GCM and QRPA

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Saclay, June 1, 2012

Collaborators and other people I bothered

P.-H. Heenen, J.-M. Yao, V. Hellemans

M. Bender, B. Avez

A. Pastore

D. Tarpanov

J. Toivanen

P.-G. Reinhard

The main codes I used

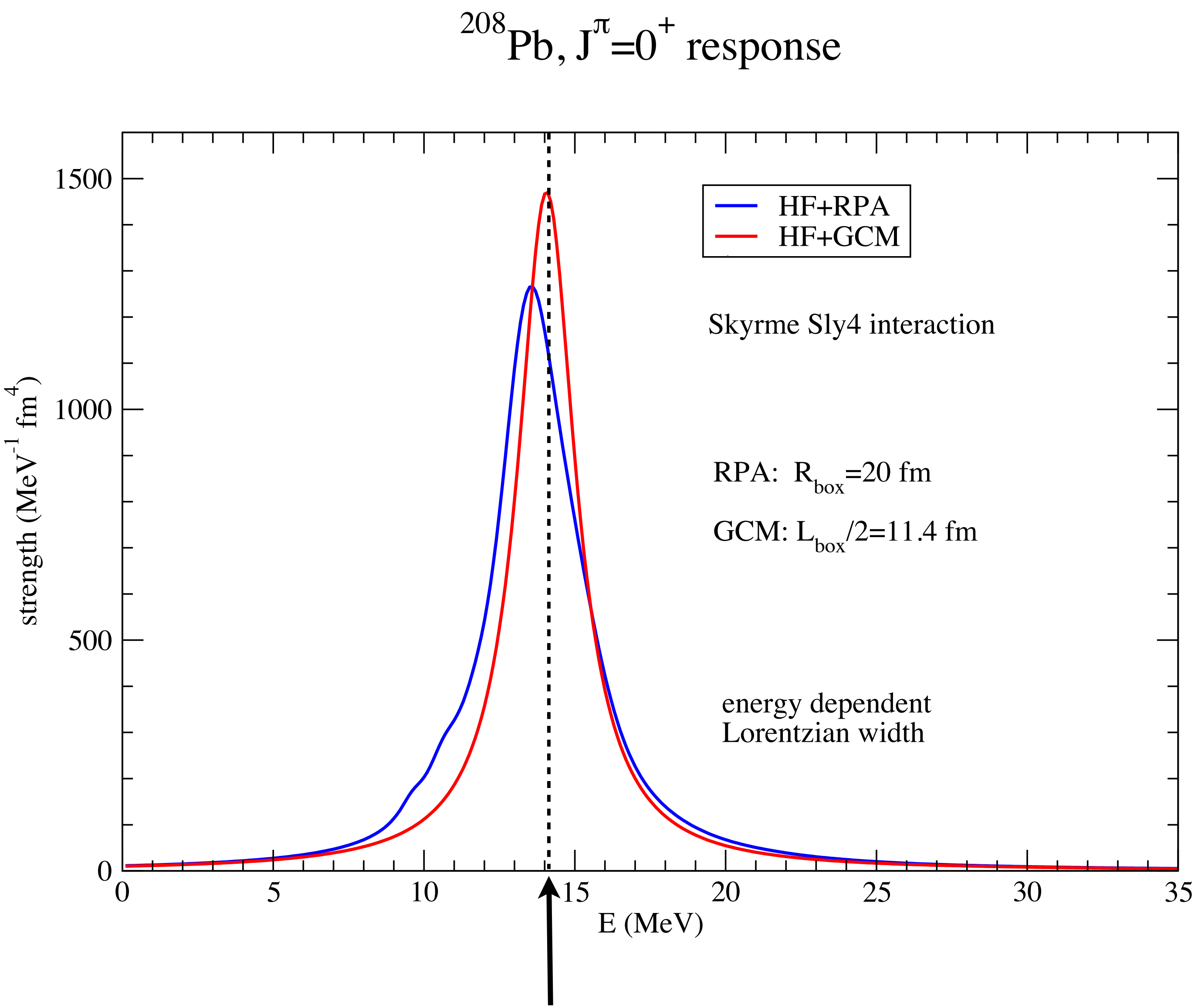
GCM side:

- HFBCS: ev8
- projection + kernel calculation: promesse
- (P. Bonche, H. Flocard, P.-H. Heenen, M. Bender)

QRPA side:

- sphHFB
- QRPA (J. Terasaki)

