

Self-consistent single-particle approximation to nuclear state densities at high excitation energy

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Introduction

- The **nuclear level density** $\rho(E)$ is a characteristic property of every nucleus and it is defined as the number of levels per unit energy at a certain excitation energy.

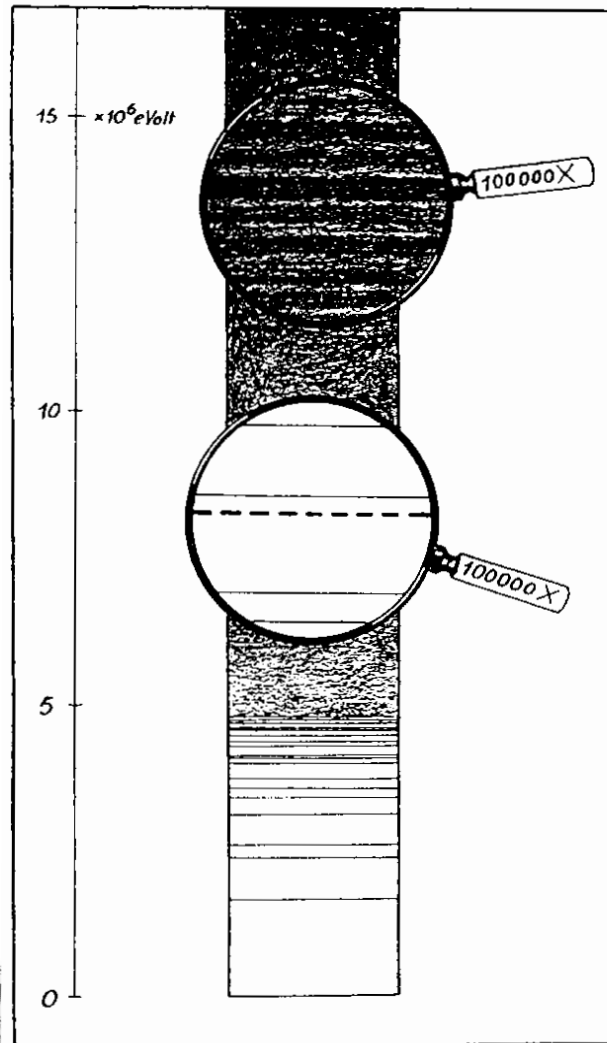
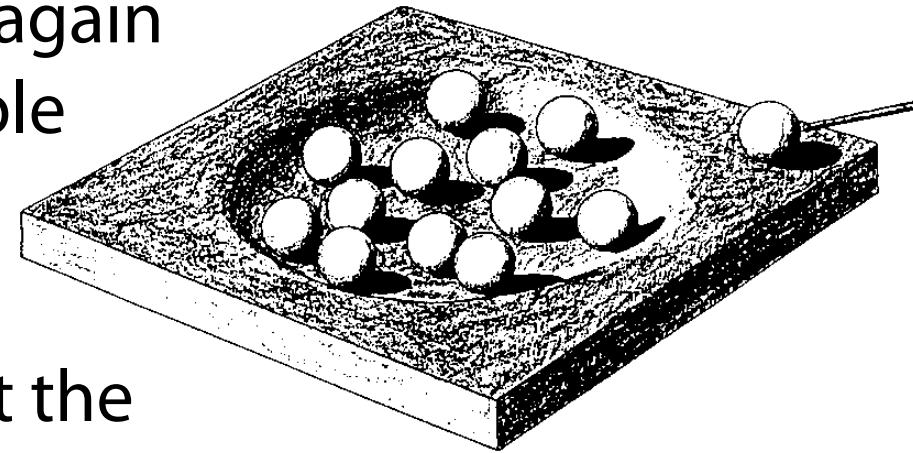
$$\rho(E) = dN/dE$$

- It is the number of different ways in which individual nucleons can be placed in the various single particle orbitals such that the excitation energy lies in the range E to $E+dE$. It increases rapidly with excitation energy.
- In the independent-particle model, the nuclear level density is determined from the neutron and proton single-particle level densities. This single-particle level density can be subdivided into **compound-nucleus and gas components**.
- The **nuclear level density ρ is an essential ingredient** in calculating the statistical decay of a compound nucleus by particle evaporation, γ -ray emission, or fission.



Introduction - compound nucleus

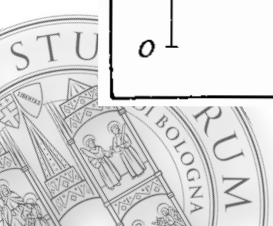
The “compound nucleus” is a state in which **the excitation energy is distributed statistically among all the available degrees of freedom**. Only as the result of a very rare fluctuation, all the excitation energy could be again concentrated on a single particle, which will then be able to leave the nucleus, which has **no memory** of the original reaction



It was known experimentally that the lowest excited states in heavy nuclei had energies of order a few hundred keV above the ground state. Bohr expected these low-lying states to reflect the normal modes of motion (surface, compressive modes, and collective rotation) of the nuclear substance.

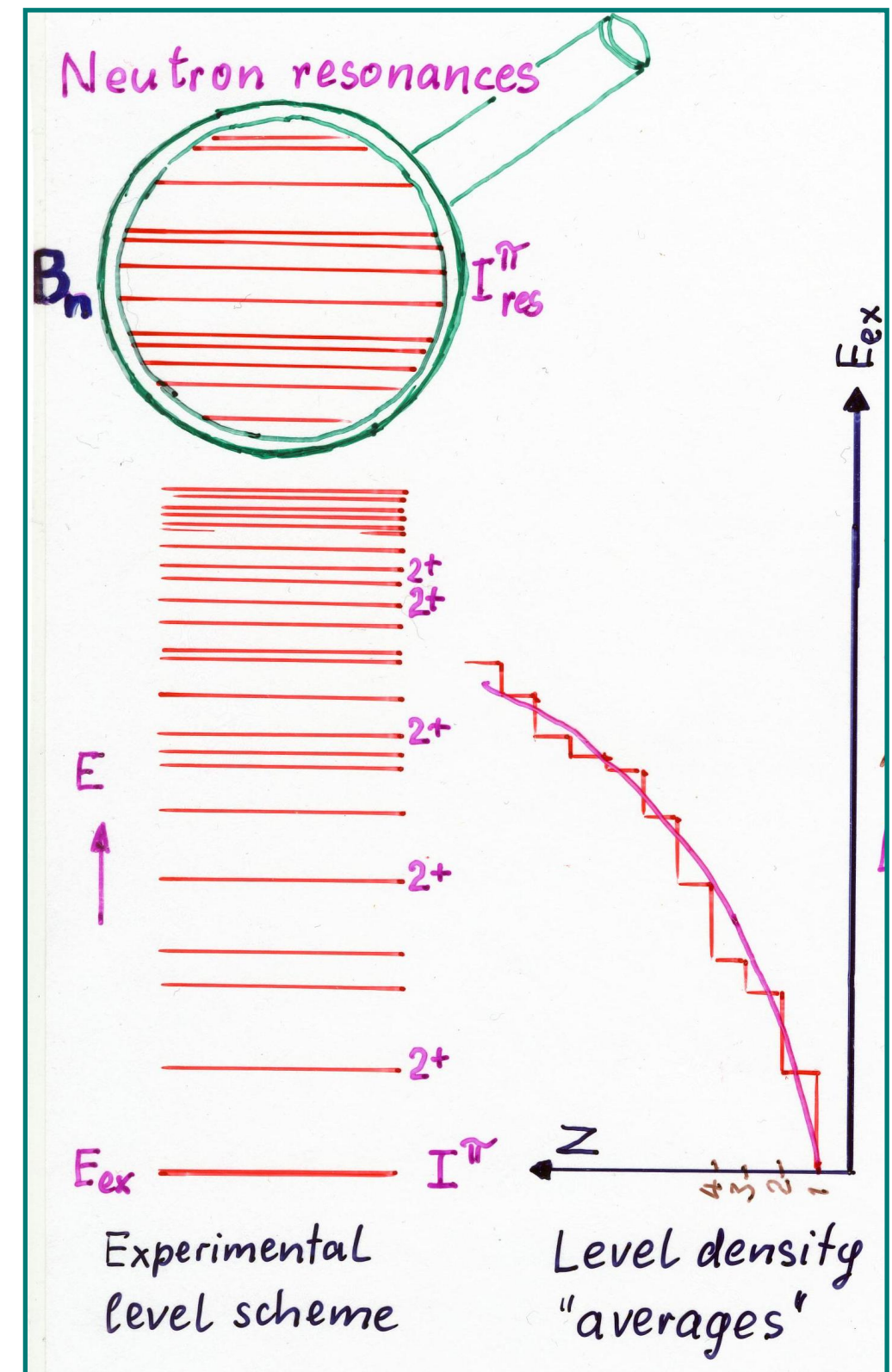
With increasing excitation energy, the number of ways in which the total energy can be divided among these different modes increase exponentially and therefore the level density of the quantum states of the compound nucleus will increase

N. Bohr, Nature **137**, 344 (1936)



Introduction - compound nucleus

The levels of a nucleus can be divided into two regions. This division arises naturally from the different approaches employed for their analysis: the spectroscopical approach for the low energy levels and the statistical approach for the high energy levels. The **low-lying nuclear excited levels** are small in number, well separated, and rather simple in structure. With increasing excitation energy, the spacing between the levels is progressively reduced. The existence of such complex levels is illustrated by the **neutron-capture resonances**. Their average spacing is about 10^6 times smaller than the average single-particle level spacing, and their widths are also 10^6 times smaller than expected for a single particle excitation.



Introduction (a simple derivation)

A simple result can be obtained within the independent-particle model. It starts with sets of single-particle levels for both neutrons and protons. **The determination of the nuclear level density is essentially a combinatorial problem**, i.e., determining how many ways these single-particle levels can be occupied to give the desired total excitation energy.

$$\rho(E^*) = \frac{\exp S}{2\pi \sqrt{D}}$$

where f are the average occupancy of a single particle level

$$f_i = \frac{1}{[1 + \exp(\beta \epsilon_i - \alpha)]}$$

Nucleon number

$$A = \frac{\partial \ln Z}{\partial \alpha} = \sum_i f_i$$

Total energy

$$E = E_{\text{gs}} + E^* = -\frac{\partial \ln Z}{\partial \beta} = \sum_i \epsilon_i f_i$$

Entropy

$$S = \beta E - \alpha N + \ln Z(\alpha, \beta)$$

$$S = \sum_i s_i$$

$$s_i = -f_i \ln f_i - (1 - f_i) \ln(1 - f_i)$$



Introduction (a simple derivation)

A simple result can be obtained within the independent-particle model. It starts with sets of single-particle levels for both neutrons and protons. **The determination of the nuclear level density is essentially a combinatorial problem**, i.e., determining how many ways these single-particle levels can be occupied to give the desired total excitation energy.

$$\rho(E^*) = \frac{\exp S}{2\pi\sqrt{D}}$$

At the saddle point

$$\ln Z = \sum_i \ln[1 + \exp(\alpha - \beta\epsilon_i)]$$

$$D = \begin{vmatrix} \frac{\partial^2 \ln Z}{\partial \alpha^2} & \frac{\partial^2 \ln Z}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \ln Z}{\partial \beta \partial \alpha} & \frac{\partial^2 \ln Z}{\partial \beta^2} \end{vmatrix}$$

Entropy $S = \beta E - \alpha N + \ln Z(\alpha, \beta)$

$$S = \sum_i s_i$$

$$s_i = -f_i \ln f_i - (1 - f_i) \ln(1 - f_i)$$

$$g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i)$$

$$\rho(E^*) = \frac{\exp S}{\sqrt{48}E^*}$$

$$S = 2\sqrt{aE^*} = 2aT$$

level-density parameter

Introduction (general definition)

AUGUST 15, 1936

PHYSICAL REVIEW

VOLUME 50

An Attempt to Calculate the Number of Energy Levels of a Heavy Nucleus

H. A. BETHE, *Cornell University*

(Received June 5, 1936)

Although the previous formula can be derived without recourse to statistical mechanics, Bethe realized there is a close analogy to the problem of a Fermi gas in contact with a heat bath of temperature $T = 1/\beta$ and with chemical potential μ .

Z is the grand partition function, S is the entropy, and thus $1/T = dS/dE^*$.

$$Z_{GC}(\beta, \alpha) = \text{Tr} \exp[-\beta \hat{H} + \alpha \hat{N}]$$

$$Z_{GC}(\beta, \alpha) = \sum_N \int_{E_0}^{\infty} \rho(E, N) e^{-\beta E + \alpha N} dE$$

$$\rho(E, N) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int_0^{2\pi} Z_{GC}(\beta + is, \alpha + i\phi) \\ \times e^{-(\alpha + i\phi)N + (\beta + is)E} d\phi ds.$$

$$\rho(E, N) \approx \frac{Z_{GC}(\beta, \alpha) e^{\beta E - \alpha N}}{[(2\pi)^2 \text{Det}(\frac{\partial^2 \ln Z_{GC}}{\partial \eta_i \partial \eta_j})]^{1/2}}$$



Introduction (a common approach)

The Fermi gas model in its various modifications is widely used for calculation of the nuclear level density. This model enables simple systematics to be established based on normalization of the energy dependence of the nuclear level density to data on the cumulative numbers of low-lying levels and the average spacings between S-wave neutron resonances at the neutron binding energy (B_n) in the nucleus.

However, the level density parameter a and excitation energy shift δ_{eff} , caused by even-odd differences in the nuclei, are considered free parameters. Since the δ_{eff} values obtained for odd-odd nuclei are negative, this approximation has been termed the **back-shifted Fermi gas model**.

total level density

$$\rho(U) = \frac{1}{12\sqrt{2}} \frac{1}{\sigma a^{1/4}} \frac{\exp \left[2\sqrt{a(U - \delta_{eff})} \right]}{(U - \delta_{eff})^{5/4}}$$

a is the level density parameter associated with the density of single particle states near the Fermi energy;

the excitation energy shift δ_{eff} is caused by even-odd differences in the nuclei



Introduction (experimental sources)

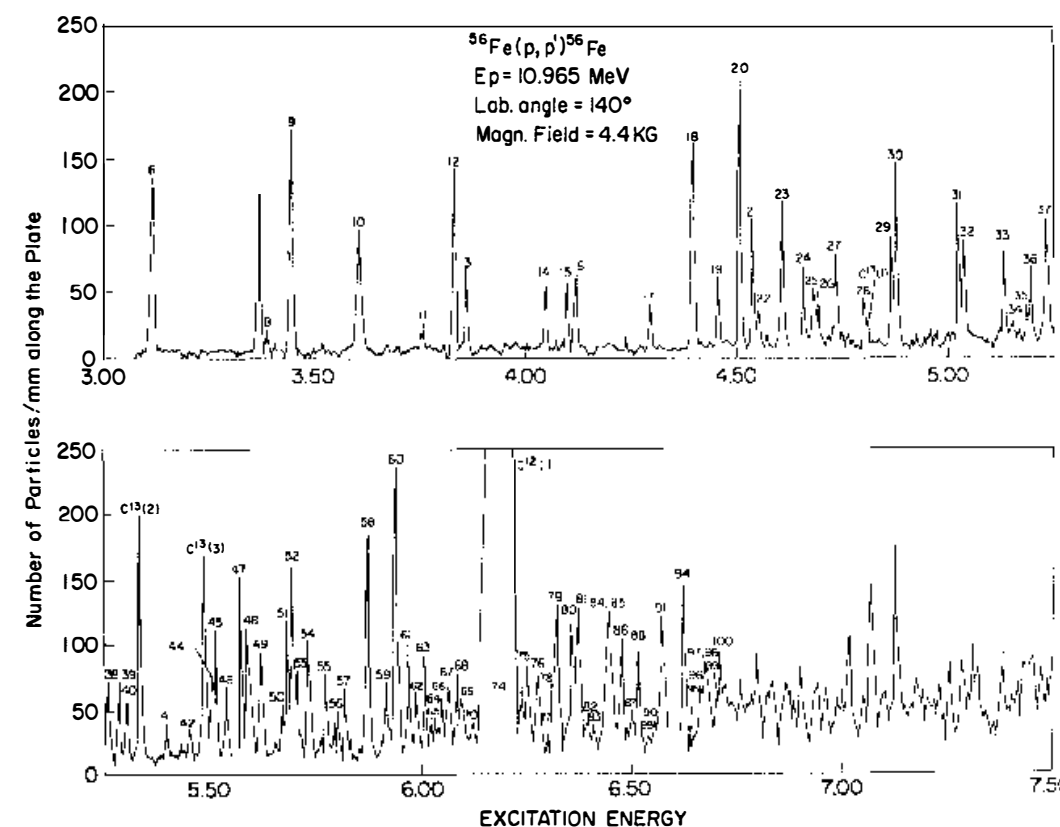
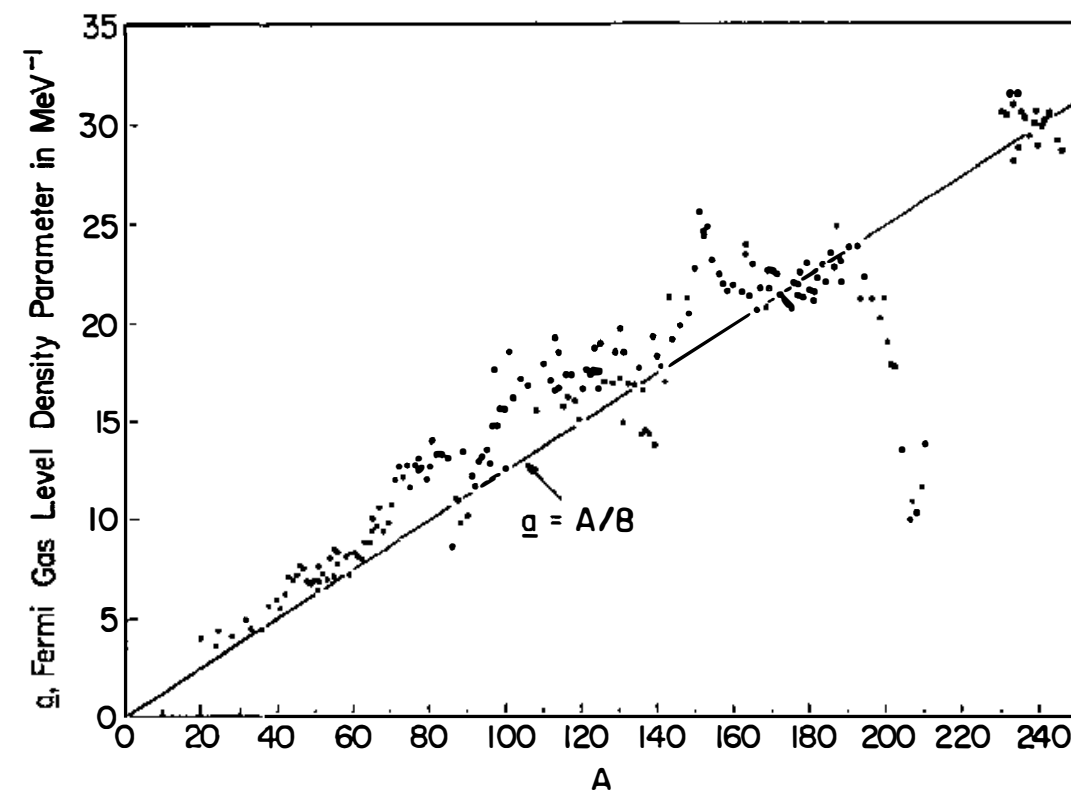
Neutron resonances

In this type of experiment the nuclear energy levels are observed at an energy just exceeding the neutron binding energy, and the number of levels is obtained by counting the resonances in a particular neutron energy interval. It is necessary in such experiments that the width Γ of each level be less than the level spacing Δ and that the experimental resolution be good enough to resolve individual levels.

