Covariance analysis & finite temperature behaviour of Skyrme functionals

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Brief Outline

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- Covariance analysis
  - Following Xavi's notes (uploaded into indico)
  - Exercise: try to reproduce SLy5
  - Detailed analysis of issues
  - What do we learn?

- EDFs at finite temperature
  - Instabilities in spin-isospin-polarized systems
  - Analysis of liquid-gas phase transition

Skyrme EDF framework

- Establish energy density functional (Skyrme EDF)

$$\mathcal{E}_T = C_T^{\rho}\rho_T^2 + C_T^{\Delta\rho}\Delta\rho_T^2 + C_T^{\tau}\rho_T\tau_T + C_T^{J}\mathcal{J}_T^2 + C_T^{\nabla J}\rho_T\nabla\cdot\mathbf{J}$$

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha}\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}') \qquad \rho_T(\mathbf{r}) = \sum_{\sigma\tau}\rho(\mathbf{r}\sigma\tau,\mathbf{r}\sigma\tau)\tau^T \qquad \tau_T(\mathbf{r}) = \nabla\cdot\nabla'\rho_T(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}$$

$$\mathcal{J}_T(\mathbf{r}) = \frac{i}{2}\left(\nabla' - \nabla\right)\rho_T(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'} \qquad \mathbf{J} = \sum_{ijk}\epsilon_{ijk}\mathcal{J}_{jk}\mathbf{e}_i$$

- Solve Kohn-Sham equations (+ BCS)

$$h_{ij} = \frac{\delta\mathcal{E}}{\delta\rho_{ij}} \Rightarrow h_{ij}\phi_\alpha = \varepsilon_\alpha\phi_\alpha$$

- Use density to compute energy

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha}\phi_\alpha(\mathbf{r})\phi_\alpha^*(\mathbf{r}') \quad \Rightarrow \quad \mathcal{E}(\rho)$$

$\Downarrow$

Observables: densities, energies, deformations

A typical Skyrme functional

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$$\mathcal{E}_T = C_T^\rho \rho_T^2 + C_T^{\Delta\rho} \Delta\rho_T^2 + C_T^\tau \rho_T \tau_T + C_T^J \mathcal{J}_T^2 + C_T^{\nabla J} \rho_T \nabla \cdot \mathbf{J}$$

T=0	T=1
$C_1^\rho = -\frac{1}{8} t_0 (1+2x_0) - \frac{1}{48} t_3 (1+2x_3) \rho^\alpha$	$C_0^\rho = \frac{3}{8} t_0 + \frac{3}{48} t_3 \rho^\alpha$
$C_1^s = -\frac{1}{8} t_0 - \frac{1}{48} t_3 \rho^\alpha$	$C_0^s = -\frac{1}{8} t_0 (1-2x_0) - \frac{1}{48} t_3 (1-2x_3) \rho^\alpha$
$C_1^\tau = -\frac{1}{16} t_1 (1+2x_1) + \frac{1}{16} t_2 (1+2x_2)$	$C_0^\tau = \frac{3}{16} t_1 + \frac{1}{4} t_2 \left(\frac{5}{4} + x_2 \right)$
$C_1^J = -\eta_J \left[-\frac{1}{16} t_1 + \frac{1}{16} t_2 \right]$	$C_0^J = -\eta_J \left[-\frac{1}{16} t_1 (1-2x_1) + \frac{1}{16} t_2 (1+2x_2) \right]$
$C_1^{\nabla J} = -\frac{1}{2} b'_4$	$C_0^{\nabla J} = -b_4 - \frac{1}{2} b'_4$

SLy5

$$t_0 = -2484.88\,, \quad x_0 = 0.778$$
$$t_1 = 483.13\,, \quad x_1 = -0.328$$
$$t_2 = -549.40\,, \quad x_2 = -1.000$$
$$t_3 = 13763.0\,, \quad x_3 = 1.267$$
$$\sigma = \frac{1}{6}\,, \quad b_4 = 63$$

Fit procedure

Given a set of m observables O used to calibrate the parameters $\mathbf{p}$ of a model, the optimum parametrization $\boldsymbol{p_0}$ is determined by a fit with global quality measure

$$\chi^2(\mathbf{p}) = \sum_{i=1}^{m} \left(\frac{O_i^{theo}(\mathbf{p}) - O_i^{ref}}{\Delta O_i^{ref}} \right)^2$$

O_i^{theo} : calculated values

O_i^{ref} : reference/experimental values

ΔO_i^{ref} : adopted errors

- Values often chosen *ad hoc* (personal bias)⇒ <u>information</u> theory?
- Weights also chosen *ad hoc* ⇒ <u>meaningul</u> errors?
- Post-optimization test: $\Delta O_i^{ref} \sim O_i^{theo} - O_i^{ref}$

Most recently: B.A. Brown, arxiv:1308.3664 (no correlation!)

Skyrme Lyon fit

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$$\chi^2 = \left(\frac{e_\infty + 16}{0.2}\right)^2 + \left(\frac{\rho_\infty - 0.16}{0.005}\right)^2$$ → Saturation

$$+ \sum_{i=1}^{11} \left(\frac{e_i^{PNM} - e_i^{UV14+UVIII}}{\Delta E_i}\right)^2$$ → Neutron matter microscopic EoS

$$+ \sum_{i=1}^{5} \left(\frac{B_i^{HF} - B_i^{exp}}{2}\right)^2$$ → Binding energies

$^{40,48}Ca$, ^{56}Ni, ^{132}Sn, ^{208}Pb

$$+ \sum_{i=1}^{4} \left(\frac{\sqrt{\langle r^2_{ch}\rangle_i}^{HF} - \sqrt{\langle r^2_{ch}\rangle_i}^{exp}}{0.02}\right)^2$$ → Charge radii

$^{40,48}Ca$, ^{56}Ni, ^{208}Pb

+ σ=1/6 + x_2=-1 (no ferromagnetism)

+ W_0, fixed to 3p neutron splitting in ^{208}Pb

Chabanat *et al.*, Nucl. Phys. A **627**, 710 (1997); *ibid* **635,** 231 (1998)

Skyrme Lyon fit

Table 4

Constraints used for the new Skyrme forces

	SLy4	SLy5	SLy6	SLy7	SLy10
UV14+UVII EOS [a]	×	×	×	×	×
Binding energies and $\langle r^2 \rangle_{ch}$	×	×	×	×	×
Splitting $3p\frac{3}{2} - 3p\frac{1}{2}$ in ^{208}Pb	×	×	×	×	×
$x_2 = -1$ [b]	×	×	×	×	×
J^2 terms		×		×	×
Two-body cm correction			×	×	×
Two components in spin–orbit					×

[a] See paper I, Section 3.3 for the discussion of these constraints.

[b] See paper I, Section 3.6 for the discussion of these constraints.

- More theoretical uncertainty coming from assumptions themselves
- (Difficult to quantify such systematic errors. How to do it?)

- Numerical uncertainty as well (generally easier to find out)

Chabanat *et al.*, Nucl. Phys. A **627**, 710 (1997); *ibid* **635,** 231 (1998)

UNEDF fit

$$\chi^2 = \sum_{i=1}^{72} \left(\frac{B_i^{theo} - B_i^{exp}}{2} \right)^2 + \sum_{i=1}^{28} \left(\frac{\sqrt{\langle r_{ch}^2 \rangle_i}^{theo} - \sqrt{\langle r_{ch}^2 \rangle_i}^{exp}}{0.02} \right)^2 + \sum_{i=1}^{8} \left(\frac{OES_i^{theo} - OES_i^{exp}}{0.02} \right)^2$$

Large pool of nuclei: 28 sph (mass+radii), 44 deformed (mass), 8 odd-even staggering

Kortelainen *et al.*, Phys. Rev. C **82**, 024313 (2010); *ibid* **85,** 024304 (2012)

Covariance analysis

- Minimum of χ^2 $$\partial_{\mathbf{p}} \chi^2(\mathbf{p})\Big|_{\mathbf{p}=\mathbf{p_0}} = 0$$
- Estimate around minimum $$\chi^2(\mathbf{p}) \sim \chi^2(\mathbf{p_0}) + (\mathbf{p}-\mathbf{p_0})_i \underbrace{\mathcal{M}_{ij}}_{\frac{1}{2}\partial_{p_i}\partial_{p_j}\chi} (\mathbf{p}-\mathbf{p_0})_j$$

Error

$$e(\mathbf{p}_i) = \sqrt{(\mathcal{M}^{-1})_{ii}}$$

```
Errors in free parameters
=============================
e_i = sqrt( Eii )

t_0 =        -2475.408000 +/-  149.455460
t_1 =          482.842000 +/-   58.537029
t_2 =         -559.374000 +/-  144.534277
t_3 =        13697.070000 +/- 1672.926947
x_0 =            0.741185 +/-    0.189191
x_1 =           -0.146374 +/-    0.468173
x_3 =            1.162688 +/-    0.340537
```

Correlation

$$\mathcal{C}_{ij} = \frac{\mathcal{M}^{-1}_{ij}}{\sqrt{\mathcal{M}^{-1}_{ii}\mathcal{M}^{-1}_{jj}}}$$

```
Correlation Matrix
====================
Cij = Eij/sqrt(Eii Ejj)
```

t_0	t_1	t_2	t_3	x_0	x_1	x_3
1.0000	0.9837	0.9854	-0.9997	-0.6766	0.8110	-0.6158
0.9837	1.0000	0.9575	-0.9870	-0.7066	0.8489	-0.6553
0.9854	0.9575	1.0000	-0.9863	-0.6601	0.7843	-0.5964
-0.9997	-0.9870	-0.9863	1.0000	0.6798	-0.8154	0.6197
-0.6766	-0.7066	-0.6601	0.6798	1.0000	-0.9327	0.9928
0.8110	0.8489	0.7843	-0.8154	-0.9327	1.0000	-0.9311
-0.6158	-0.6553	-0.5964	0.6197	0.9928	-0.9311	1.0000

Covariance analysis

- **Minimum of χ^2** $\partial_{\mathbf{p}} \chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p_0}} = 0$

- **Estimate around minimum** $\chi^2(\mathbf{p}) \sim \chi^2(\mathbf{p_0}) + (\mathbf{p}-\mathbf{p_0})_i \underbrace{\mathcal{M}_{ij}}_{\frac{1}{2}\partial_{p_i}\partial_{p_j}\chi} (\mathbf{p}-\mathbf{p_0})_j$

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Covariance analysis: observables

- Observable: dependence on parameters

$$A(\mathbf{p}) = A(\mathbf{p_0}) + (\mathbf{p} - \mathbf{p_0})\partial_{\mathbf{p}} A(\mathbf{p})|_{\mathbf{p_0}} + \mathcal{O}(\delta\mathbf{p}^2)$$

- Gaussian distribution of parametrizations around minimum

$$\mathcal{P}(\mathbf{p}) = \mathcal{N} \exp\left(\frac{1}{2}\delta\mathbf{p}_i \mathcal{M}_{ij} \delta\mathbf{p}_j\right)$$

- Average of observable

$$\langle A \rangle = \int \mathrm{d}\mathbf{p}\, A(\mathbf{p})\mathcal{P}(\mathbf{p}) \sim A(\mathbf{p_0})$$

- Correlations

$$C_{AB} = \langle (A(\mathbf{p}) - \langle A \rangle)\,(B(\mathbf{p}) - \langle B \rangle) \rangle \sim \partial_{\mathbf{p}_i} A(\mathbf{p})|_{\mathbf{p_0}}\,(\mathcal{M})^{-1}_{ij}\,\partial_{\mathbf{p}_j} B(\mathbf{p})|_{\mathbf{p_0}}$$

- Pearson correlations coefficient $\mathcal{C}_{AB} = \frac{C_{AB}}{\sqrt{C_{AA}C_{BB}}}$

Numerical details

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- Derivatives up to first order

$$\mathcal{M}_{ij} = \frac{1}{2}\partial_{p_i}\partial_{p_j}\chi \sim \sum_{k=1}^{m} \frac{\partial_{\mathbf{p}_i} O_k^{theo}}{\Delta O_k^{ref}} \frac{\partial_{\mathbf{p}_j} O_k^{theo}}{\Delta O_k^{ref}}$$

- Finite differences (valid to 2nd order)

$$\partial_{\mathbf{p}_i} O \sim \frac{O(\ldots, p_{0i} + \Delta p_i, \ldots) - O(\ldots, p_{0i} - \Delta p_i, \ldots)}{2\Delta p_i}$$

