

Uncertainty evaluation of peak energy of giant dipole resonance propagated from uncertainties of Skyrme parameters

The workshop on photonuclear science in 2025

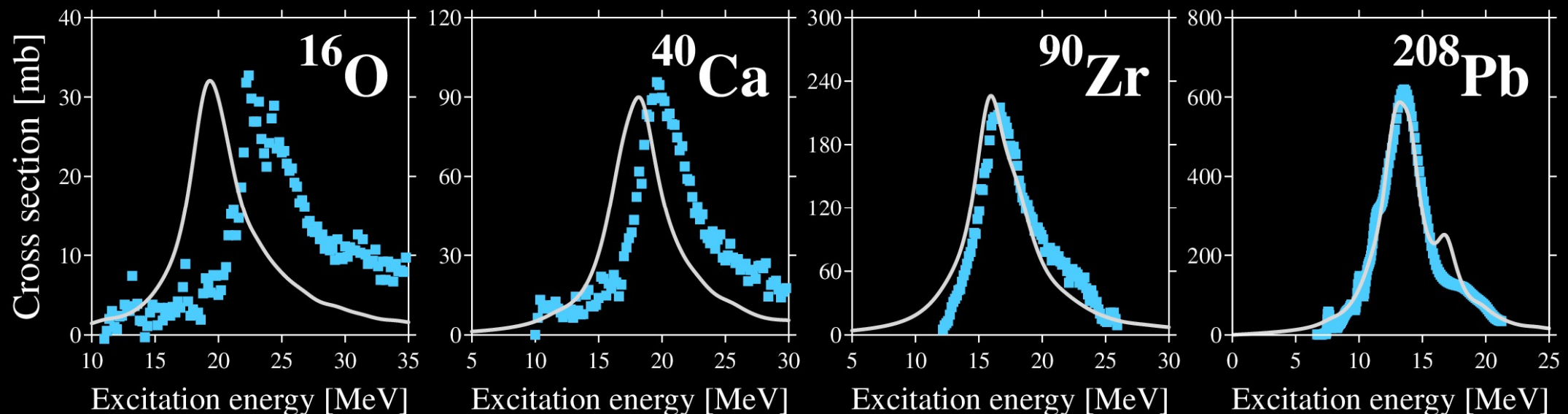
**Fudan University, Shanghai, China
and online**

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Underestimation of GDR peak energy

- GDR is systematically calculated by Skyrme-RPA / Skyrme-QRPA.
- Underestimated by **2-4 MeV in light nuclei**.
- Adjust parameters to reproduce GDR peak energy.
 - ⇒ Evaluating uncertainty of GDR peak energy calculated with Skyrme-RPA using Monte Carlo calculation.



Skyrme interaction

$$\begin{aligned}
 V_{\text{Skyrme}} = & \textcolor{red}{t}_0(1+\textcolor{red}{x}_0P_\sigma)\delta(r_i-r_j) && \dots \text{Attractive} \\
 & + \frac{\textcolor{red}{t}_1}{2}(1+\textcolor{red}{x}_1P_\sigma) [\delta(r_i-r_j)k^2 + k'^2\delta(r_i-r_j)] && \dots \text{Non-local} \\
 & + \textcolor{red}{t}_2(1+\textcolor{red}{x}_2P_\sigma)k' \cdot \delta(r_i-r_j)k && \dots \text{Non-local} \\
 & + \frac{\textcolor{red}{t}_3}{2}(1+\textcolor{red}{x}_3P_\sigma)\rho^\alpha \left(\frac{r_i+r_j}{2} \right) \delta(r_i-r_j) && \dots \text{Density-dep repulsive} \\
 & + i\textcolor{red}{W}_0(\sigma_1+\sigma_2) \cdot [k' \times \delta(r_i-r_j) \cdot k] && \dots \text{Spin-orbit}
 \end{aligned}$$

$$P_\sigma = \frac{1 + \sigma_i \cdot \sigma_j}{2}, \quad k = \frac{1}{2i} (\vec{\nabla}_i - \vec{\nabla}_j), \quad k' = \frac{-1}{2i} (\overleftarrow{\nabla}_i - \overleftarrow{\nabla}_j)$$

10 parameters $\textcolor{red}{t}_\#, \textcolor{red}{x}_\#, \alpha, \textcolor{red}{W}_0$ are fitted to reproduce experimental data such as binding energy, radius, and so on.

Parameter set: SkM*, SLy4, UNEDF1,

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Parameter set: SkM*, SLy4, UNEDF1,

⇒ Each parameter has **best-fit value & uncertainty**,
and is **correlated with other parameters**.

