Workshop on "Pairing degrees of freedom in nuclei and the nuclear medium"
Institute for Nuclear Theory, UW Seattle, November 14-18, 2005

Correcting for self-pairing and poles in the particle-number projected Hartree-Fock-Bogoliubov method:

II. Preliminary results of work in progress

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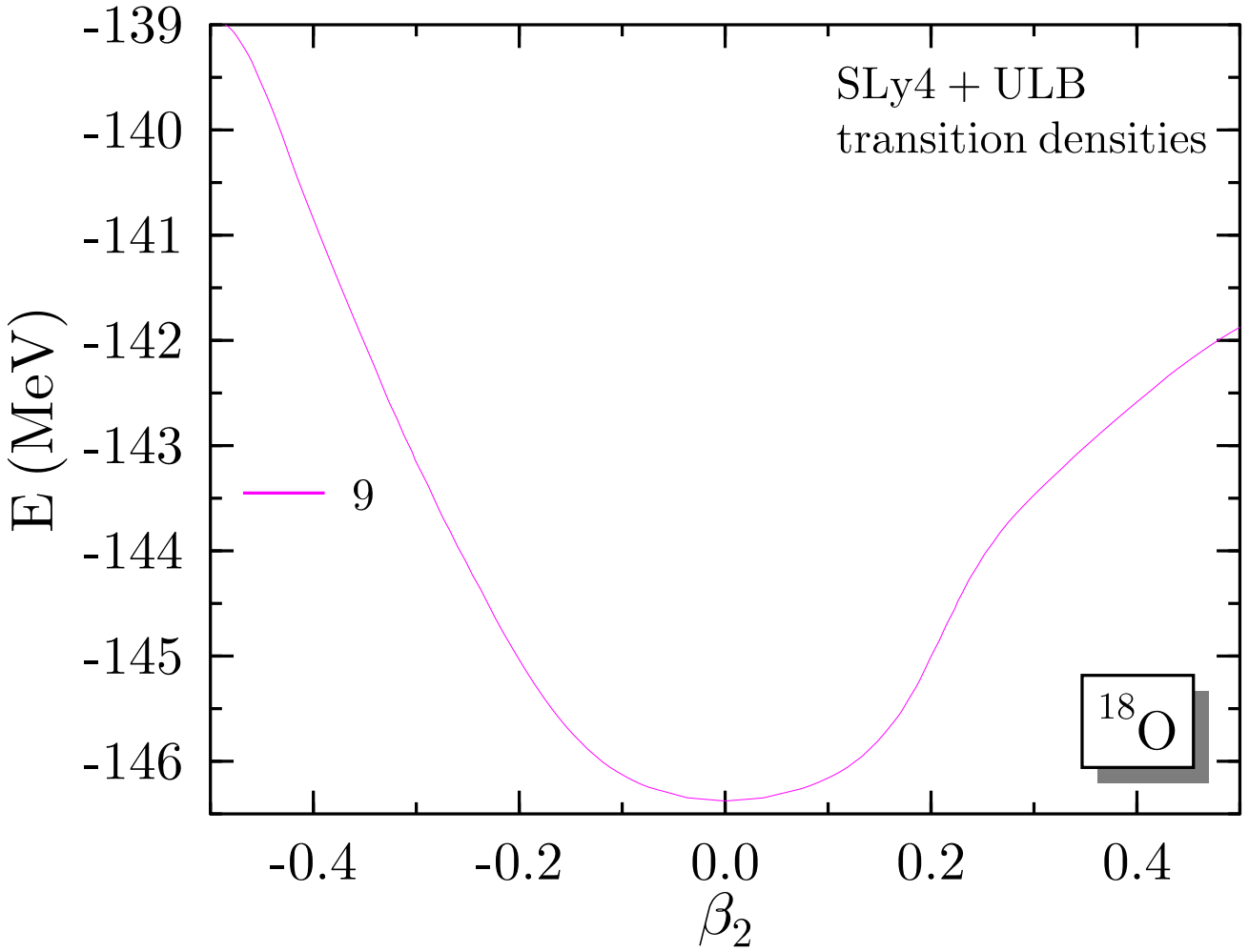
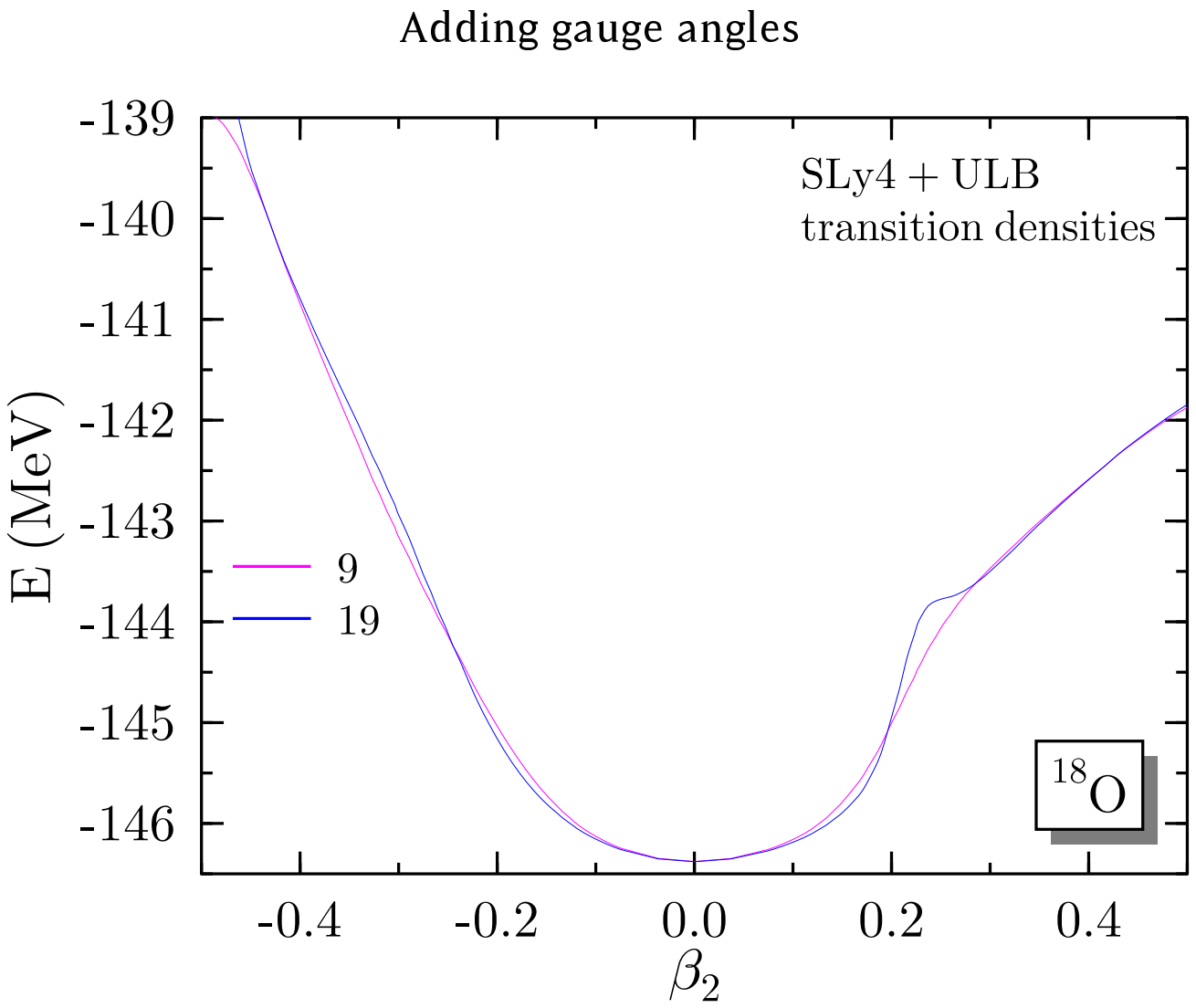
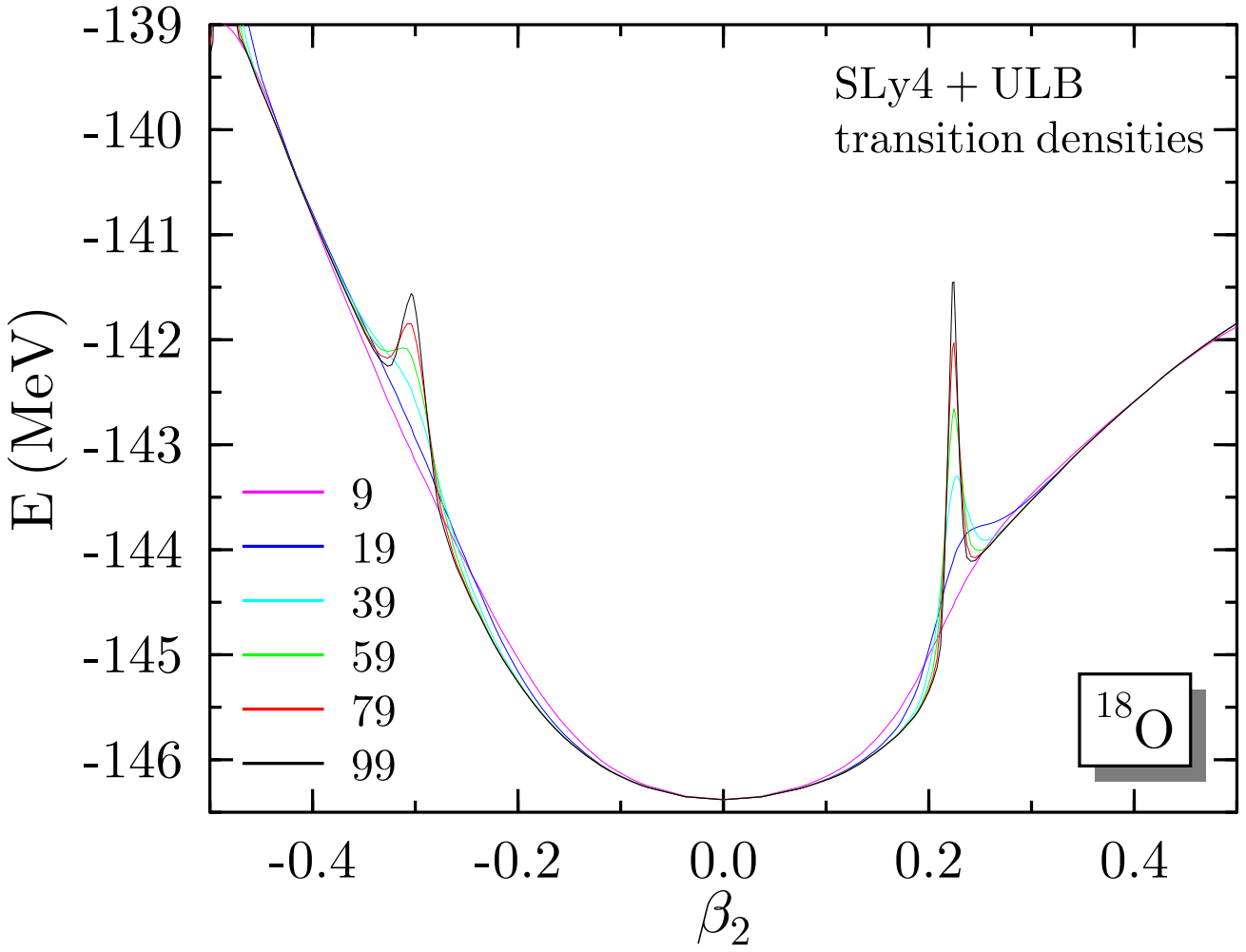
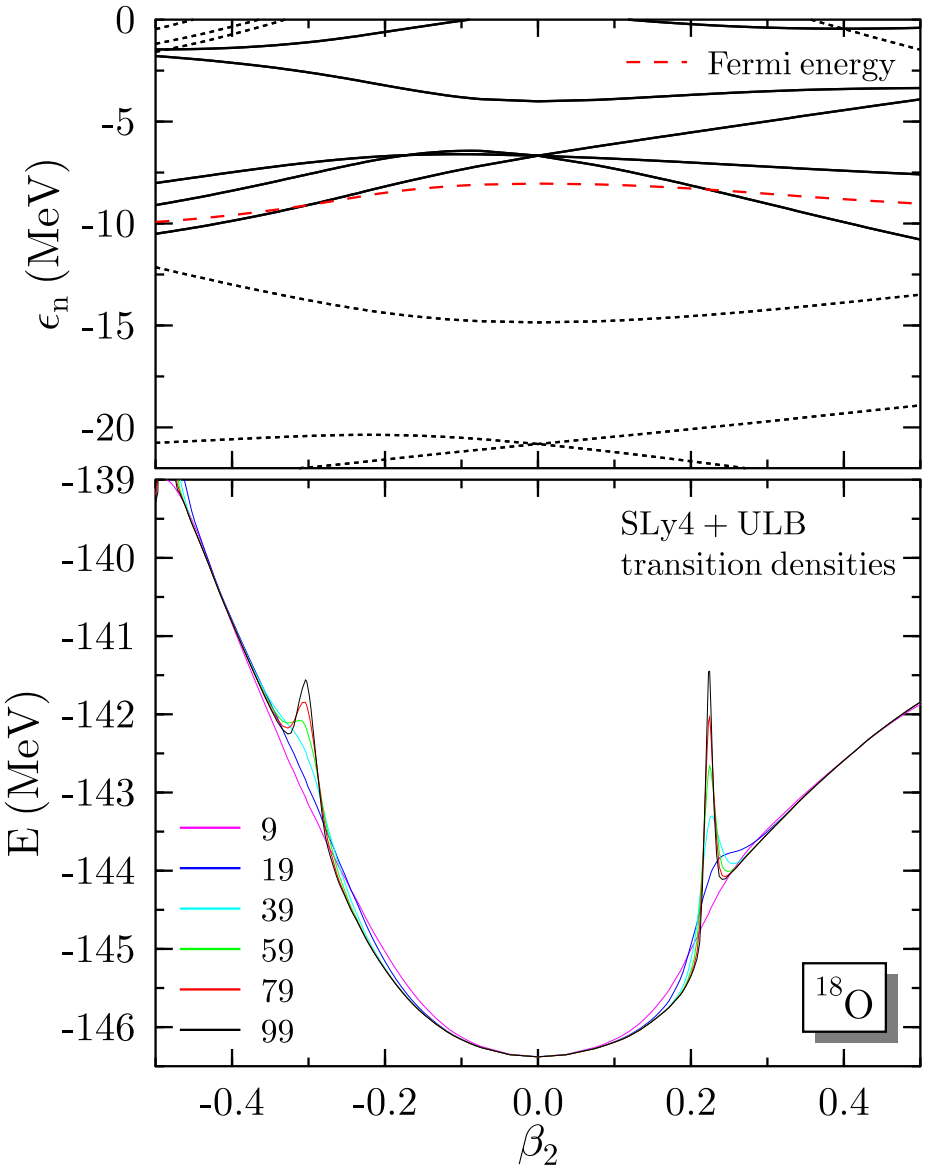
A regular projected HFB calculation discretizing the integrals using 9 gauge angles




