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Optimization and parameter reduction in nuclear EDFs

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Energy Density Functionals

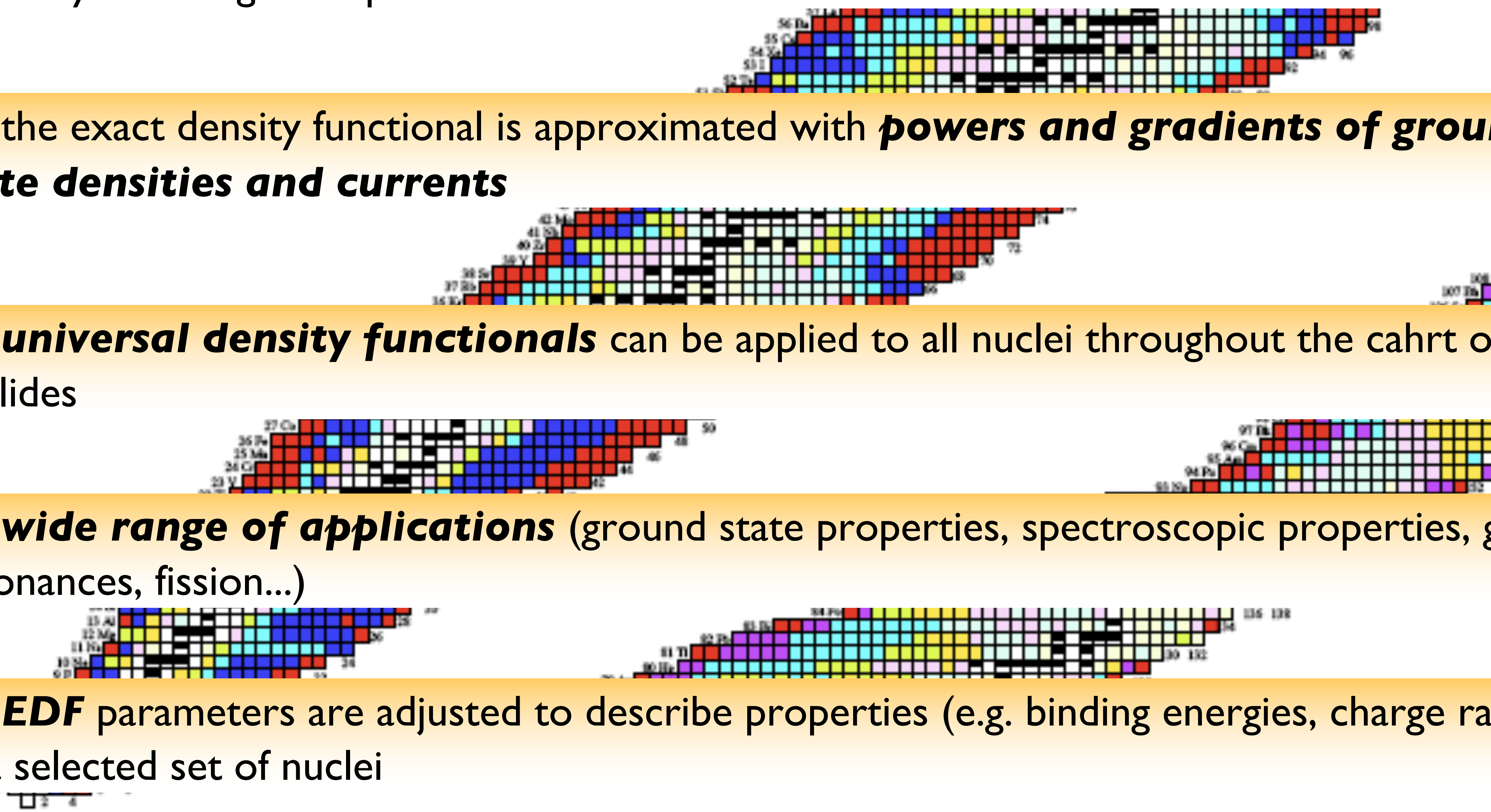
the nuclear many-body problem is effectively mapped onto a ***one-body problem*** without explicitly involving inter-particle interactions

the exact density functional is approximated with ***powers and gradients of ground-state densities and currents***

universal density functionals can be applied to all nuclei throughout the cahrt of nuclides

wide range of applications (ground state properties, spectroscopic properties, giant resonances, fission...)