Skyrme parameters and their uncertainties

Best-fit values
(mean value) **Uncertainties**
(standard deviation)

SLy5-min				
p	p_0		$\sqrt{\mathcal{E}_{ii}}$	units
t_0	-2475.408	$\pm$	149.455	MeV fm ³
t_1	482.842	$\pm$	58.537	MeV fm ⁵
t_2	-559.374	$\pm$	144.534	MeV fm ⁵
t_3	13697.07	$\pm$	1672.93	MeV fm ^{3+3α}
x_0	0.741185	$\pm$	0.189191	
x_1	-0.146374	$\pm$	0.468173	
x_2	-1		fixed	
x_3	1.162688	$\pm$	0.340537	
W_0	126		fixed	MeV fm ⁵
W'_0	126		fixed	MeV fm ⁵
α	1/6		fixed	

Correlation Matrix

=====

$C_{ij} = E_{ij}/\sqrt{E_{ii} E_{jj}}$

Covariance

(correlation matrix)

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

- Almost all Skyrme interactions :
Only **best-fit values**
(SkM*, SLy series,)
- Some recently-designed Skyrme interactions :
best-fit values and **uncertainties**
(SAMi series, SV- series,)
- Only a few Skyrme interactions :
best-fit values, **uncertainties** and **covariances**.
(SLy5-min, UNEDF-series)

SLy5-min: Roca-Maza, Paar, and Colo,
J. Phys. G: Nucl. Part. Phys. 42 034033 (2015)

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(mean value)

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best-fit values, **uncertainties** and **covariances**.
(SLy5-min, UNEDF-series)

t_0 : strength of attraction,
 t_3 : strength of repulsion
correlation: -0.9997

⇒ strengthening attraction (t_0) causes
automatically strengthening repulsion (t_3).

Uncertainty evaluation for GDR peak energy

Monte Carlo calculation evaluating uncertainty of GDR peak energy propagated from uncertainties of Skyrme parameters.

SLy5-min parameter

SLy5-min				
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α	1/6		fixed	

1. Generating uncorrelated random numbers following normal distribution $N(0, 1)$, $X = (x_1, x_2, \dots)^T$
2. Creating **correlated random numbers** by acting Q , which is obtained from correlation matrix C by singular value decomposition ($C = Q^T Q$), QX
3. Using SLy5-min values p_0 and its standard deviations $\Delta p (= \sqrt{\mathcal{E}_{ii}})$, generating **correlated randomized parameter set**, $p_0 + (QX)\Delta p$
4. Generating 2500 randomized parameter sets.
5. Employing these 2500 parameter sets, performing **RPA calculations 2500 times** using **skyrme_rpa**.
6. Evaluating uncertainty of GDR peak energy E_{GDR} from the results.

Correlation Matrix

=====

$C_{ij} = E_{ij}/\sqrt{E_{ii} E_{jj}}$

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Computer Physics Communications

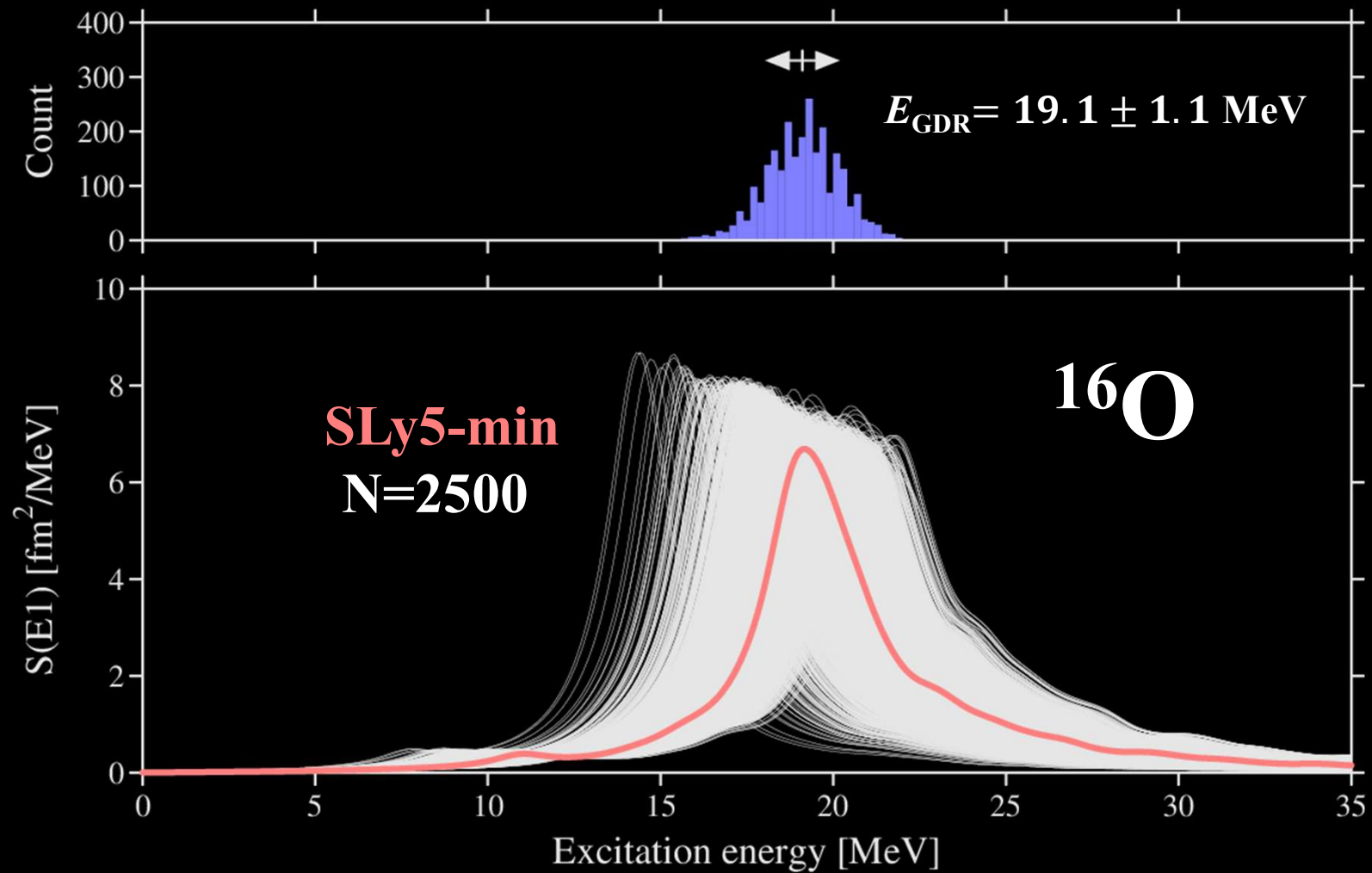
journal homepage: www.elsevier.com/locate/cpc