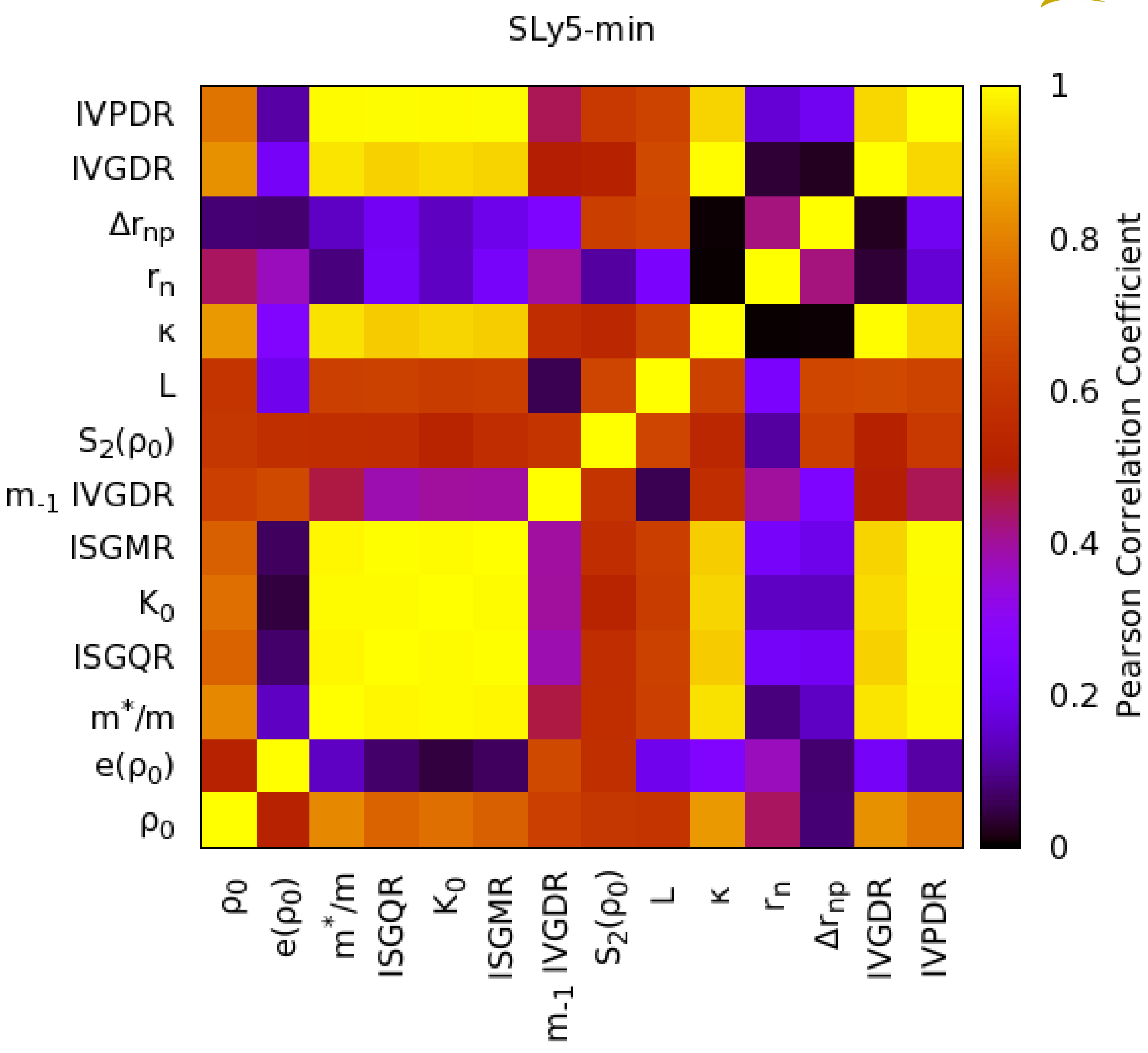
$$\partial^2_{\mathbf{p}_i} O \sim \frac{O(\ldots, p_{0i} + \Delta p_i, \ldots) - 2O(\mathbf{p_0}) + O(\ldots, p_{0i} - \Delta p_i, \ldots)}{(\Delta p_i)^2}$$ (error estimate)

- Step sizes: $\Delta\chi^2(\mathbf{p}) \sim 1$

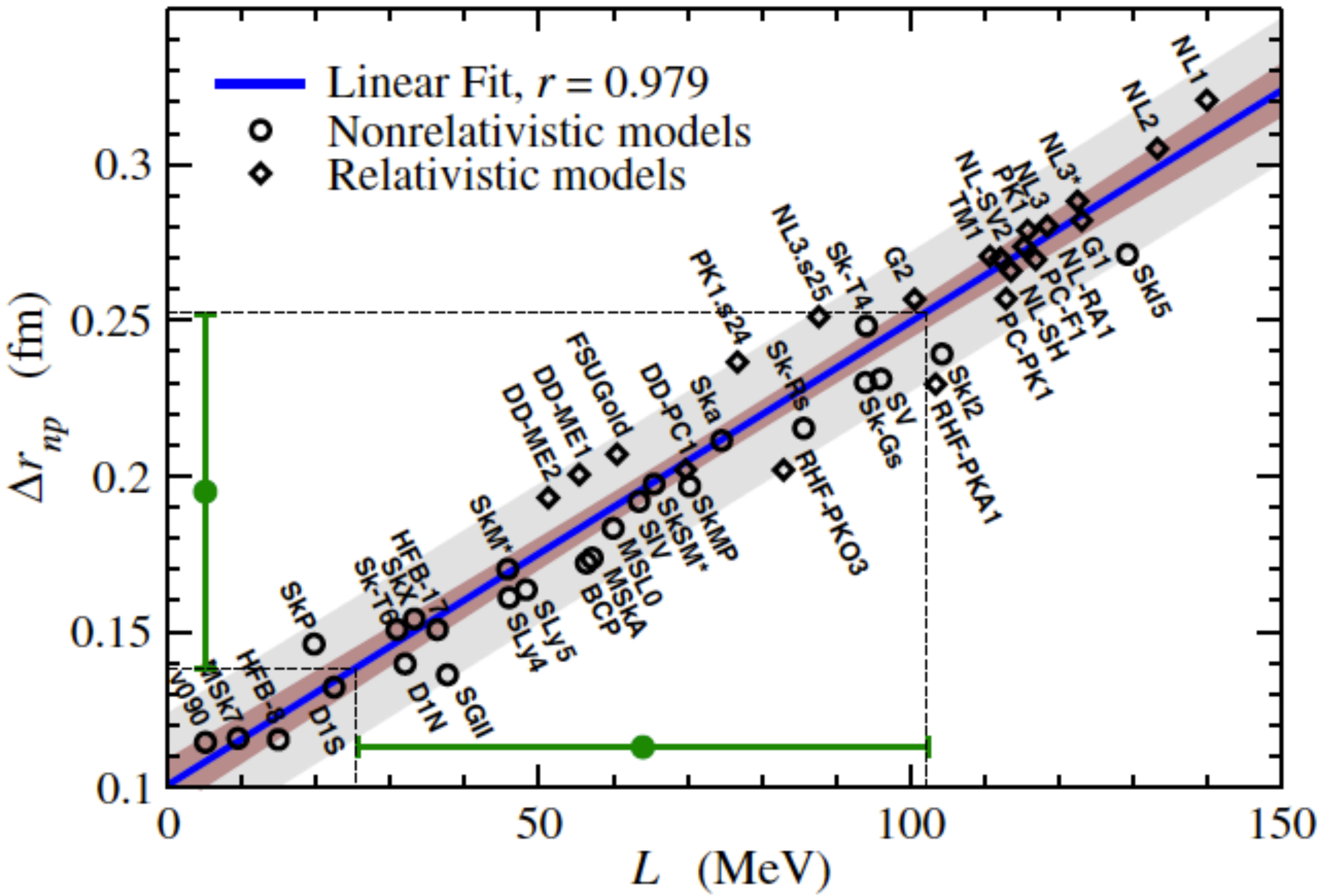
$$(\Delta p_i)^2 \equiv e(p_i) = \left(\mathcal{M}^{-1}\right)_{ii} = 2\left(\partial^2_{p_i}\chi^2\right)^{-1}$$

$$\sim 2h^2 \left(\chi_{p_i - h} - 2\chi_0 + \chi_{p_i + h}\right)^{-1}$$

Correlations I

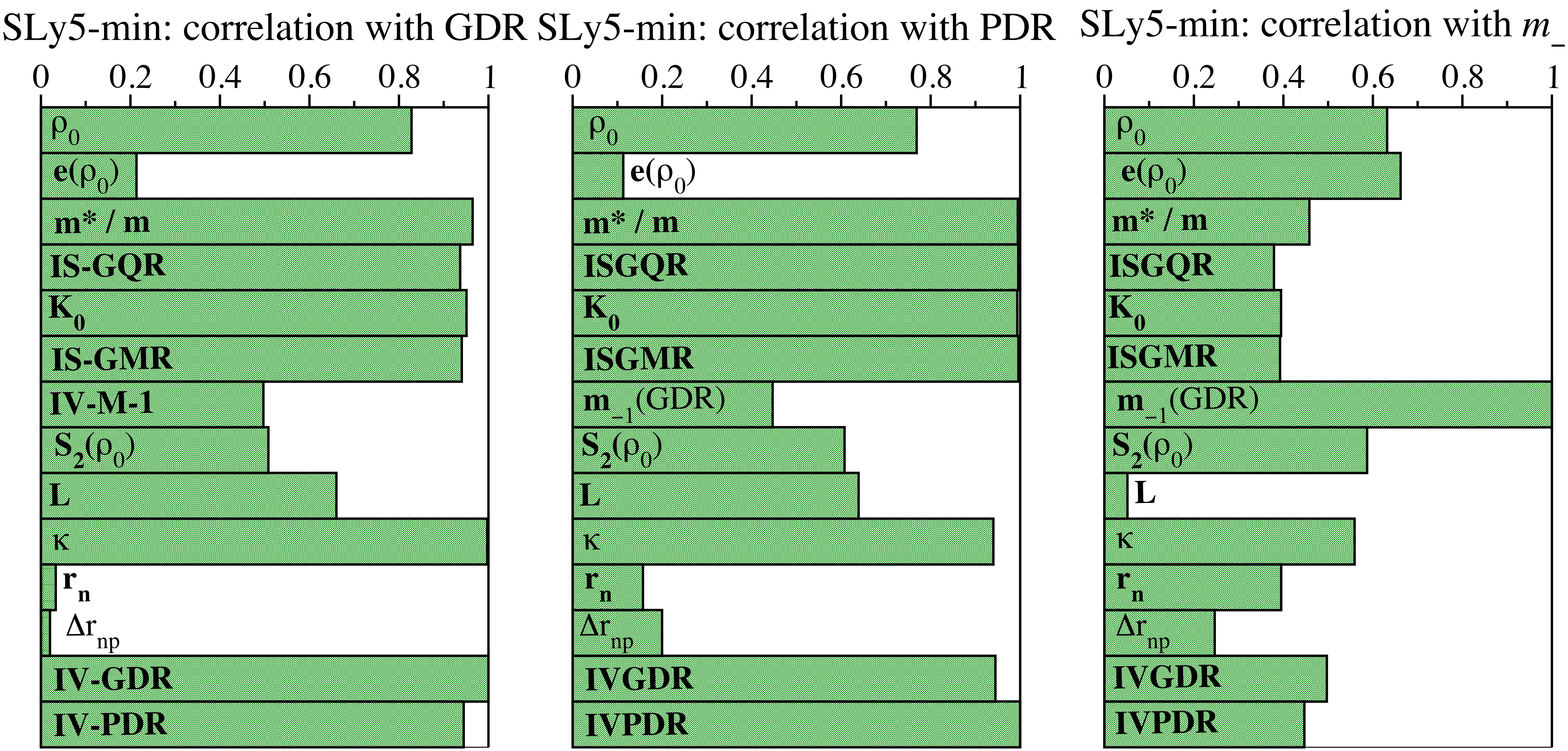


Correlations II



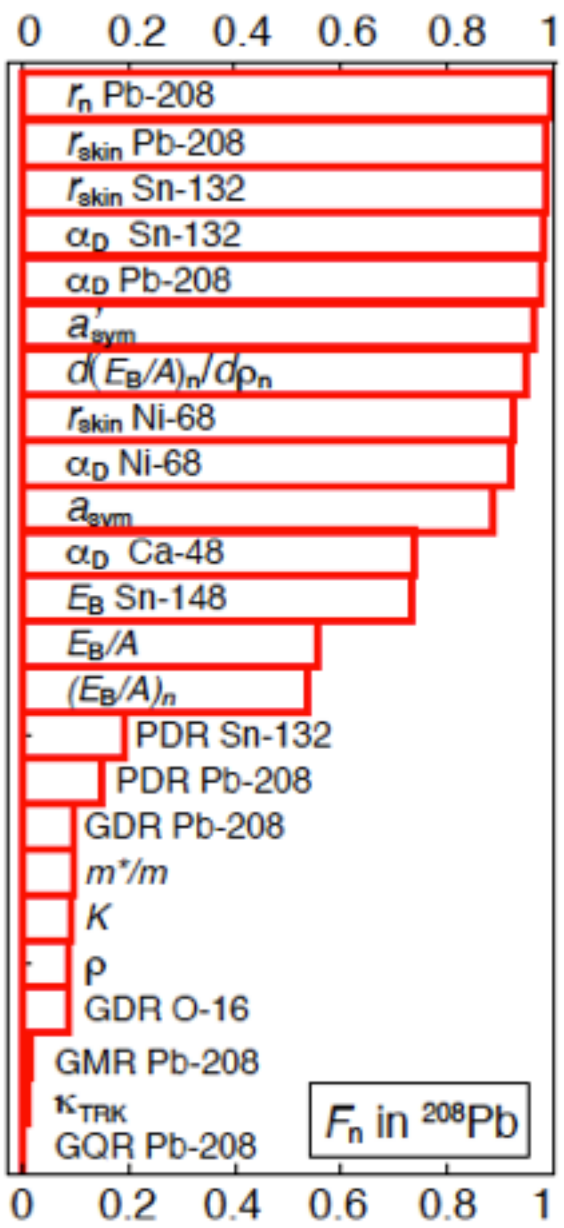
Roca-Maza *et al.*, Phys. Rev. Lett. **106** 252501 (2011)