Adding gauge angles
SLy4 + ULB
transition densities
9
19
^{18}O
E (MeV)
-139
-140
-141
-142
-143
-144
-145
-146
-0.4
-0.2
0.0
0.2
0.4
β_2

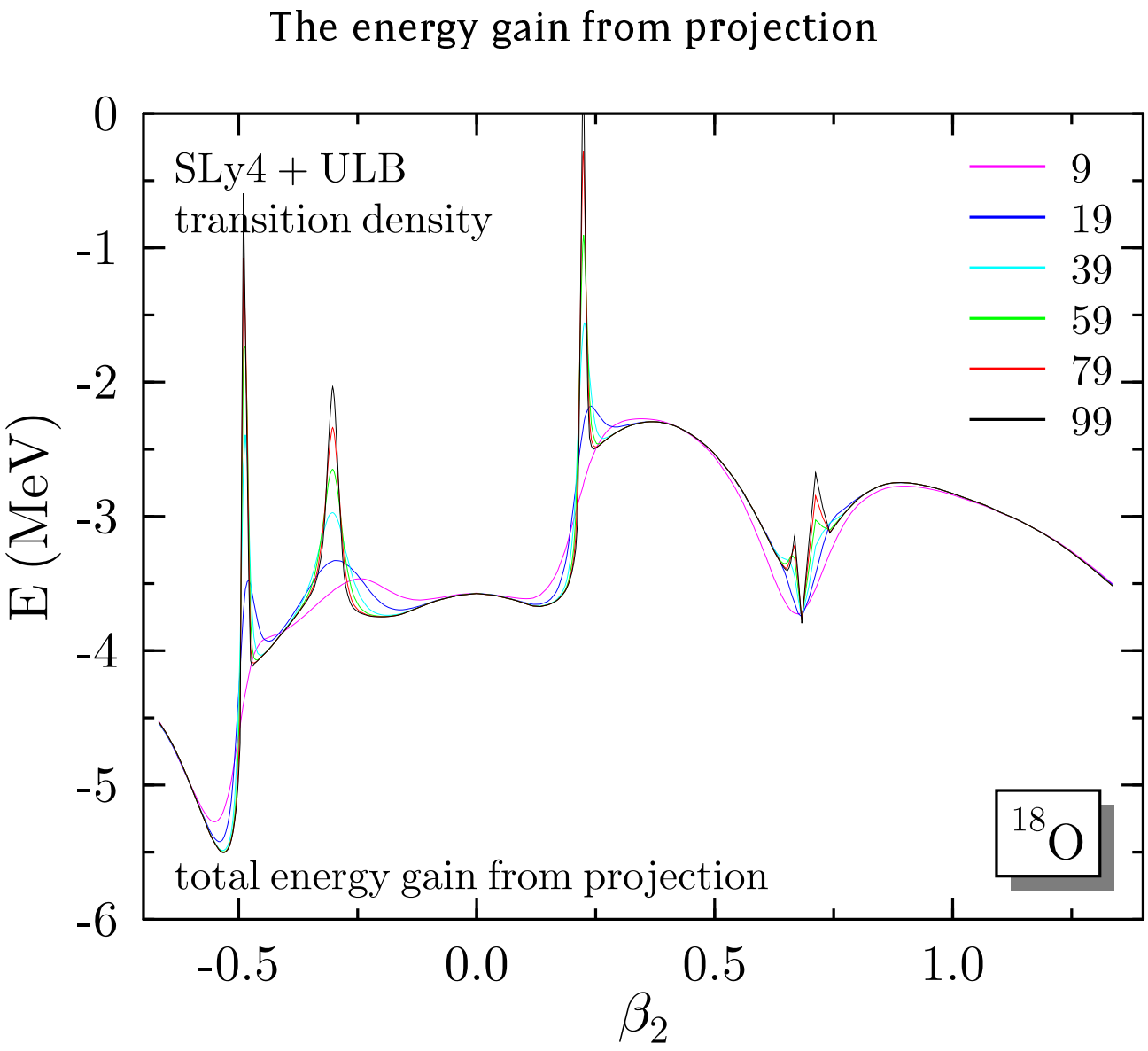
Varying the number of discrete gauge angles from 9 to 99 reveals a divergence