Inelastic scattering and nuclear reactions to resolved levels

The resolution obtained in these experiments is orders of magnitude poorer than that achieved with s-wave neutron spectroscopy. With such experiments, it is possible to study isolated levels up to an excitation energy of approximately 5 to 6 MeV for a nucleus with atomic mass around 60. Typical nuclear reactions are the (p, p') , (n, n') , (α, α') and (p, α) reactions.

and others...



Our project

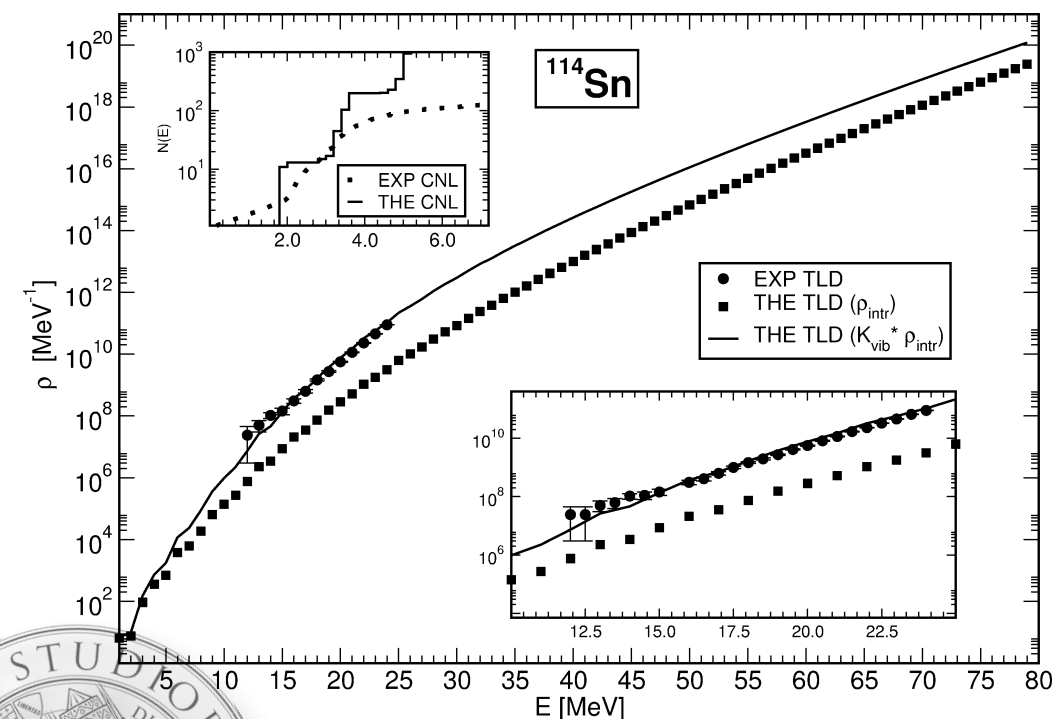
Relativistic
mean field

input

Frozen bound states

Subtraction method

Combinatorial method



Pezer, **Ventura** and Vretenar, NPA **717** (2003) 21-43

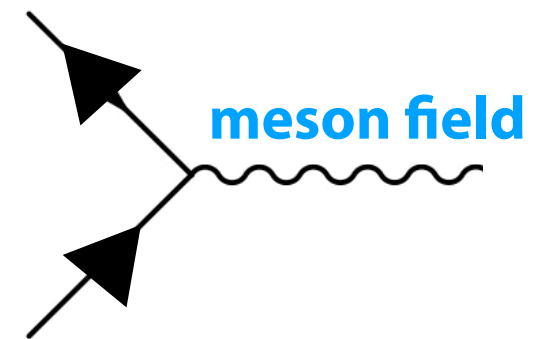
ρ

Relativistic mean field (I)

Finelli et al., PRC **66**, 024306 (2002)

Lagrangian density

$$\begin{aligned} \mathcal{L} = & \bar{\psi} \left[i\gamma^\mu \partial_\mu - M - g_\sigma \sigma - g_\omega \gamma^\mu \omega_\mu - g_\rho \gamma^\mu \vec{\tau} \cdot \vec{\rho}_\mu - e\gamma^\mu A_\mu \frac{1 - \tau_3}{2} \right] \psi \\ & + \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - U_\sigma(\sigma) - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + U_\omega(\omega_\mu) - \frac{1}{4} \vec{R}^{\mu\nu} \cdot \vec{R}_{\mu\nu} + U_\rho(\vec{\rho}_\mu) \\ & - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}, \end{aligned}$$



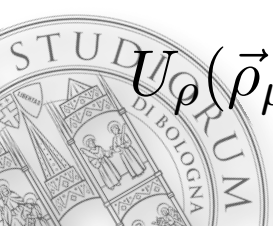
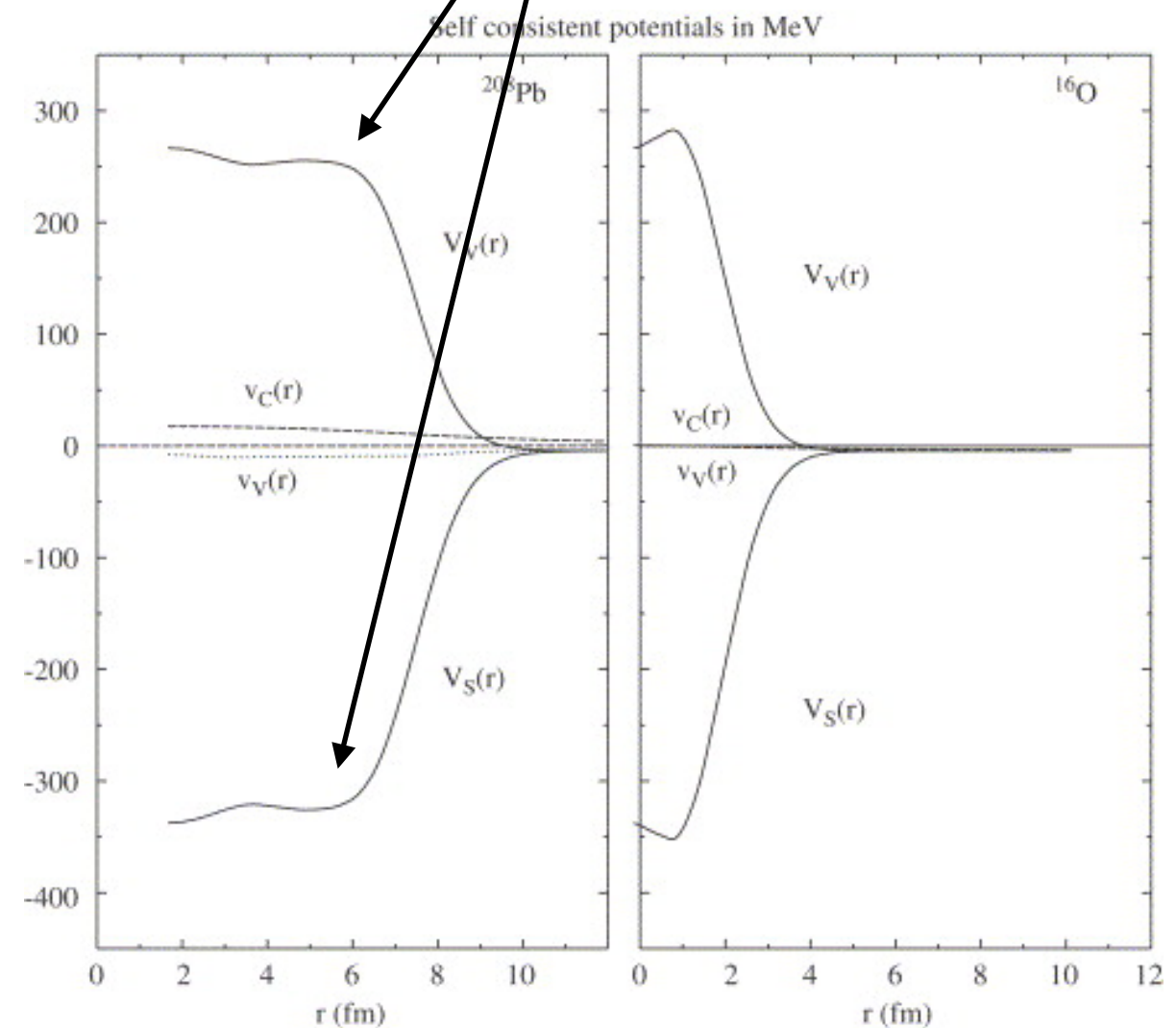
Meson fields

$$\begin{aligned} -\nabla^2 \sigma + U'_\sigma(\sigma) &= -g_\sigma \rho_s, \\ -\nabla^2 \omega_0 + U'_\omega(\omega_0) &= g_\omega \rho_v, \\ -\nabla^2 \rho_0^3 + U'_\rho(\rho_0^3) &= g_\rho \rho_3, \\ -\nabla^2 A_0 &= e\rho_c. \end{aligned}$$

non linear terms

$$\begin{aligned} U_\sigma(\sigma) &= \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4, \\ U_\omega(\omega_\mu) &= \frac{1}{2} m_\omega^2 \omega^\mu \omega_\mu + \frac{1}{4} c_3 (\omega^\mu \omega_\mu)^2, \\ U_\rho(\vec{\rho}_\mu) &= \frac{1}{2} m_\rho^2 \vec{\rho}^\mu \cdot \vec{\rho}_\mu + \frac{1}{4} d_3 [\vec{\rho}^\mu \cdot \vec{\rho}_\mu]^2. \end{aligned}$$

sigma and omega fields have opposite signs



Relativistic mean field (II)

Finelli et al., PRC **66**, 024306 (2002)

Mean field

$$|\Phi\rangle = \prod_{i=1}^A c_i^\dagger |0\rangle \quad \langle\Phi|\Phi\rangle = 1$$

$$E_{\text{RMF}}(\rho, \phi) = \langle\Phi|\mathcal{H}|\Phi\rangle$$

$$= \int d^3x \text{Tr} \left[\beta \left(\gamma \cdot \mathbf{p} + M + g_\sigma \sigma + g_\omega \omega^\mu \gamma_\mu + g_\rho \vec{\tau} \cdot \vec{\rho}_\mu \gamma^\mu + \frac{1}{2} e(1 - \tau_3) A_\mu \gamma^\mu \right) \rho \right] \\ + \int d^3x \left\{ -\frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma + U_\sigma(\sigma) + \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} - U_\omega(\omega_\nu) + \frac{1}{4} \vec{R}^{\mu\nu} \cdot \vec{R}_{\mu\nu} - U_\rho(\vec{\rho}_\nu) + \frac{1}{4} F^{\mu\nu} F_{\mu\nu} \right\}$$

Spinor wave function for spherical symmetry

$$\psi_{\alpha\kappa m}(\mathbf{r}, t) = \begin{pmatrix} i \frac{G_\alpha^\kappa(r)}{r} \\ \frac{F_\alpha^\kappa(r)}{r} \boldsymbol{\sigma} \cdot \hat{\mathbf{r}} \end{pmatrix} Y_{jm}^l(\theta, \phi) \chi_{t_\alpha}(t)$$

$$\epsilon_\alpha G_\alpha^\kappa = \left(-\frac{d}{dr} + \frac{\kappa}{r} \right) F_\alpha^\kappa + (M + S(r) + V(r)) G_\alpha^\kappa,$$

$$\epsilon_\alpha F_\alpha^\kappa = \left(+\frac{d}{dr} + \frac{\kappa}{r} \right) G_\alpha^\kappa - (M + S(r) - V(r)) F_\alpha^\kappa,$$

$$S(r) = g_\sigma \sigma,$$

$$V(r) = g_\omega \omega_0 + g_\rho \tau_3 \rho_0^3 + \frac{1}{2} e(1 - \tau_3) A_0.$$

central potential

spin-orbit potential



Relativistic mean field (III)

Finelli et al., PRC **66**, 024306 (2002)

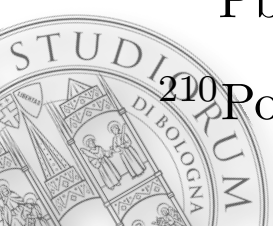
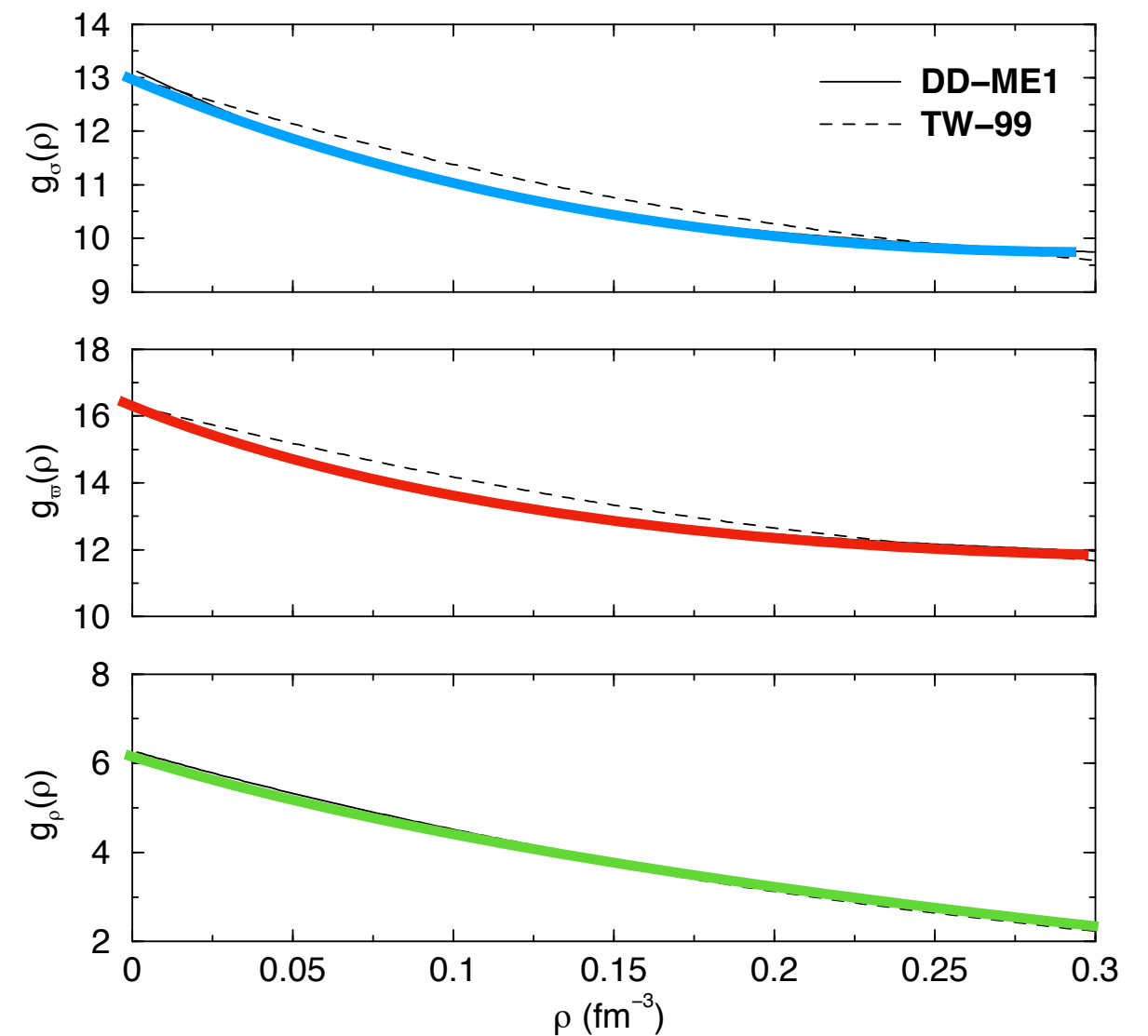
Density-dependent extension

$$g_i(\rho_v) = g_i(\rho_{\text{sat}}) f_i(x)$$

$$f_i(x) = a_i \frac{1 + b_i(x + d_i)^2}{1 + c_i(x + d_i)^2} \quad x = \rho/\rho_{\text{sat}}$$

$$g_\rho = g_\rho(\rho_{\text{sat}}) \exp[-a_\rho(x - 1)]$$

	E/A (MeV)	r_{ch} (fm)	$r_n - r_p$ (fm)
^{16}O	-7.974 (-7.976)	2.730 (2.730)	-0.03
^{40}Ca	-8.576 (-8.551)	3.464 (3.485)	-0.05
^{48}Ca	-8.631 (-8.667)	3.482 (3.484)	0.19
^{90}Zr	-8.704 (-8.710)	4.294 (4.272)	0.06
^{112}Sn	-8.501 (-8.514)	4.586 (4.596)	0.11
^{116}Sn	-8.516 (-8.523)	4.616 (4.626)	0.15 (0.12)
^{124}Sn	-8.462 (-8.467)	4.671 (4.674)	0.25 (0.19)
^{132}Sn	-8.352 (-8.355)	4.720	0.27
^{204}Pb	-7.885 (-7.880)	5.500 (5.486)	0.18
^{208}Pb	-7.884 (-7.868)	5.518 (5.505)	0.20 (0.20)
^{214}Pb	-7.764 (-7.772)	5.568 (5.562)	0.27
^{210}Po	-7.857 (-7.834)	5.553	0.18