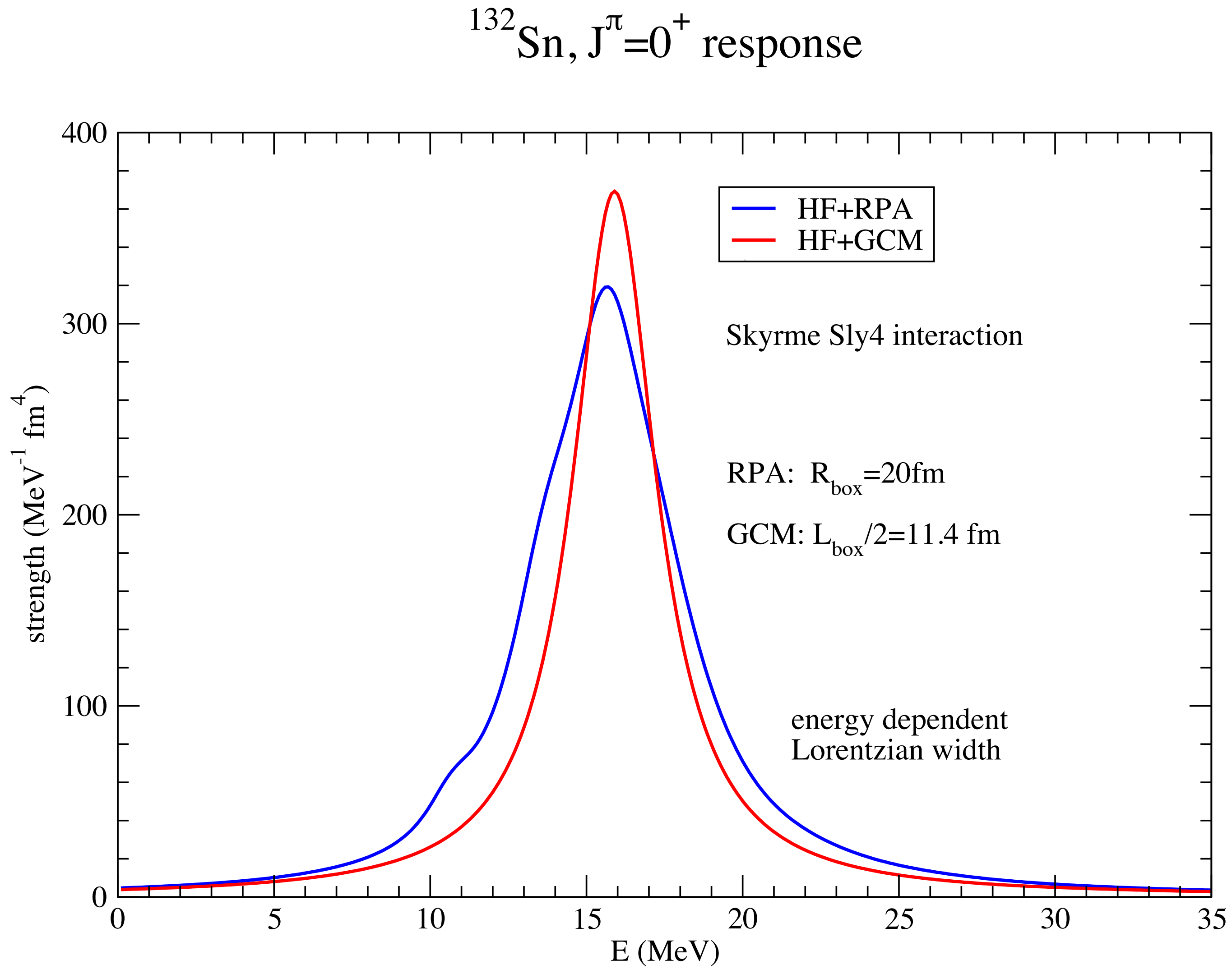
Monopole response



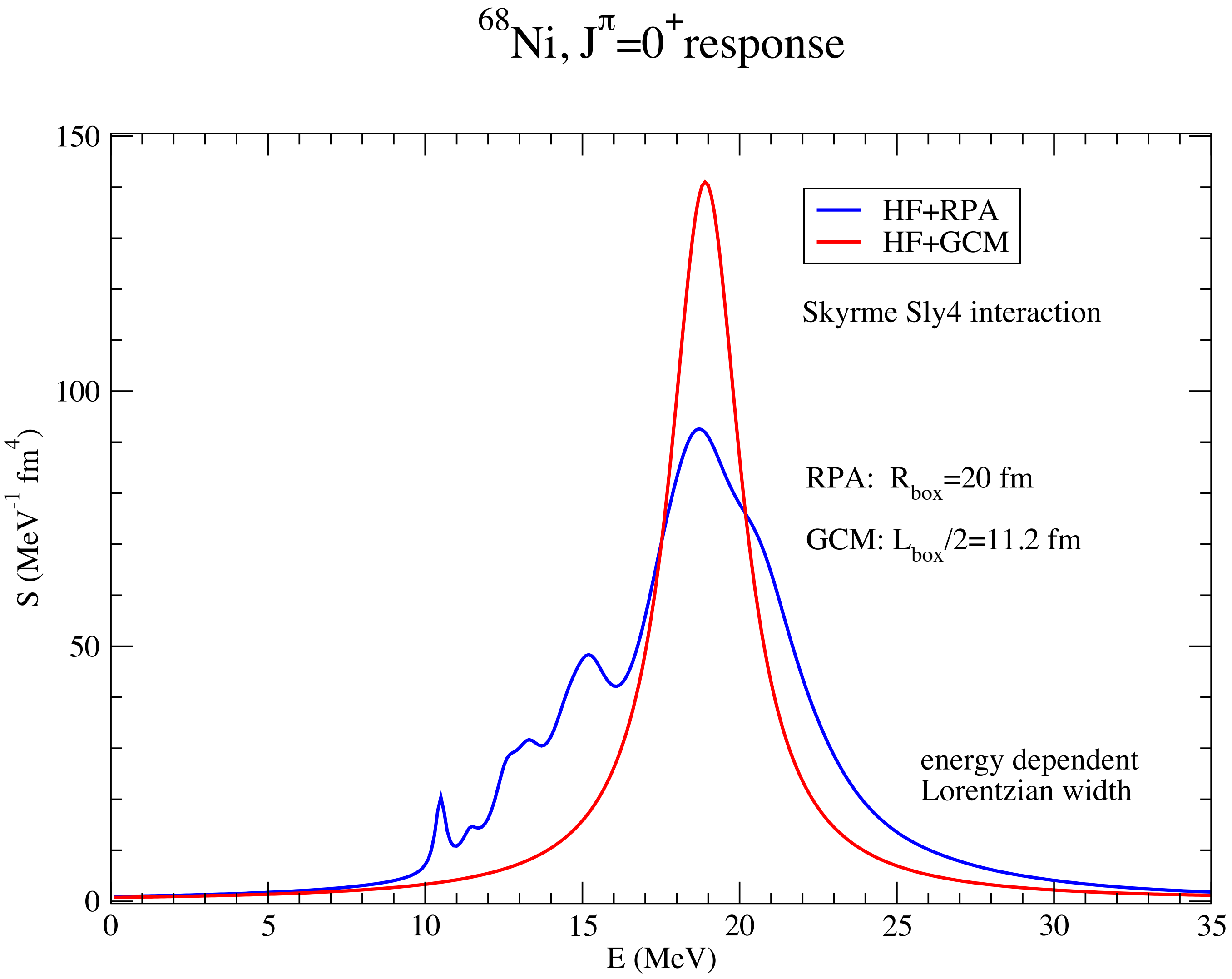
experimental $m_1/m_0 = 14.18 \pm 0.11$ MeV

(Youngblood et al, PRL82 (1999))

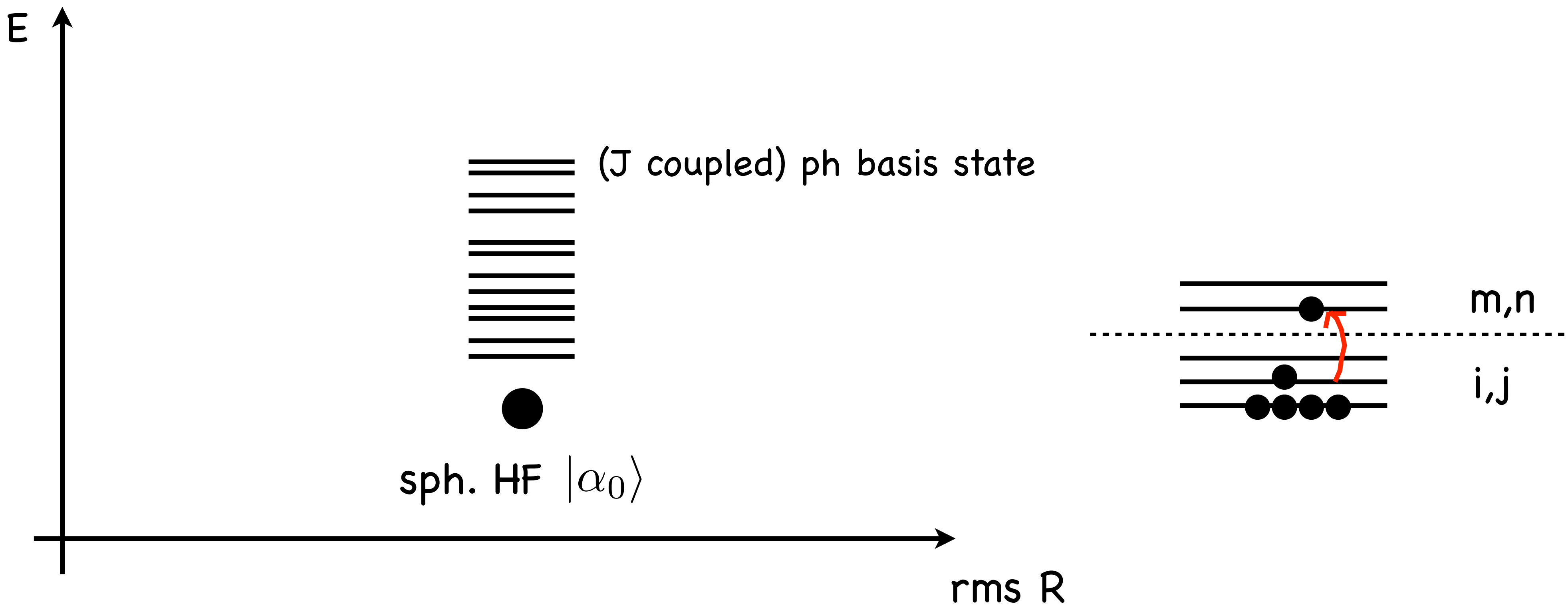
Monopole response



Monopole response



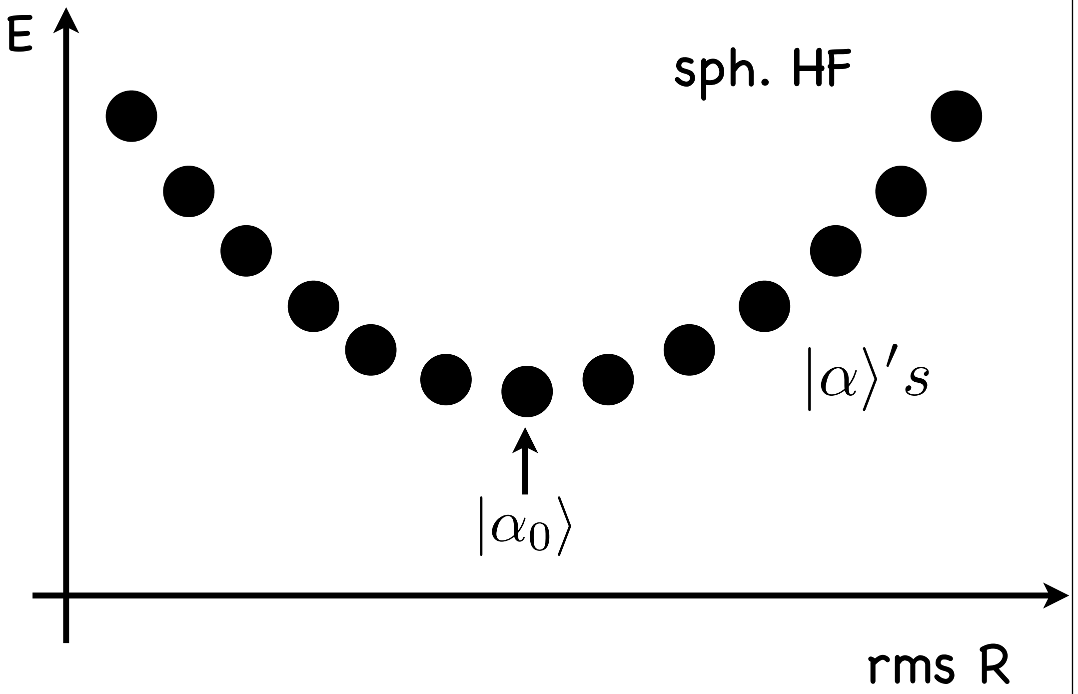
Single reference (RPA) vs. Multi reference (GCM)



$$|RPA(k)\rangle = \sum_{mi} \left(X^k_{mi} \left(a^\dagger_m a_i \right)^{J^\pi} - Y^k_{mi} \left(a^\dagger_i a_m \right)^{J^\pi} \right) |RPA_{gs}\rangle$$

Single reference (RPA) vs. Multi reference (GCM)