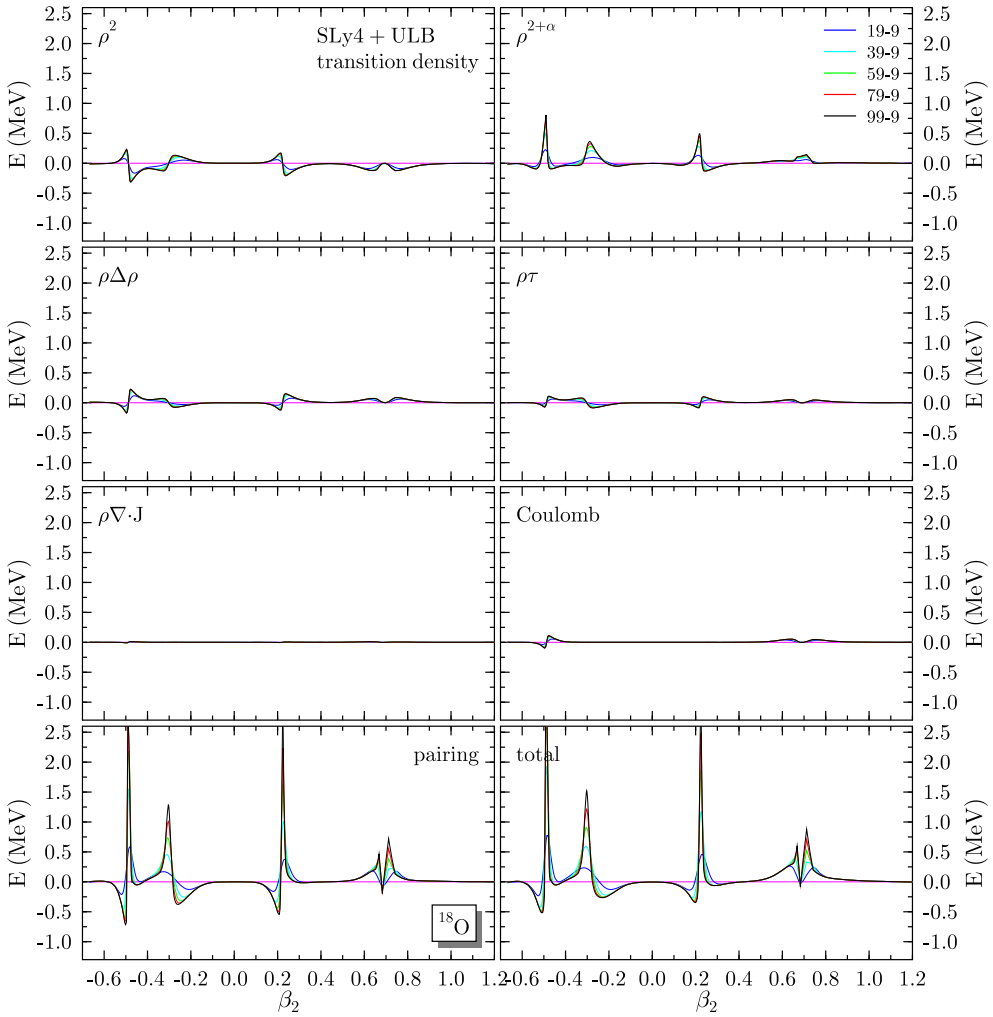


- The divergence appears where single-particle levels cross the Fermi energy

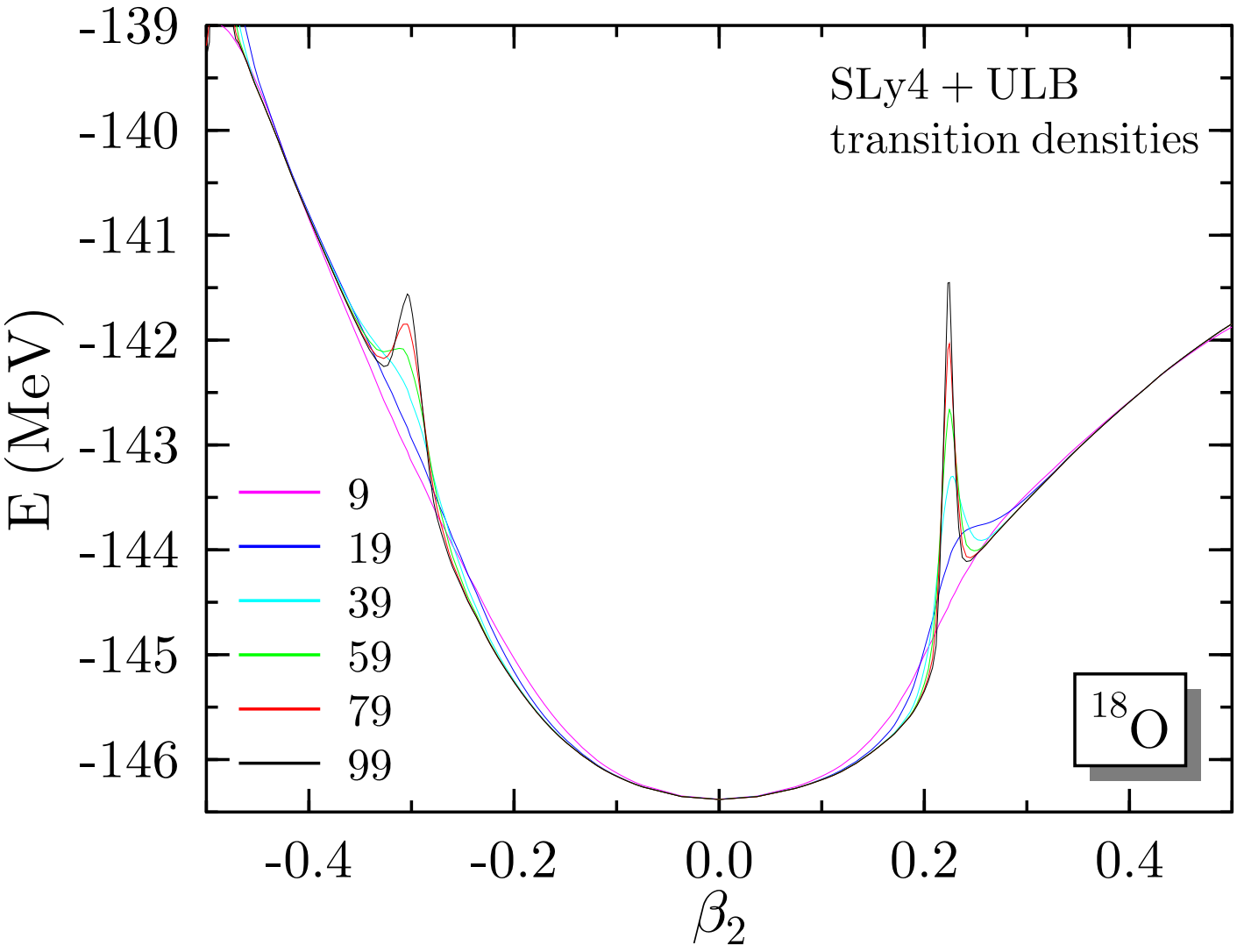
- In a calculation where the integrals over gauge angles are discretized using an odd number of gauge angles (as is usual practise and done here), the divergence of the projected energy manifests itself as a dependence of the projected energy on the number of points, as the divergence at $\pi/2$ gets better and better resolved.


The energy gain from projection
SLy4 + ULB
transition density
9
19
39
59
79
99
^{18}O
total energy gain from projection
E (MeV)
β_2
0
-1
-2
-3
-4
-5
-6
-0.5
0.0
0.5
1.0

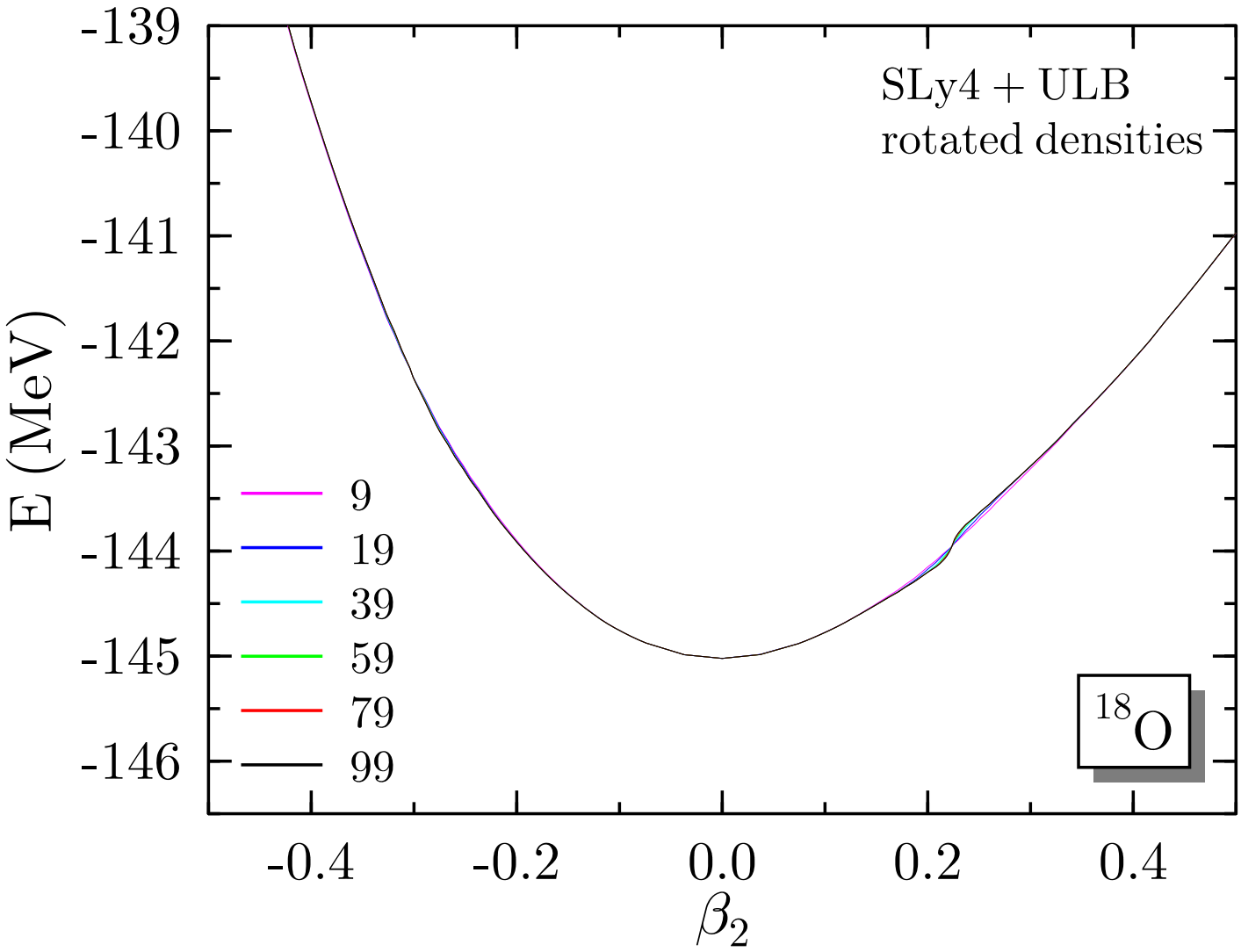
The divergence term by term using transition densities for the density-dependent coupling constants