Correlations II



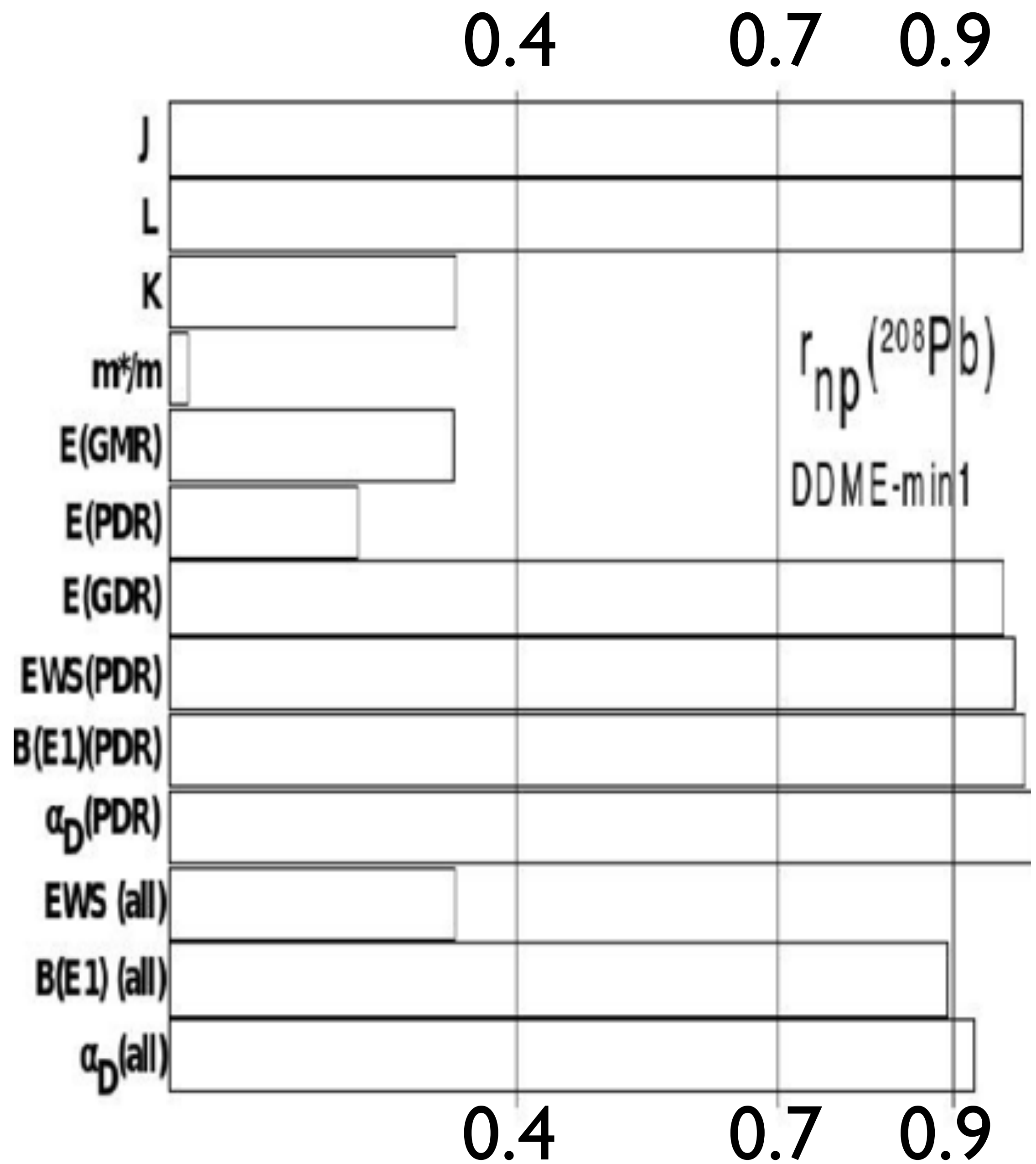
Correlations III

SV-min EDF



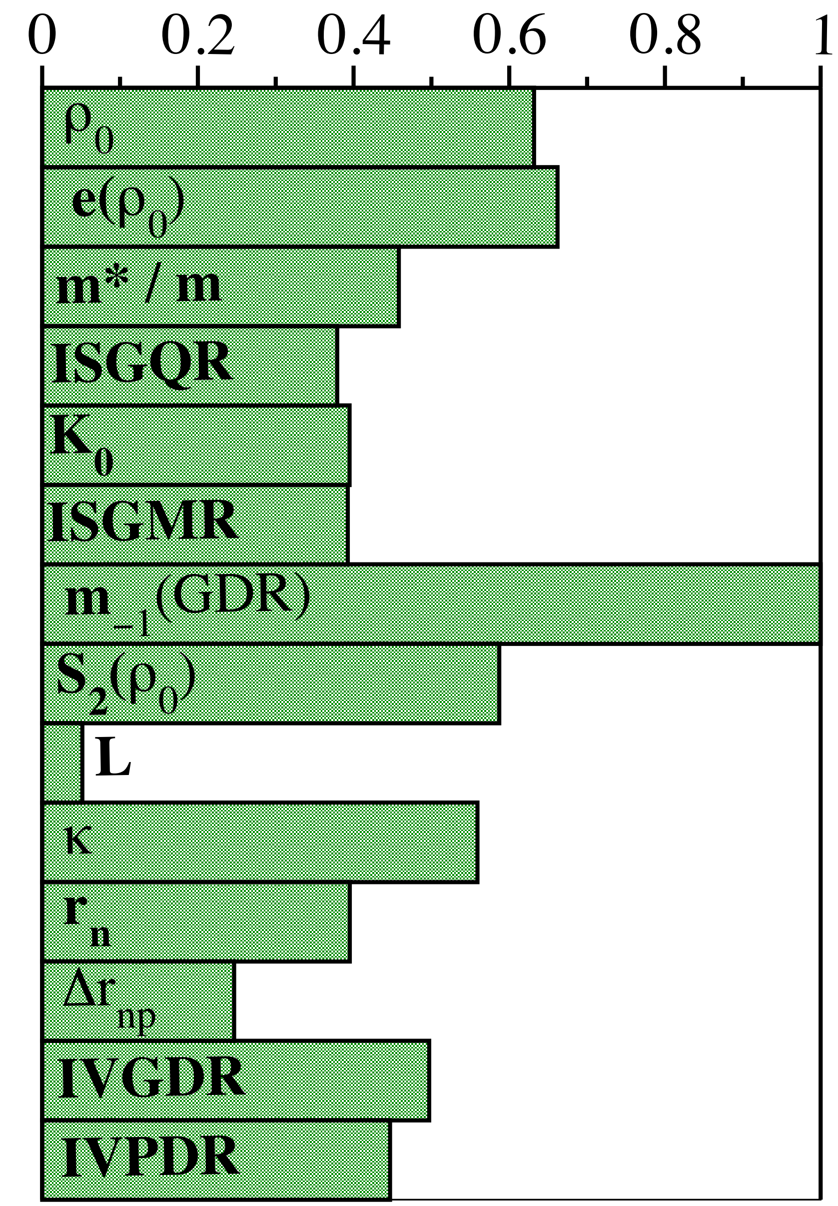
Reinhard and Nazarewicz., Phys. Rev. C **81**, 051303 (2010)

Relativistic mean-field



N. Paar, INPC 2013

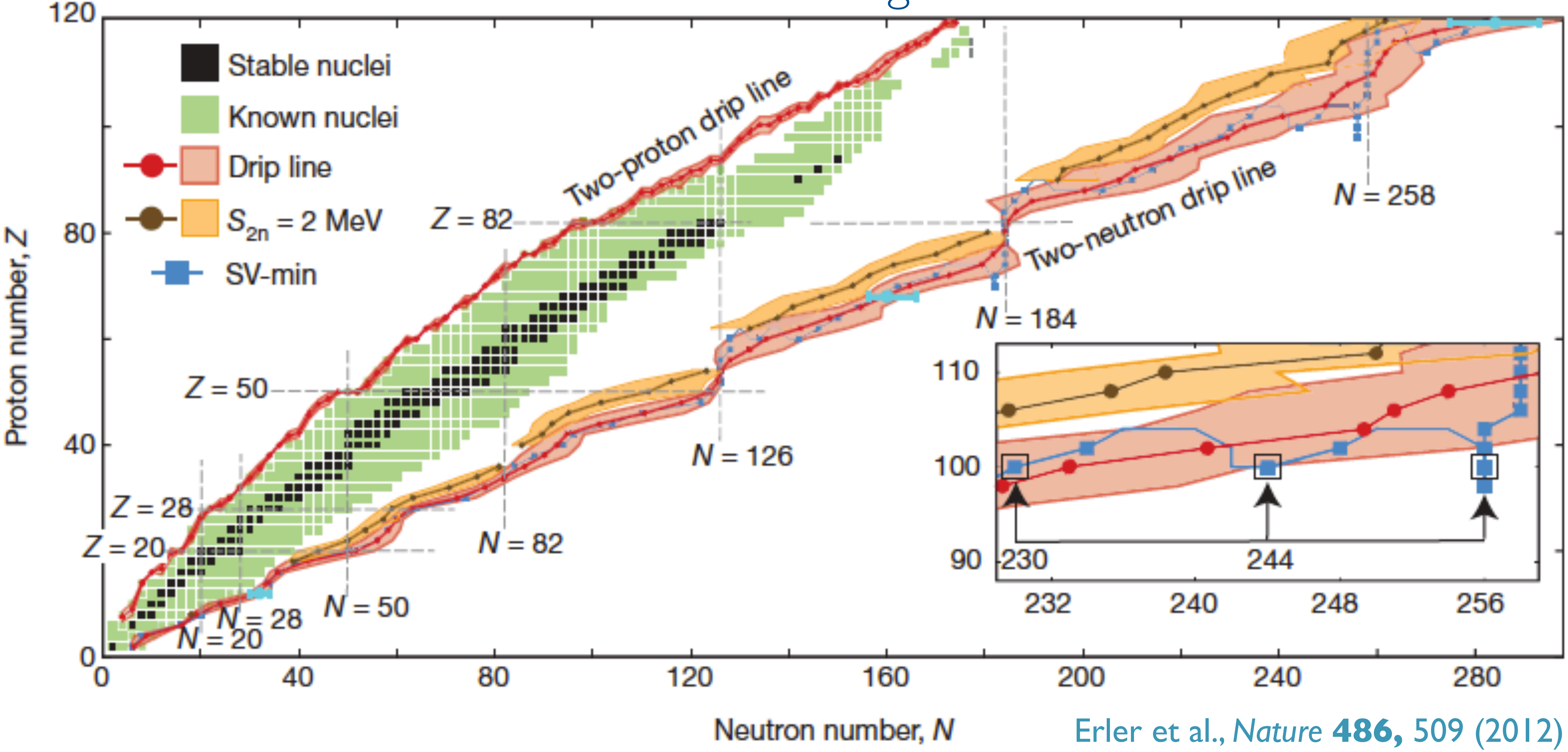
SLy5-min: correlation with m_{-1}



Roca-Maza

Theoretical predictions

Theoretical Segre chart



Erler et al., *Nature* **486,** 509 (2012)

- Nuclear energy density functional
- Compute all even-even isotopes simultaneously
- ≈7000 bound nuclides

Symmetry energy?