Relativistic mean field (finite T)

The temperature dependent equations are derived by the minimization of the thermodynamical potential Ω ,

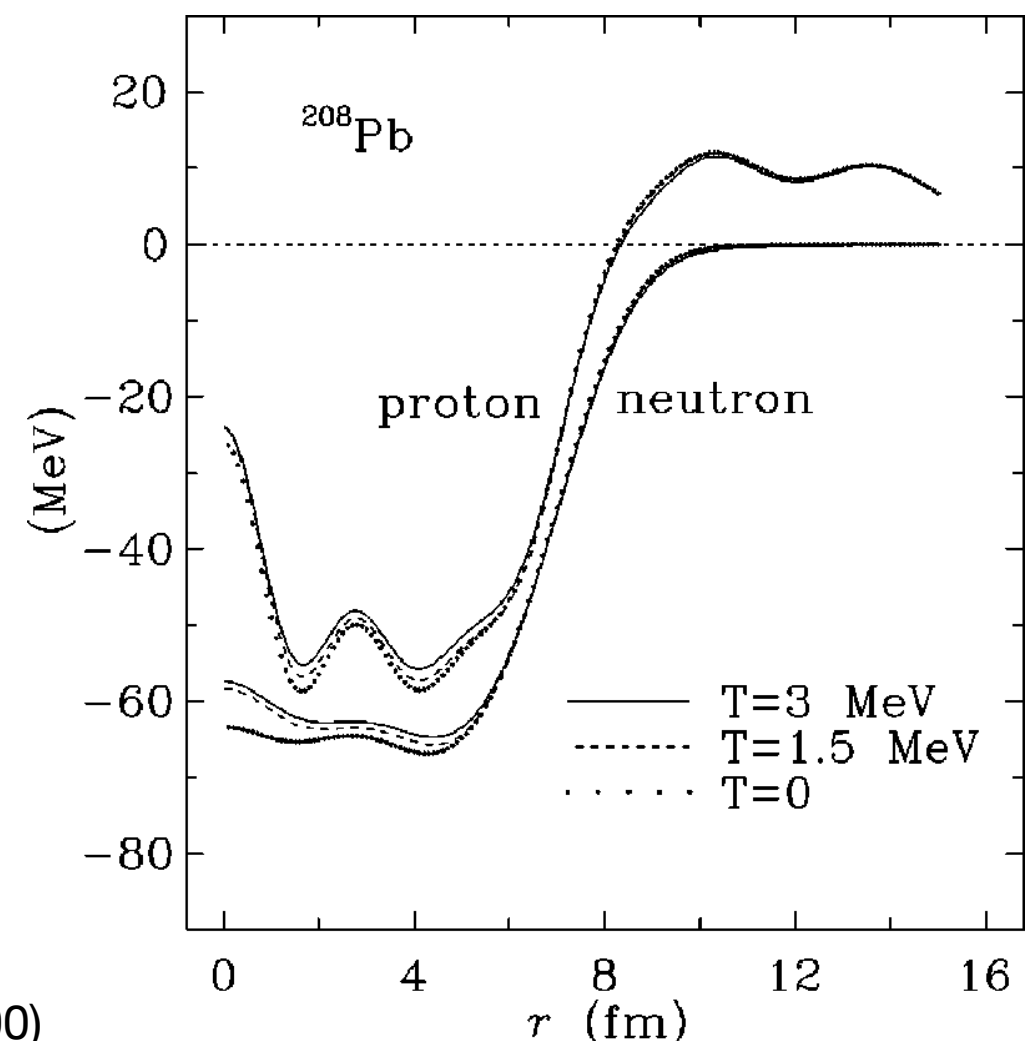
$$\Omega = E - TS - \mu N$$

where E being the energy, T is the thermodynamic temperature which is introduced through the statistical Fermi occupation probabilities n_i

$$n_i = \left[1 + \exp\left(\frac{\varepsilon_i - \mu}{kT}\right) \right]^{-1}$$

$$S = - \sum_i [n_i \ln n_i + (1 - n_i) \ln(1 - n_i)]$$

$$E^*(T) = E(T) - E(T=0)$$



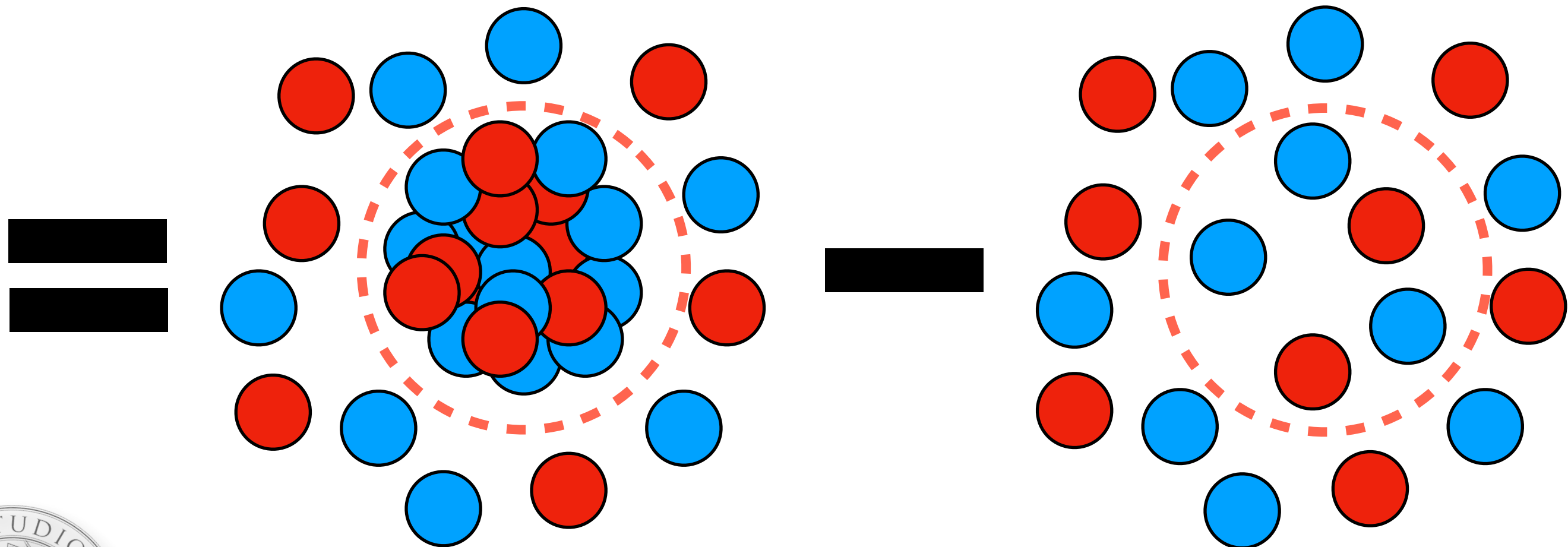
Subtraction method

Bonche-Levit-Vautherin procedure

A vapor subtraction procedure is used to account for unbound states and to remove long range Coulomb repulsion between the hot nucleus and the gas as well as the contribution of the external nucleon gas.

Nucleus + vapor

vapor



Bonche, Levit, and Vautherin, NPA **427**, 278 (1984); **436**, 265 (1985)



Subtraction method

Bonche-Levit-Vautherin procedure

They observed that the mean field equations have two solutions for a given chemical potential and temperature. One of these can be associated with a **nucleus in equilibrium with the evaporated nucleons (nucleus+gas)** while the other consists of a **gas of nucleons alone**.

They determined the properties of the hot nucleus in terms of the difference between quantities associated with the the nucleus+gas and those of the gas.

Formally, this is done by defining a subtracted thermodynamic potential as the difference between that of the nucleus+gas and that of the gas, with the exception of the Coulomb contribution. In particular, the baryon and proton numbers of the hot nucleus are then

$$A = \int d^3r [\rho_{B,n+g}(\vec{r}) - \rho_{B,g}(\vec{r})],$$

$$Z = \int d^3r [\rho_{p,n+g}(\vec{r}) - \rho_{p,g}(\vec{r})],$$

Bonche, Levit, and Vautherin, NPA **427**, 278 (1984); **436**, 265 (1985)



Subtraction method

Bonche-Levit-Vautherin procedure

The Coulomb contribution to the thermodynamic potential must be treated differently due to its long range. **The Coulomb term must be modified in order that the only contribution is from protons in the hot nucleus.** This is done by replacing the difference between the two Coulomb contributions in the thermodynamic potential by a term taking into account only the contribution of those protons,

$$\begin{aligned} & \frac{1}{2} \int d^3r [\rho_{p,n+g}(\vec{r}) V_C \rho_{p,n+g}(\vec{r}') - \rho_{p,g}(\vec{r}) V_C \rho_{p,g}(\vec{r}')] \\ & \rightarrow \frac{1}{2} \int d^3r \{ [\rho_{p,n+g}(\vec{r}) - \rho_{p,g}(\vec{r})] V_C \\ & \quad \times [\rho_{p,n+g}(\vec{r}') - \rho_{p,g}(\vec{r}')] \}. \end{aligned}$$

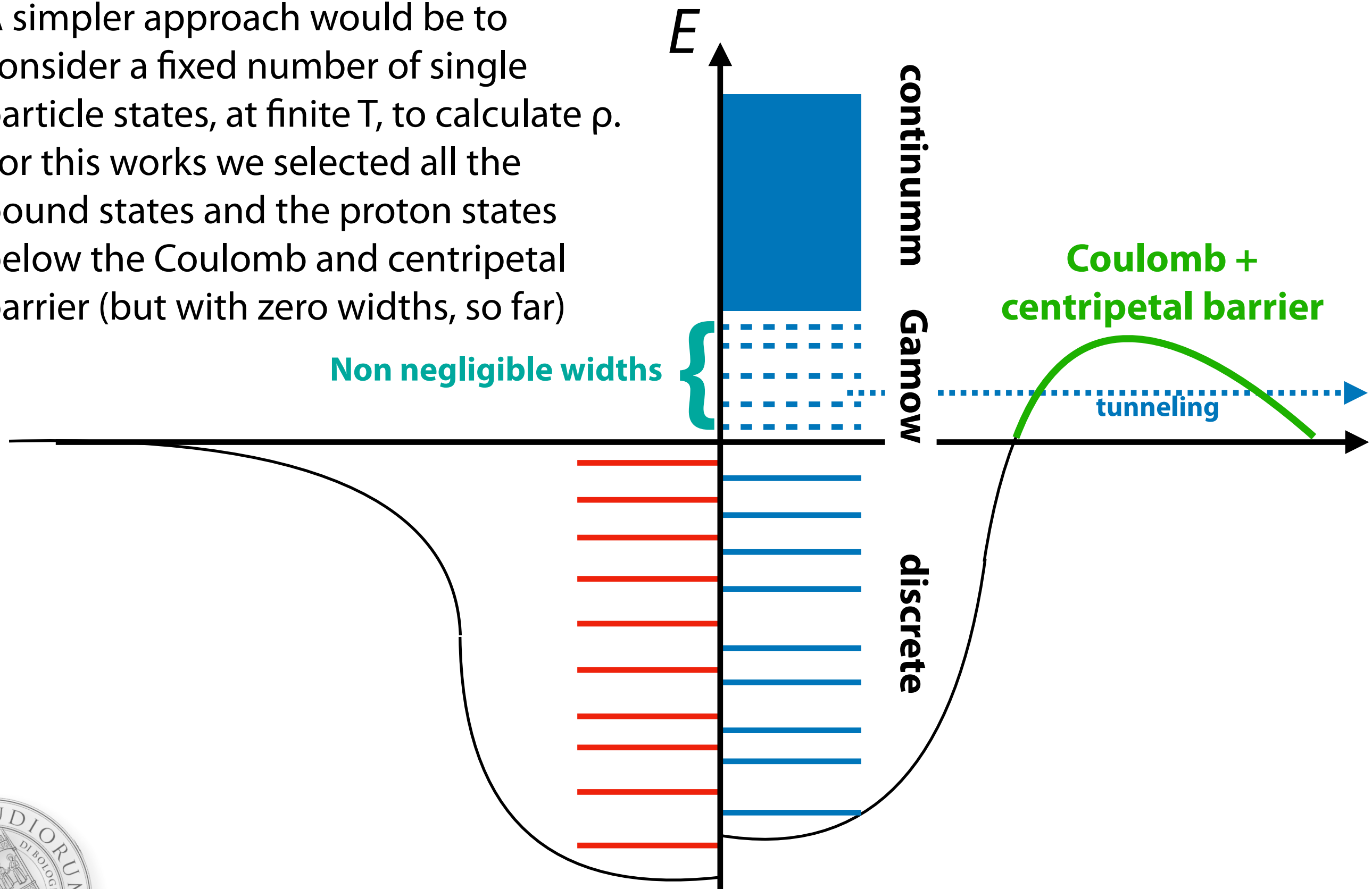
Note that, with this substitution, the evaporated protons of the nucleon+gas and gas solutions are still subject to the Coulomb repulsion of the hot nucleus, as would be expected for protons leaving the hot system.

Bonche, Levit, and Vautherin, NPA **427**, 278 (1984); **436**, 265 (1985).



Bound-state method

A simpler approach would be to consider a fixed number of single particle states, at finite T , to calculate ρ . For this work we selected all the bound states and the proton states below the Coulomb and centripetal barrier (but with zero widths, so far)



Preliminary results

^{16}O , ^{40}Ca , ^{60}Ni , ^{90}Zr , ^{114}Sn , and ^{208}Pb



Benchmark

Fermi-Gas Model Parametrization of Nuclear Level Density

Alberto MENGONI[†] and Yutaka NAKAJIMA

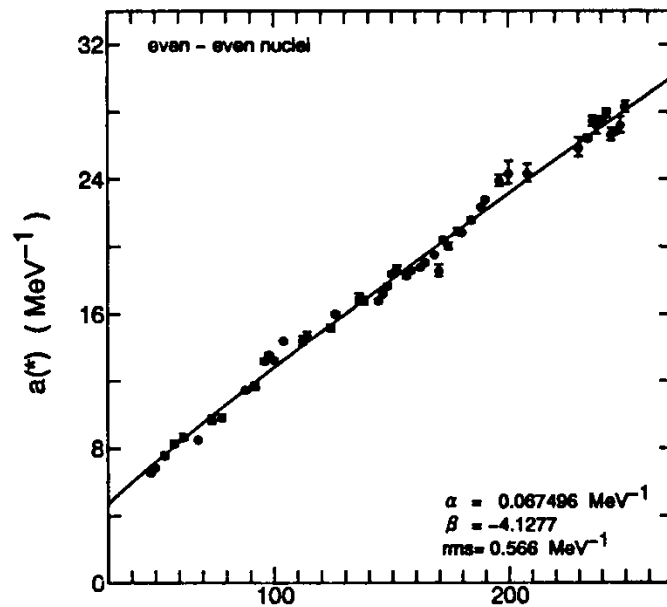
Journal of Nuclear Science and Technology, **31:2**, 151-162 (1994)

Pairing correction

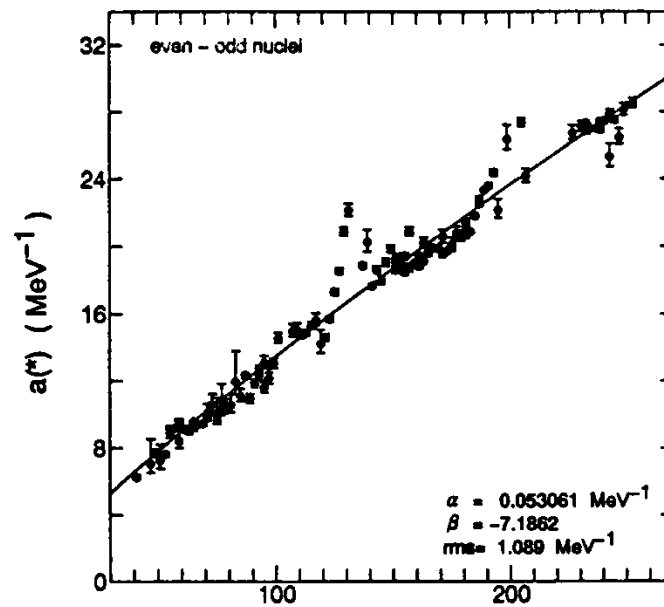
$$U \rightarrow U - \delta \begin{cases} = 2\delta & \text{even - even} \\ = \delta & \text{odd} \\ = 0 & \text{odd - odd} \end{cases}$$