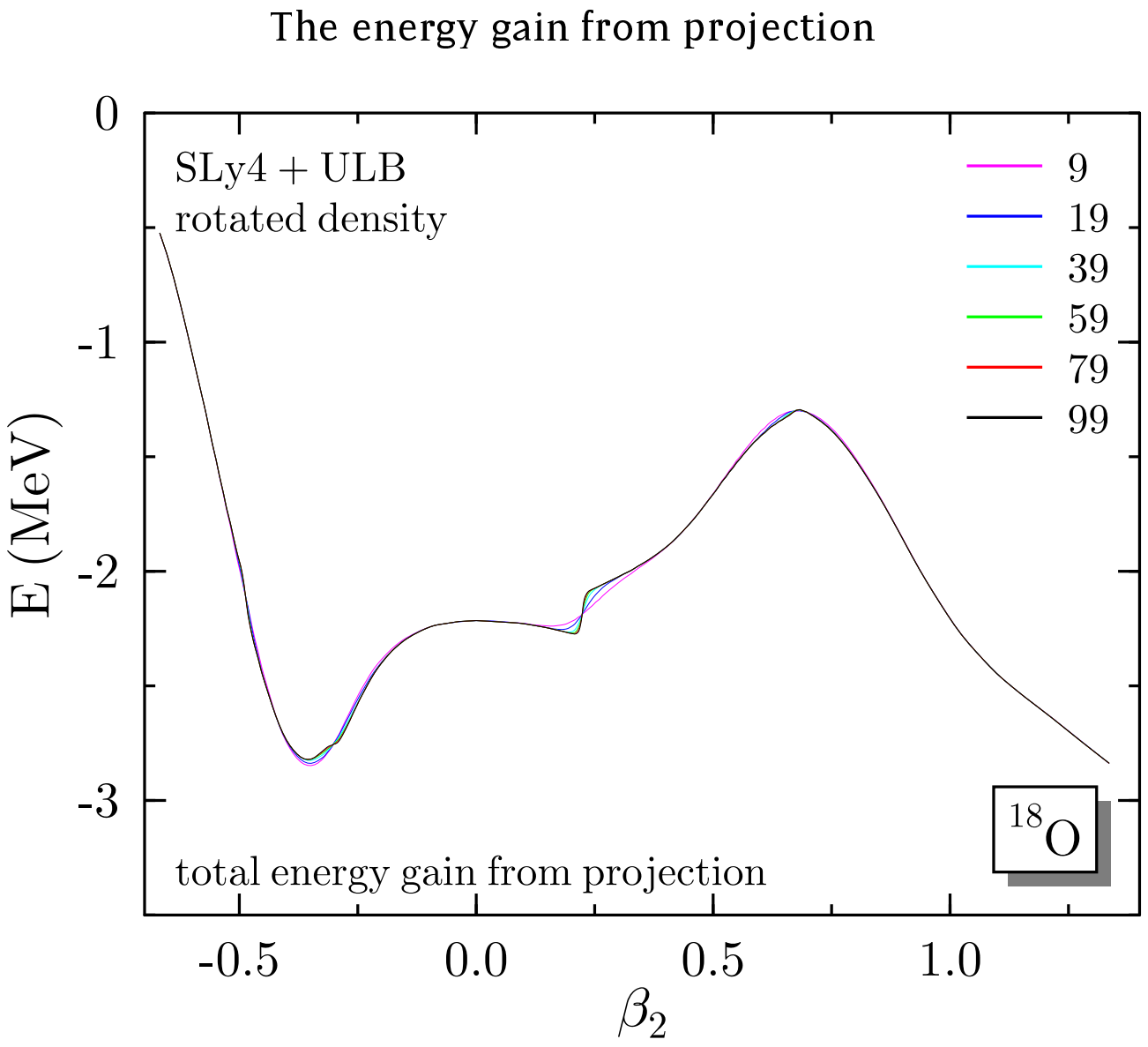


Using the transition density for the density-dependent coupling constants

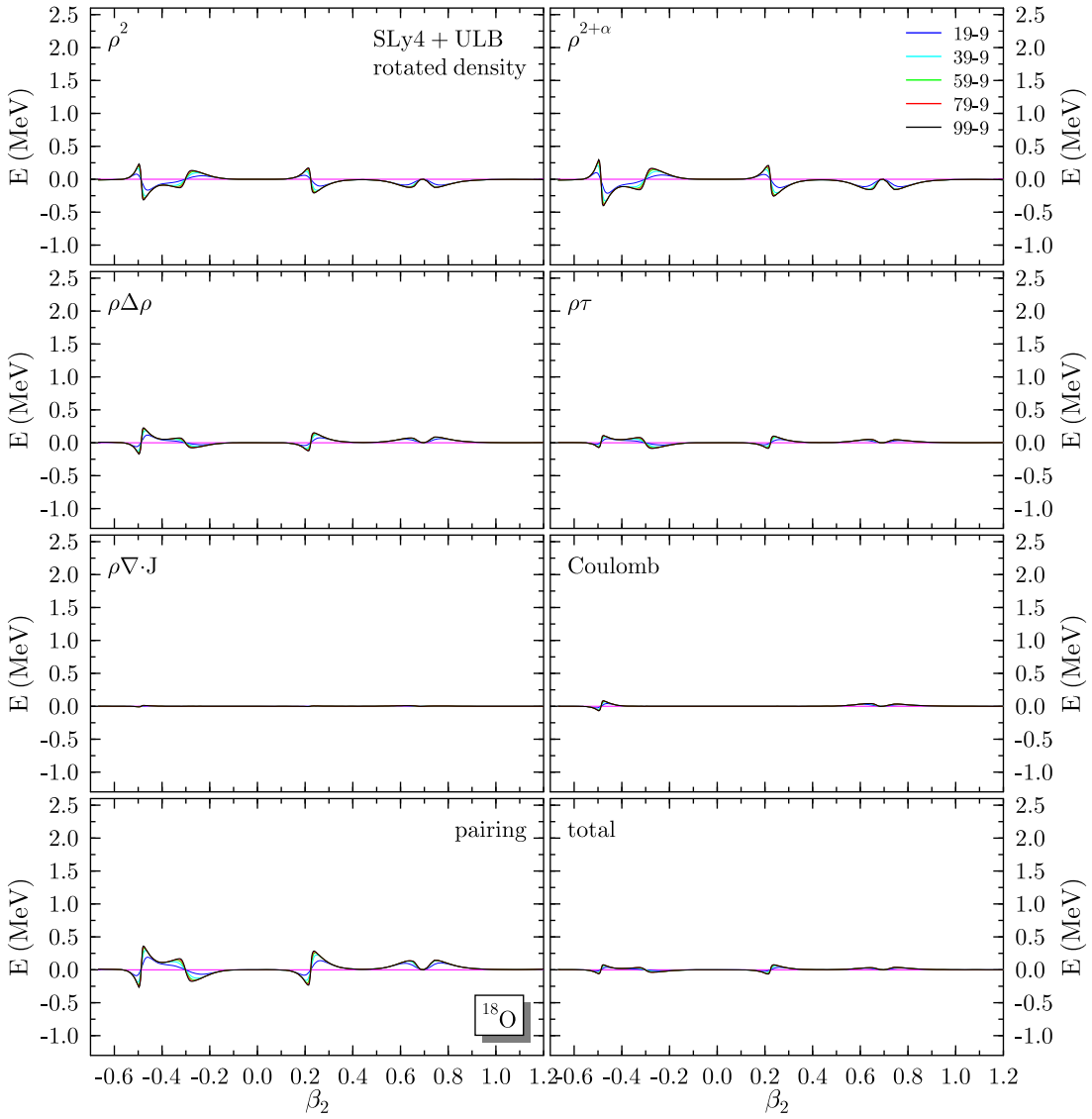


Using the rotated (= mean-field) density instead for the density-dependent coupling constants