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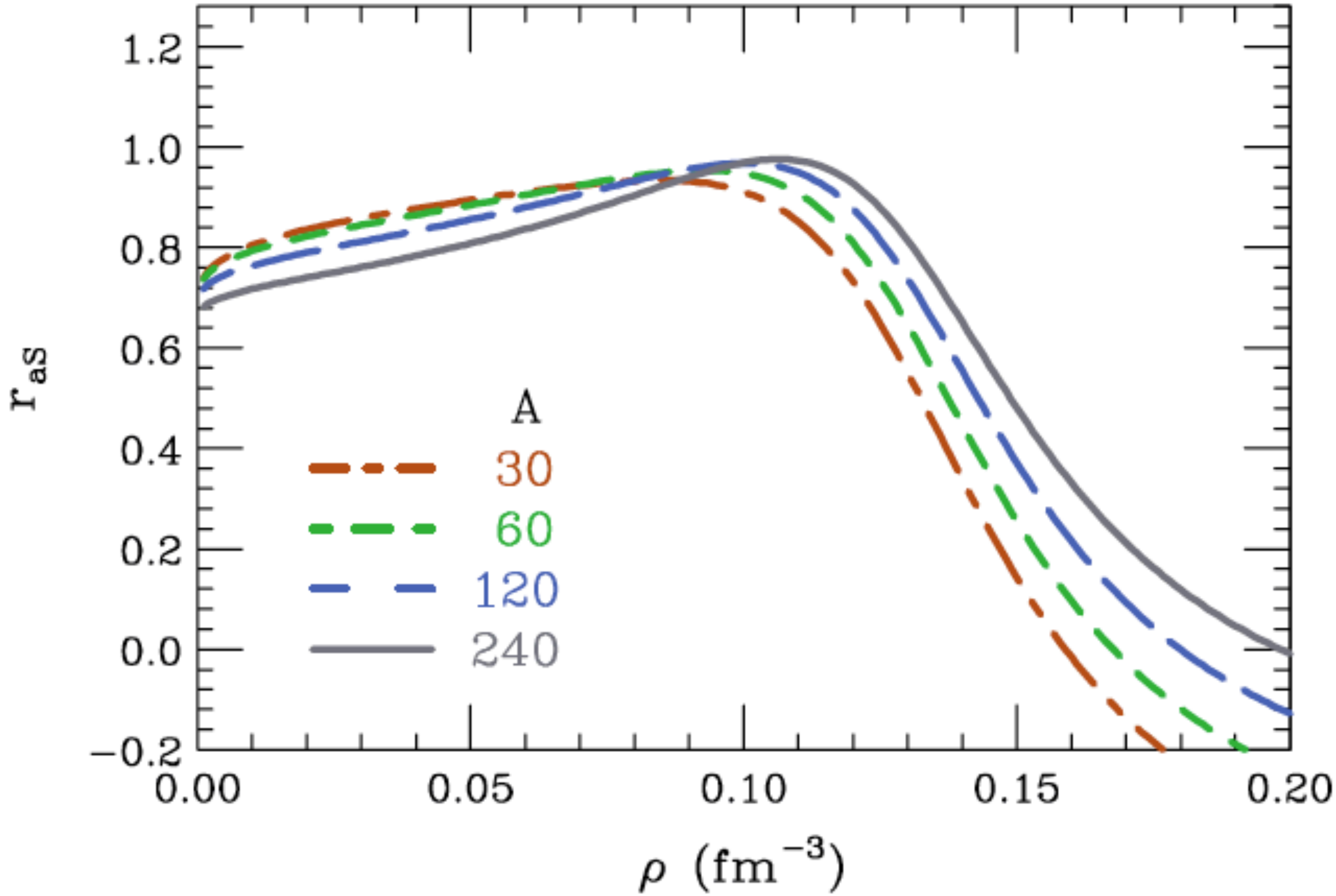
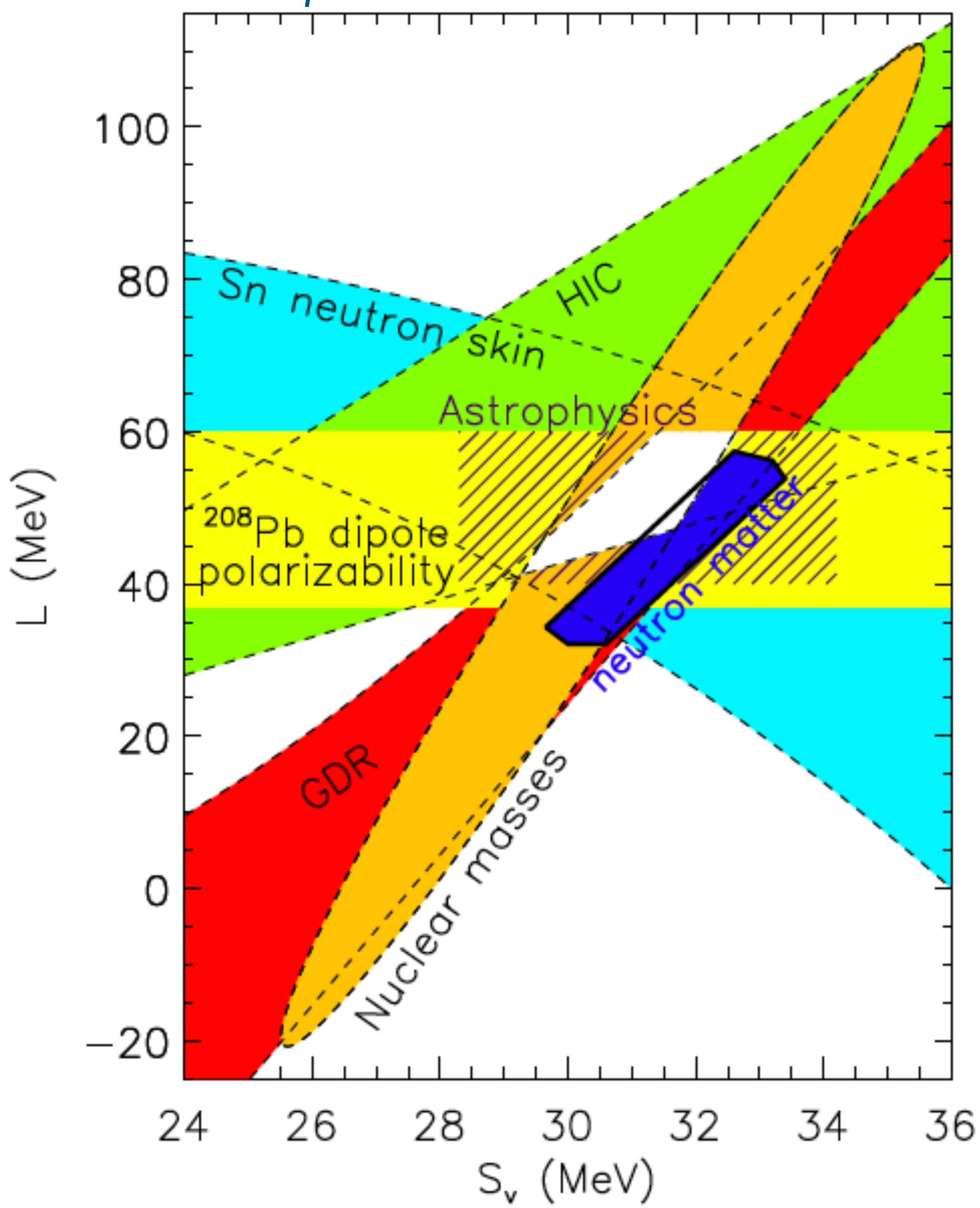
Correlation between $S(\rho)$ & $a_a(A)$



Danielewicz & Lee, arxiv:1307.4130

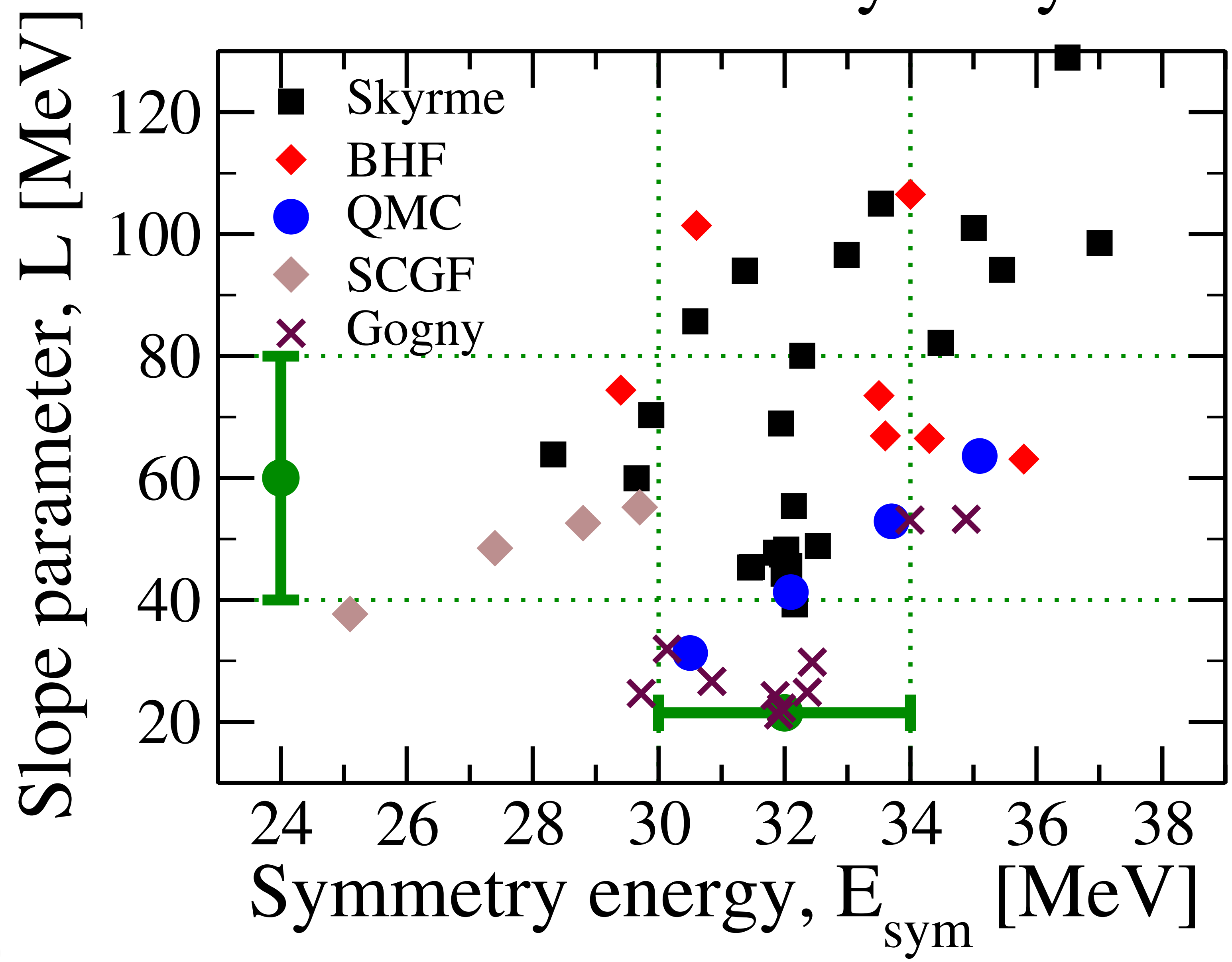
Isovector correlations

Empirical determination



Lattimer & Lim, ApJ **771**, 51 (2013)

Correlations from many-body theory



Gogny

- Somewhat bad isospin properties
- Covariance analysis?
- Rosh Sellahewa's PhD Thesis

Conclusions

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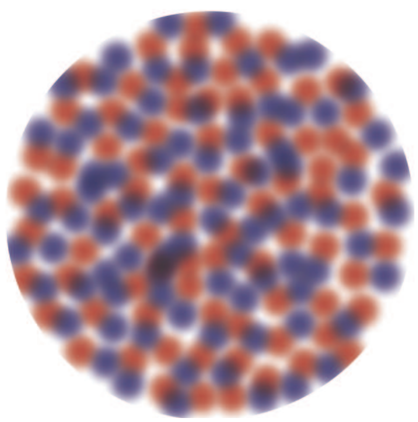
- Covariance analysis able to identify underlying connections
- Can be used to break correlations
- But error matrices need to be published!
- And then need to be used

- Following: easy example of what to do with these

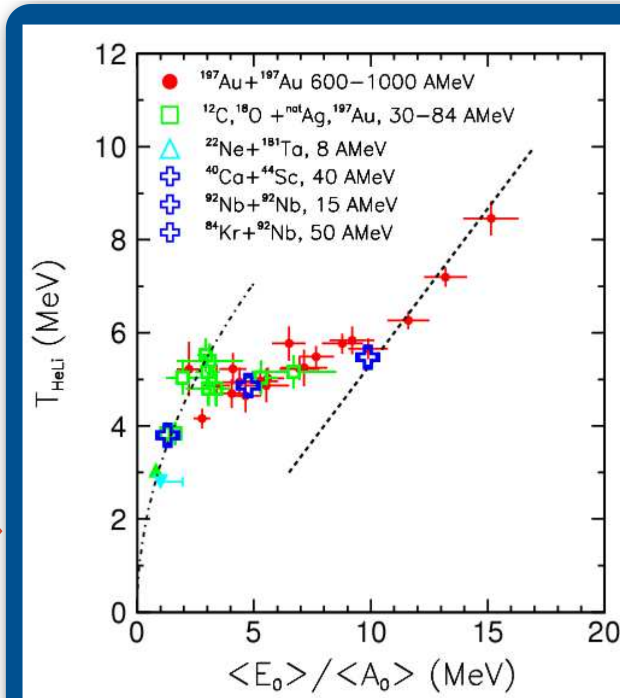
Heating nuclei up?