Self-consistent RPA calculations with Skyrme-type interactions:
The skyrme_rpa program^{*}

Gianluca Colò^{a,*}, Ligang Cao^{b,c,a}, Nguyen Van Giai^d, Luigi Capelli^{a,1}

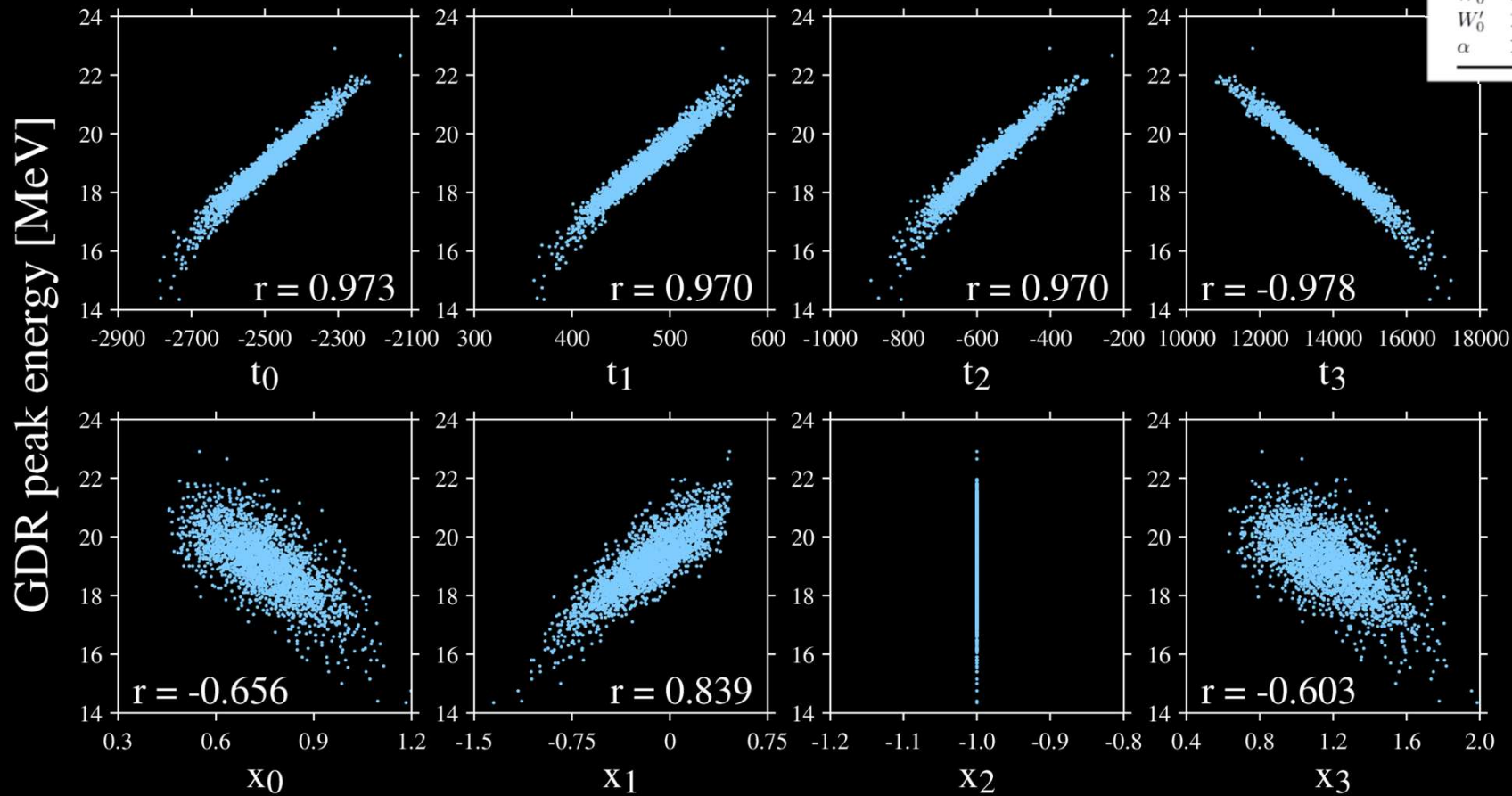
Colo, Cao, Giai, Capelli, Comp. Phys. Comm. 184, 142