Shell correction

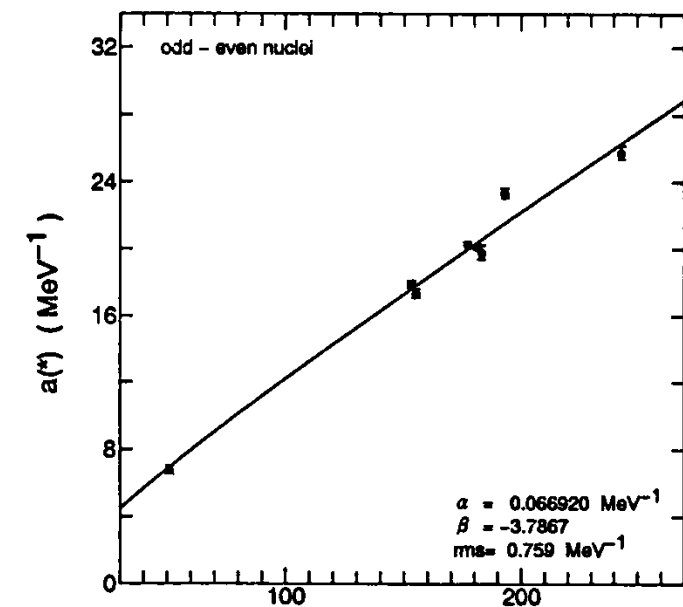
$$a(U) = a(*) \left[1 + \frac{E_{sh}}{U} (1 - e^{-rU}) \right]$$



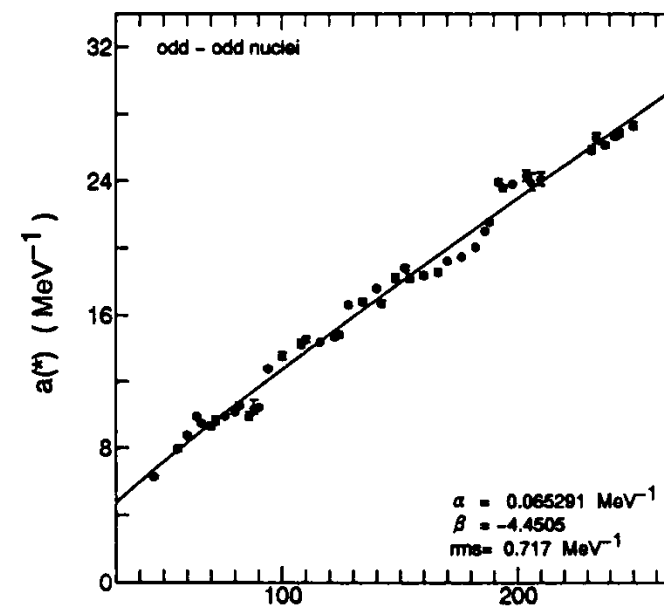
Mass number A
(a) Even Z-even N nuclei



Mass number A
(b) Even Z-odd N nuclei



Mass number A

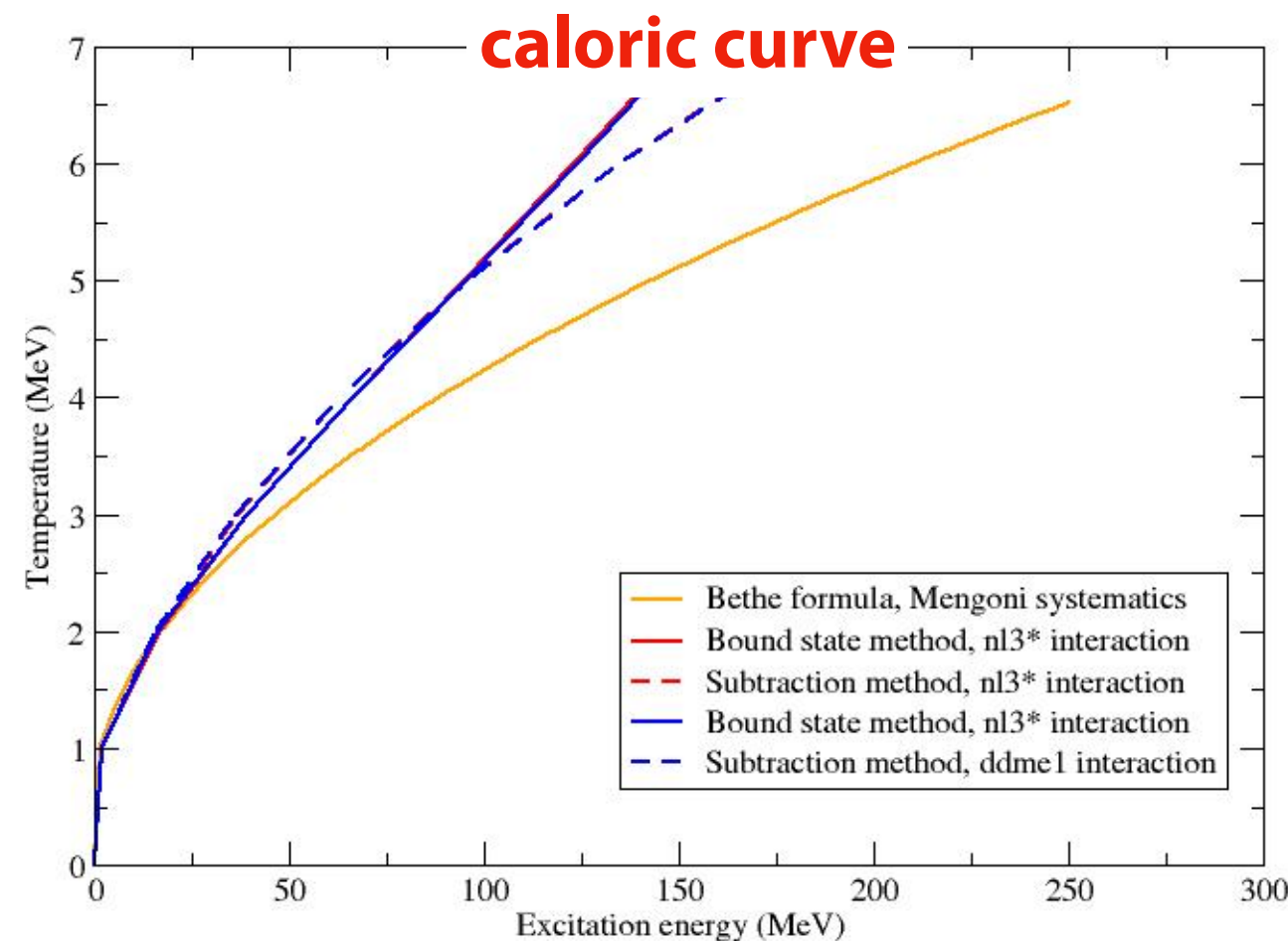
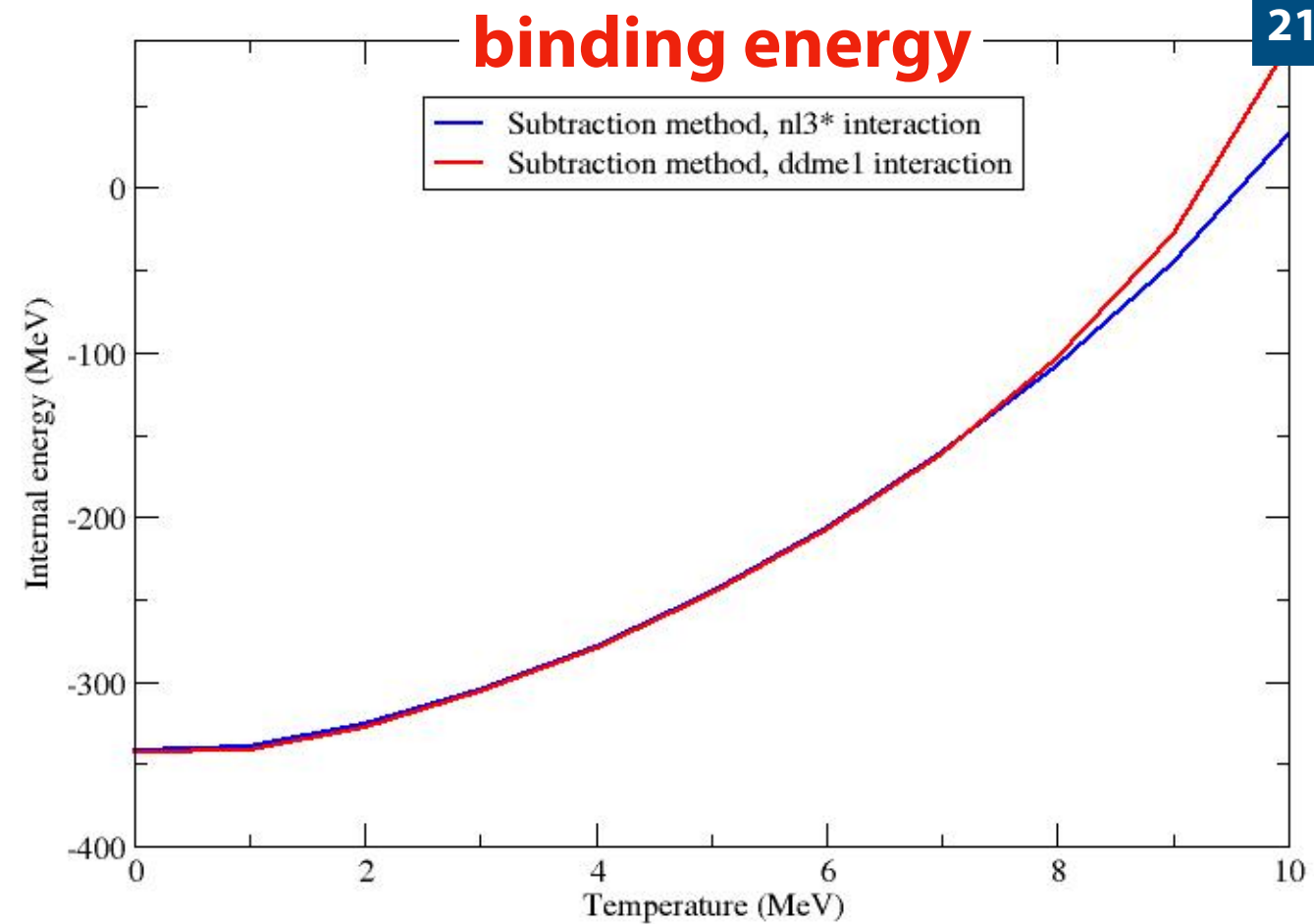
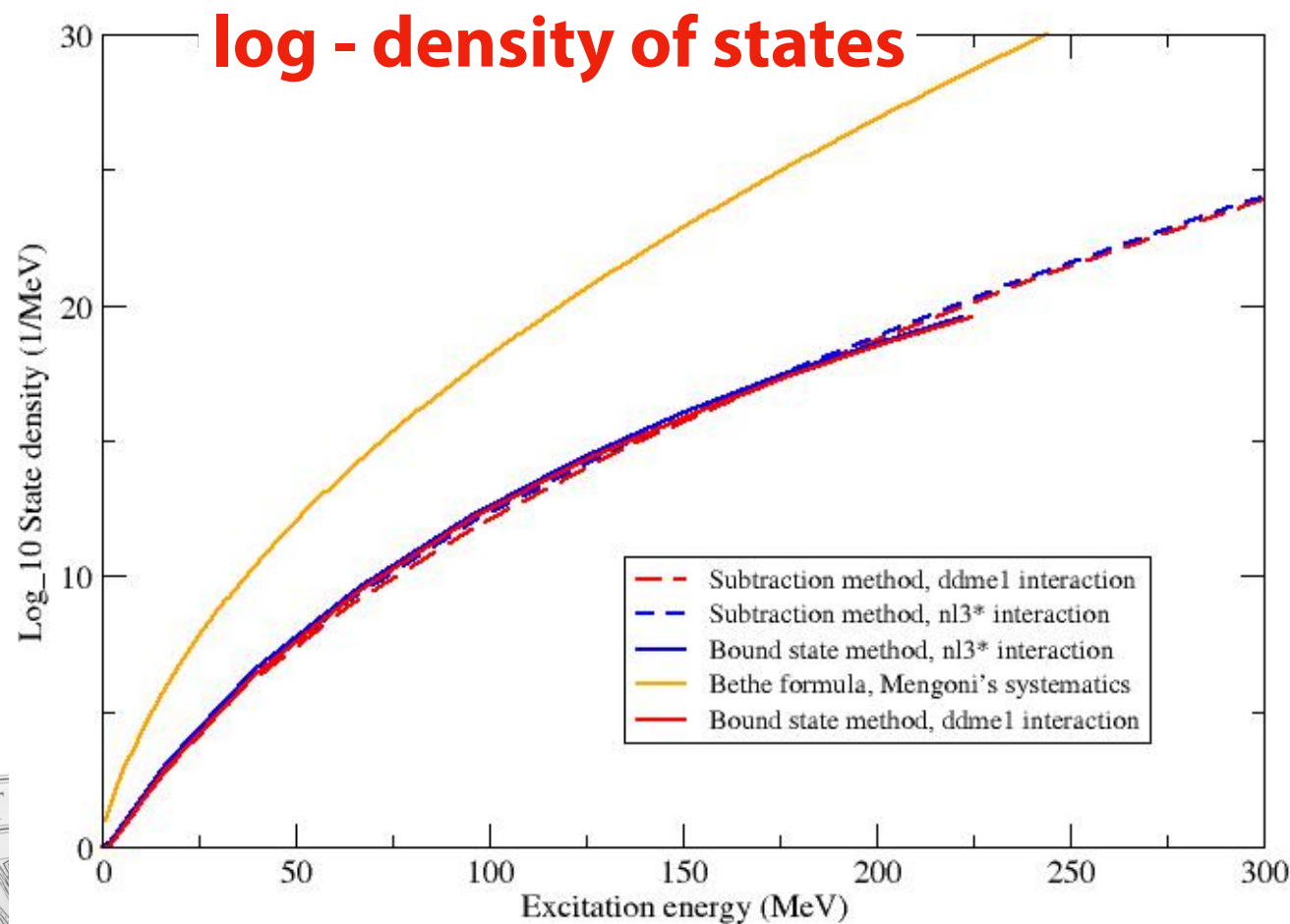


Mass number A



^{40}Ca

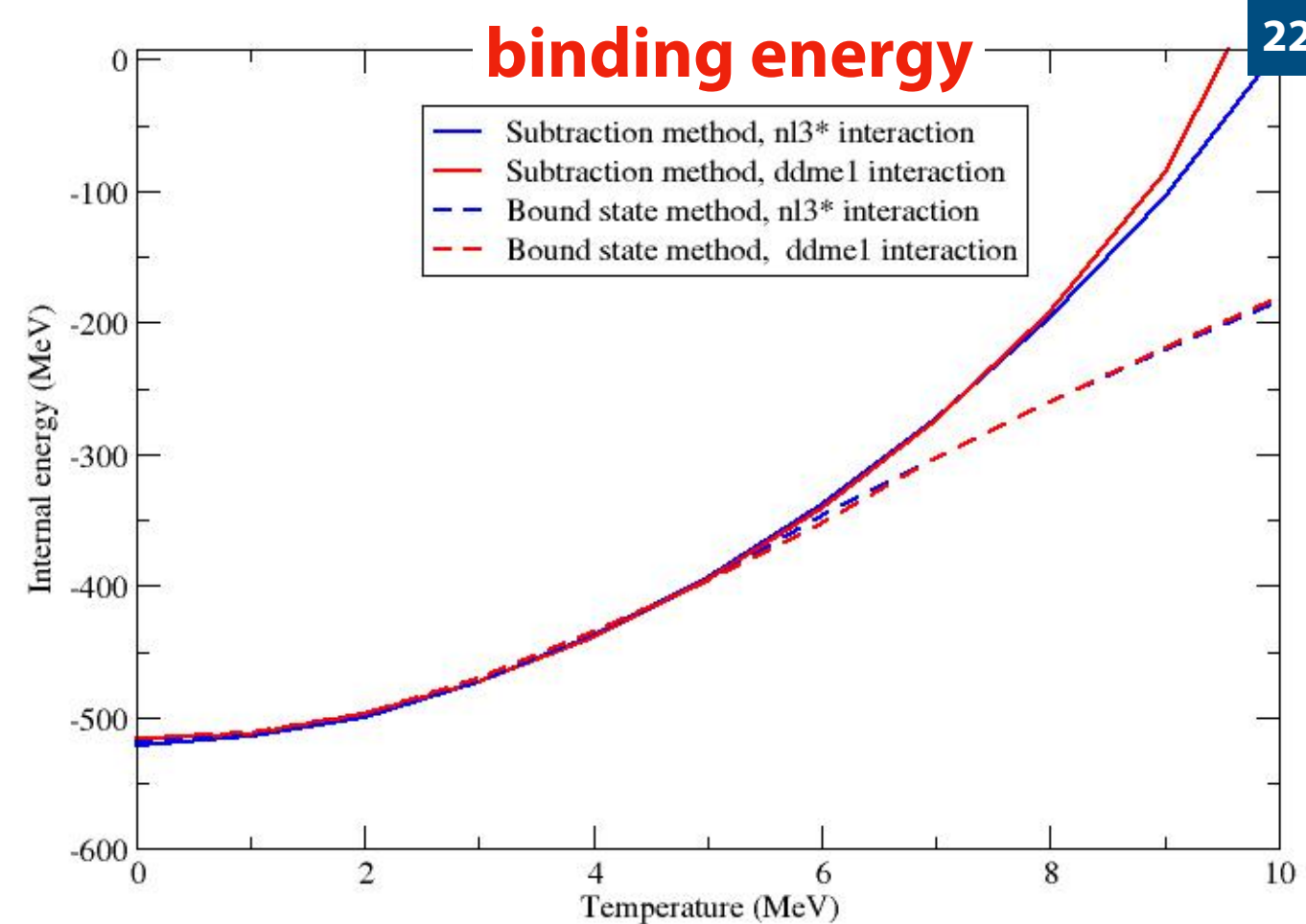
- weak dependence on the interaction (non-linear vs. density dependent)
- \log_{10} density of states substantially underestimated respect to phenomenological approaches
- no appreciable differences between the two methods