Cooking the nuclear soup



Temperatures

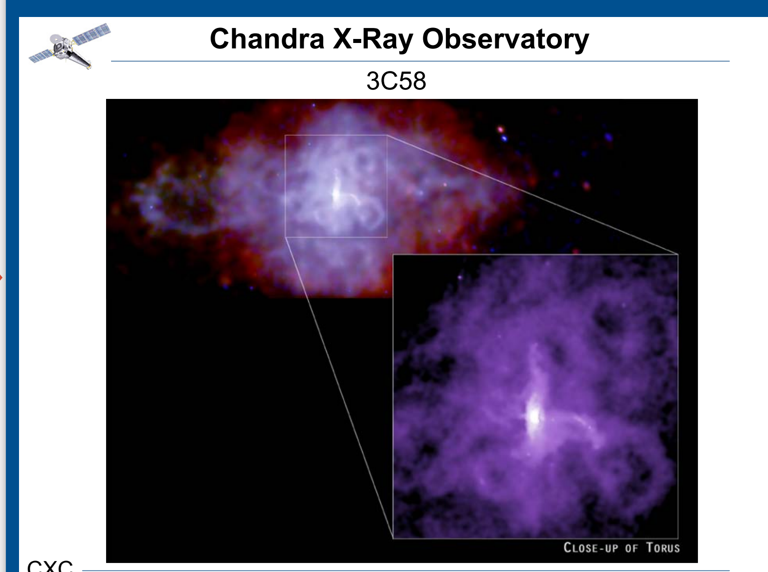
1 MeV~10^{11} K



Pochodzalla *et al*, PRL 75 1040 (1995)

Heavy ion collisions

- ✦N~Z systems
- ✦Hot for a short time
- ✦Finite systems



SN 1181 remnant (SNR3C58)
Pulser PSRJ0205+6449

Neutron stars

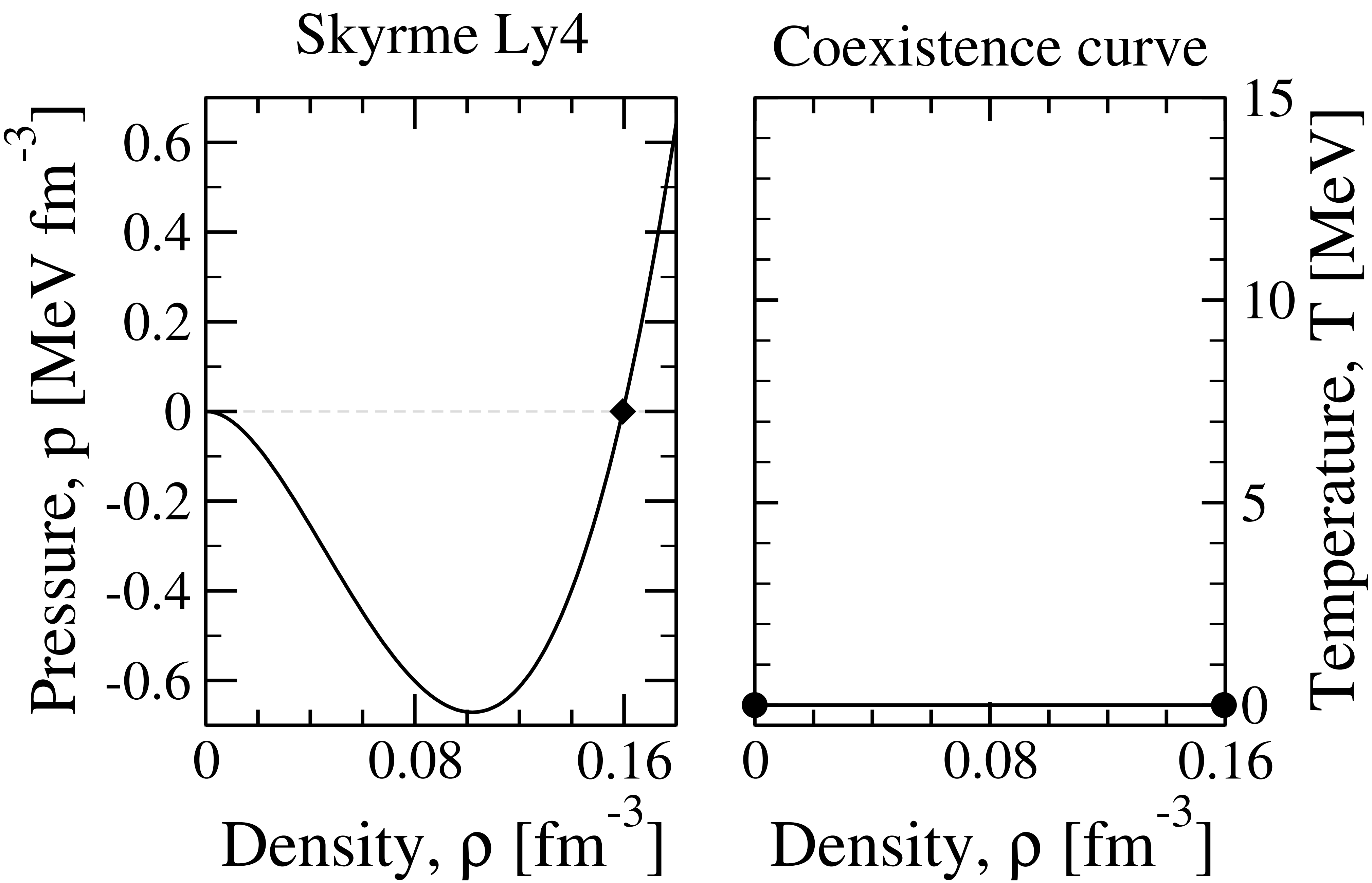
- ✦N>>Z systems
- ✦Hot for a short time
- ✦Infinite system

β=0

$$\beta = \frac{N-Z}{N+Z}$$

β=1

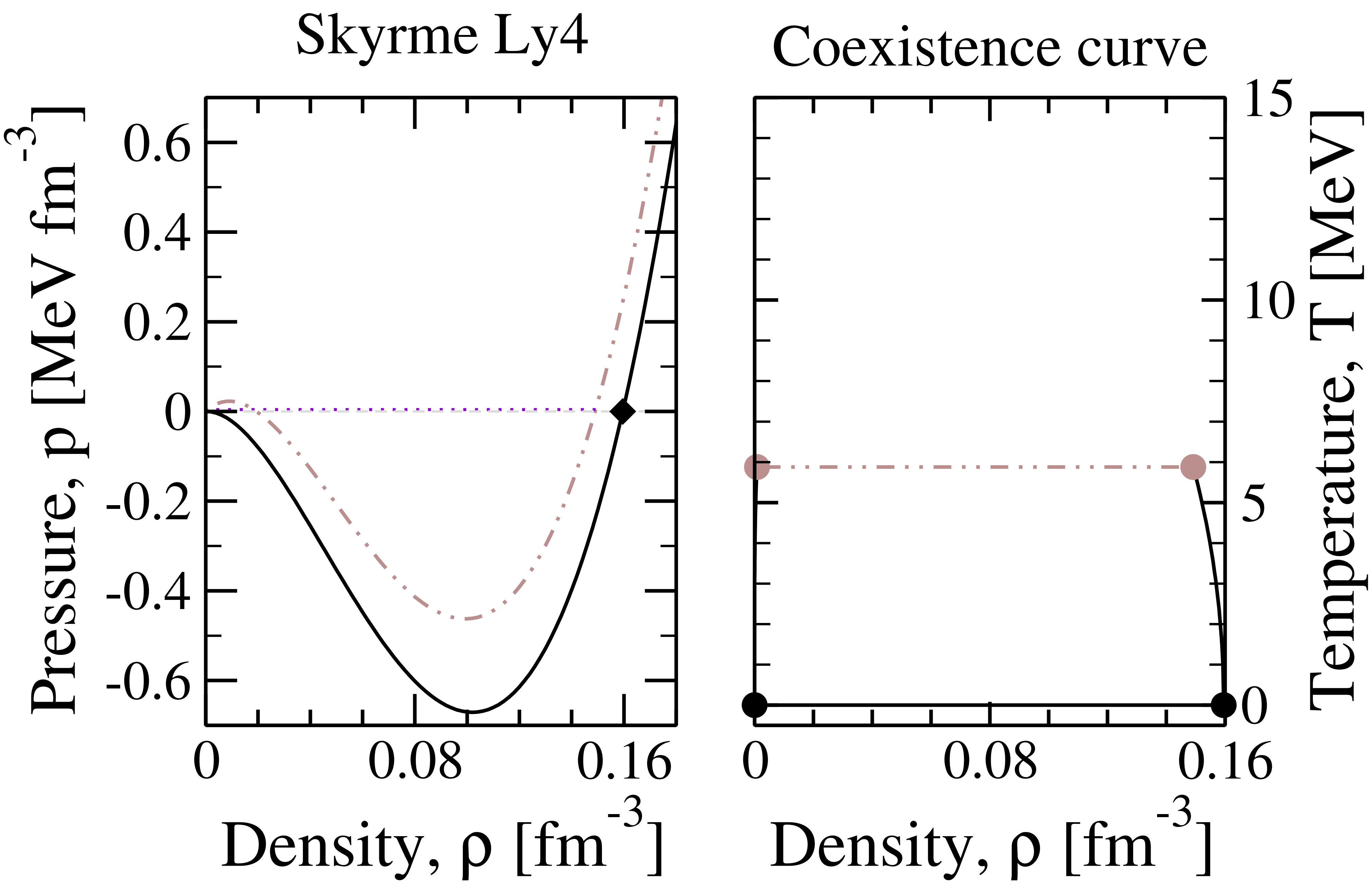
Phase coexistence



- Maxwell criterion: $\mu_g = \mu_l \, , \quad P_q = P_l$
- Simultaneous description of gas and liquid phase
- 3 points of physical importance

