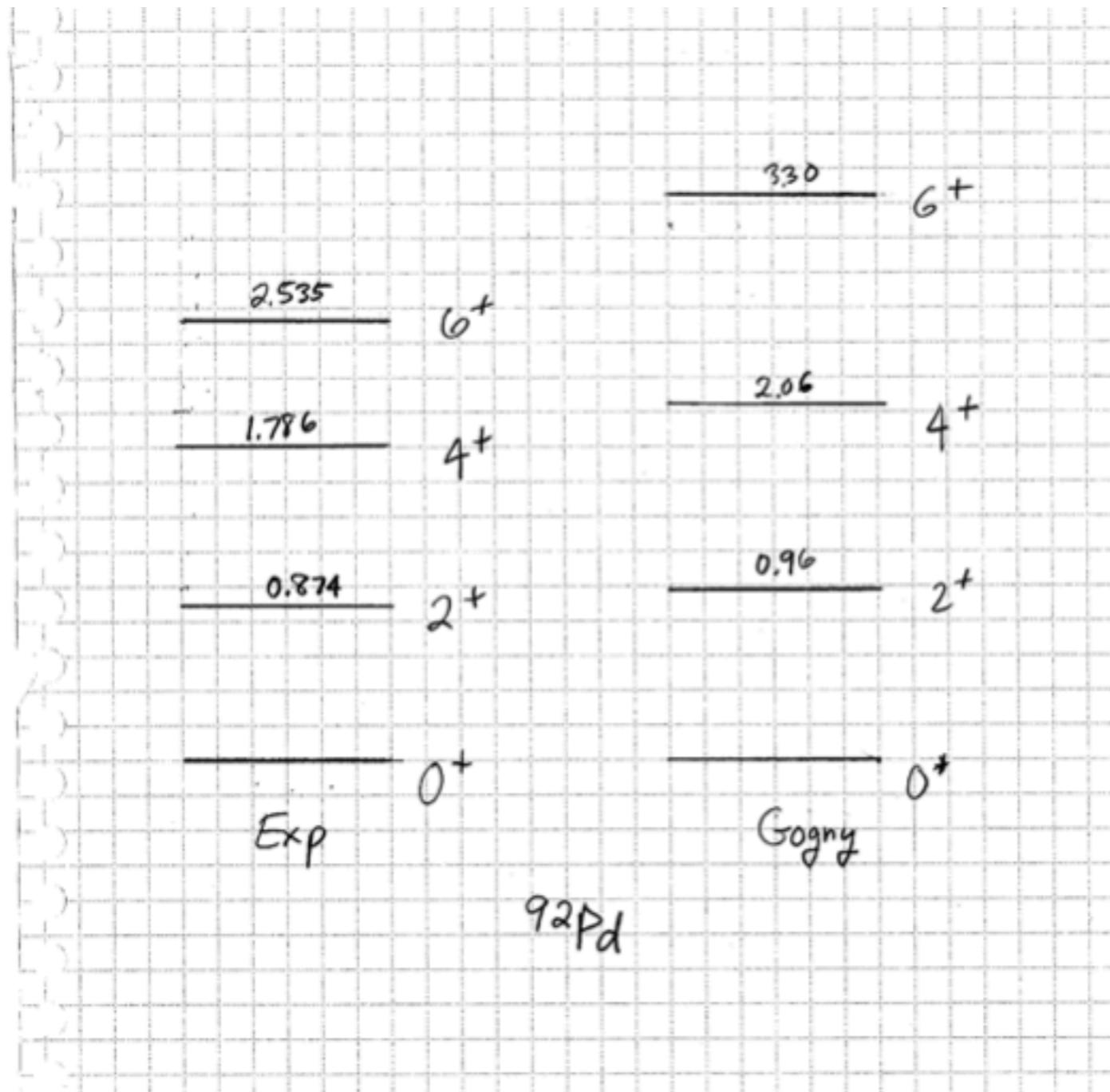


J-P. Delaroche, M. Girod, J. Libert, H. Goutte, S. Hilaire, S. Peru, N.
Pillet, and G.F. Bertsch,
Phys. Rev. C 81 014303 (2010)

Evidence for a spin-aligned neutron–proton paired phase from the level structure of ^{92}Pd