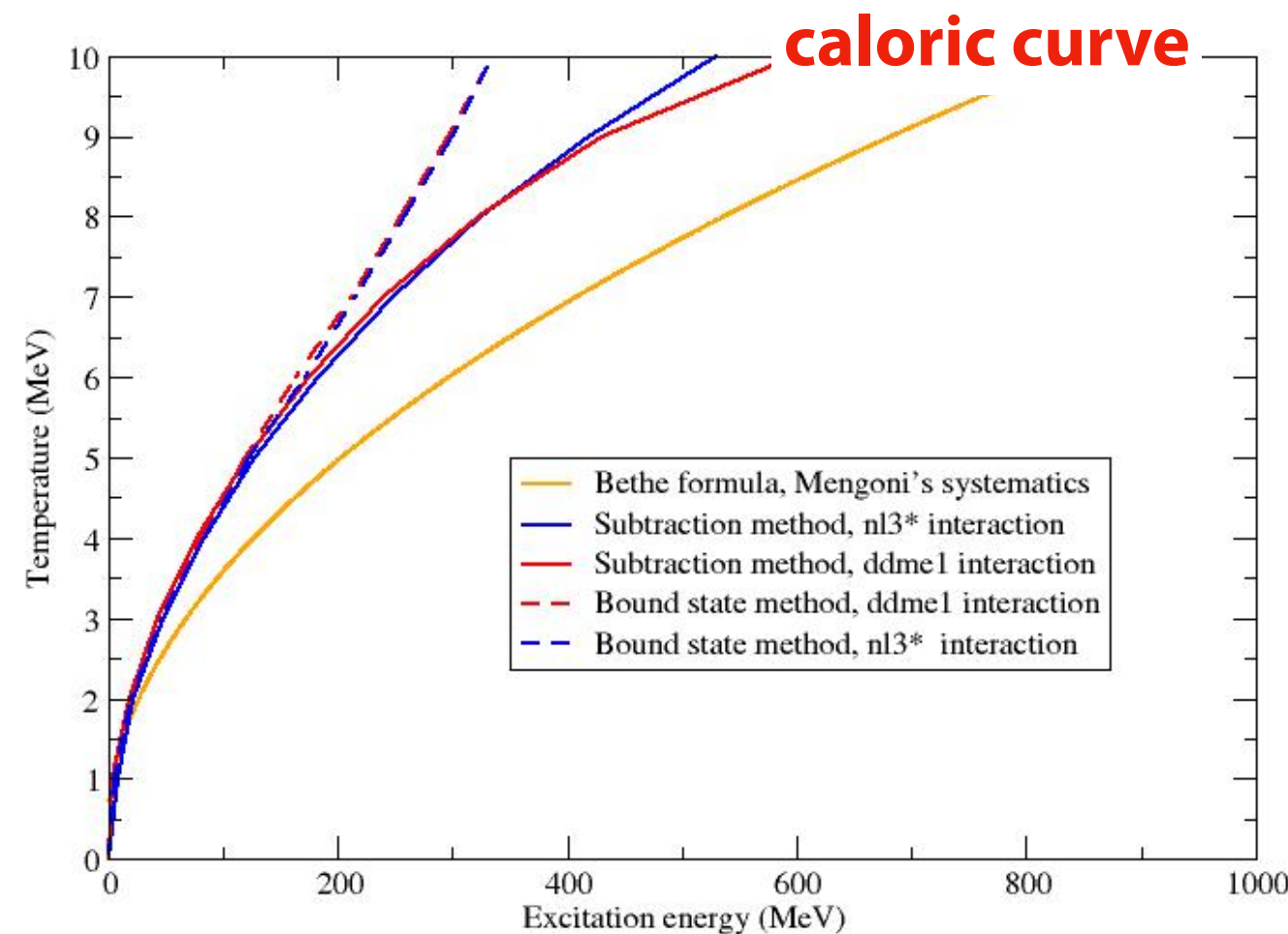
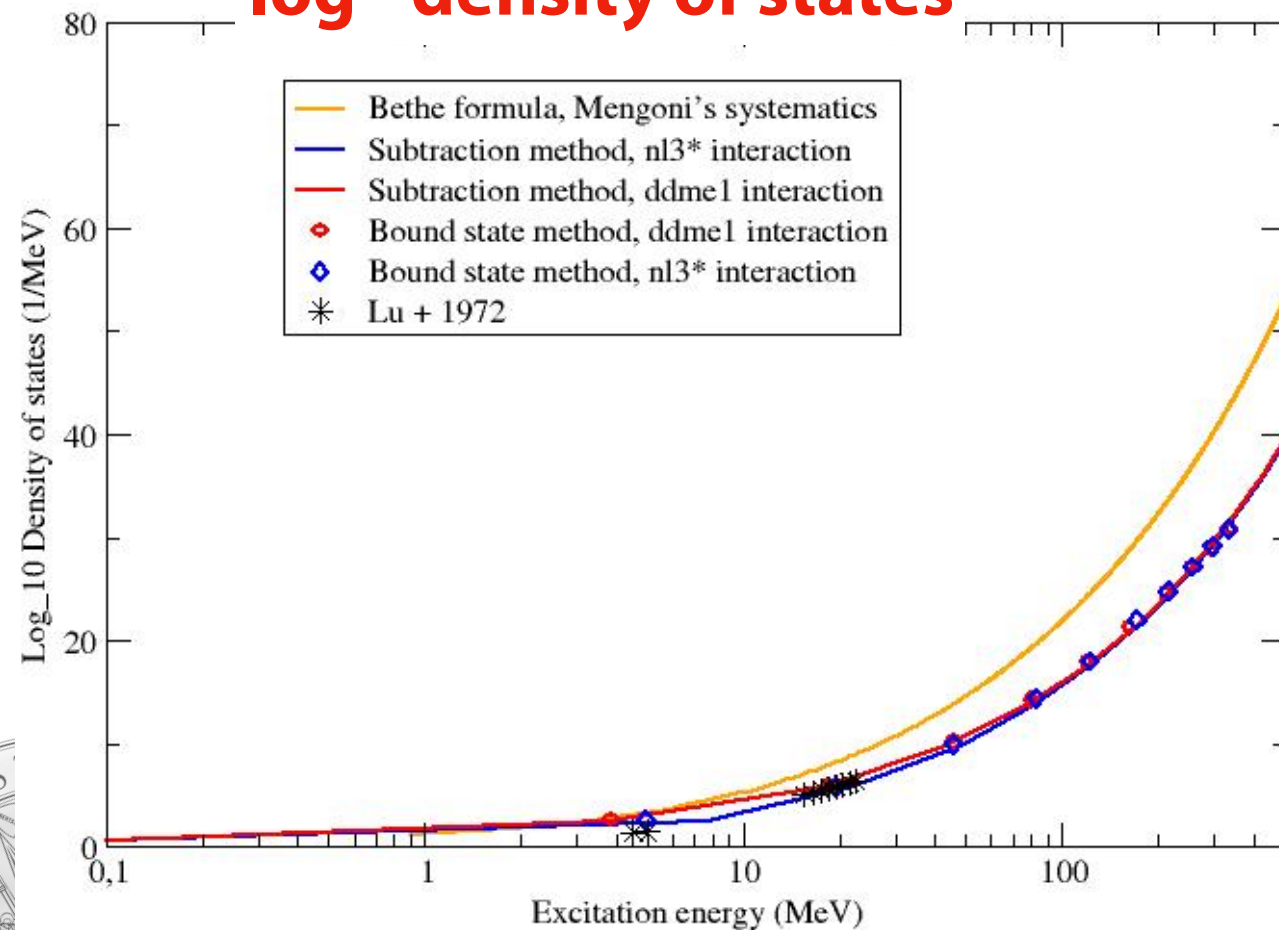
^{60}Ni

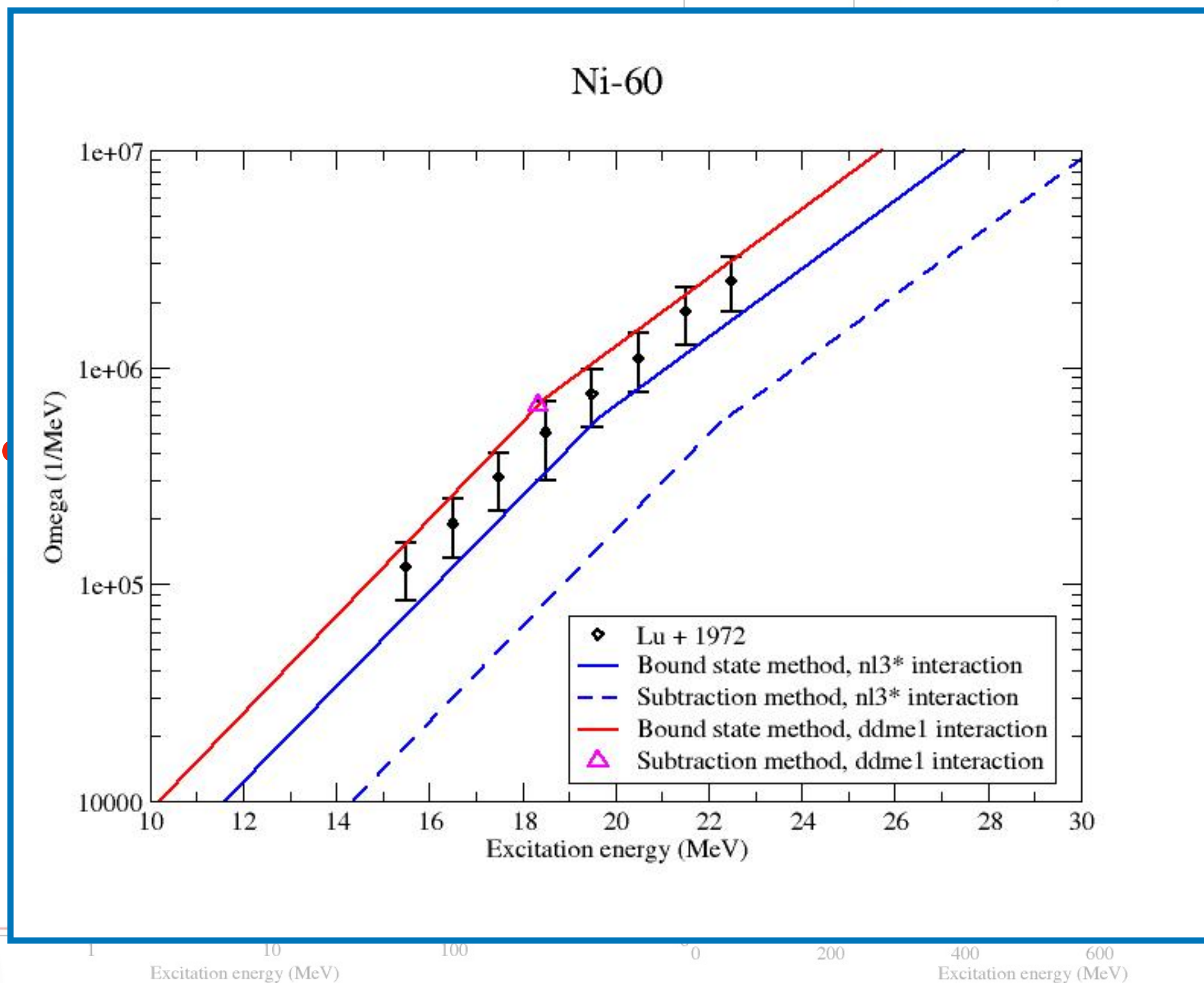
- weak dependence on the interaction (non-linear vs. density dependent)
- \log_{10} density of states closer to phenomenological estimates
- appreciable differences between the two methods for higher excitation energies