A. Rios, Nucl. Phys. A **845**, 58 (2010)

Phase coexistence



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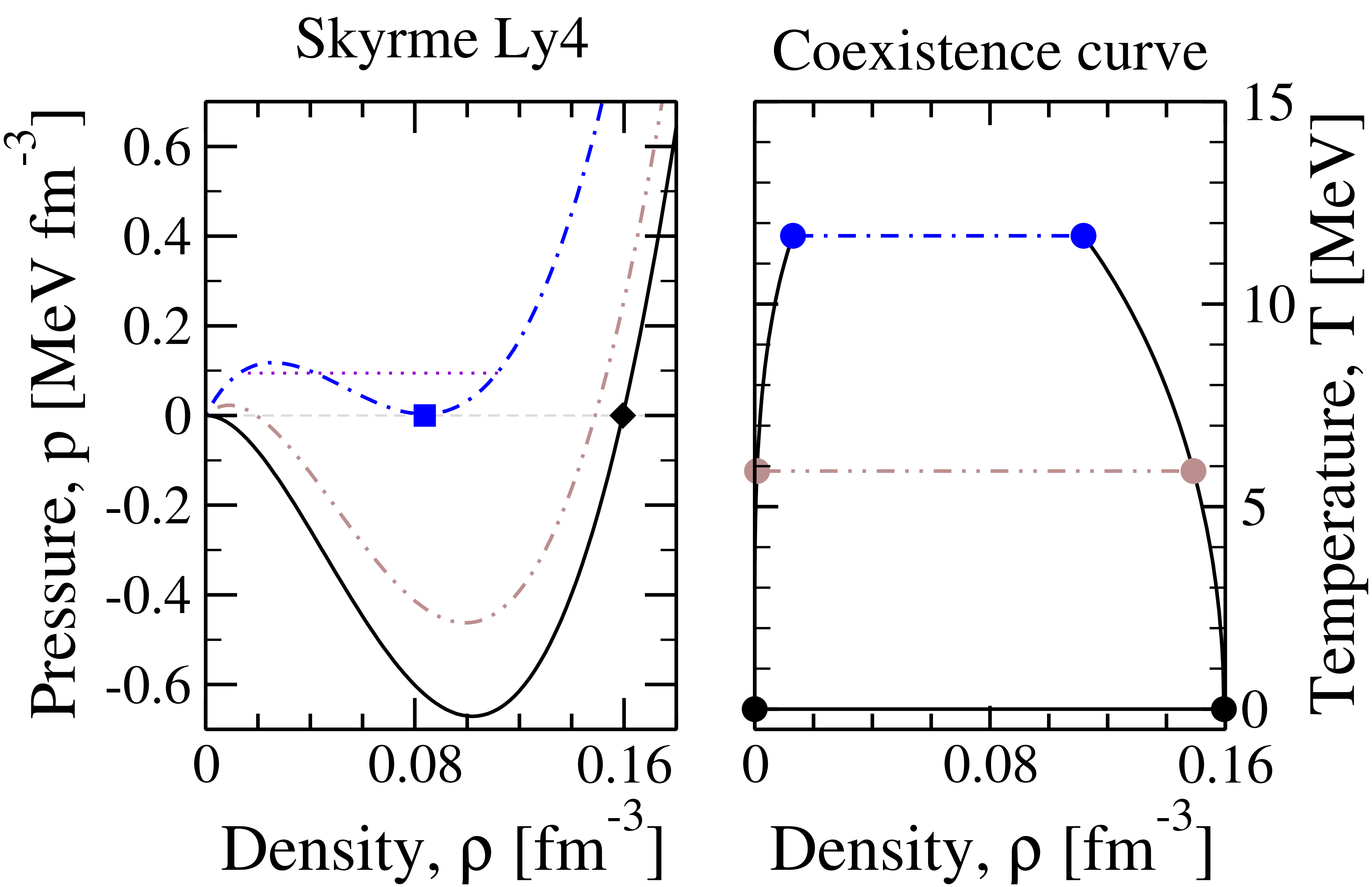

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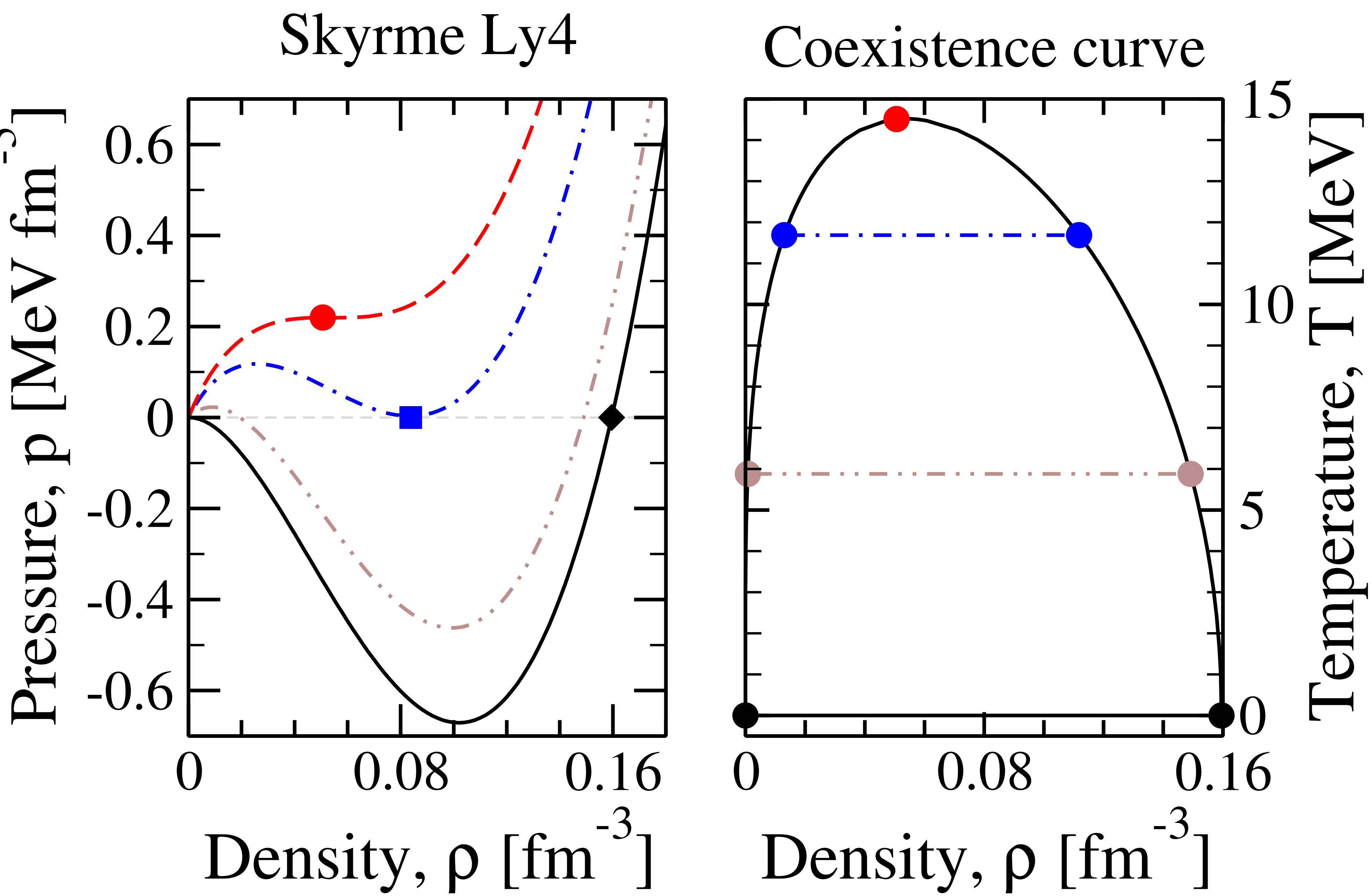

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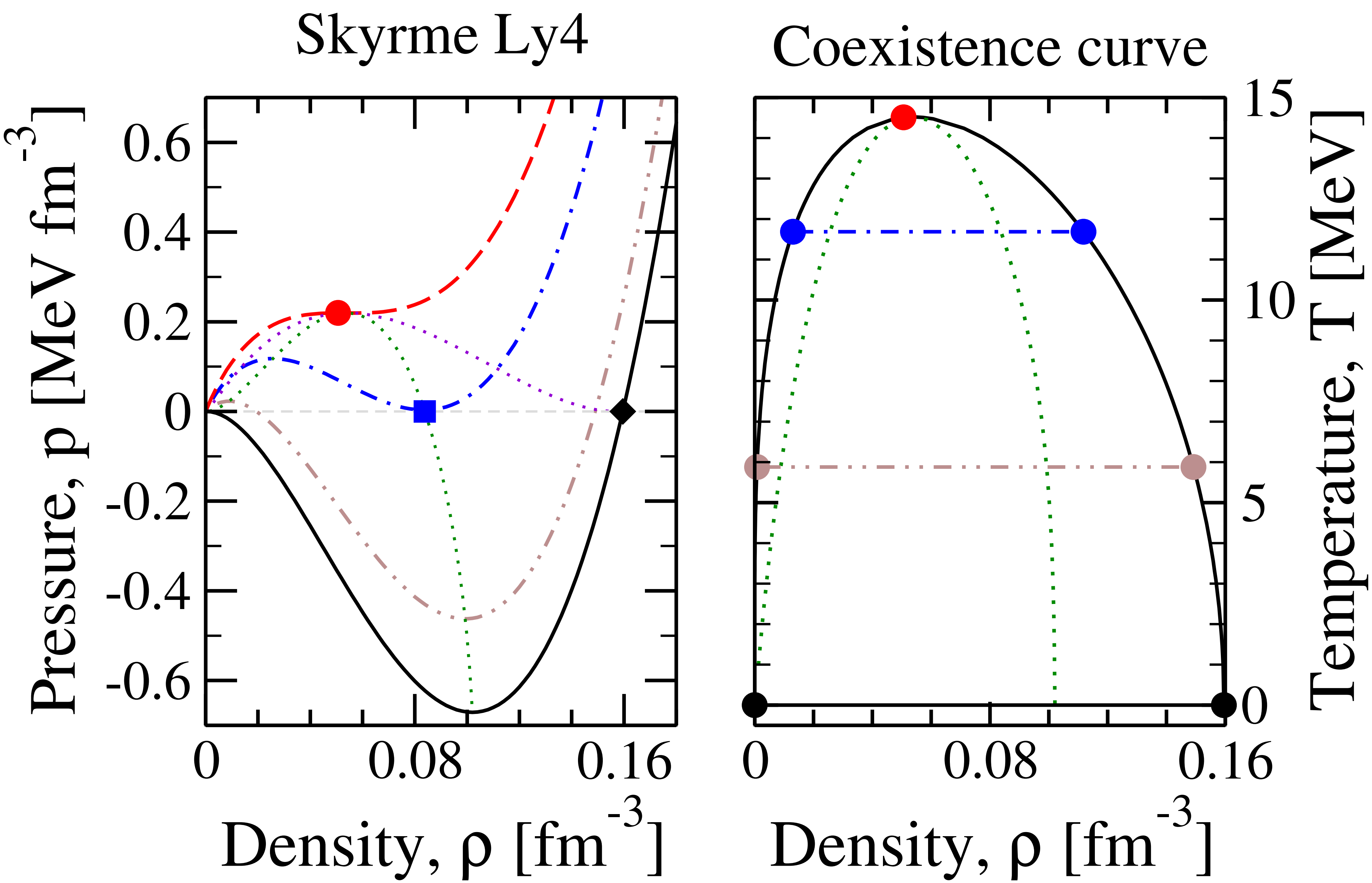

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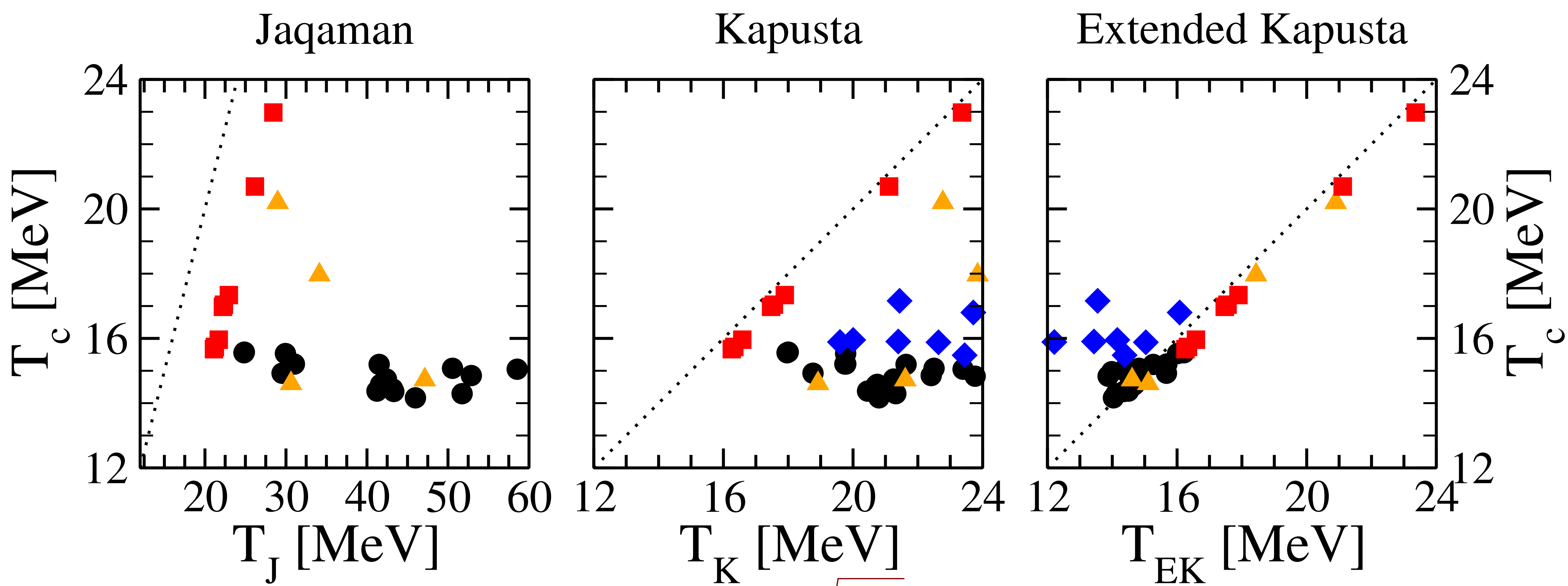
Prediction of critical point