Randomized GDR in ^{16}O



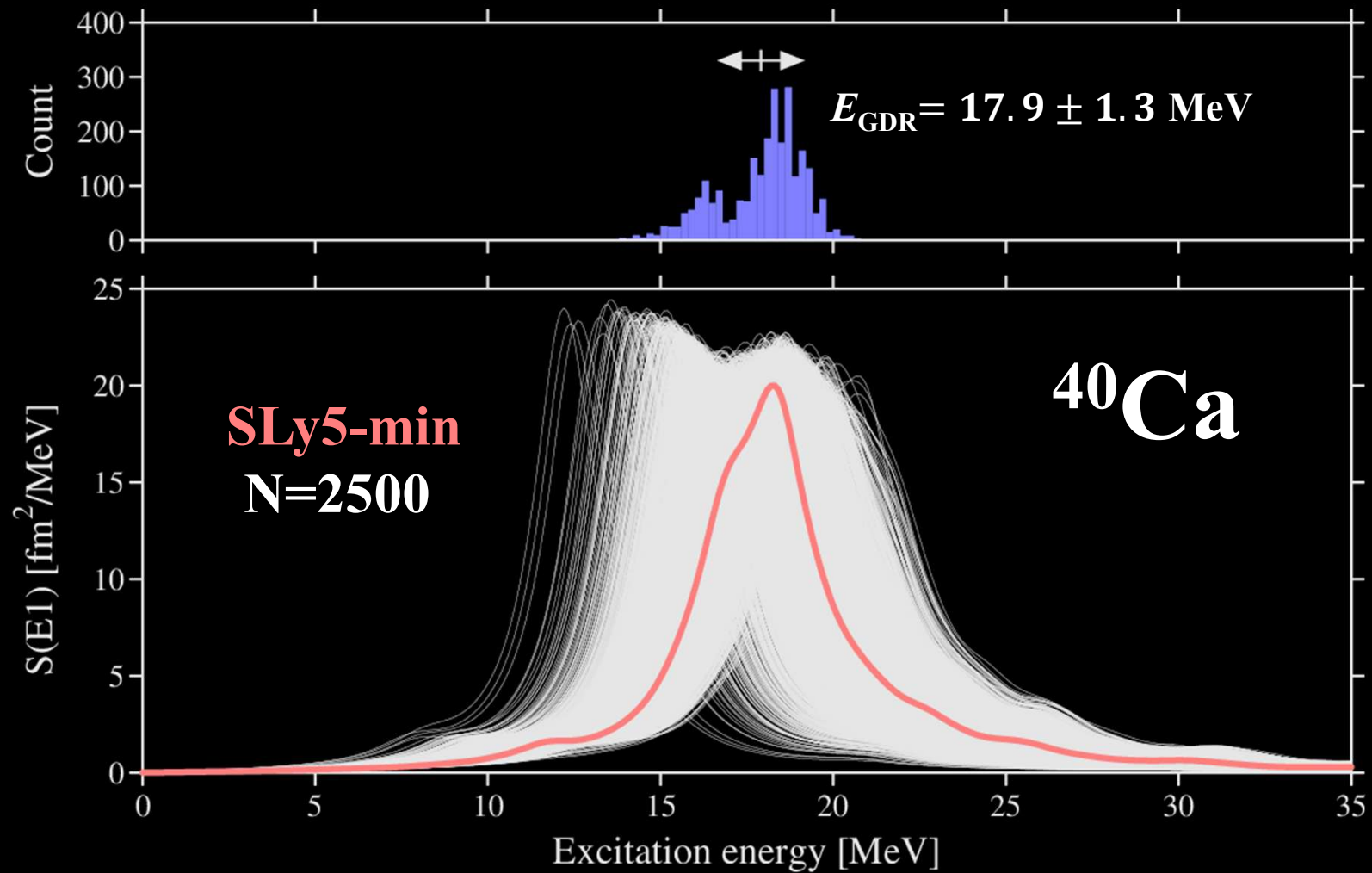
Correlations between GDR peak energies & Skyrme parameters in ^{16}O