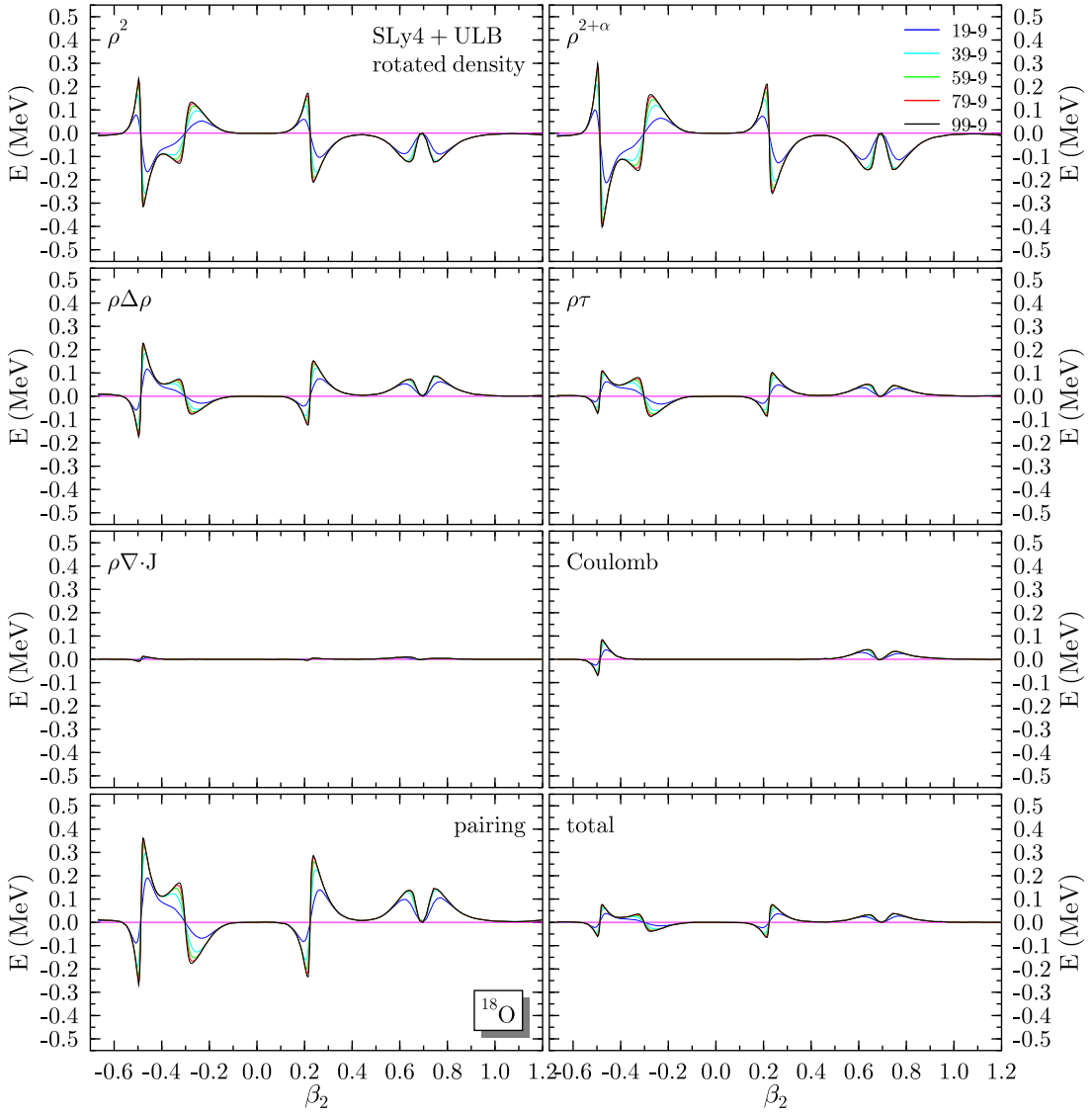



The energy gain from projection
SLy4 + ULB
rotated density
9
19
39
59
79
99
^{18}O
total energy gain from projection
E (MeV)
β_2
0
-1
-2
-3
-0.5
0.0
0.5
1.0

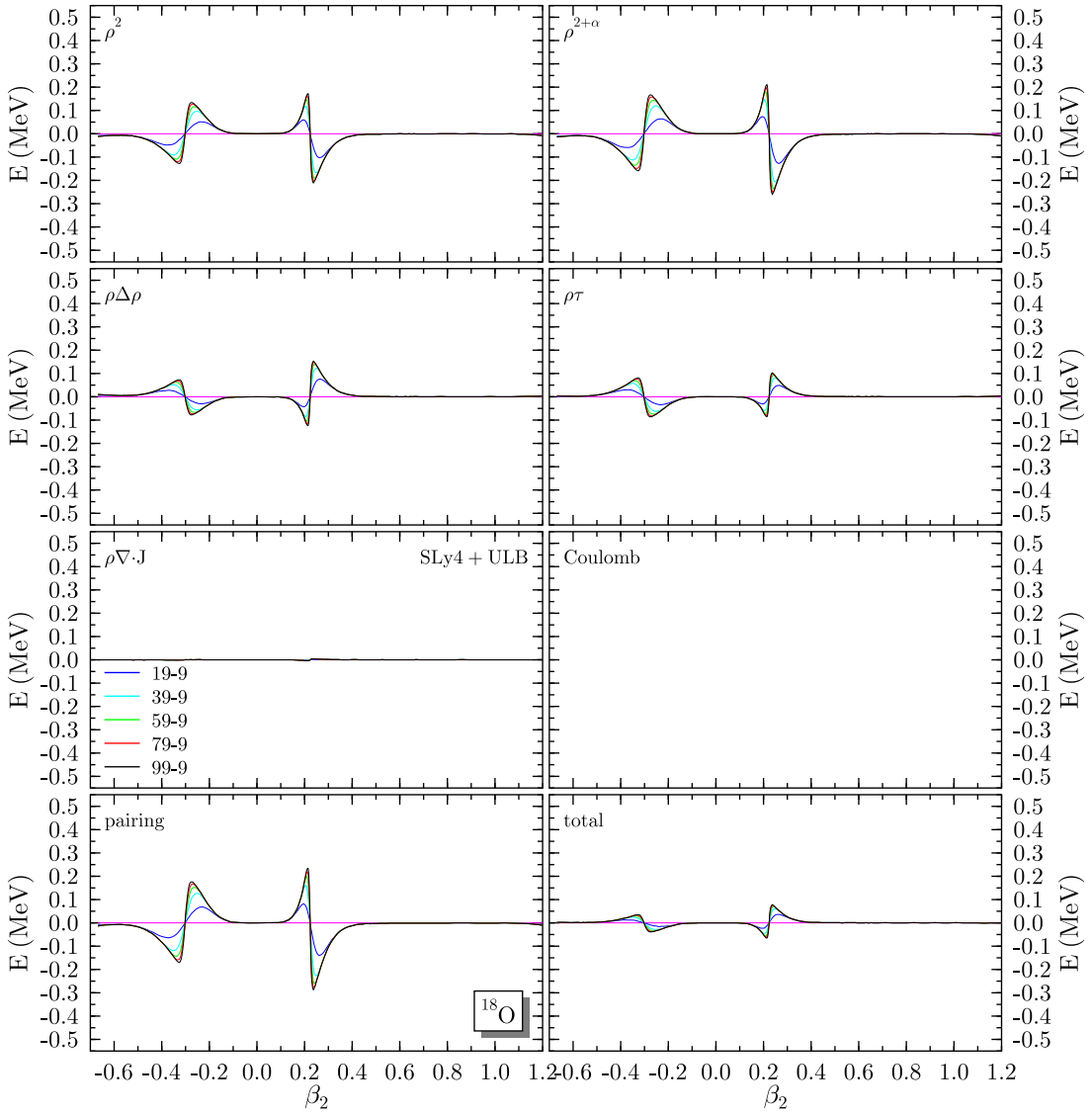
The divergence term by term using rotated densities for the density-dependent coupling constants