Predicted vs calculated critical temperature



$$T_J = \frac{3}{4}\frac{\alpha}{\alpha+1}t_0\rho_c$$

$$T_K = 0.326\sqrt{\frac{K_0}{m_0^*}}\rho_0^{1/3}$$

$$T_{EK} = \frac{m^*(5\rho_0/12)}{m}T_K$$

Semiclassical t_0-t_3 force

Degenerate constant m^*

Degenerate Skyrme m^*

Squares: old Skyrme $m^*=m$

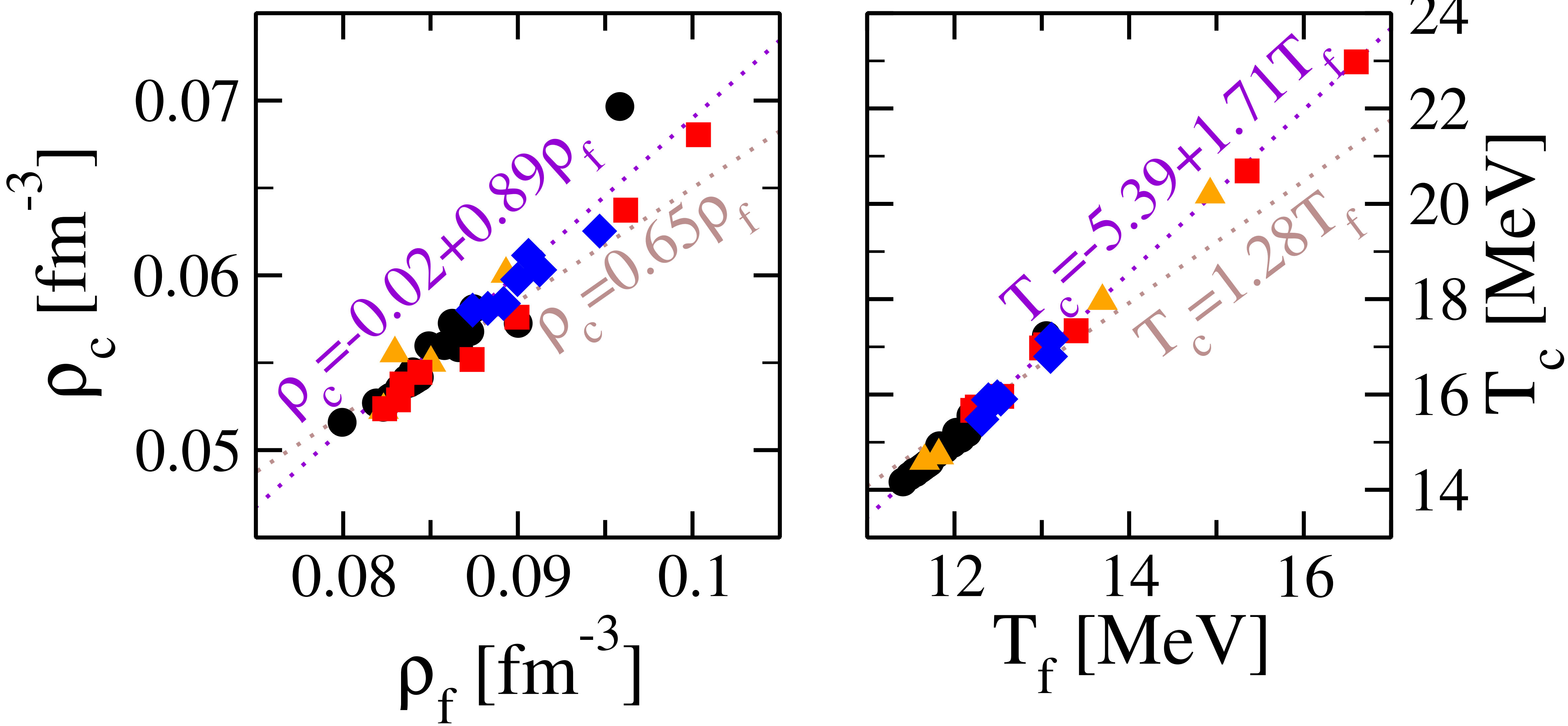
Triangles: old Skyrme $m^*\neq m$

Circles: modern Skyrme $m^*\neq m$

Diamonds: Gogny

Empirical correlations

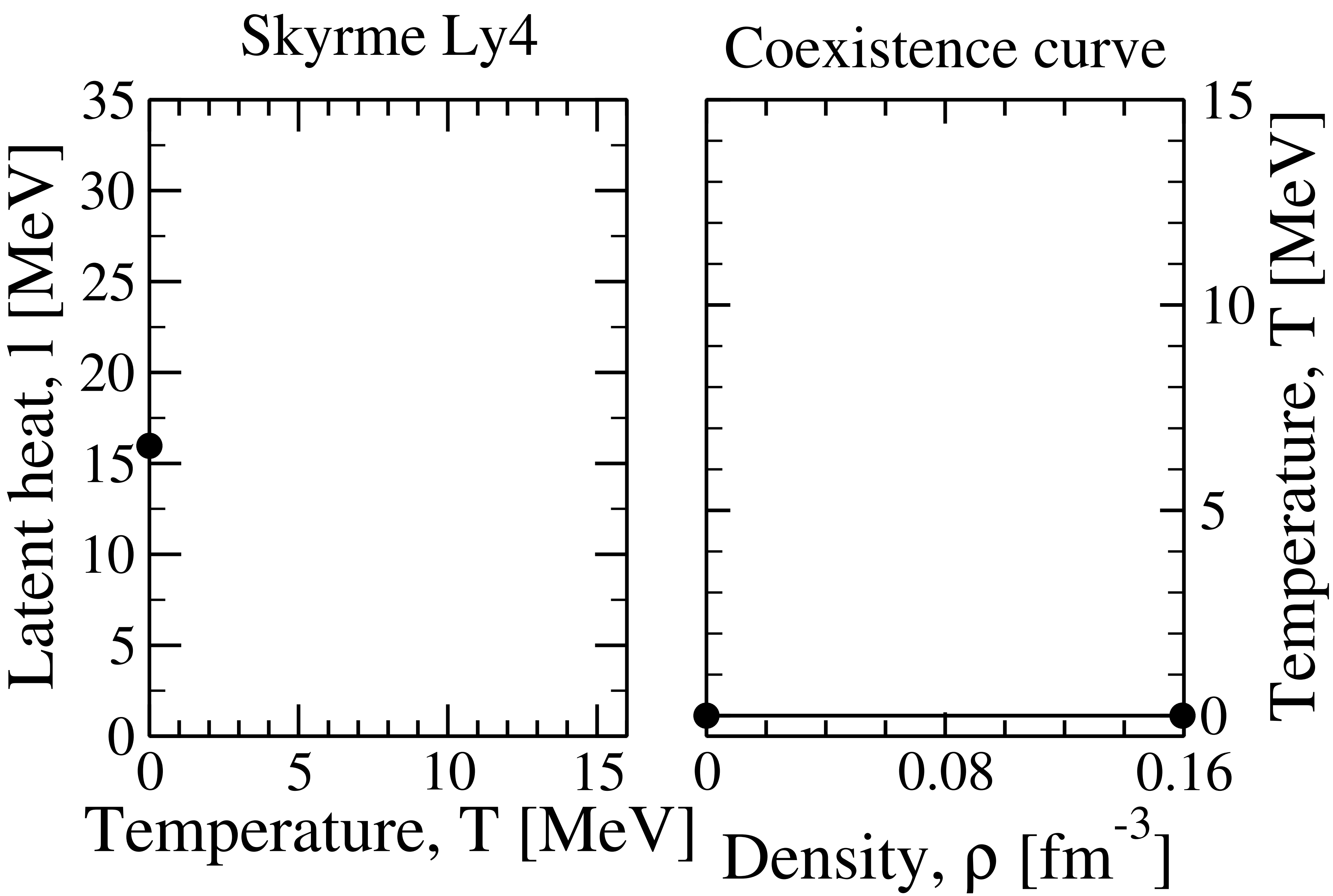
Correlation between flashing and critical points



$$\rho_c = \frac{2}{3}\rho_f \qquad T_c = (1.3 - 1.75)T_f$$

Are these built-in the parametrization?

Latent heat

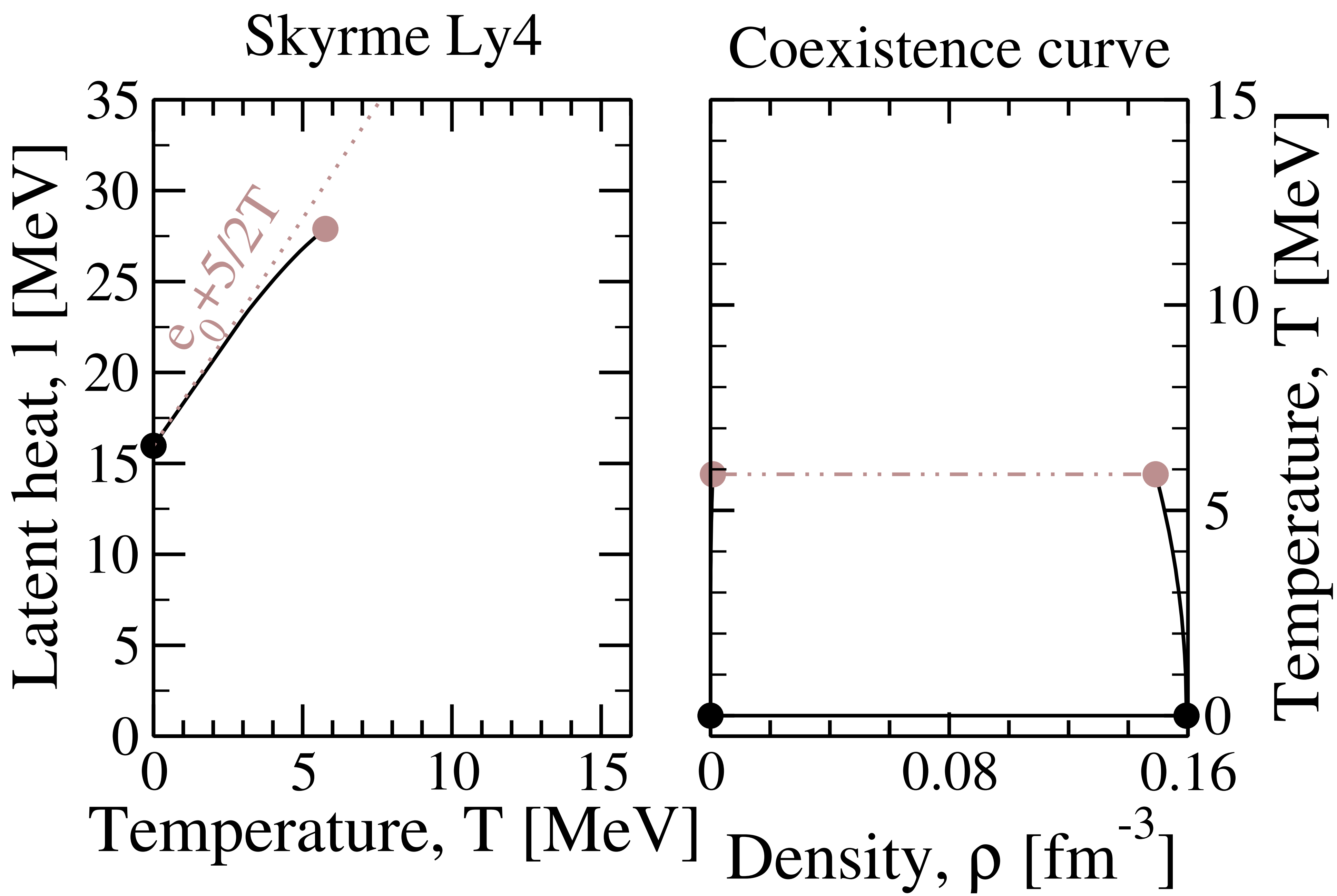


$$l = T(s_g - s_l)$$

$$l = T\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right) \left.\frac{\mathrm{d}p}{\mathrm{d}T}\right|_{\mathrm{coex}}$$