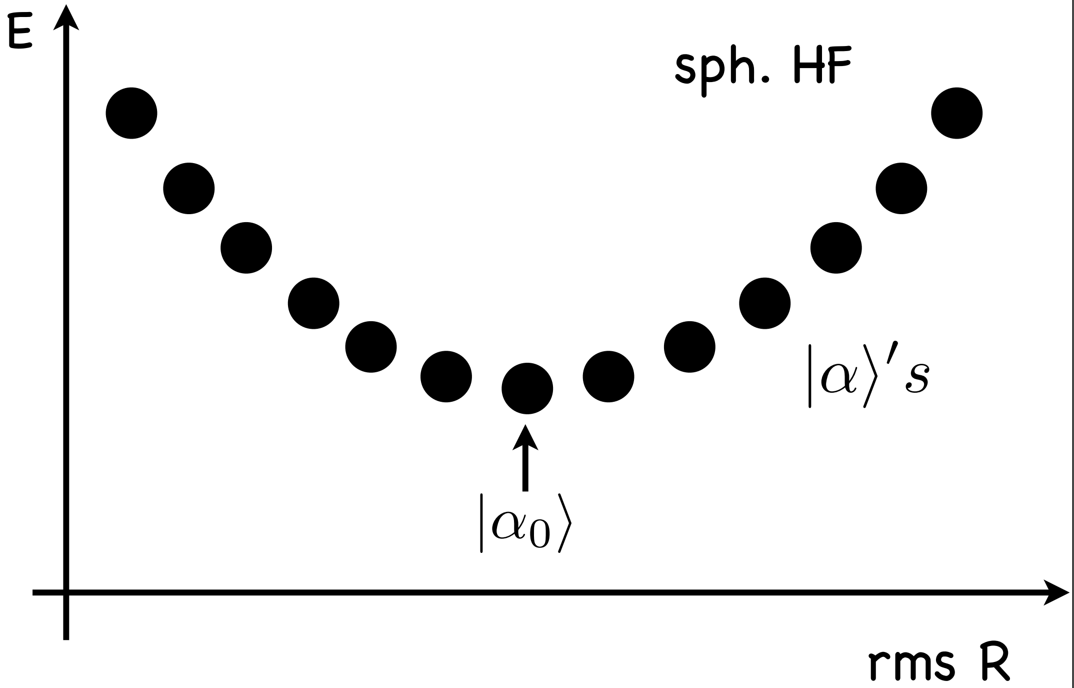
$$|GCM(k)\rangle = \sum_{\alpha} f_{k\alpha}|\alpha\rangle$$



Single reference (RPA) vs. Multi reference (GCM)

$$|GCM(k)\rangle = \sum_\alpha f_{k\alpha}|\alpha\rangle$$

$$|\alpha_0\rangle = \prod_{i=1}^{A} a_i^\dagger|0\rangle$$



$$|\alpha\rangle = \prod_{i=1}^{A}\prod_{m=A+1}^{\infty}\left(1 + C^\alpha_{mi}a^\dagger_m a_i\right)|\alpha_0\rangle$$

$$= |\alpha_0\rangle + \sum_{mi} C^\alpha_{mi}a^\dagger_m a_i|\alpha_0\rangle + \sum_{mi}\sum_{m'i'} C^\alpha_{mi}C^\alpha_{m'i'}a^\dagger_m a_i a^\dagger_{m'} a_{i'}|\alpha_0\rangle + \ldots$$

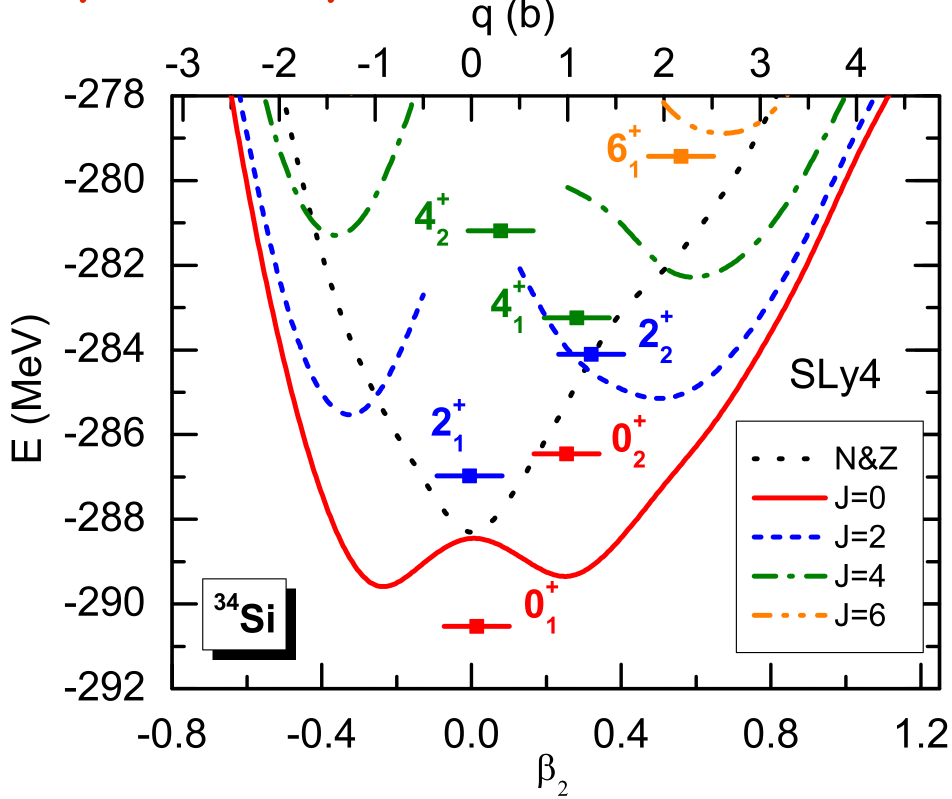
(Thouless, NP21 (1960) 225)

$$|GCM(k)\rangle = \sum_\alpha f_{k\alpha}|\alpha_0\rangle + \sum_{mi}\left(\sum_\alpha f_{k\alpha}C^\alpha_{mi}\right)a^\dagger_m a_i|\alpha_0\rangle$$

$$+\sum_{mi}\sum_{m'i'}\left(\sum_\alpha f_{k\alpha}C^\alpha_{mi}C^\alpha_{m'i'}\right)a^\dagger_m a_i a^\dagger_{m'} a_{i'}|\alpha_0\rangle + \ldots$$

- both g.s. and excited states
- richer than RPA

Symmetry restoration in GCM



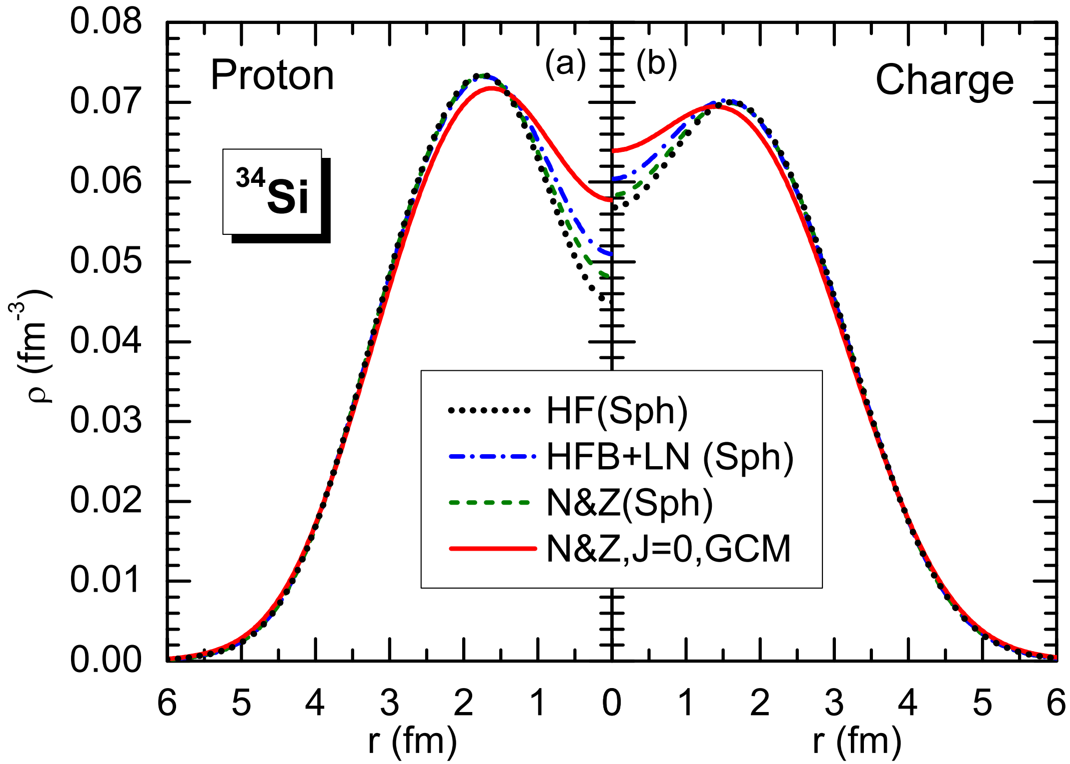
(J.-M. Yao, S. Baroni, M. Bender, P.-H. Heenen, arXiv:1205.2262)

q-constrained HFB : $|\alpha\rangle \equiv |q\rangle$

symmetry restoration : $|NZJMq\rangle = \dfrac{\hat{P}^J_{M0}\hat{P}_N\hat{P}_Z|q\rangle}{\sqrt{\langle q|\hat{P}^J_{00}\hat{P}_N\hat{P}_Z|q\rangle}}$