22



log - density of states



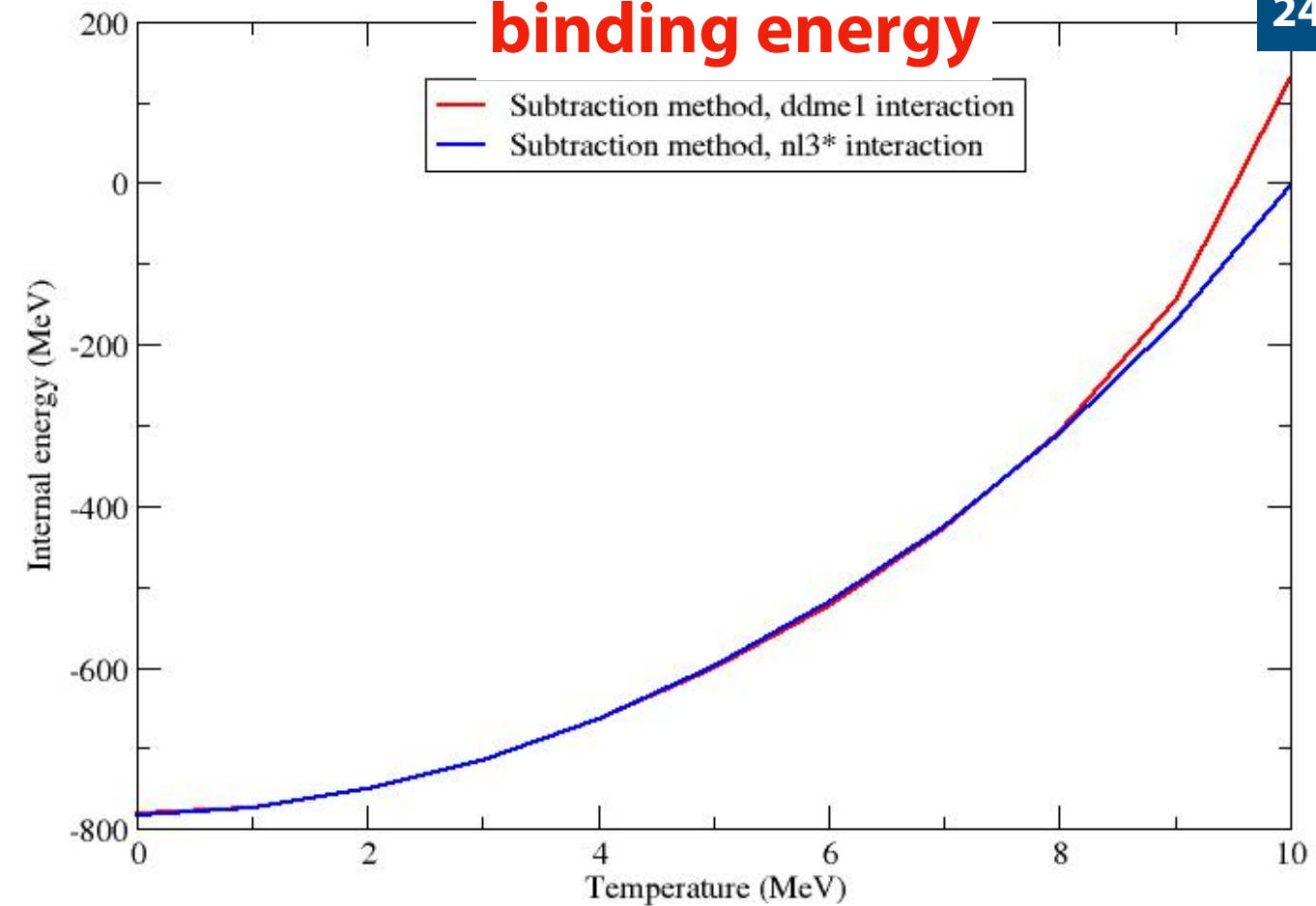


^{90}Zr

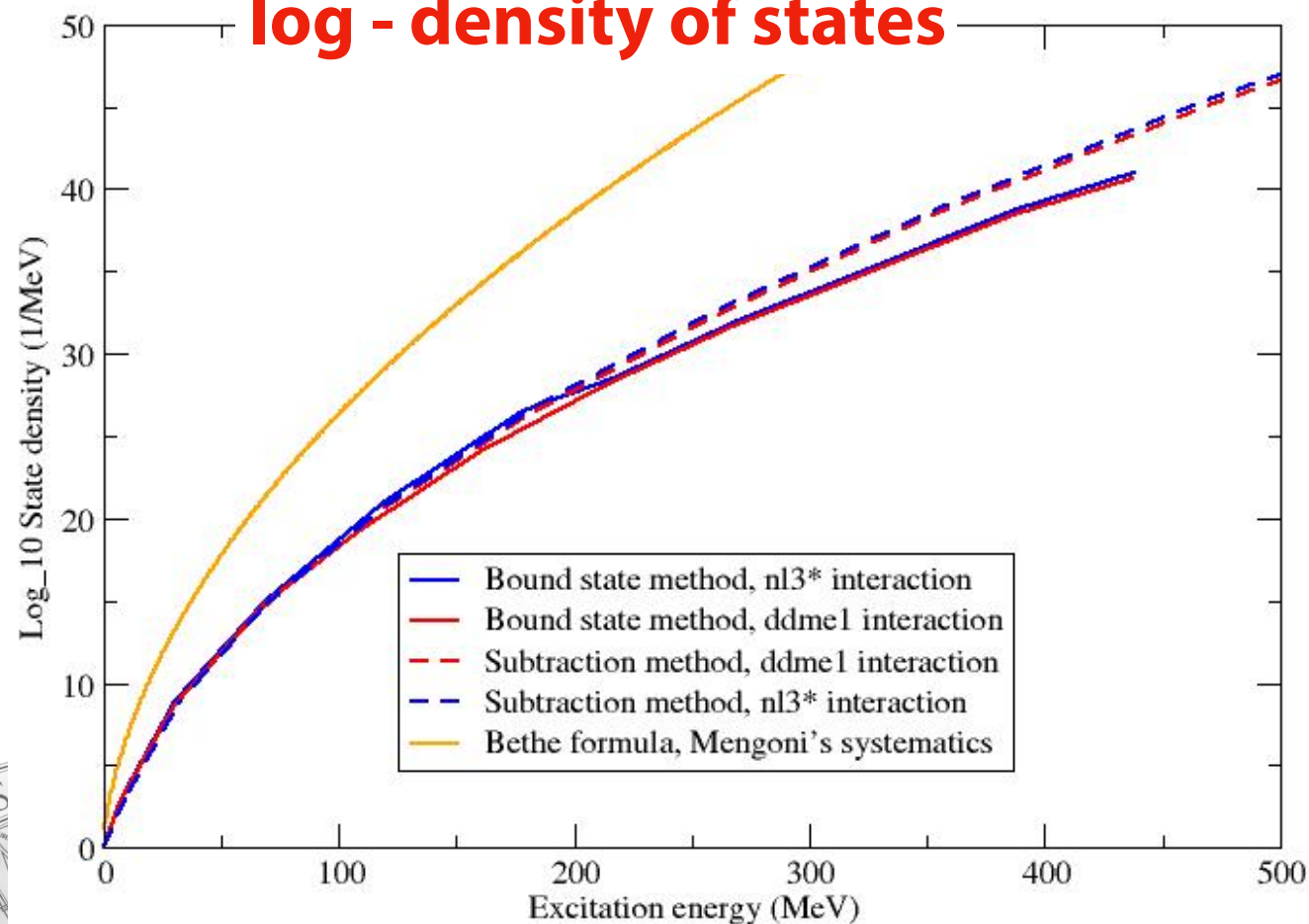
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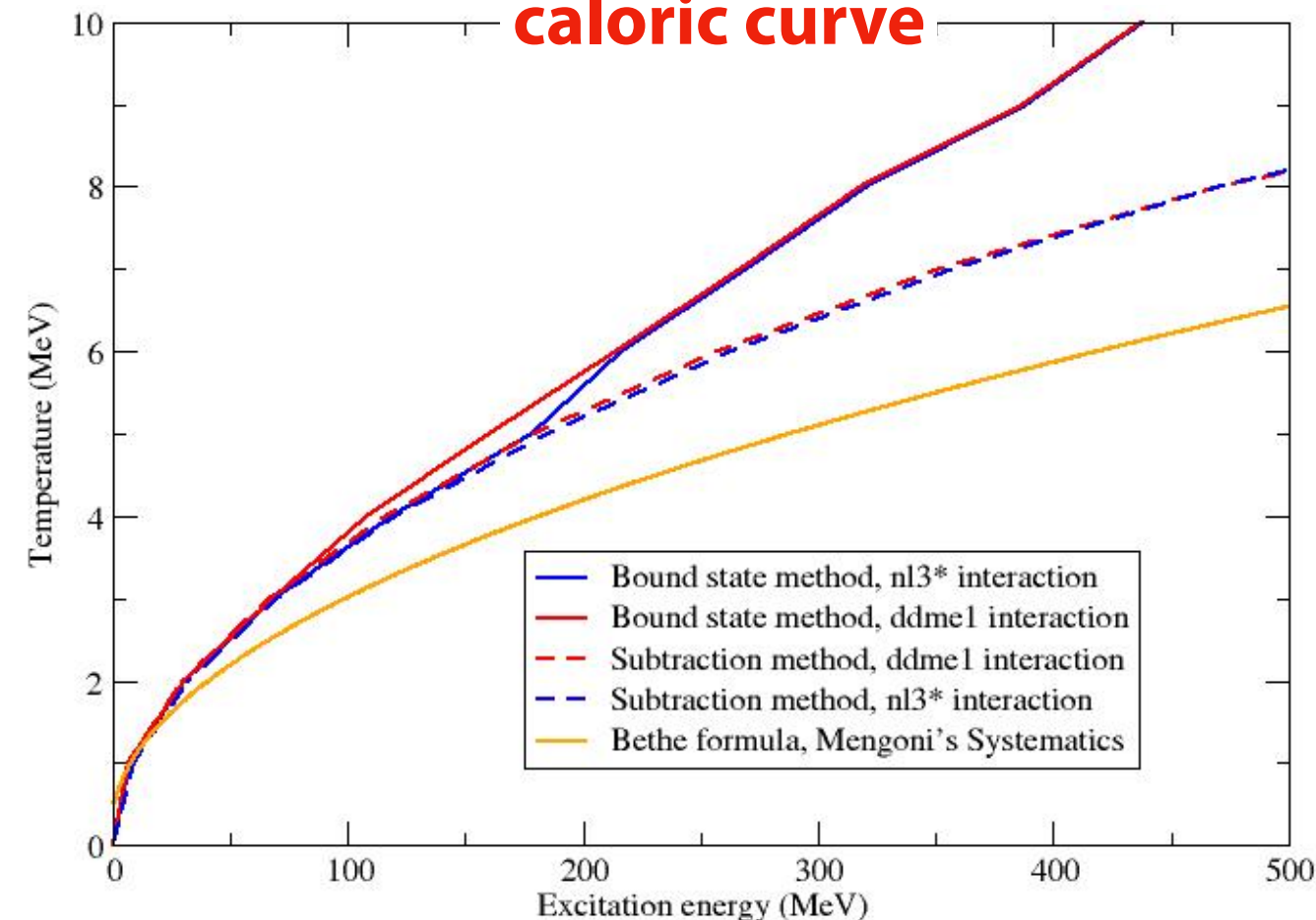
binding energy



log - density of states



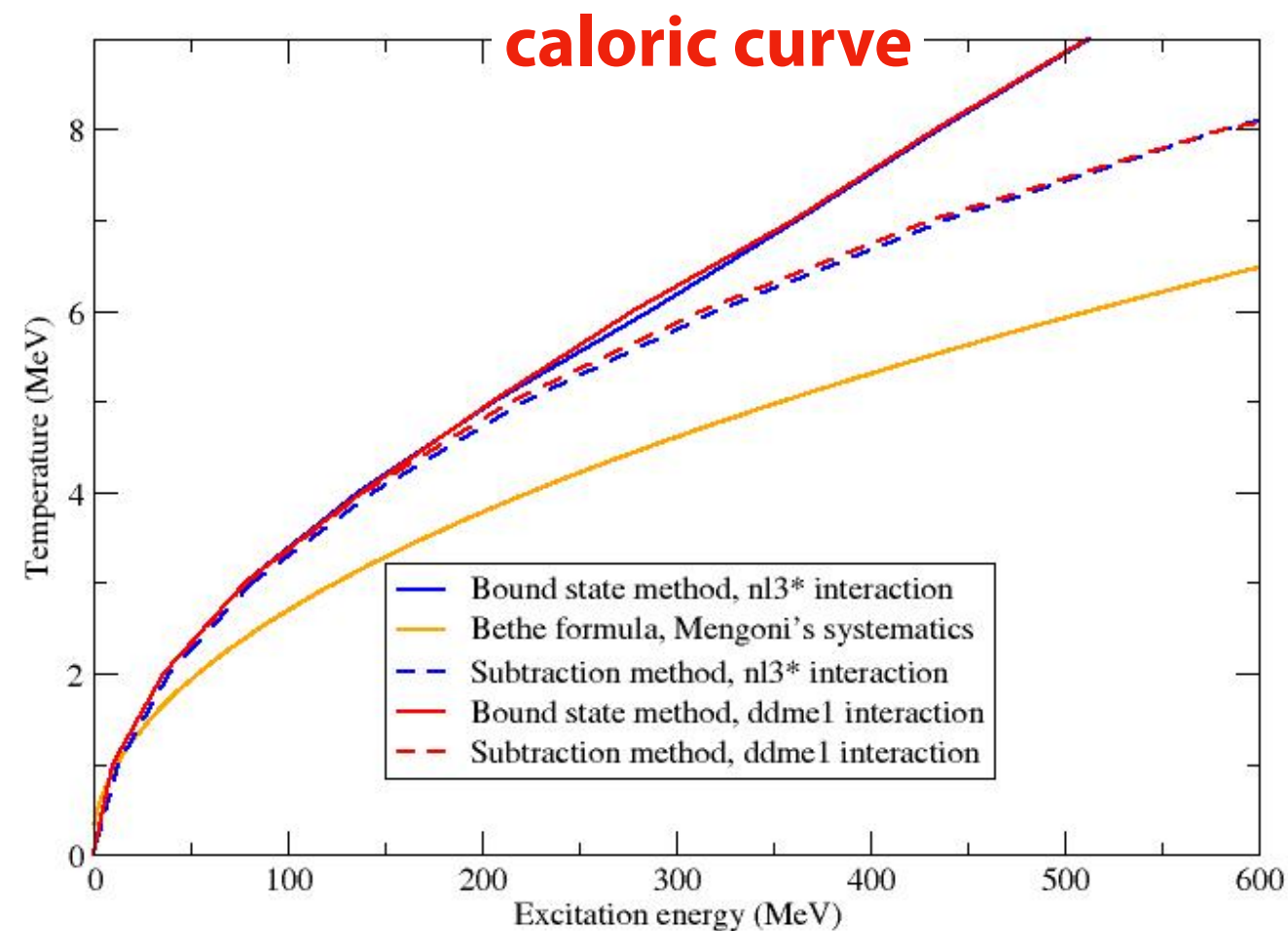
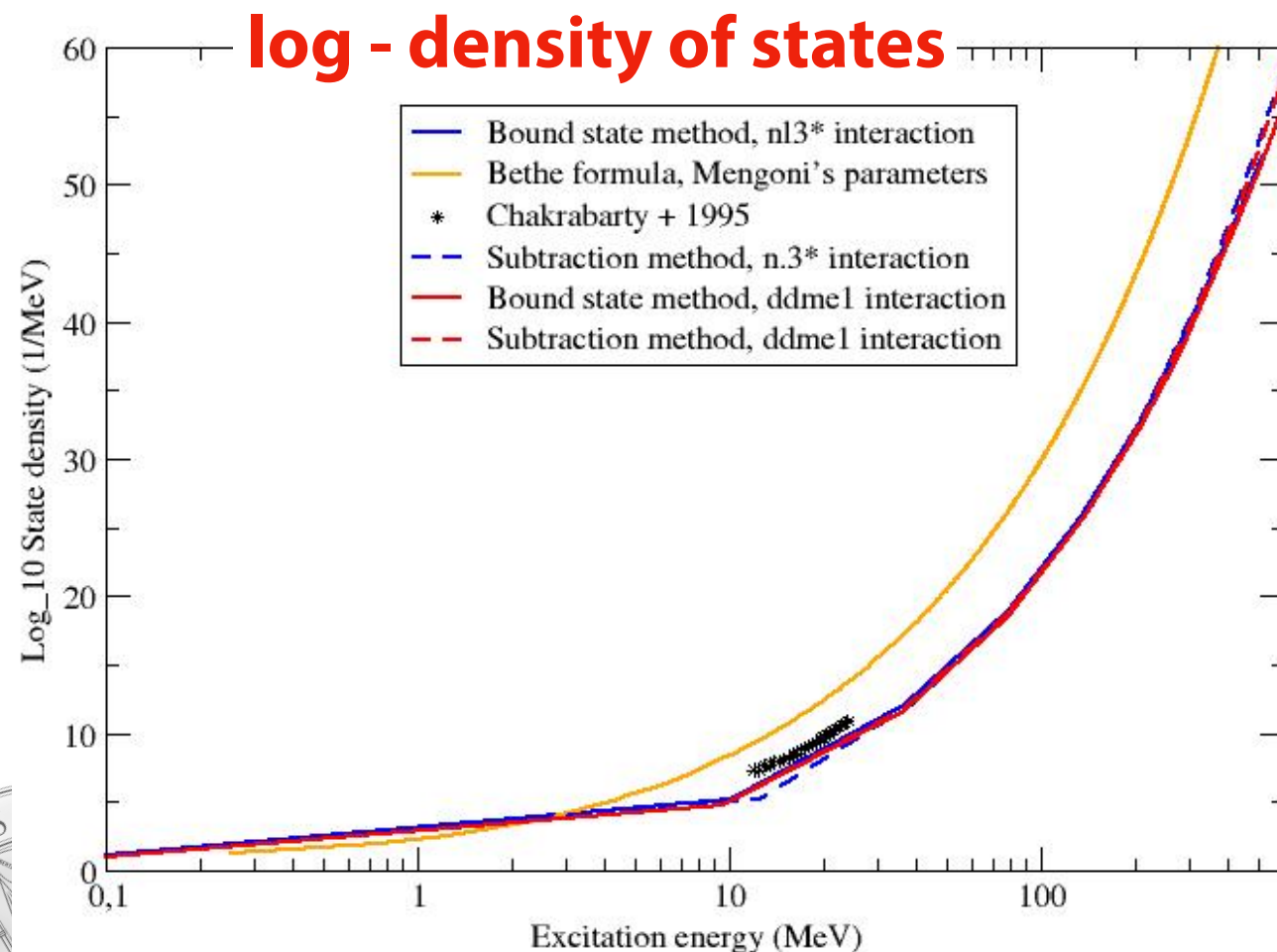
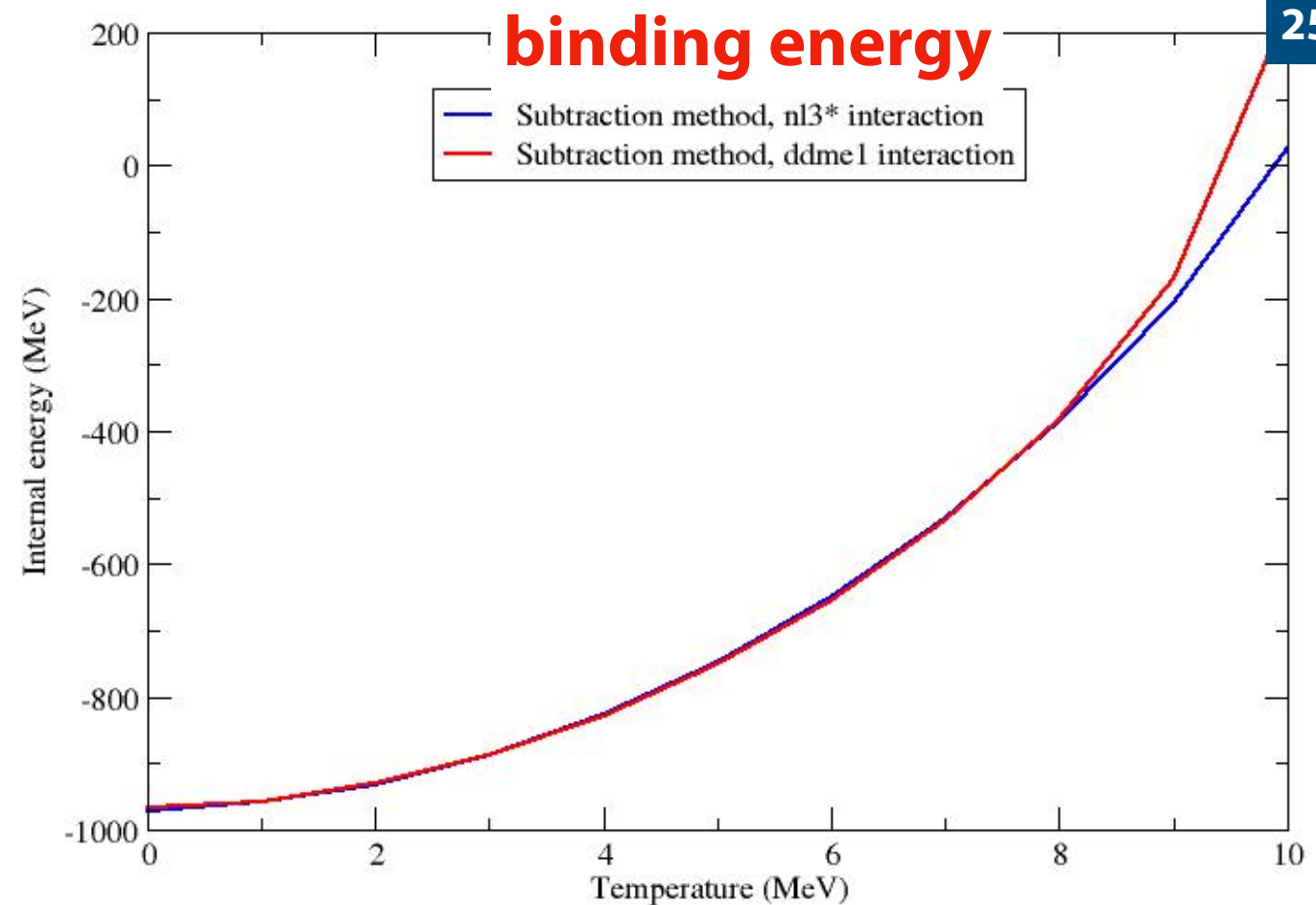
caloric curve



^{114}Sn

- weak dependence on the interaction (non-linear vs. density dependent)
- \log_{10} density of states closer to phenomenological estimates
- appreciable differences between the two methods for higher excitation energies