A. Carbone, A. Polls, A. Rios, I. Vidaña, Phys. Rev. C **83**, 024308 (2011)

Latent heat



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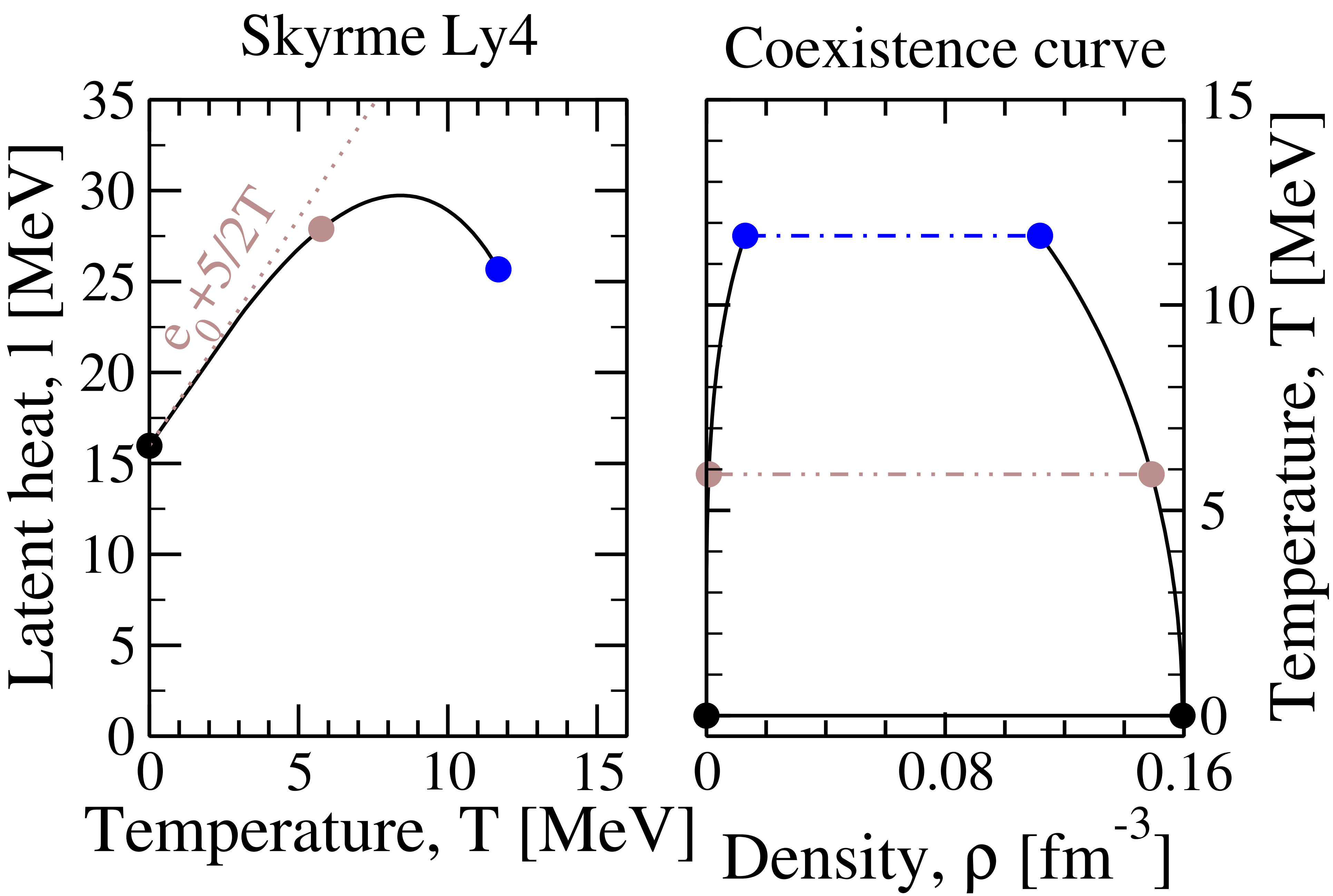

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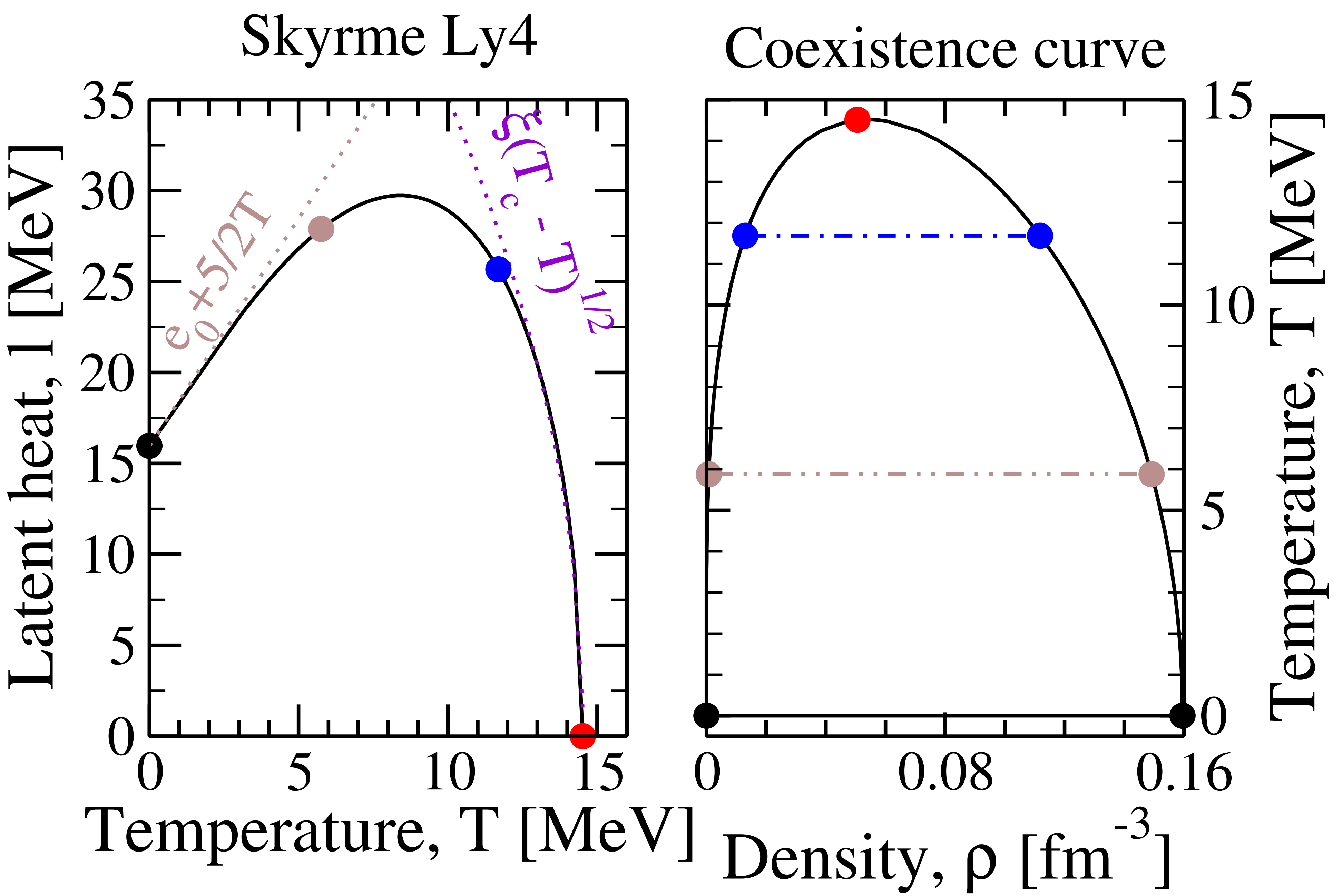
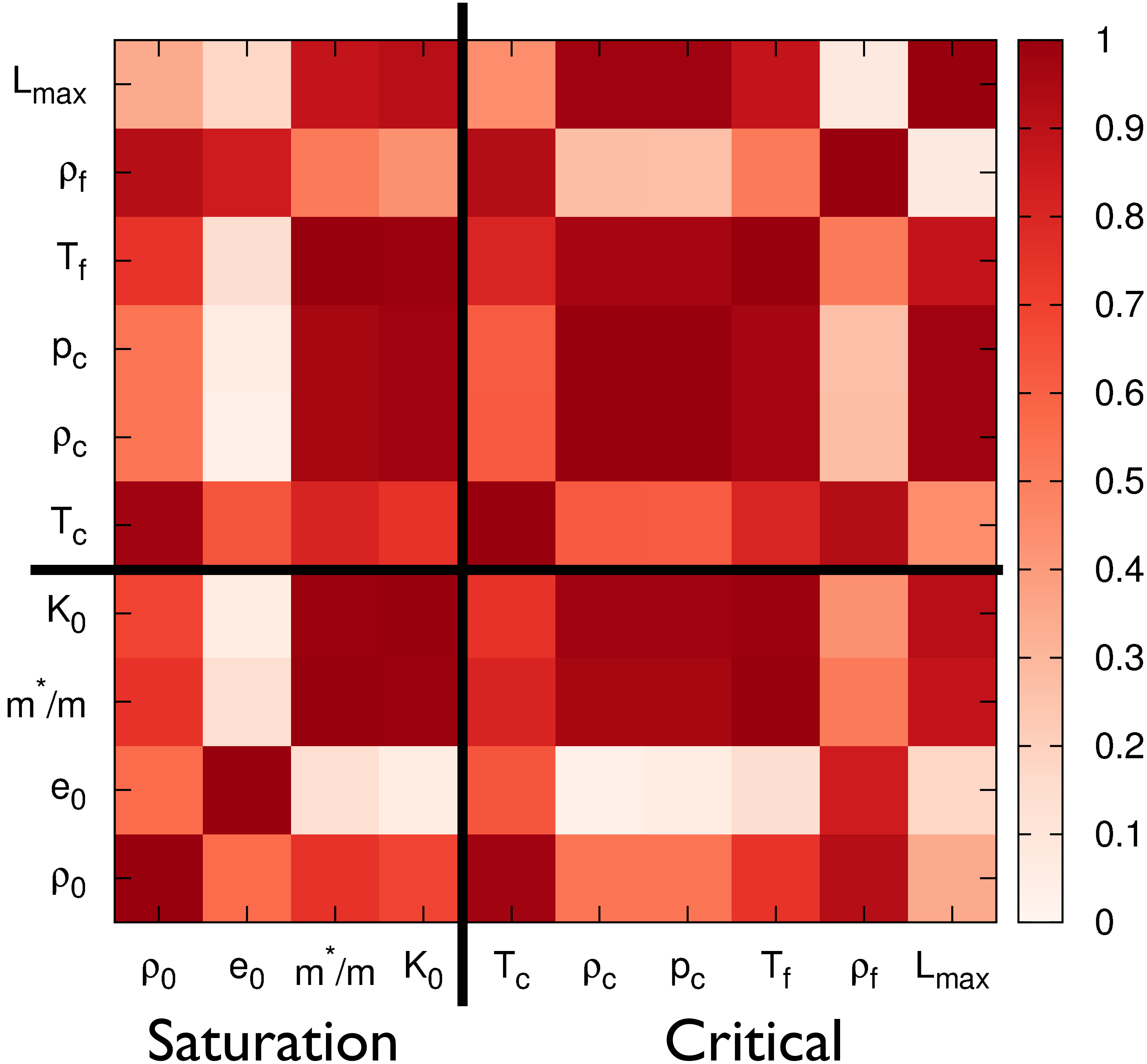


$$l = T(s_g - s_l)$$

$$l = T\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right) \left.\frac{\mathrm{d}p}{\mathrm{d}T}\right|_{\mathrm{coex}}$$

A. Carbone, A. Polls, A. Rios, I. Vidaña, Phys. Rev. C **83**, 024308 (2011)

Correlations at finite T: SLy5-min



$$T_c = 14.6 \pm 0.1 \text{ MeV}$$

$$\rho_c = 0.054 \pm 0.002 \text{ fm}^{-3}$$

$$T_f = 11.73 \pm 0.06 \text{ MeV}$$

$$\rho_f = 0.085 \pm 0.001 \text{ fm}^{-3}$$

$$L_{\max} = 29.8 \pm 0.4 \text{ MeV}$$

Science & Technology Facilities Council

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Thank you!

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+ 2014 IoP Nuclear Physics Conference (April)

***Continue** the discussion there!*