B. Cederwall¹, F. Ghazi Moradi¹, T. Bäck¹, A. Johnson¹, J. Blomqvist¹, E. Clément², G. de France², R. Wadsworth³, K. Andgren¹, K. Lagergren^{1,4}, A. Dijon², G. Jaworski^{5,6}, R. Liotta¹, C. Qi¹, B. M. Nyakó⁷, J. Nyberg⁸, M. Palacz⁵, H. Al-Azri³, A. Algora⁹, G. de Angelis¹⁰, A. Ataç¹¹, S. Bhattacharyya^{2†}, T. Brock³, J. R. Brown³, P. Davies³, A. Di Nitto¹², Zs. Dombrádi⁷, A. Gadea⁹, J. Gál⁷, B. Hadinia¹, F. Johnston-Theasby³, P. Joshi³, K. Juhász¹³, R. Julin¹⁴, A. Jungclaus¹⁵, G. Kalinka⁷, S. O. Kara¹¹, A. Khaplanov¹, J. Kownacki⁵, G. La Rana¹², S. M. Lenzi¹⁶, J. Molnár⁷, R. Moro¹², D. R. Napoli¹⁰, B. S. Nara Singh³, A. Persson¹, F. Recchia¹⁶, M. Sandzelius^{1†}, J.-N. Scheurer¹⁷, G. Sletten¹⁸, D. Sohler⁷, P.-A. Söderström⁸, M. J. Taylor³, J. Timár⁷, J. J. Valiente-Dobón¹⁰, E. Vardaci¹² & S. Williams¹⁹

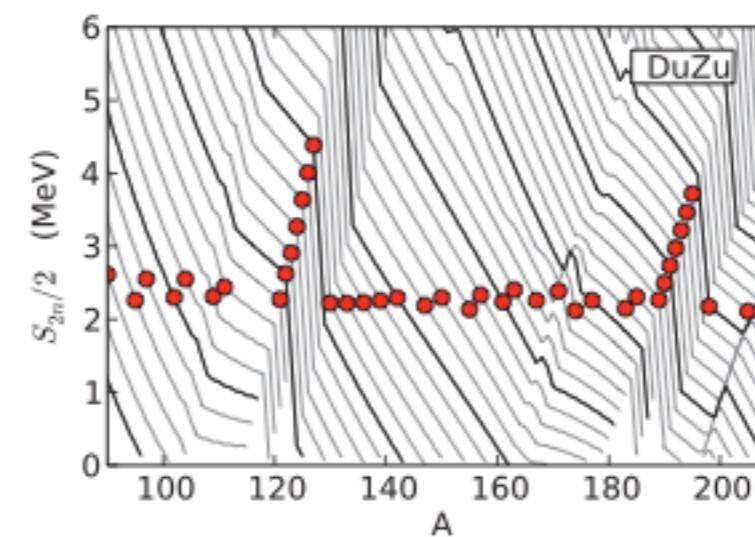
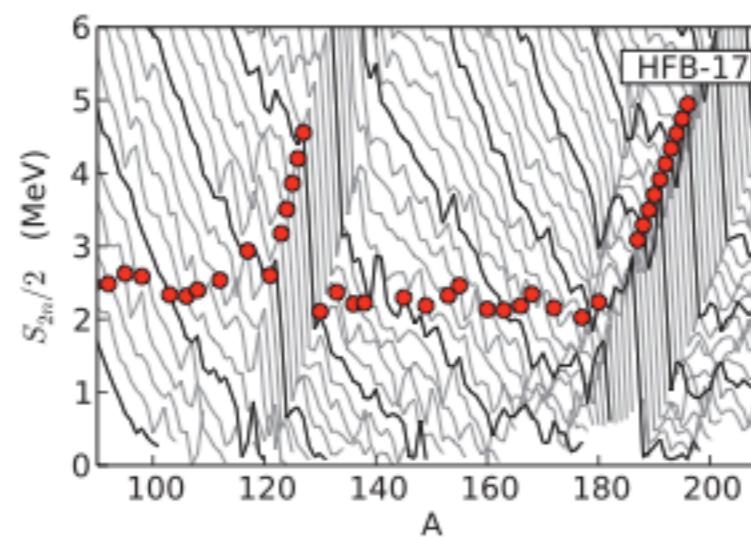
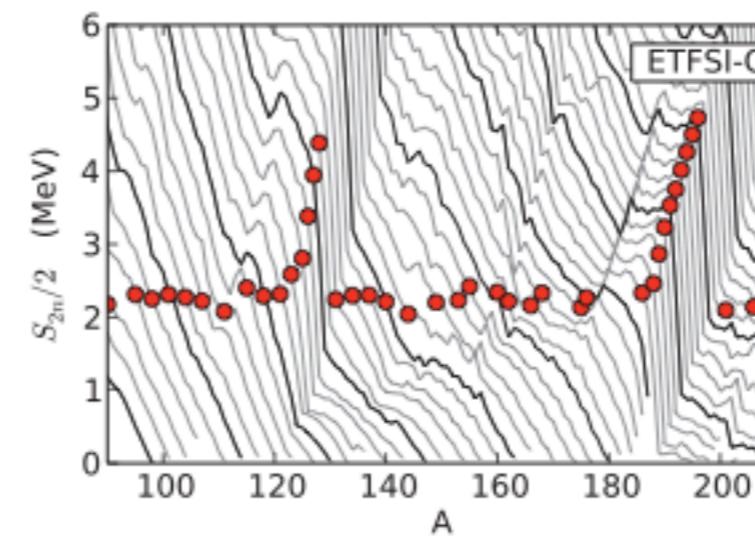
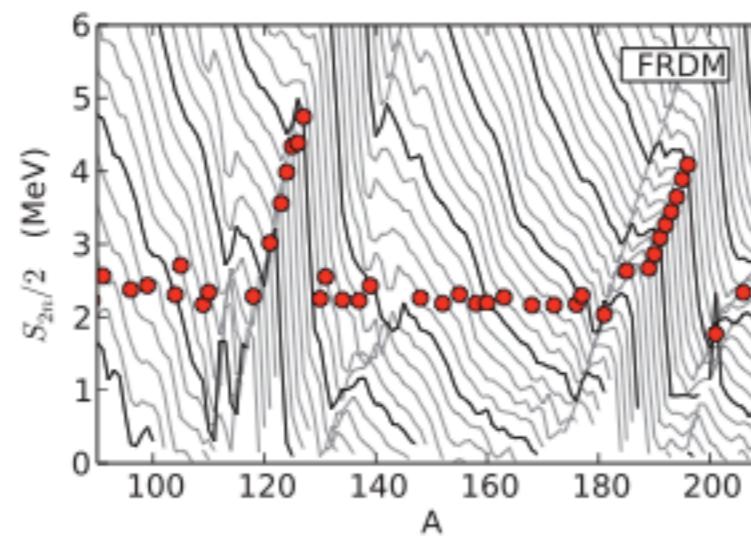