configuration mixing : $|GCM^{NZJM}(k)\rangle = \sum_q f^J_{kq}|NZJMq\rangle$

Ground-state properties in GCM

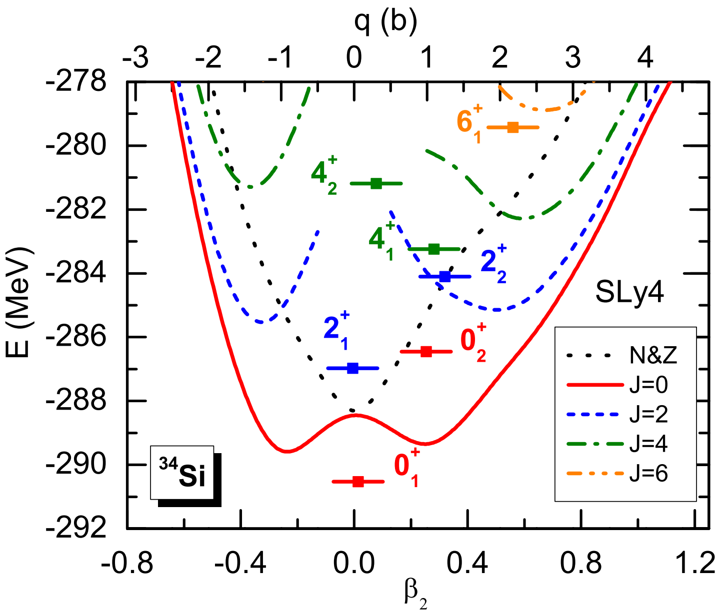


Bubble nuclei?
There's no such a thing!

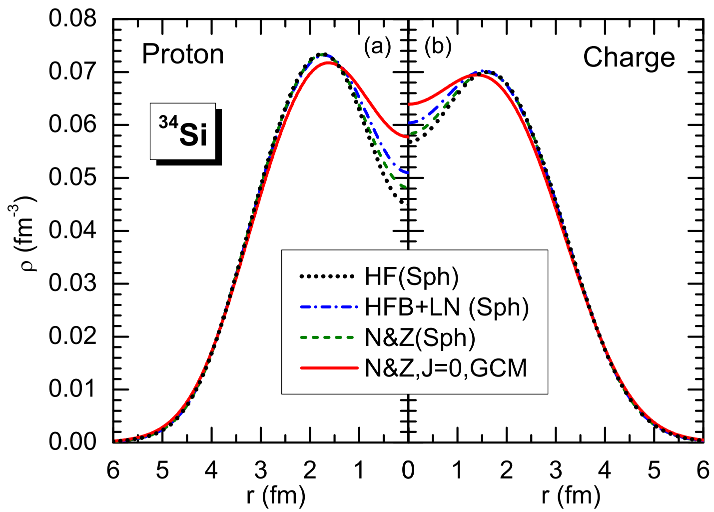
(J.-M. Yao, S. Baroni, M. Bender, P.-H. Heenen, arXiv:1205.2262)

- ground-state correlations accessible
- effect of pairing, deformation, symmetry restoration on gs properties

GCM and RPA

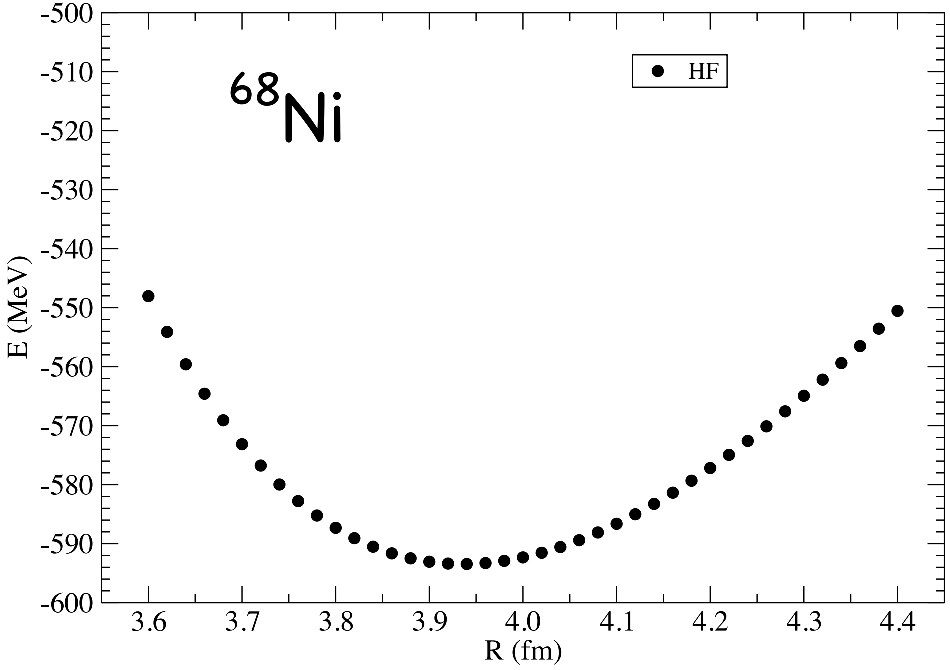


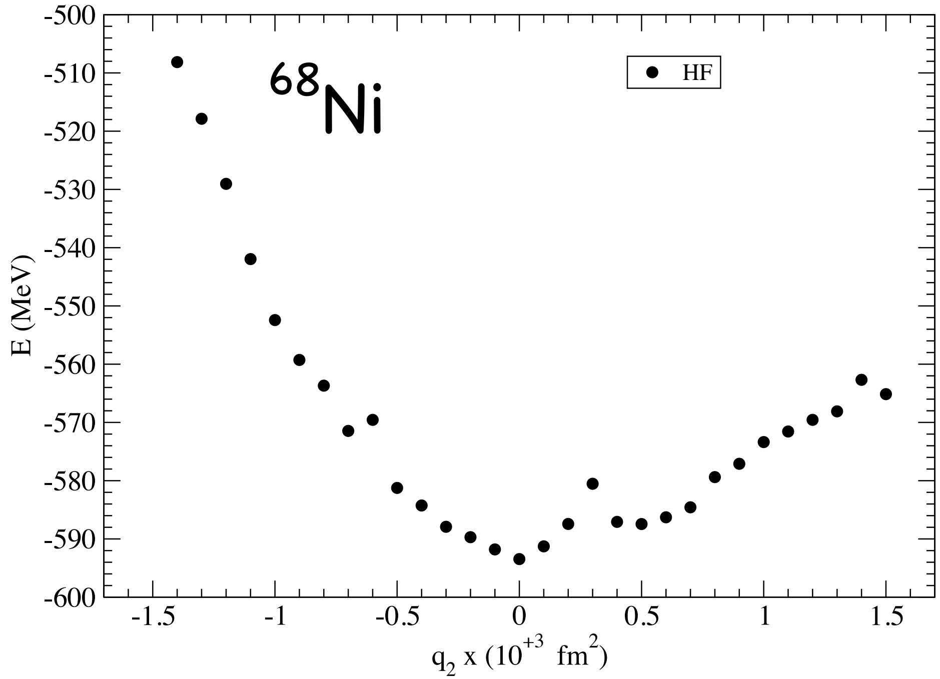
- Symmetry-restored GCM states
- RPA gives g.s. correlation energies separately for each mode, w/o coupling them



- g.s. correlations accessible in GCM
- GCM can handle shape mixing
- proper pairing treatment beyond mean field