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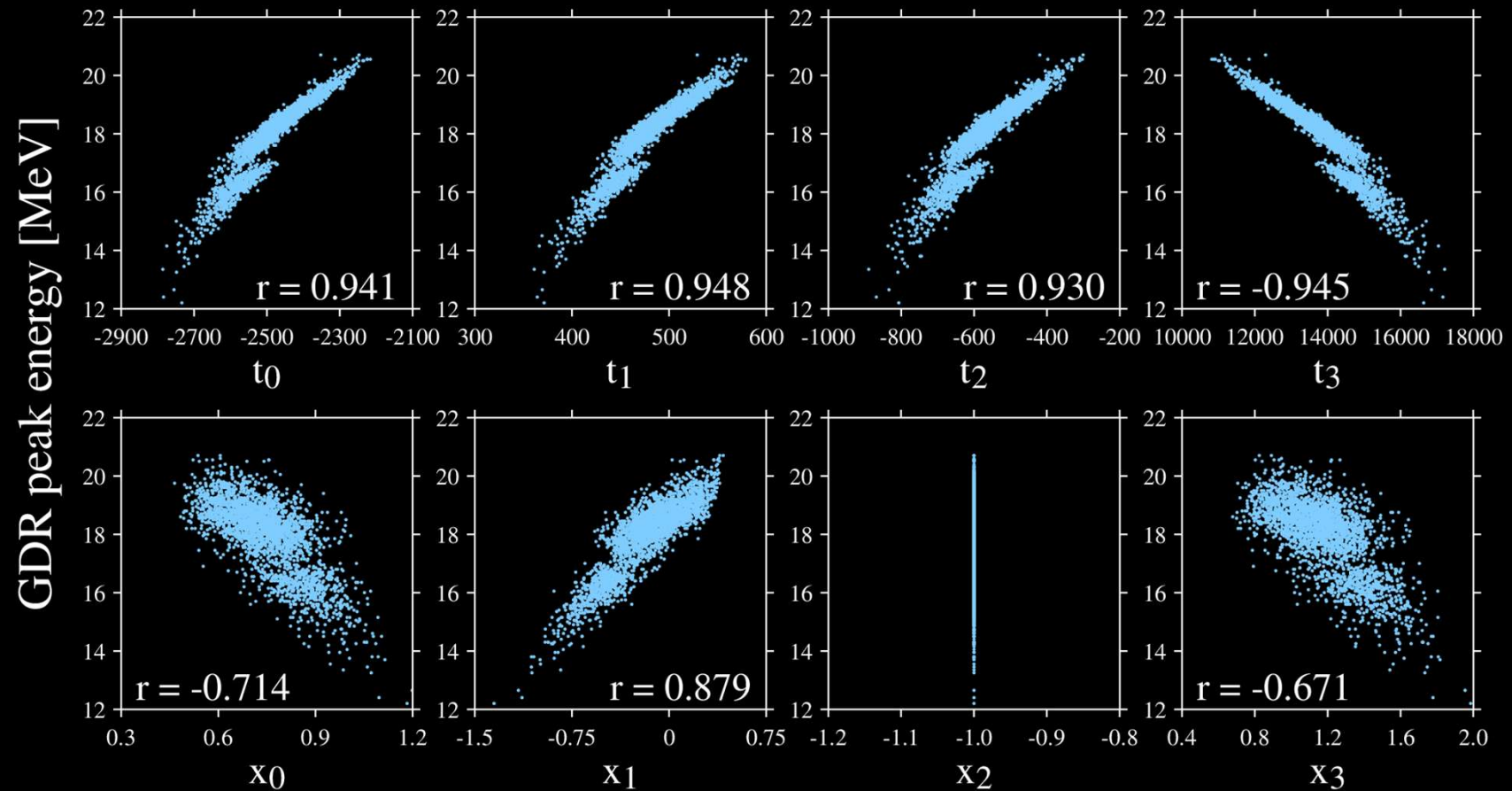