Problems with the standard functionals

1. Smoothness
2. Not reliably extendable

2-nucleon separation energies



Hamiltonian vs Energy Functional

We would like to have an effective Hamiltonian:

$$H = ta^\dagger a + v^{(2)}a^\dagger a^\dagger aa + v^{(3)}a^\dagger a^\dagger a^\dagger aaa$$

but we use up to now is an energy functional of the form:

$$H = ta^\dagger a + v^{(2)}(r - r')a_r^\dagger a_{r'}^\dagger a_{r'} a_r + t_3 \rho(r)^{1/3} v^{(3)} a_r^\dagger a_{r'}^\dagger a_r a_r$$

Skyrme: $v(2)$ is contact with up to two derivatives.

Gogny: $v(2)$ is a two-term Gaussian.

Why the power 1/3 in the density-dependent term?

--incompressibility

--many-body theory of weakly interacting Fermi gas

Example of Pb-208

^{208}Pb energy	Ska	D1S
Kinetic	3863	3920
Coulomb direct/exchange	831/-31	832/-31
Spin-orbit	-97	-105
Central 2B	-12480	-12783
t_3	6274	6530
Total	-1640	-1637

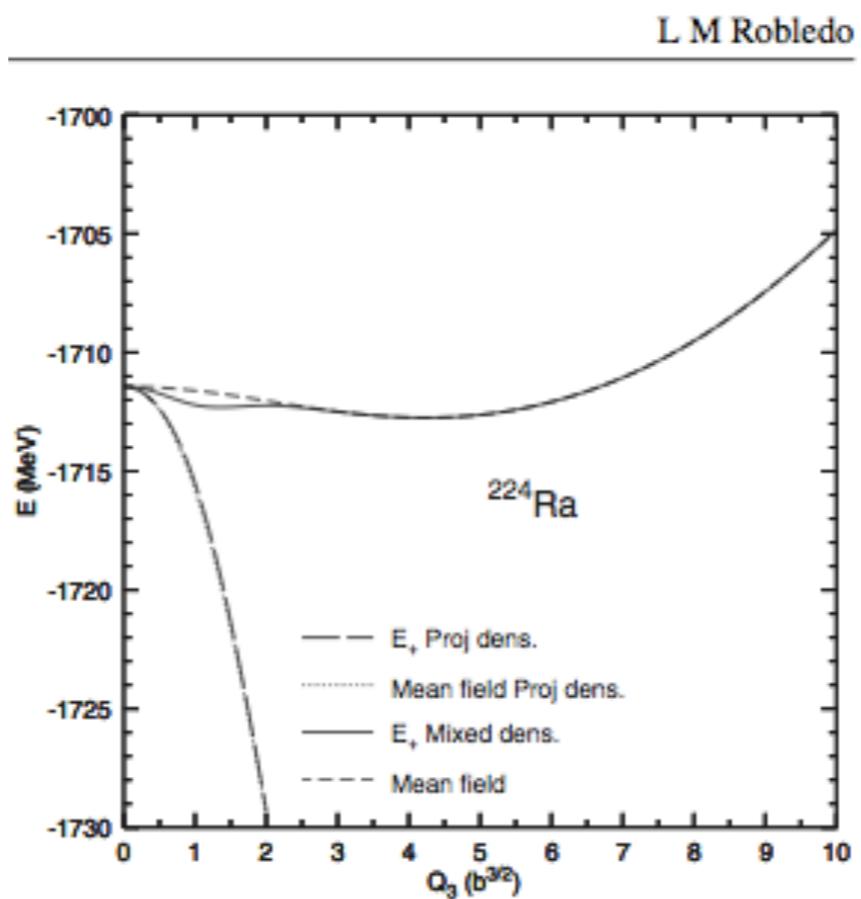
What $\rho(r)$ goes into \hat{H} for the wave function $|\psi\rangle = \sum_{\alpha} c_{\alpha} |HFB_{\alpha}\rangle$?

Choices:

a) $\rho(r) = \langle \psi | \hat{\rho}(r) | \psi \rangle$

b) $\rho(r) = \langle HFB_{\alpha} | \hat{\rho}(r) | HFB_{\beta} \rangle$ for computing $c_{\alpha} c_{\beta} \langle HFB_{\alpha} | \hat{H} | HFB_{\beta} \rangle$

Consequences of the choices:



L.M. Robledo, J.Phys. G 37 064020 (2010)

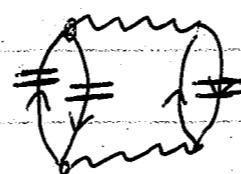
Induced 3-body Interaction

Lee/Yang/Galitskii 1958 - see Fetter & Walecka

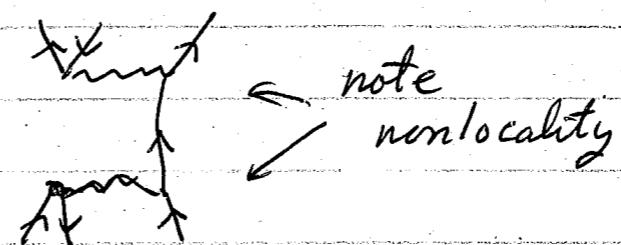
$$E/N = \frac{3}{5} \frac{k_F^2}{2m} + C_1 a k_F + C_2 a^2 k_F^4 + \dots$$

a is scattering length

Arises from



Operator in Fock space



Coordinate-space reduction: $\langle \cdot \cdot \cdot \rangle = \frac{1}{w - k^2/2m}$ set $w=0$.