The choice of the generator coordinate





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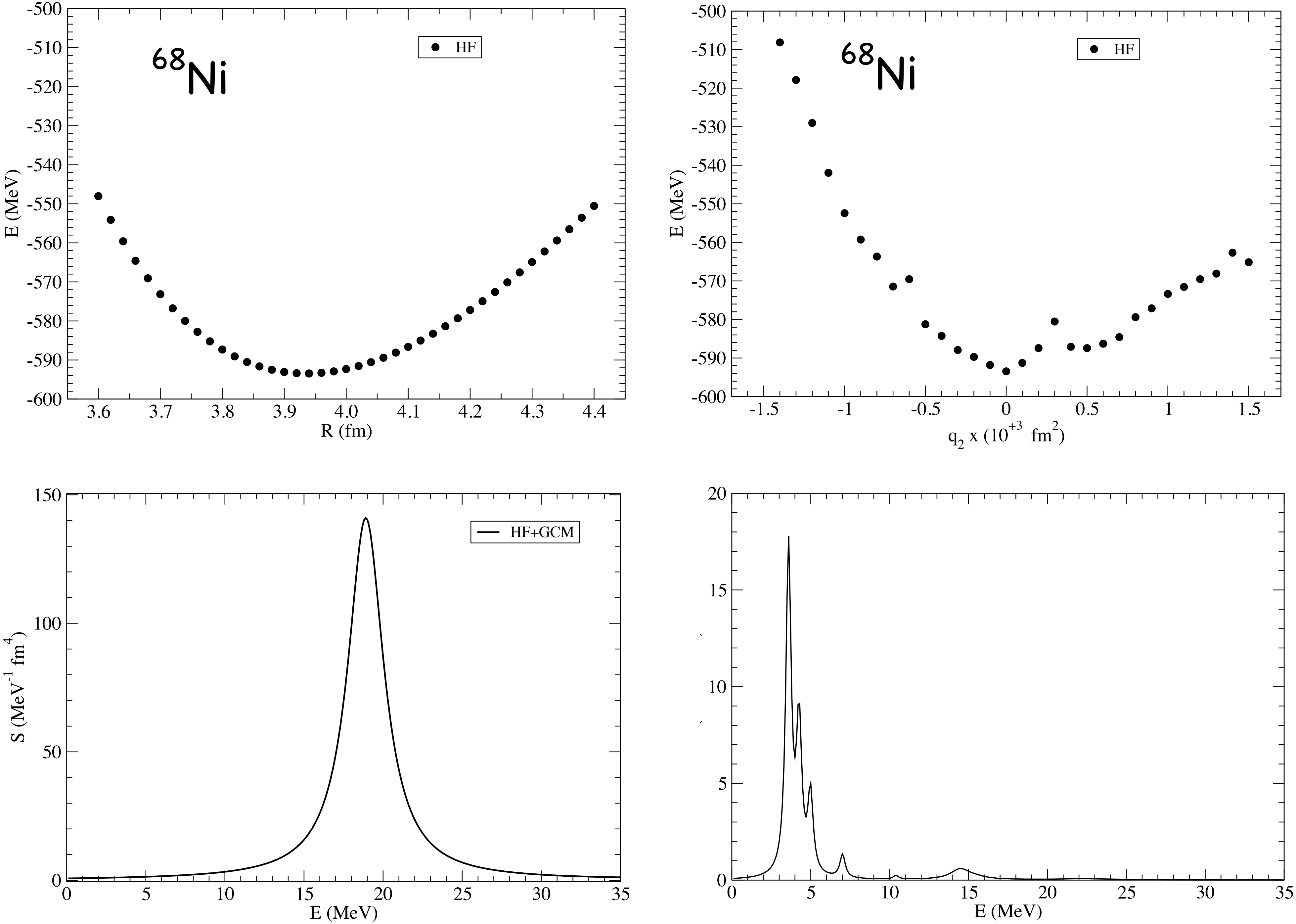

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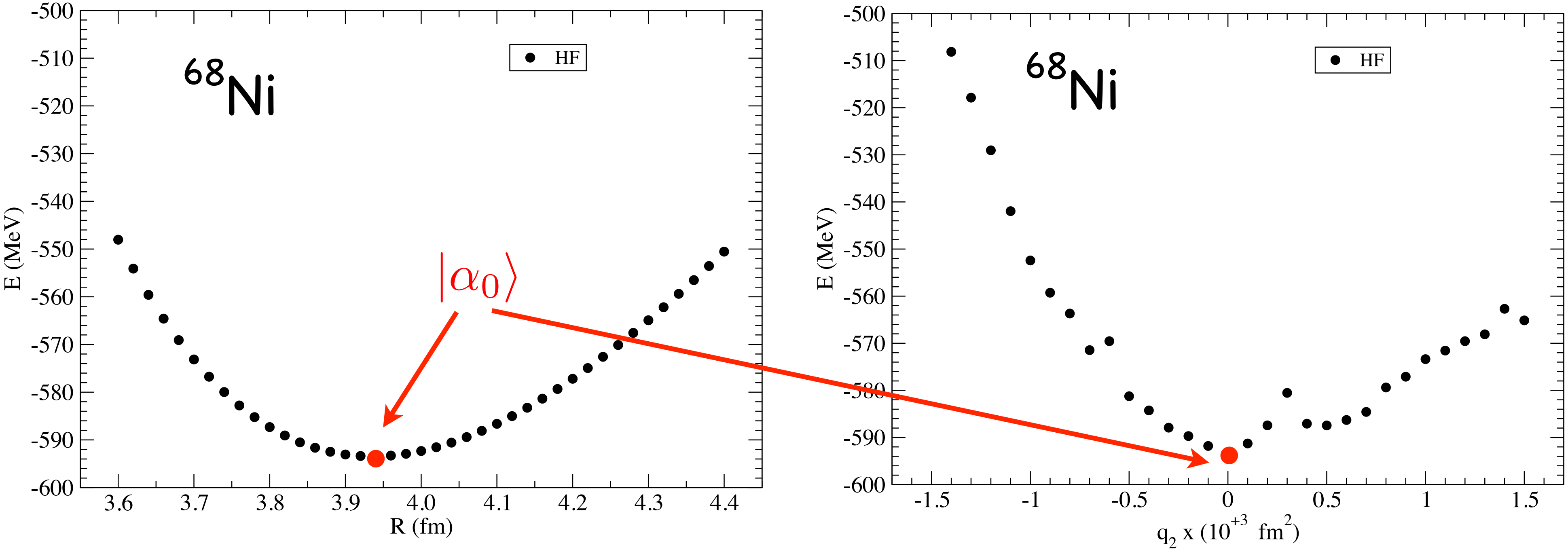
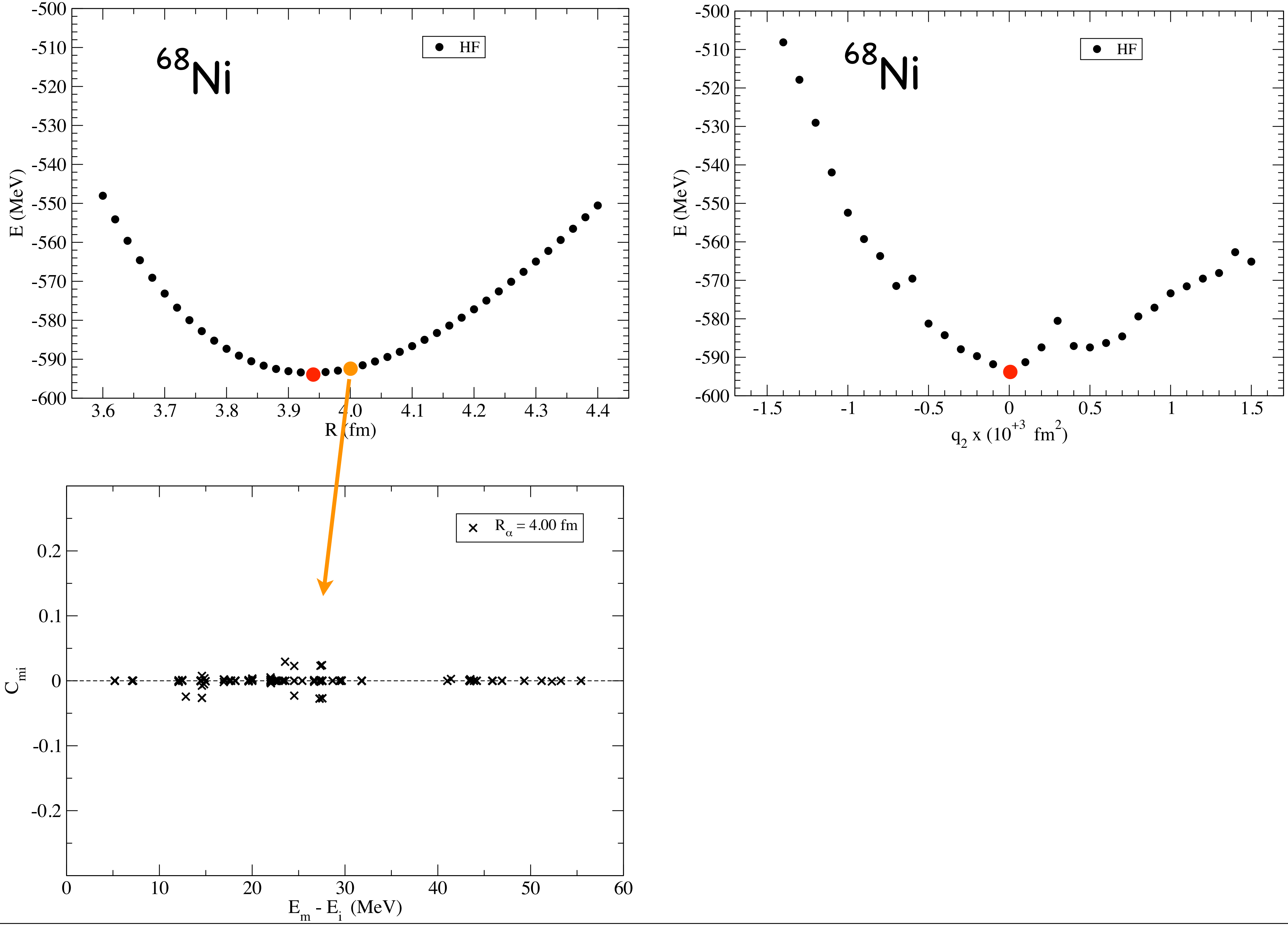


$$|\alpha\rangle = \prod_{i=1}^{A} \prod_{m=A+1}^{\infty} \left(1 + C^{\alpha}_{mi} a^{\dagger}_{m} a_i\right) |\alpha_0\rangle$$

$$= |\alpha_0\rangle + \sum_{mi} C^{\alpha}_{mi} a^{\dagger}_{m} a_i |\alpha_0\rangle + \sum_{mi} \sum_{m'i'} C^{\alpha}_{mi} C^{\alpha}_{m'i'} a^{\dagger}_{m} a_i a^{\dagger}_{m'} a_{i'} |\alpha_0\rangle + \dots$$