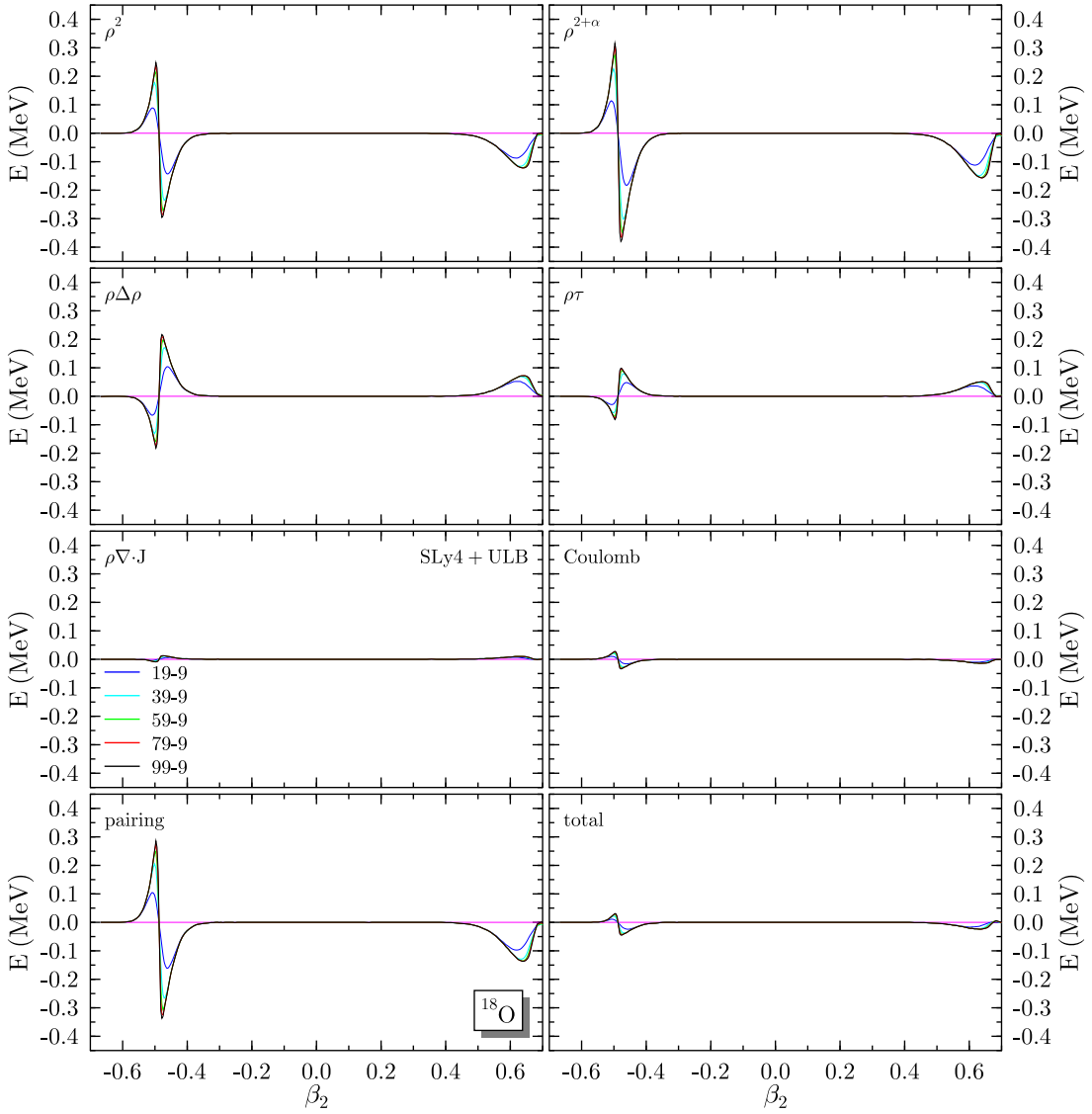
The divergence term by term using rotated densities for the density dependence