↓

$$C \int d^3r d^3r' \frac{\rho^3(r, r')}{|r - r'|}$$

The effective one-body Hamiltonian

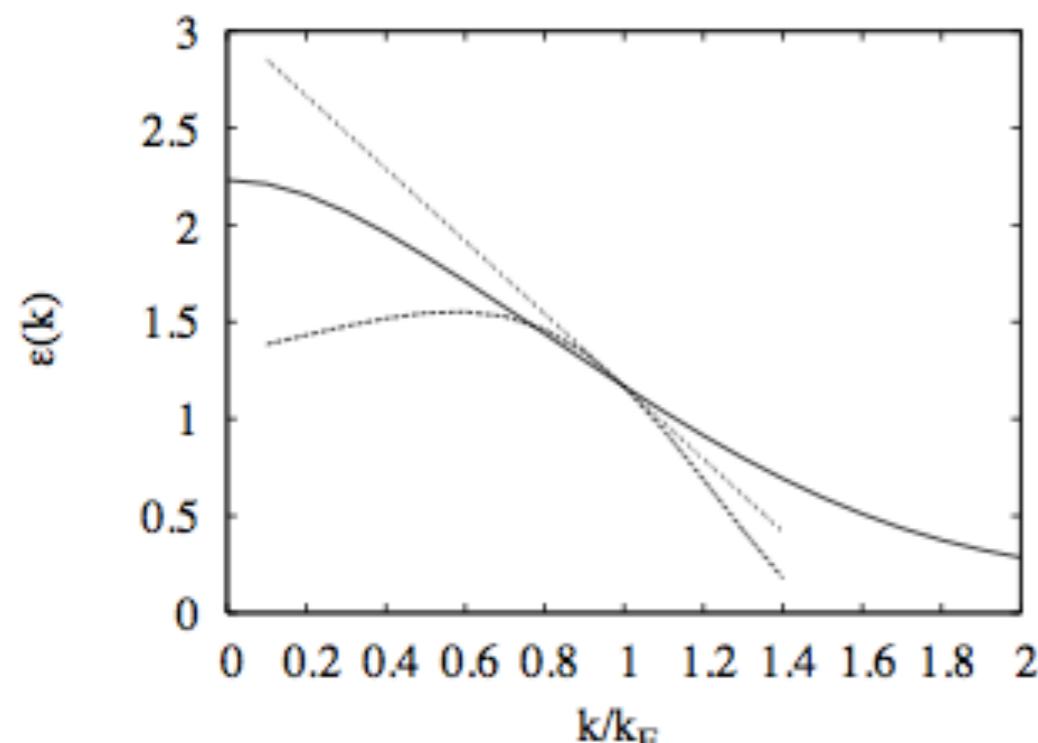


TABLE VIII. The same as Table VII, except for the UNEDF0.

k	Par.	\hat{x}	95% CI	% of Int.	σ
1	ρ_c	0.160526	[0.160,0.161]	10	0.001
2	E^{NM}/A	-16.0559	[-16.146,-15.965]	45	0.055
3	K^{NM}	230	-	-	-
4	$a_{\text{sym}}^{\text{NM}}$	30.5429	[25.513,35.573]	126	3.058
5	$L_{\text{sym}}^{\text{NM}}$	45.0804	[-20.766,110.927]	219	40.037
6	$1/M_s^*$	0.9	-	-	-
7	$C_0^{\rho\Delta\rho}$	-55.2606	[-58.051,-52.470]	9	1.697
8	$C_1^{\rho\Delta\rho}$	-55.6226	[-149.309,38.064]	94	56.965
9	V_0^n	-170.374	[-173.836,-166.913]	3	2.105
10	V_0^p	-199.202	[-204.713,-193.692]	6	3.351
11	$C_0^{\rho\nabla J}$	-79.5308	[-85.160,-73.901]	16	3.423
12	$C_1^{\rho\nabla J}$	45.6302	[-2.821,94.081]	65	29.460

“UNEDF0” Phys. Rev. C 82 024313 (2010)

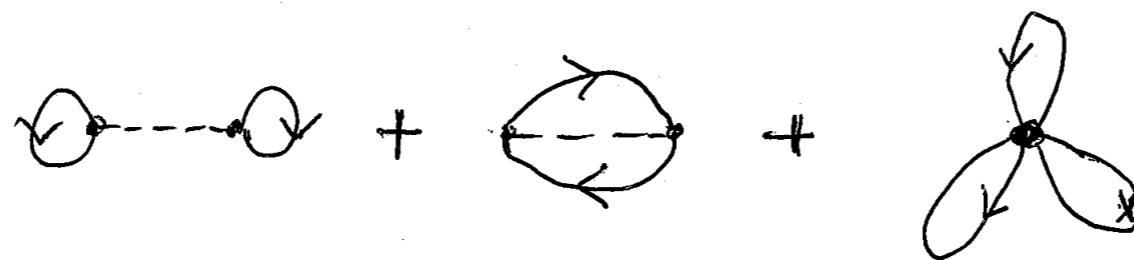
What should be in the next generation HFB theory?

1. Replace energy density functional by an effective Hamiltonian.
2. Get rid of contact interactions.
3. Allow maximum nonlocality consistent with computational feasibility. Should one keep Galilean invariance?
 - (+) conservation laws
 - (--) tuning to nuclear matter

Robledo Codes

$\text{---} = \text{sum of Gaussians}$

$$e^{-r^2} = e^{-x^2} e^{-y^2} e^{-z^2} \quad \text{Brink/Boeker/Talman/Bogolyubov}$$



An easy extension

$$\text{---} \Rightarrow \text{---} = \text{---} + \text{---}$$