The choice of the generator coordinate



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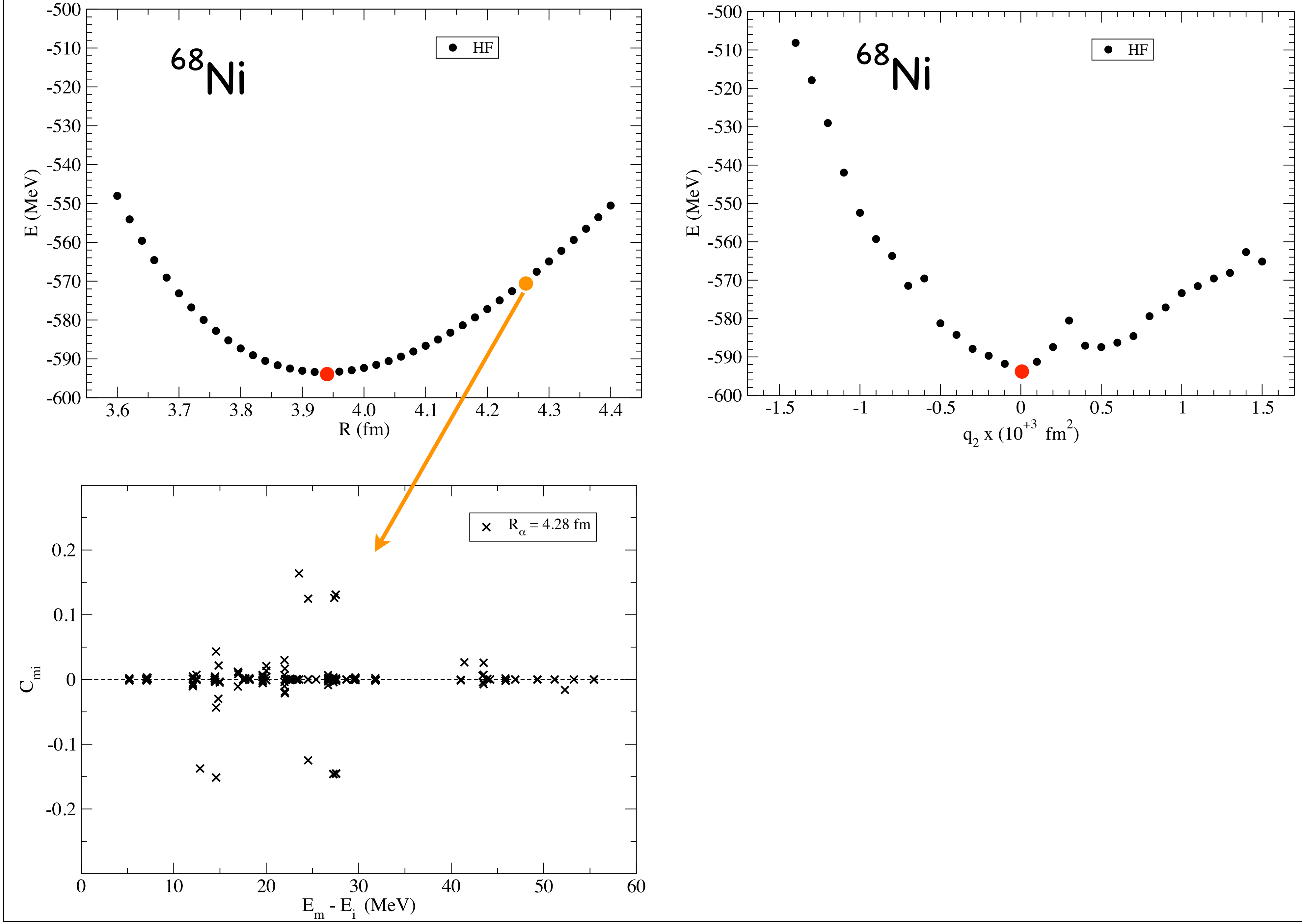

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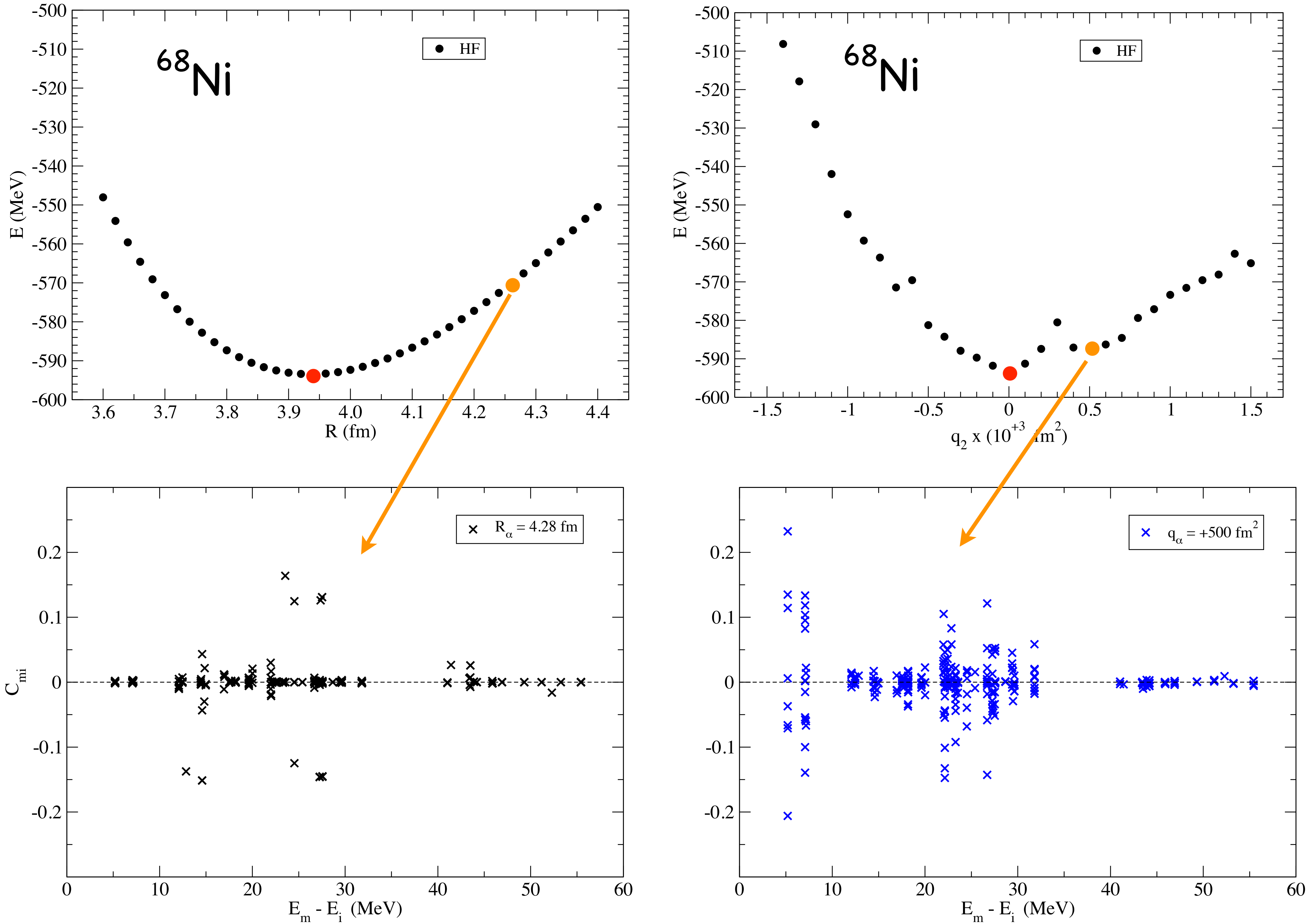