SLy5-min
N=2500

Randomized GDR in ^{40}Ca



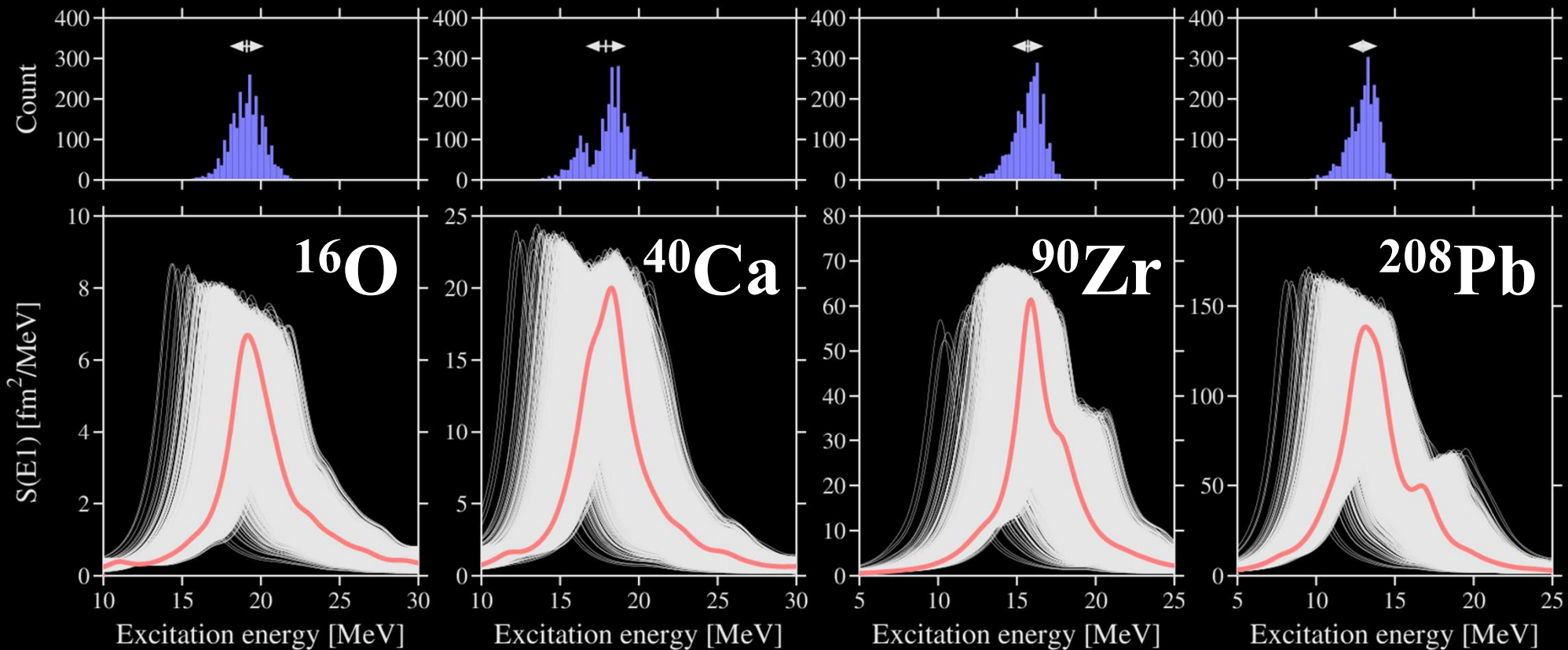
Correlations between GDR peak energies & Skyrme parameters in ^{40}Ca