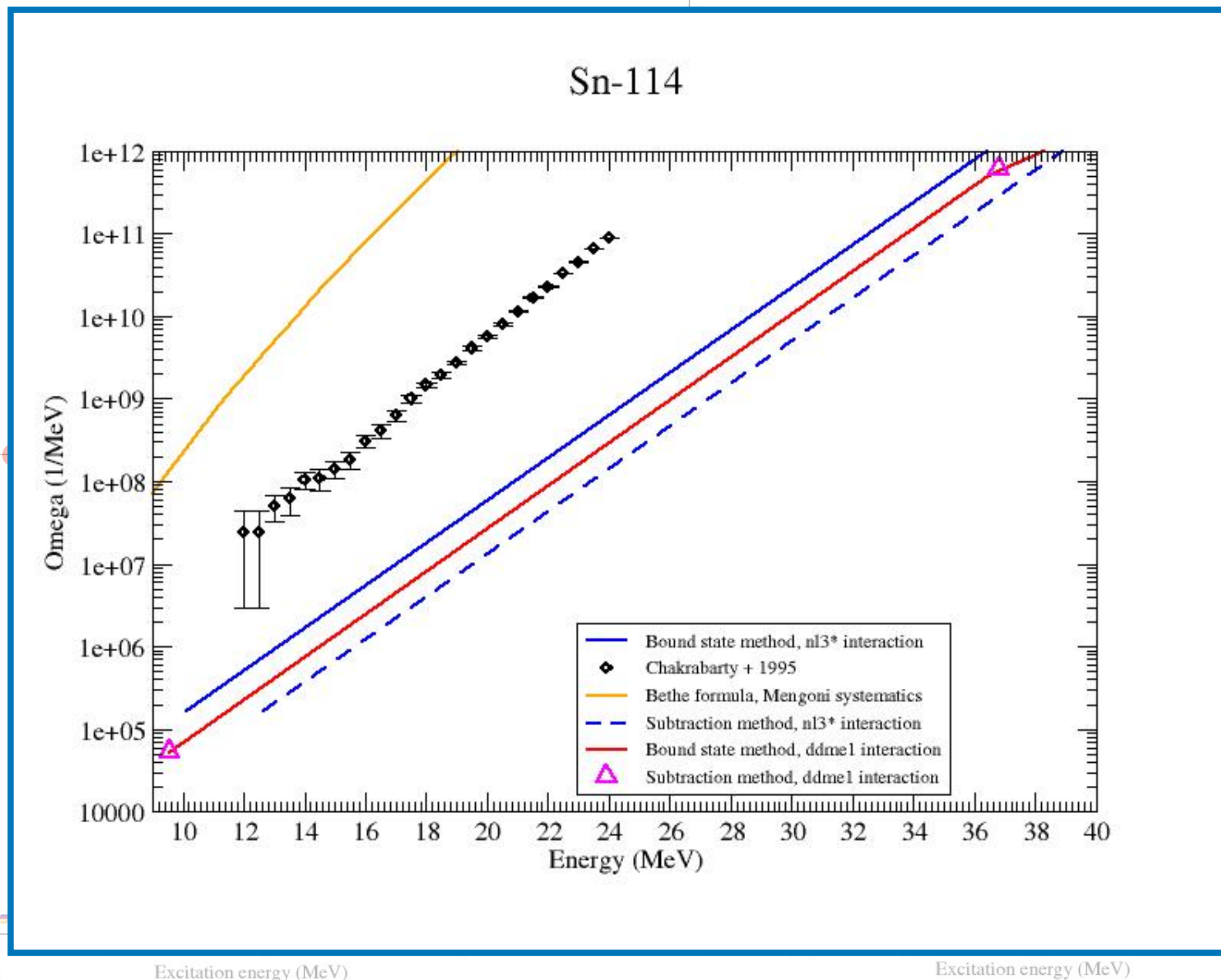
25



^{114}Sn

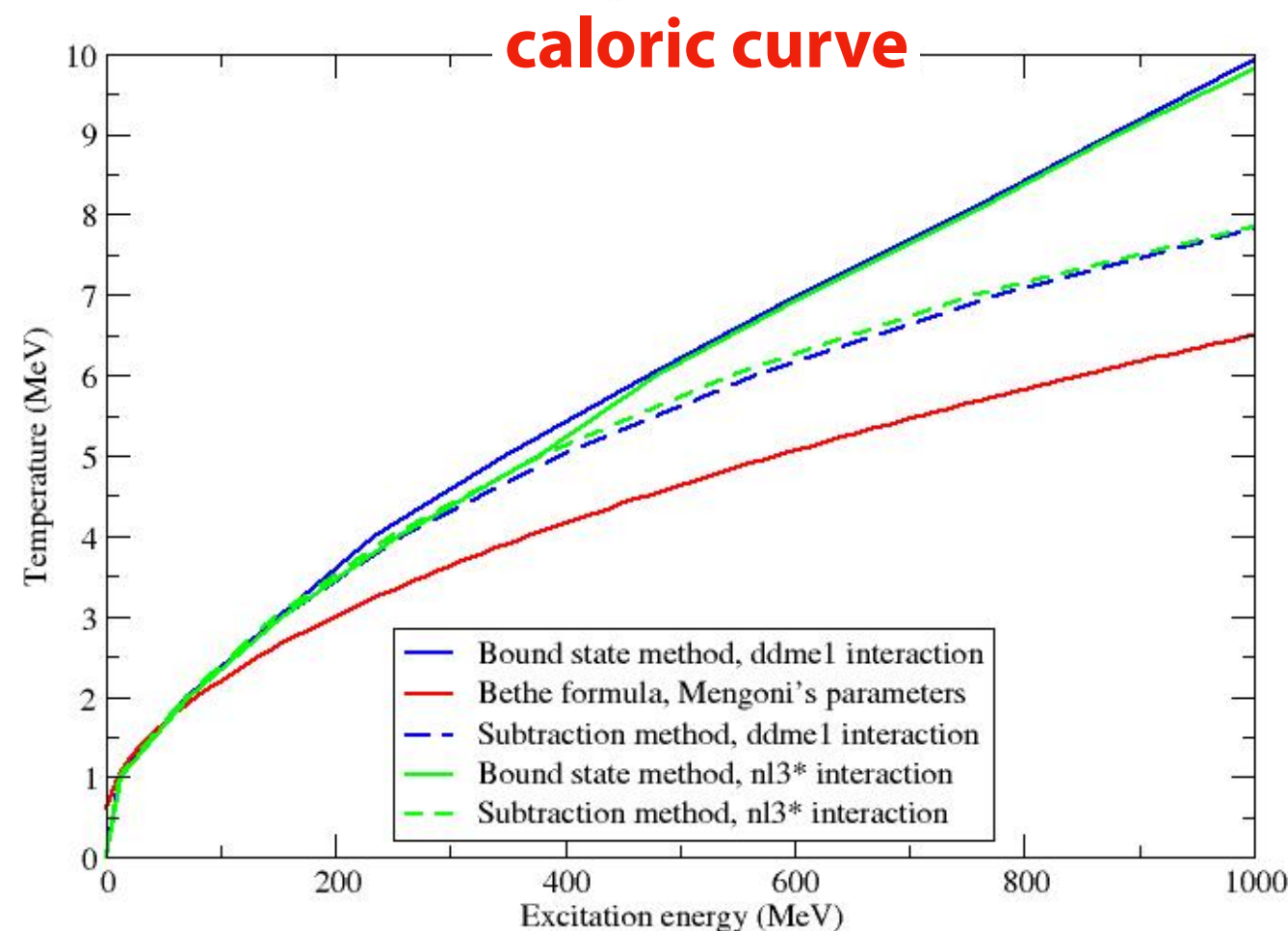
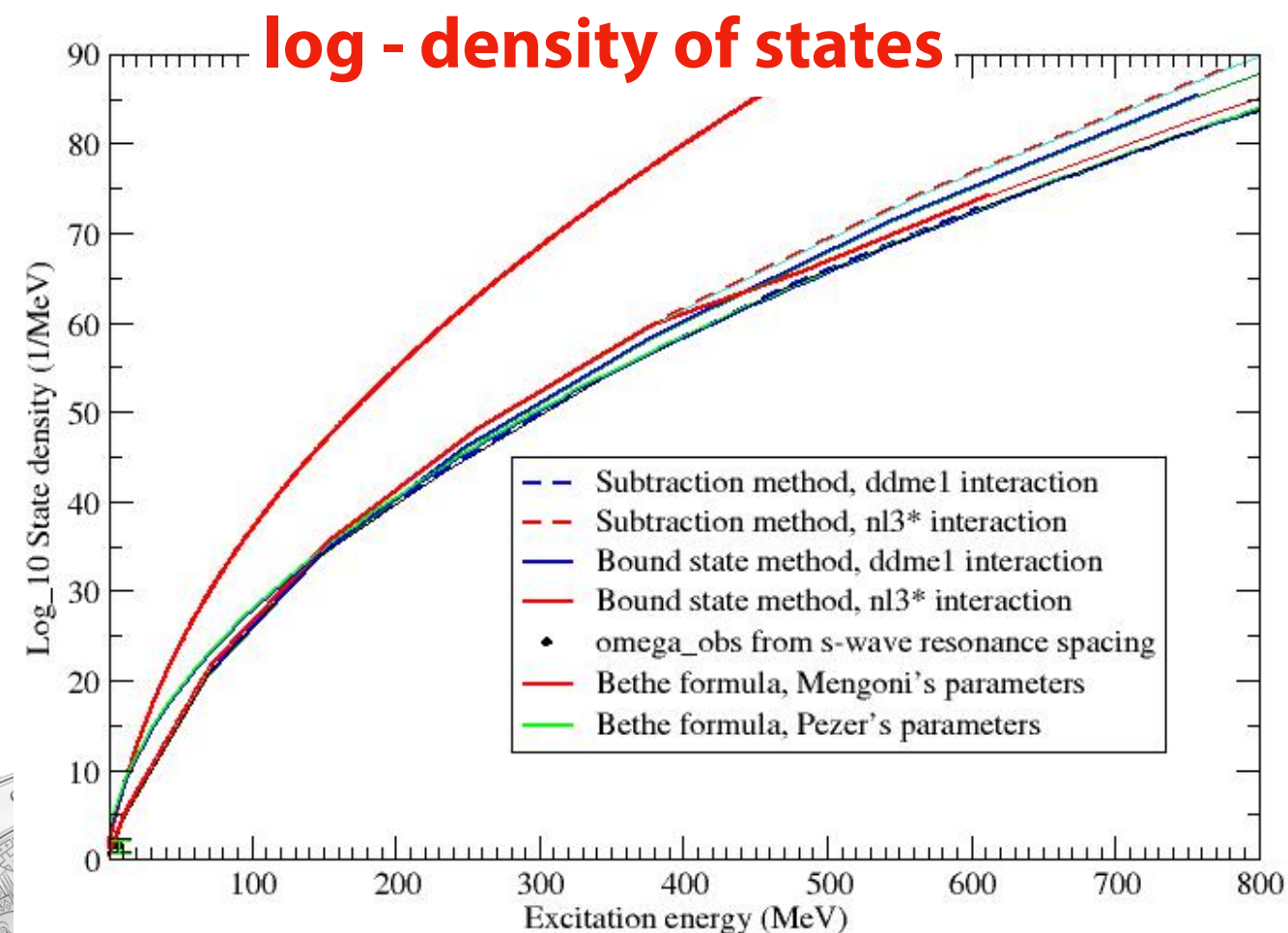
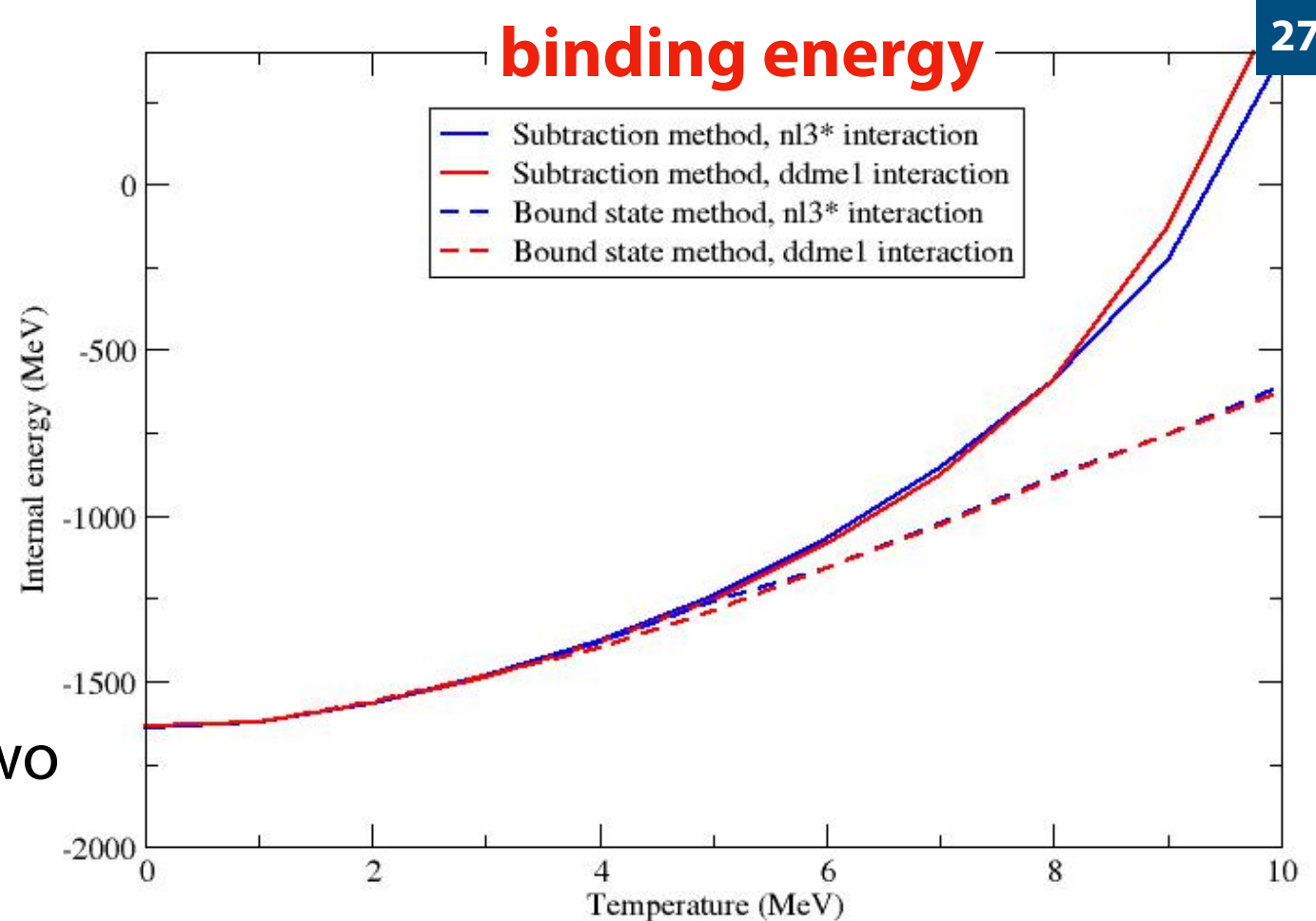
26

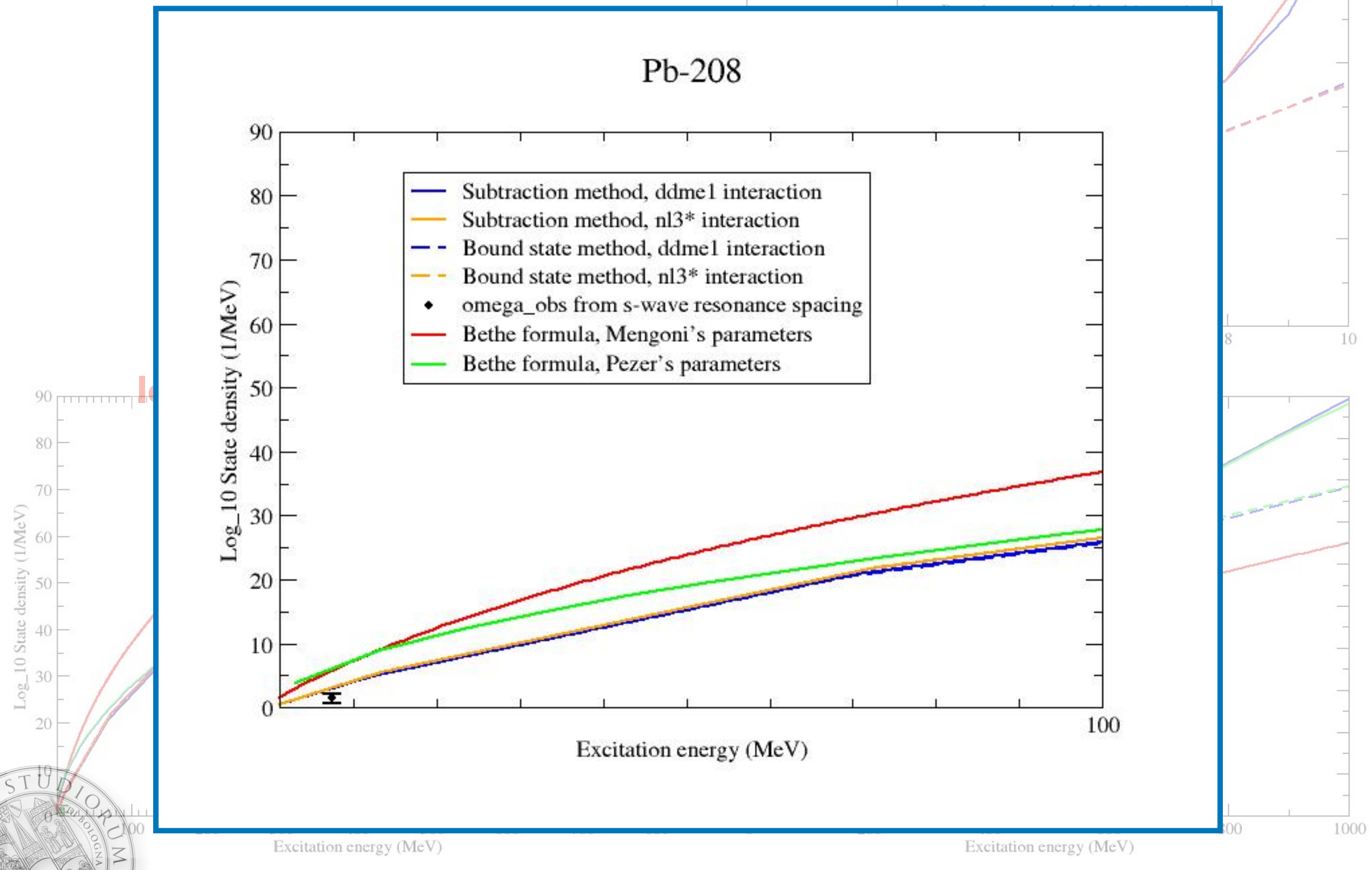
binding energy



208Pb

- mild dependence on the interaction (non-linear vs. density dependent)
- \log_{10} density of states substantially underestimated respect to phenomenological approaches (Mengoni but not Pezer)
- appreciable differences between the two methods for higher excitation energies