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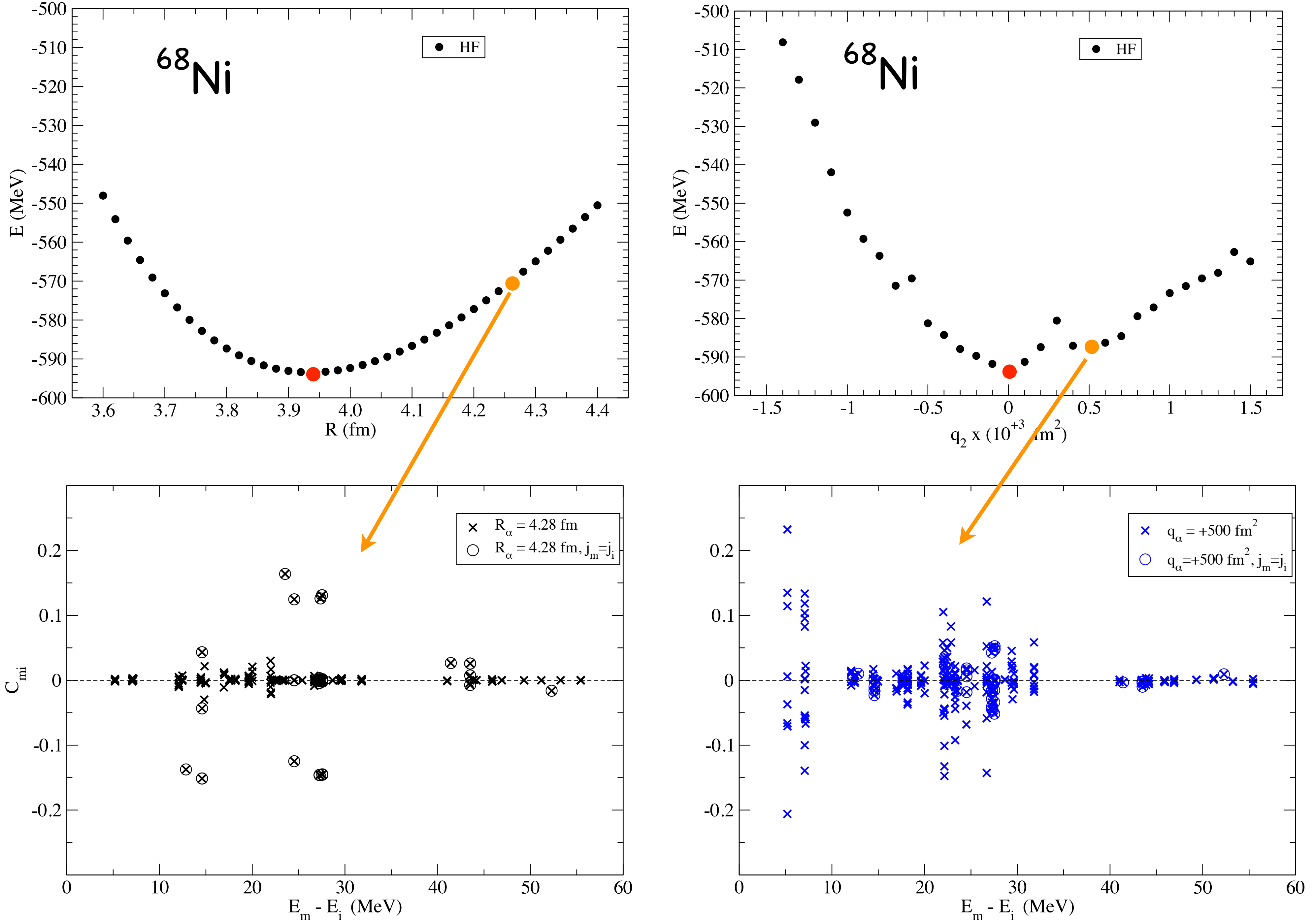

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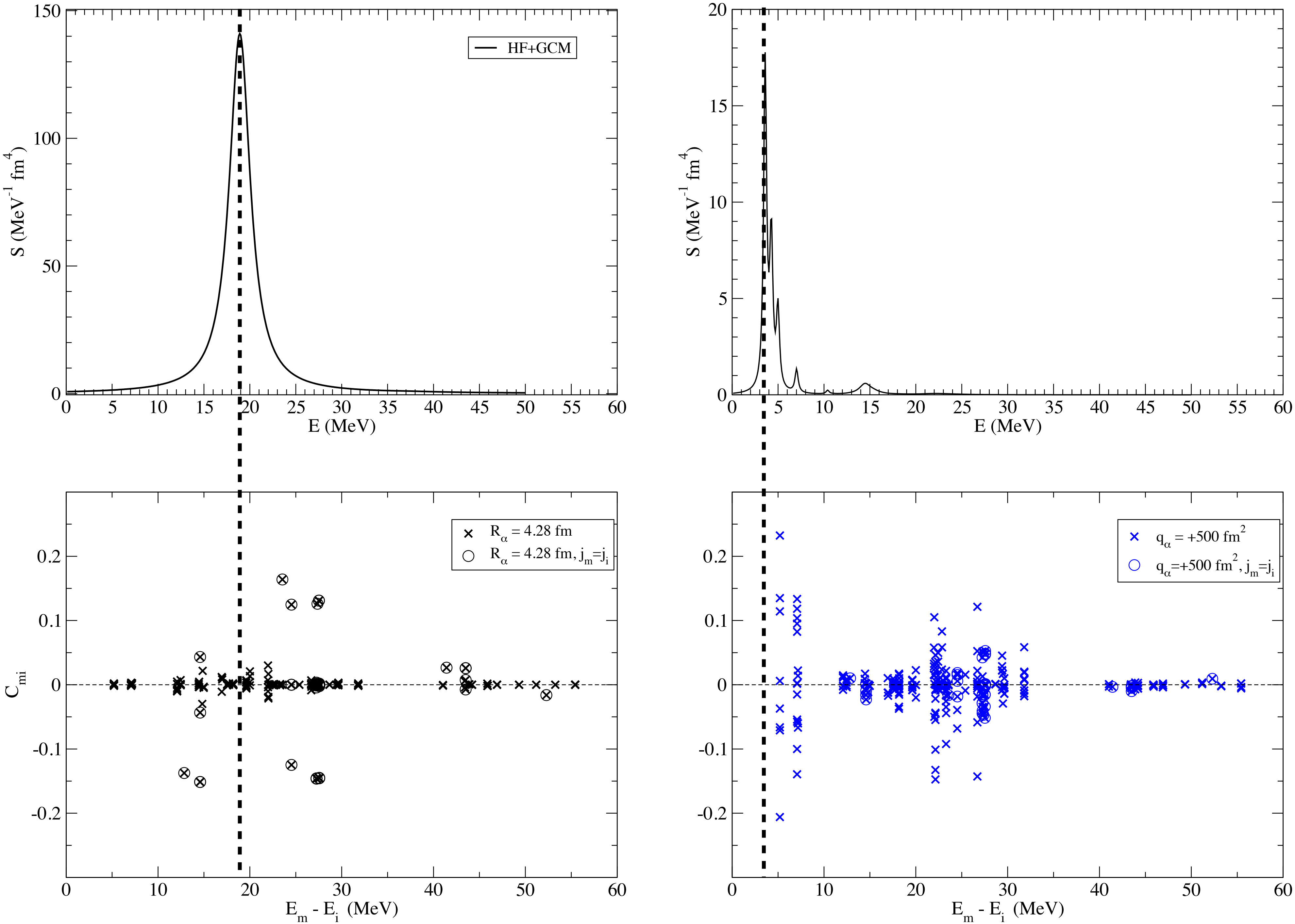