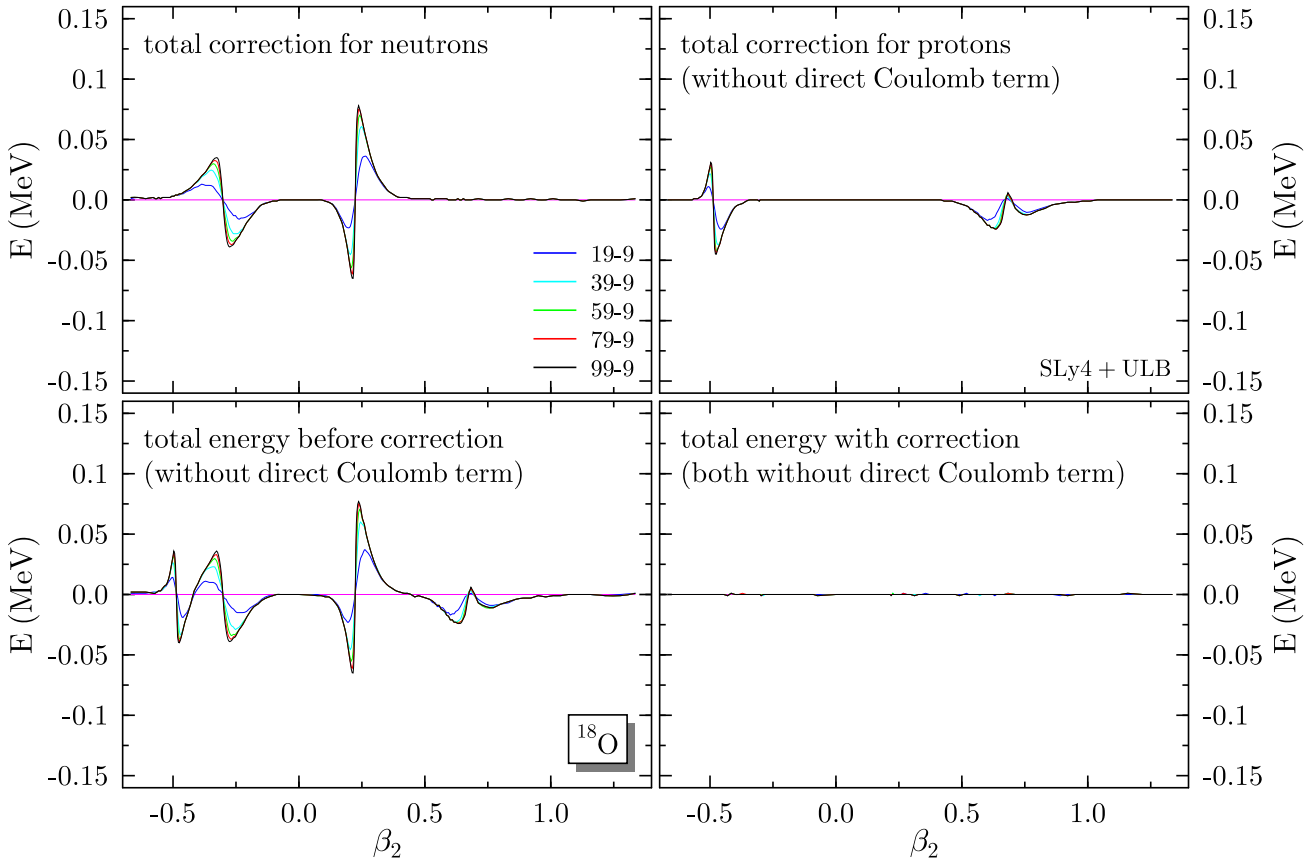
Correction for neutrons



Correction for protons

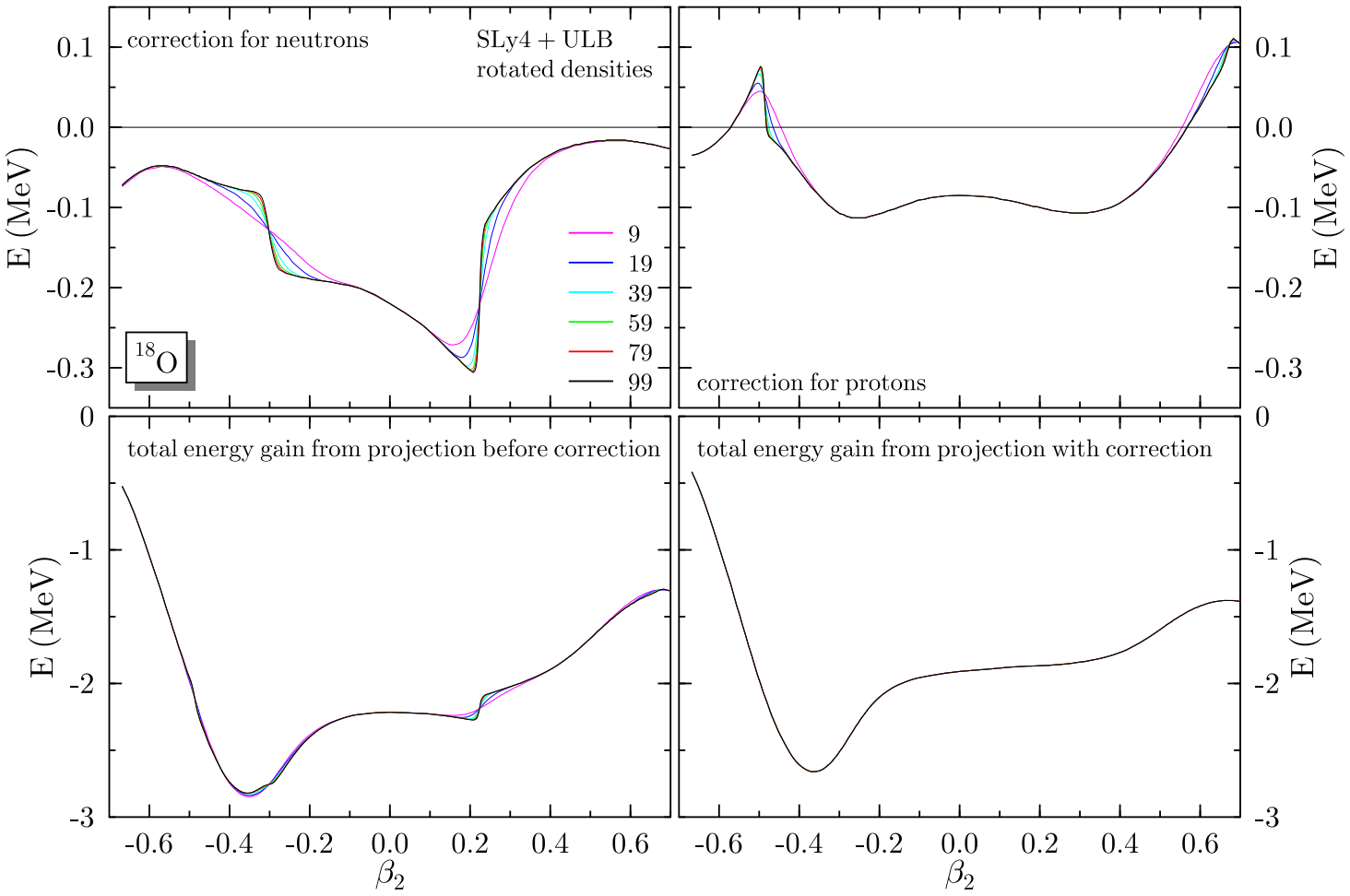


Summing all up

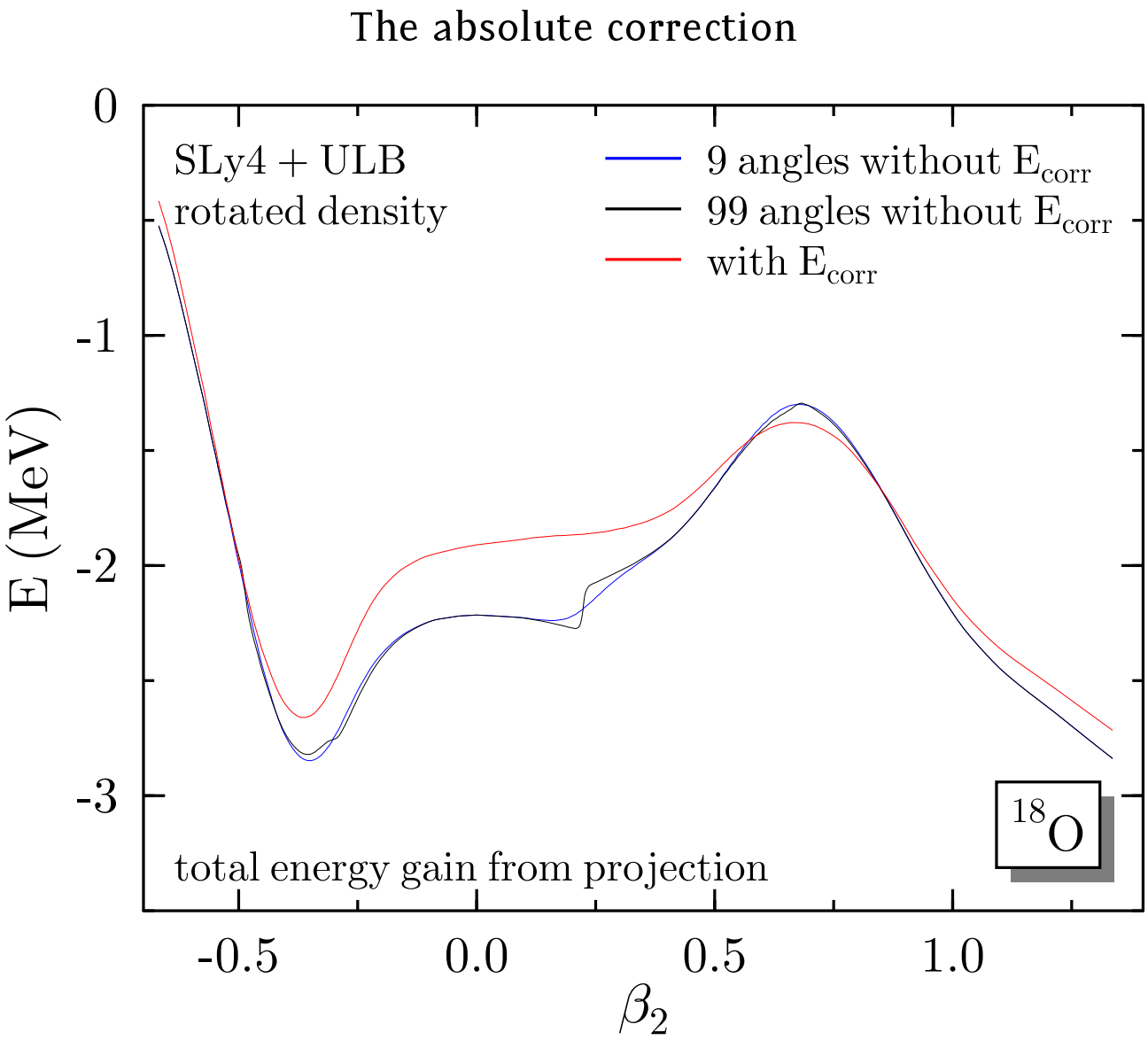


$\Rightarrow$ after correction, the total energy is independent on the number of integration points

The absolute correction



⇒ There is a non-divergent spurious contribution to the projected energy that is also corrected for


The absolute correction
SLy4 + ULB
rotated density
9 angles without E_corr
99 angles without E_corr
with E_corr
total energy gain from projection
18O
E (MeV)
β2
0
-1
-2
-3
-0.5
0.0
0.5
1.0

Summary and premature conclusions

- We propose a scheme to remove spurious contributions from the particle-number projected energy in the framework of DFT.
- The correction removes the divergence of the particle-number projected energy when occupations are close to 0.5 *and* a non-divergent spurious energy, that varies with deformation.
- After correction, the results are independent on the number of integration points on a scale of 1 keV.
- The correction decreases with mass number (based on test calculations not shown).

Open points to be worked out

- Correction for direct Coulomb term (work in progress)
- Correction for 3-body forces (work in progress)
- Set up correction scheme for variation after projection.
- How to correct non-diagonal projected GCM kernels? What will be the impact on GCM?
- Using the rotated densities for the density-dependend terms in connection with existing Skyrme interactions spoils the results for angular-momentum projected GCM.

Acknowledgements

This work was initialized by stimulating discussions with Mario Stoitsov, Witek Nazarewicz, Jacek Dobaczewski and P.-G. Reinhard.

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. . . to be continued