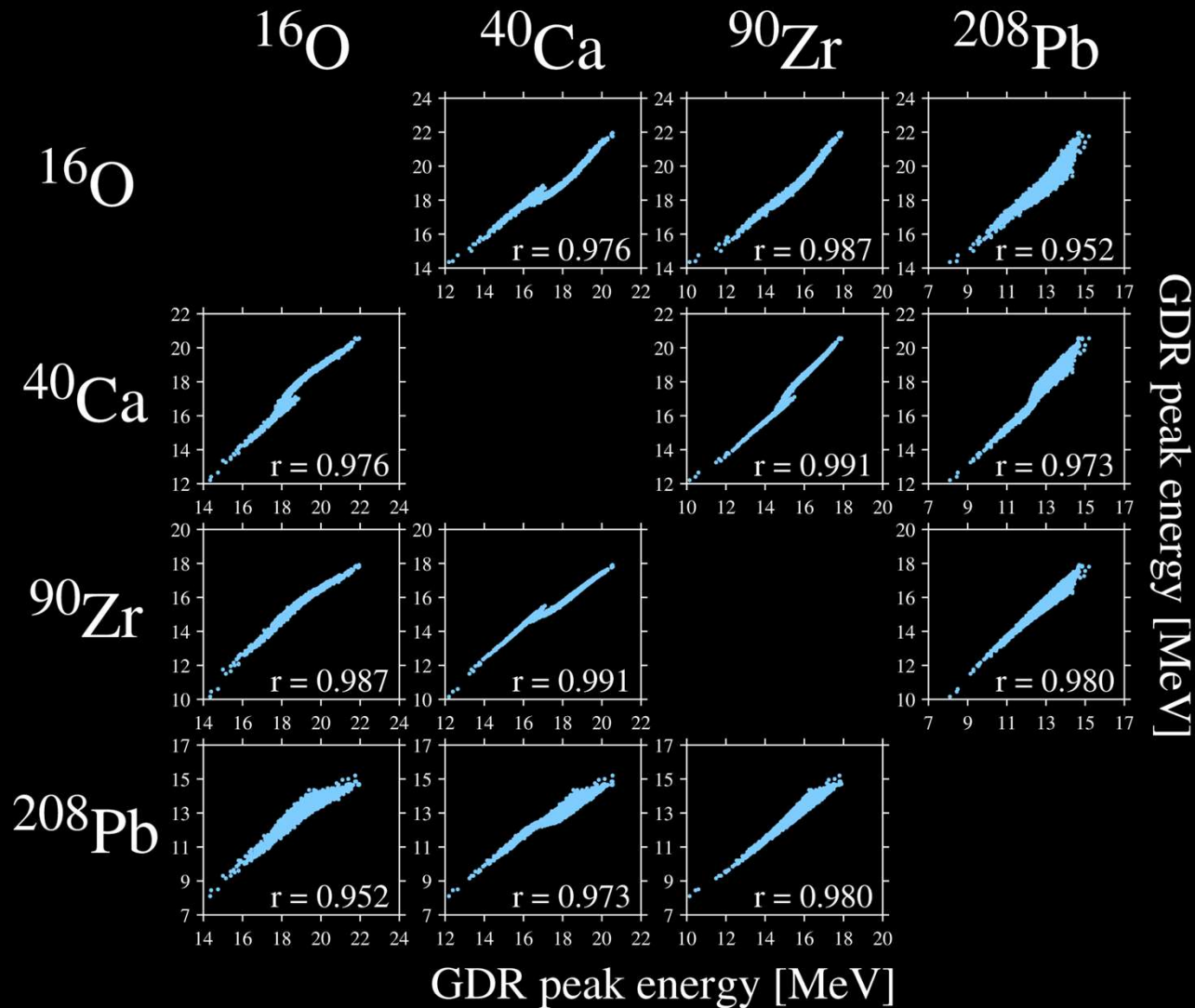
E_{GDR} and uncertainty

	E_{GDR} [MeV]
^{16}O	19.1 ± 1.1
^{40}Ca	17.9 ± 1.3
^{90}Zr	15.7 ± 1.0
^{208}Pb	13.0 ± 0.9

E_{GDR} uncertainty is $\sim 1\text{MeV}$,
irrespective of mass.



Correlations between randomized GDR peak energies



Strong correlations
between GDR peak energies
in ^{16}O , ^{40}Ca , ^{90}Zr , ^{208}Pb .

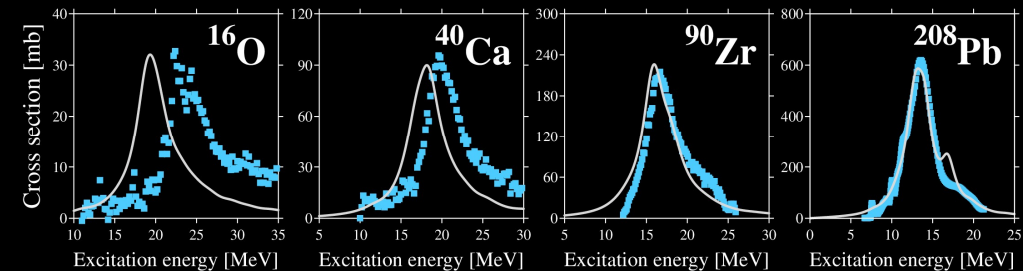
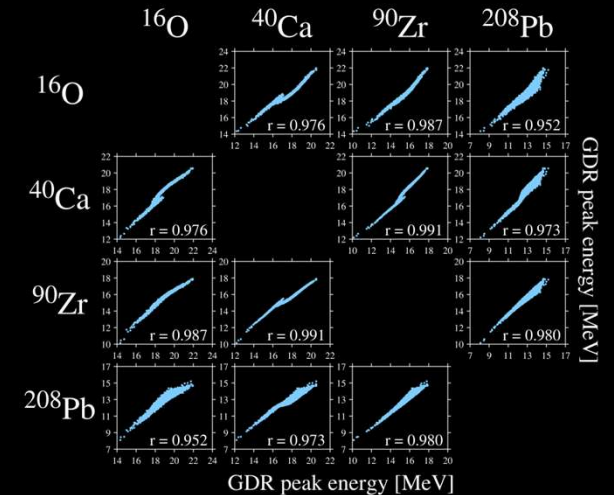
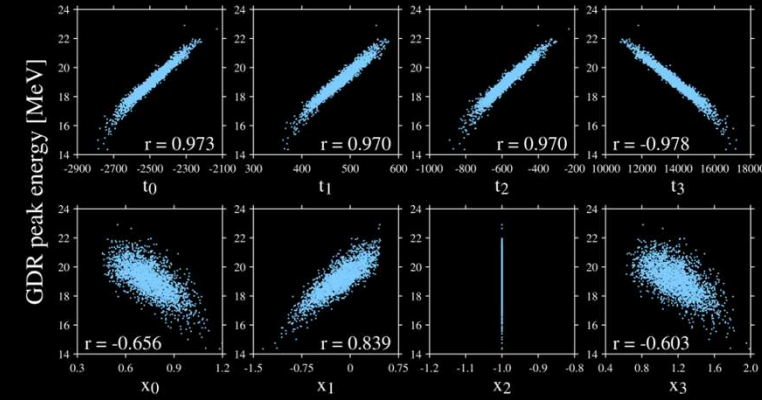
For new parameter set

Short summary

- E_{GDR} can be shifted by adjusting parameters.
- Adjusting parameters shift E_{GDR} simultaneously.
- E_{GDR} uncertainty is almost irrespective of mass.
- Disagreement is larger in light nuclei

⇒ Adjusting parameters
by large shifting in light nuclei
and by small shifting in heavy nuclei.