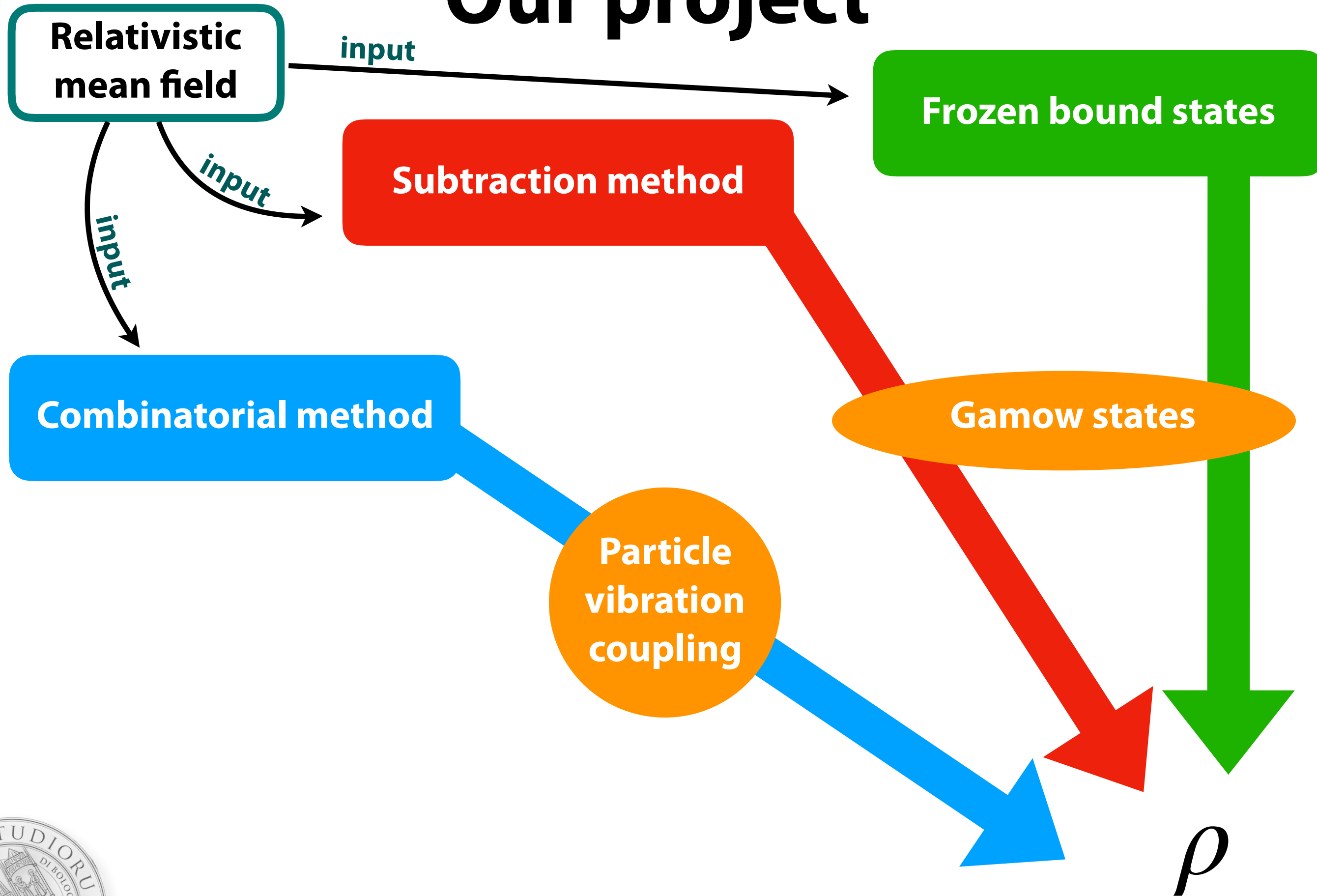


Open issues

1. Importance of the **effective mass**
2. **Non negligible widths** for resonance states
3. Corrections for low excitation energies
4. Extension of the combinatorial approach to higher energies



Our project



Extensions - CSM (work in progress)

Complex scaling method

Y. K. Ho, Phys. Rep. **99**, 1 (1983); A. T. Kruppa et al., Phys. Rev. C **37**, 383 (1988); Guo et al., CPC **181**, 500 (2010), Guo et al., PRC **82**, 034318 (2010)

The starting point of the CSM is a transformation of the Hamiltonian H . First one defines the unbounded non-unitary scaling operator $U(\theta)$ where θ is real

$$U(\theta) = \begin{pmatrix} e^{i\theta\hat{S}} & 0 \\ 0 & e^{i\theta\hat{S}} \end{pmatrix} \quad \hat{S} = r \frac{\partial}{\partial r}$$

The transformed complex scaled Hamiltonian is of the form

$$H_\theta = \begin{pmatrix} V(re^{i\theta}) + S(re^{i\theta}) + M & e^{-i\theta} \left(-\frac{d}{dr} - \frac{1}{r} + \frac{\kappa}{r} \right) \\ e^{-i\theta} \left(\frac{d}{dr} + \frac{1}{r} + \frac{\kappa}{r} \right) & V(re^{i\theta}) - S(re^{i\theta}) - M \end{pmatrix}$$

The corresponding complex scaled equation is

$$H_\theta \psi_\theta = \epsilon_\theta \psi_\theta$$

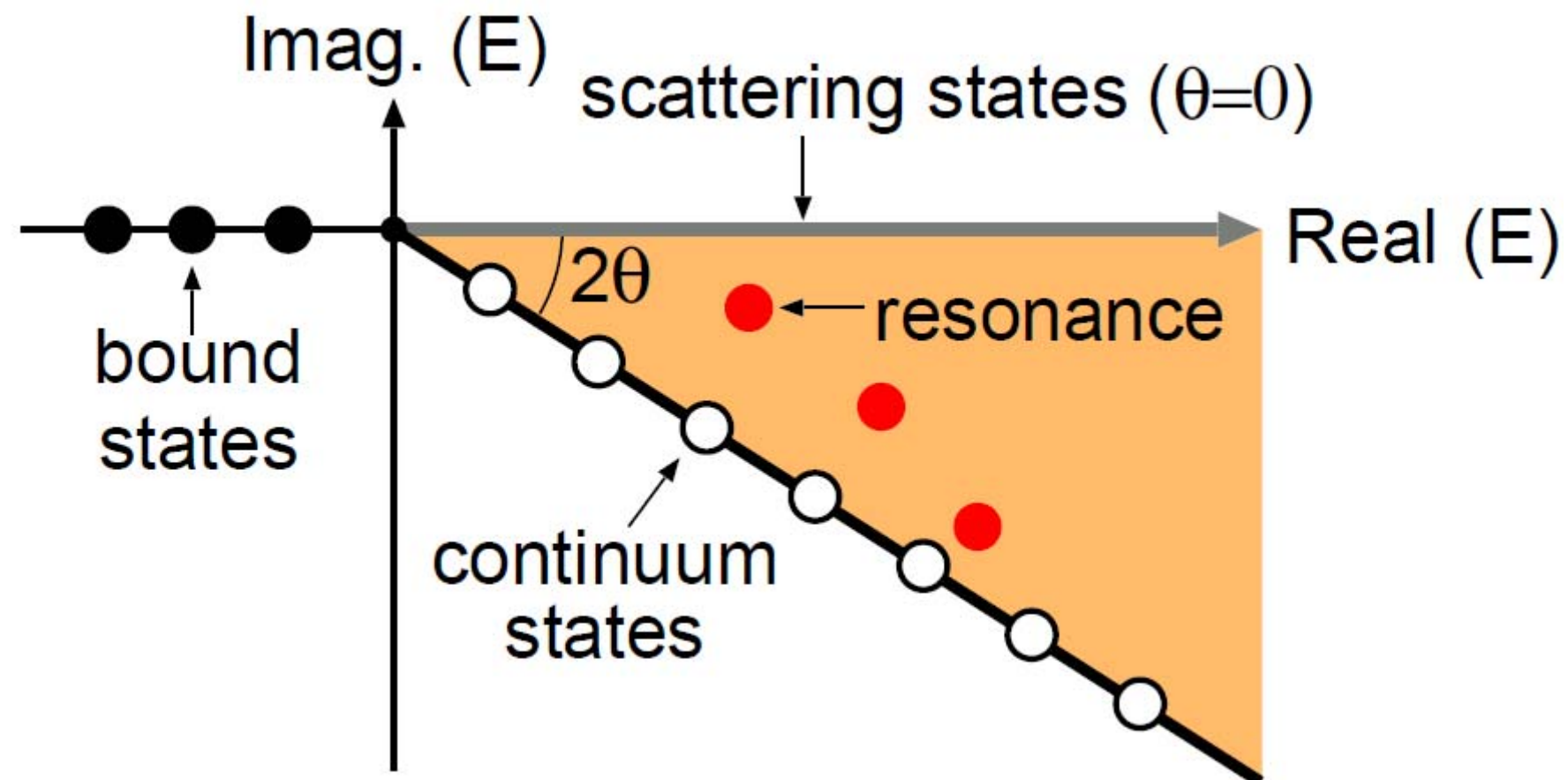


Extensions - CSM (work in progress)

Complex scaling method

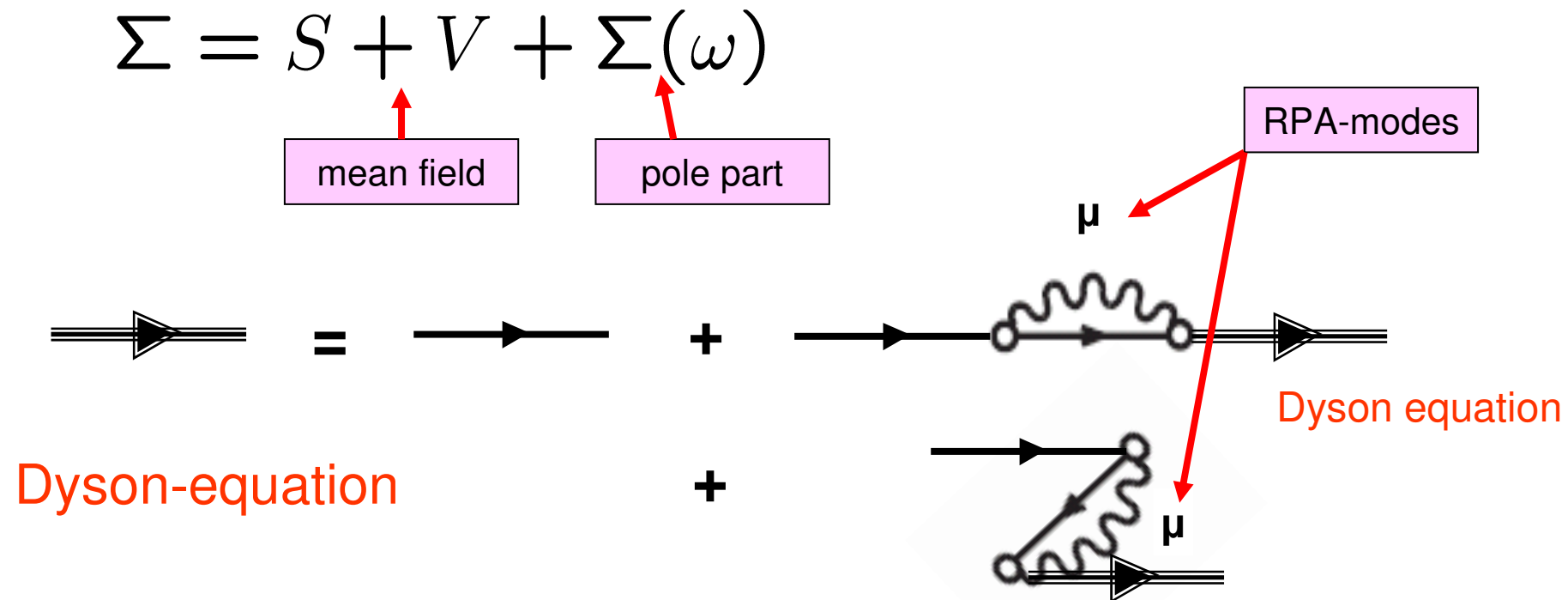
Y. K. Ho, Phys. Rep. **99**, 1 (1983); A. T. Kruppa et al., Phys. Rev. C **37**, 383 (1988); Guo et al., CPC **181**, 500 (2010),
Guo et al., PRC **82**, 034318 (2010)

- A bound state eigenvalue of H remains also an eigenvalue of H_θ
- A **resonance pole $\varepsilon = E - i\Gamma/2$ of the Green-operator of H is an eigenvalue of H_θ**
- The continuous part of the spectrum of H_θ is rotated down into the complex energy plane by the angle θ

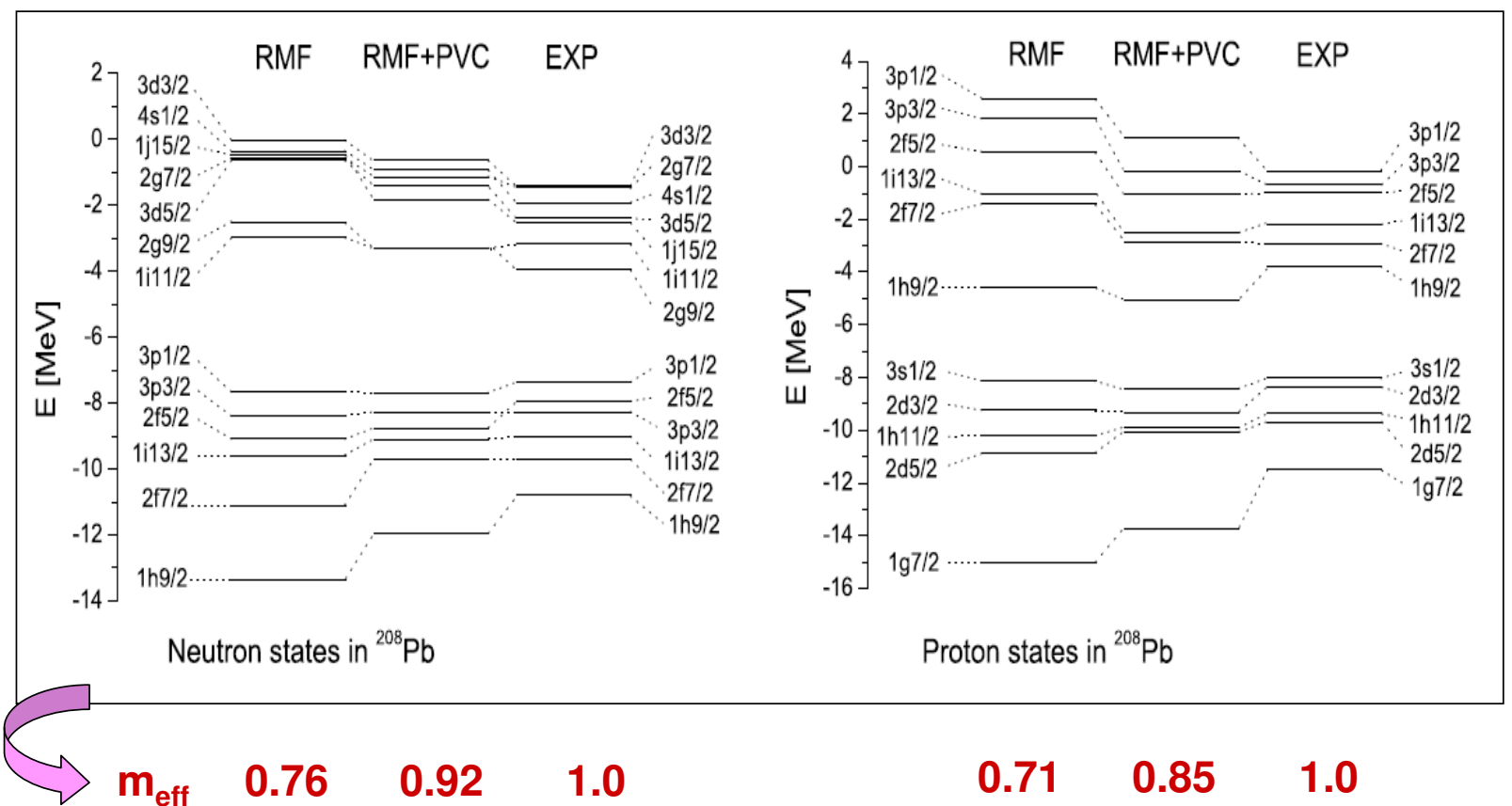


Extensions - PVC (work in progress)

Litvinova and Ring, PRC **73**, 44328 (2006), Ring talk @ 2011 KLFTP-BLTP Joint Workshop



The density of states above and below the Fermi surface is increased



Thank you very much