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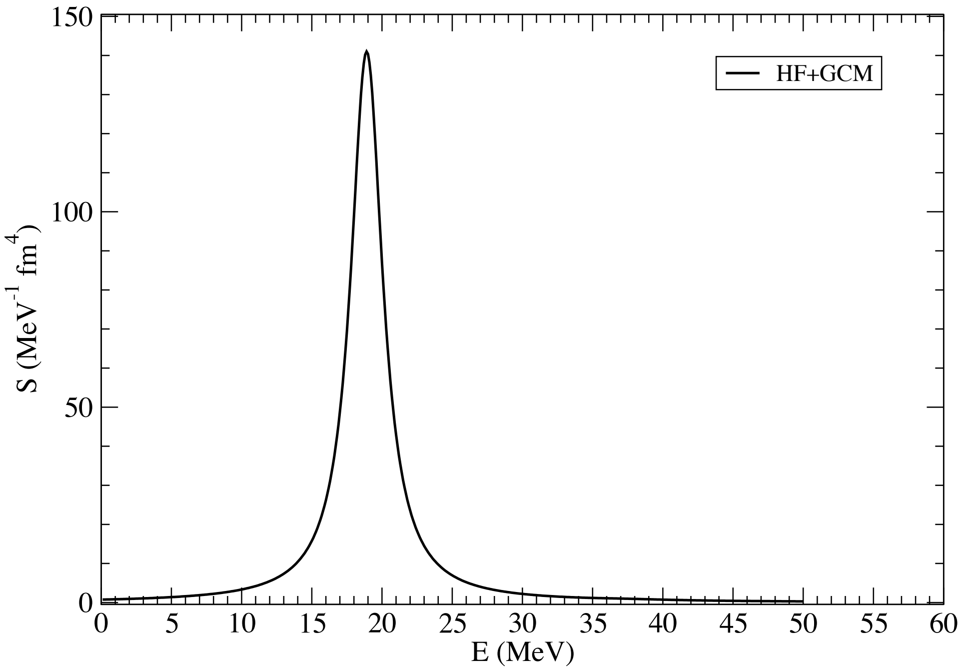
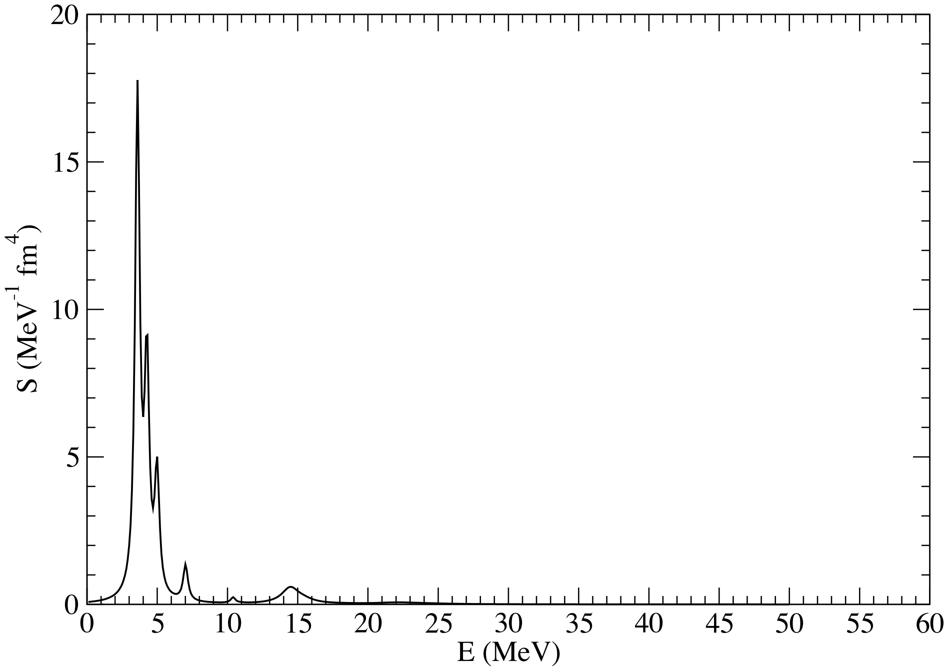
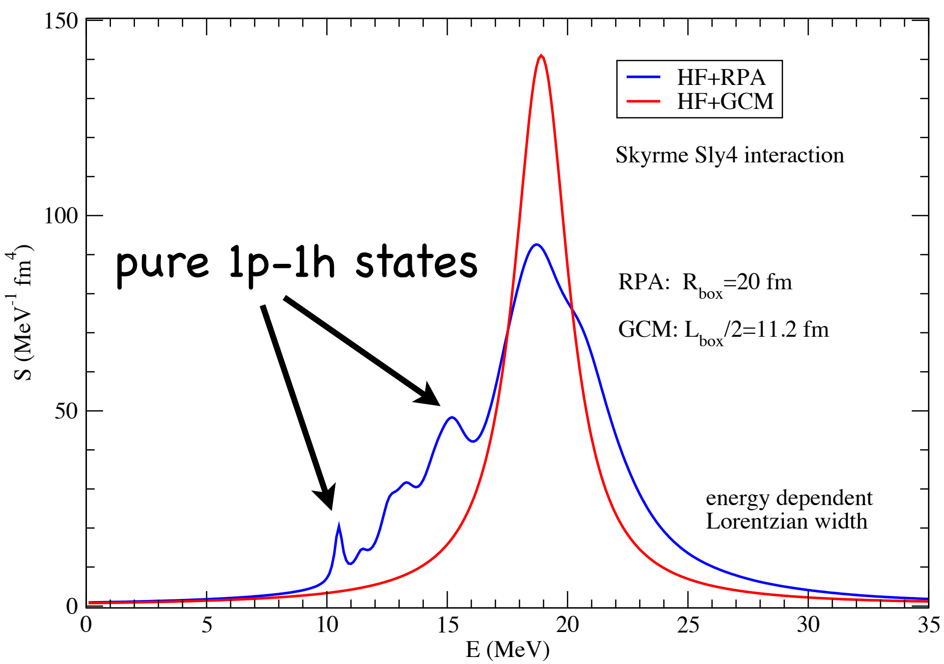






- RPA does not need to couple different J=0 responses
- one generator coordinate seems to capture almost all physics in GCM
- RPA can handle non-collective states

A link between GCM and RPA

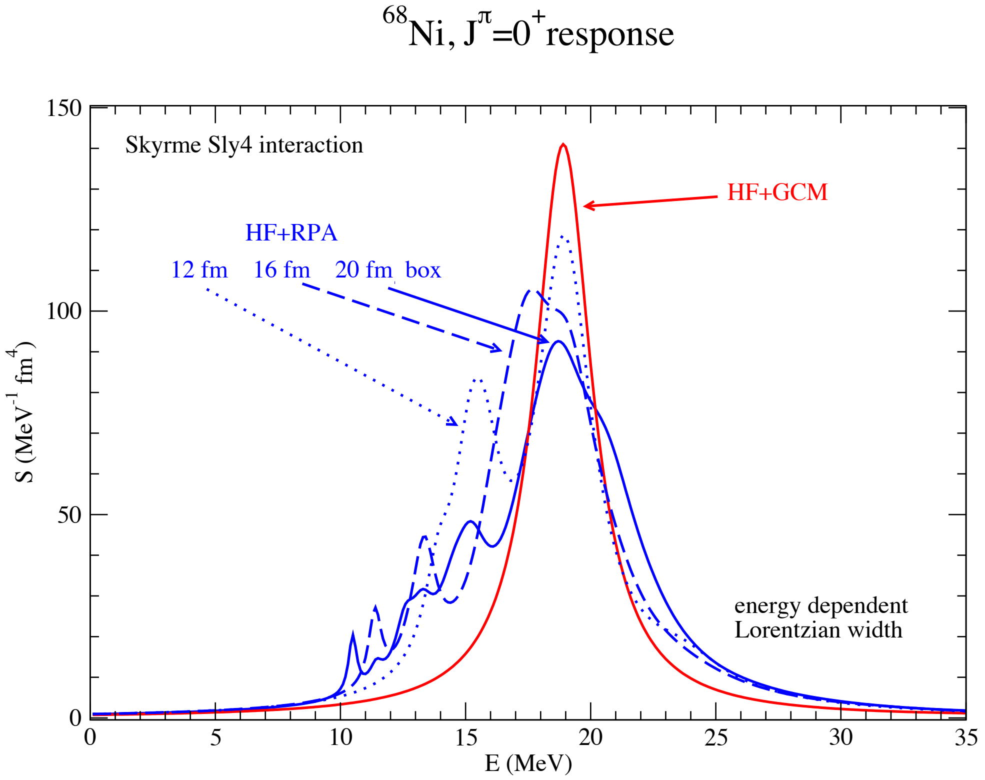
$$|RPA(k)\rangle = \sum_{mi} \left(X^k_{mi} \left(a^\dagger_m a_i \right)^{J^\pi} - Y^k_{mi} \left(a^\dagger_i a_m \right)^{J^\pi} \right) |RPA_{gs}\rangle$$

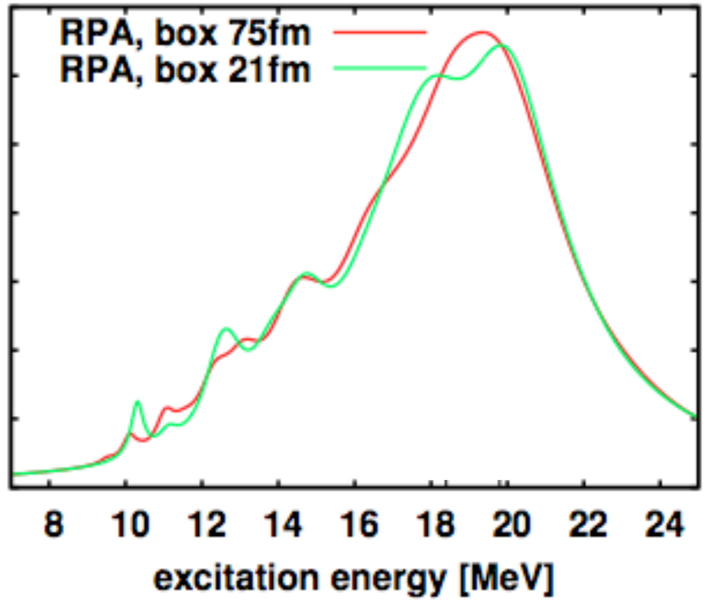
$$|GCM(k)\rangle = \sum_\alpha f_{k\alpha} |\alpha_0\rangle + \sum_{mi} \left(\sum_\alpha f_{k\alpha} C^\alpha_{mi} \right) a^\dagger_m a_i |\alpha_0\rangle + \sum_{mi} \sum_{m'i'} \left(\sum_\alpha f_{k\alpha} C^\alpha_{mi} C^\alpha_{m'i'} \right) a^\dagger_m a_i a^\dagger_{m'} a_{i'} |\alpha_0\rangle + \ldots$$

$$|GCM(k)\rangle \approx \sum_{mi} \left(X^k_{mi} \left(a^\dagger_m a_i \right)^{J^\pi} - Y^k_{mi} \left(a^\dagger_i a_m \right)^{J^\pi} \right) |GCM_{gs}\rangle$$

- how big are correlations beyond 1p-1h in GCM?

The continuum





P.-G. Reinhard, private comm.

- GCM does not need an explicit treatment of the continuum
- RPA needs states at E>0 ==> box dependence

Other pros and cons of GCM

- GCM can study large-A deformed systems with no extra effort

- GCM has problems with light nuclei (A < 60 ?)
  requires regularizable functionals
  requires forces
- GCM calculations take longer than RPA (spherical case)
- pp and hh excitations?
  pairing vibrations?
  ex: 208Pb 0+ state at about 4MeV
  68Ni 0+ state at 1.8 MeV