	E_{GDR} [MeV]
^{16}O	19.1 ± 1.1
^{40}Ca	17.9 ± 1.3
^{90}Zr	15.7 ± 1.0
^{208}Pb	13.0 ± 0.9



New parameter set

$$p = p_0 + Q \Delta p \cdot f / A$$

p_0 : original SLy5-min parameter set (best-fit values)

Δp : standard deviations of parameters (uncertainties, $\sqrt{\varepsilon_{ii}}$)

Q : factorized correlation matrix, $C = Q^T Q$ (covariance)

f : free parameter

Best-fit values Uncertainties
(standard deviation)

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SLy5-min parameter

New parameter set

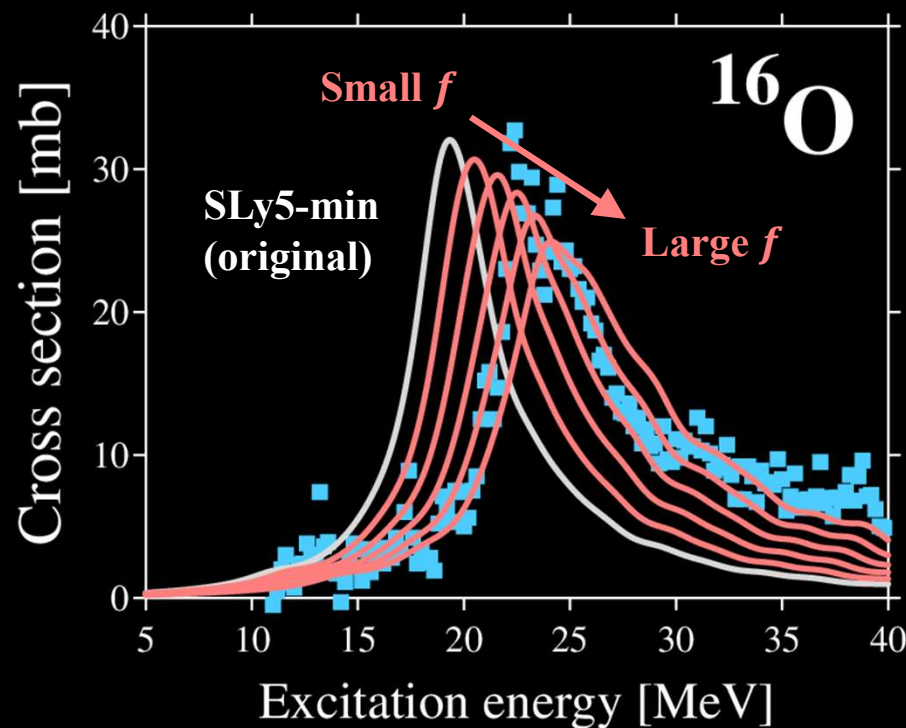
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Best-fit values Uncertainties
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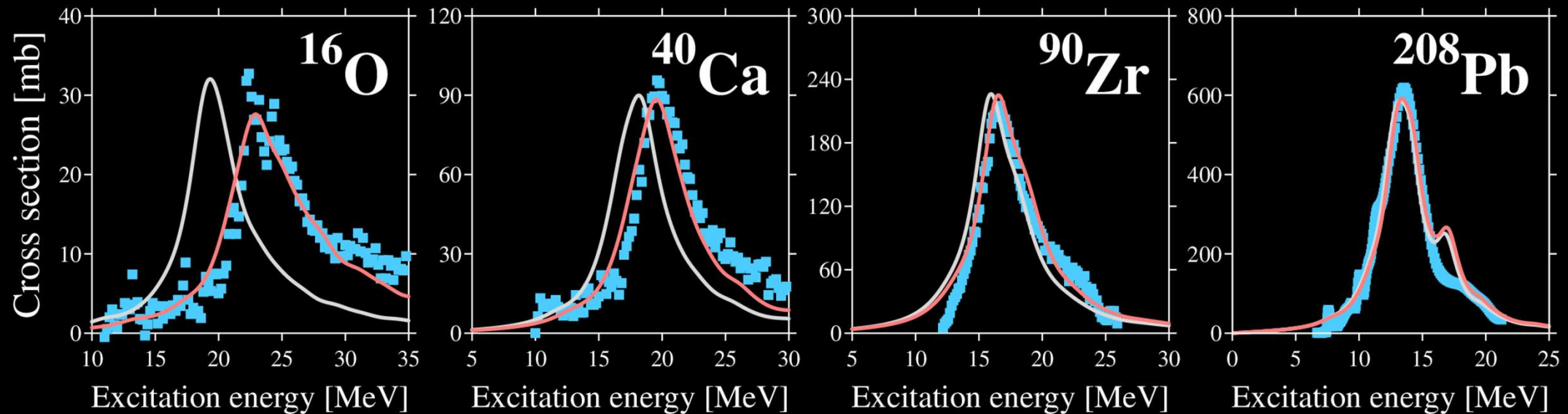
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$\Delta\mathbf{p}$: standard deviations of parameters (uncertainties, $\sqrt{\varepsilon_{ii}}$)

$\mathbf{Q}$: factorized correlation matrix, $\mathbf{C} = \mathbf{Q}^T \mathbf{Q}$ (covariance)

$\mathbf{f}$: free parameter, $f = 35$



Takeaways

- **Uncertainty of GDR peak energy propagated from uncertainty of Skyrme parameters is evaluated** using Total Monte Carlo calculations.
 - In the case of SLy5-min interaction, uncertainty of GDR peak energy is ~ 1 MeV, irrespective of mass.
 - GDR peak energy is strongly correlated with Skyrme parameters when the correlations between Skyrme parameters are considered.
- **A new Skyrme parameter set which reproduces well GDR peak energy is proposed.**

Perspective

- Deformed nuclei