EDF parameters are adjusted to describe properties (e.g. binding energies, charge radii...) of a selected set of nuclei



Relativistic energy density functionals:

The elementary building blocks are two-fermion terms of the general type:

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \qquad \mathcal{O}_\tau \in \{1, \tau_i\} \qquad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

... isoscalar and isovector four-currents and scalar densities:

$$\begin{aligned}
j_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\psi_k \ , \\
\vec{j}_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\vec{\tau}\psi_k \ , \\
\rho_S &= \langle\phi_0|\overline{\psi}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\psi_k \ , \\
\vec{\rho}_S &= \langle\phi_0|\overline{\psi}\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\vec{\tau}\psi_k
\end{aligned}$$

$|\phi_0\rangle$ is the nuclear ground state.

Energy density functional:

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}[\kappa, \kappa^*]$$

Kinetic energy term:

$$\mathcal{E}_{kin} = \sum_k v_k^2 \int \psi_k^\dagger(\mathbf{r}) \left(-\mathbf{i}\alpha\nabla + m\right) \psi_k(\mathbf{r})$$

Pairing contribution:
finite-range separable pairing

Second order terms:

$$\mathcal{E}_{2nd} = \frac{1}{2} \int \left(\alpha_v(\rho_v)\rho_v^2 + \alpha_s(\rho_v)\rho_s^2 + \alpha_{tv}(\rho_v)\rho_{tv}^2\right)$$

Derivative term:

$$\mathcal{E}_{der} = \frac{1}{2} \int \delta_s \rho_s \triangle \rho_s d^3r$$

Functions of density described by
model parameters, some examples are listed:

$$\alpha_i(\rho_v) = a_i + (b_i + c_i x)e^{-d_i x}, \ x = \rho_v/\rho_{sat}$$

$$\alpha_i(\rho_v) = a_i + b_i x + c_i x^2$$

$$\alpha_i(\rho_v) = a_i \frac{1 + b_i(x + d_i)^2}{1 + c_i(x + d_i)^2}$$

Coulomb term:

$$\mathcal{E}_{coul} = \frac{e}{2} \int j_\mu^p A^\mu d^3r$$

Least-square fit to the data

…N data points and the model depends on F dimensionless parameters.

…maximizing the log-likelihood corresponds to minimizing the cost function $\chi^2(\mathbf{p})$:

$$\chi^2(\mathbf{p}) = \sum_{n=1}^{N} r_n(\mathbf{p})^2$$

➟ the residuals: $$r_n(\mathbf{p}) = \frac{\mathcal{O}_n^{(mod)}(\mathbf{p}) - \mathcal{O}_n}{\Delta\mathcal{O}_n}$$

➟ the ***best*** model: minimum of χ^2 on the model manifold (manifold of predictions embedded in the data space)

$$\left.\frac{\partial\chi^2(\mathbf{p})}{\partial p_\mu}\right|_{\mathbf{p}=\mathbf{p}_0} = 0, \quad \forall\, \mu = 1,\ldots,F$$

In the quadratic approximation of the cost function χ^2 around the best-fit point:

$$\Delta\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}) - \chi^2(\mathbf{p}_0) = \frac{1}{2}\Delta\mathbf{p}^T\hat{\mathcal{M}}\Delta\mathbf{p}$$

$$\Delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0$$

Data could include: nuclear matter properties, properties of finite nuclei (binding energies, charge radii, diffraction radii, surface thickness…)

The symmetric Hessian matrix of second derivatives: $$\mathcal{M}_{\mu\nu} = \left.\frac{\partial^2 \chi^2}{\partial p_\mu \partial p_\nu}\right|_{\mathbf{p}=\mathbf{p}_0}$$

Diagonalization ⇒ $$\Delta\chi^2(\mathbf{p}) = \frac{1}{2}\Delta\mathbf{p}^T\left(\mathcal{A}\mathcal{D}\mathcal{A}^T\right)\Delta\mathbf{p} = \frac{1}{2}\xi^T\mathcal{D}\xi = \frac{1}{2}\sum_{\alpha=1}^{F}\lambda_\alpha\xi_\alpha^2$$

Stiff direction ⟹ large eigenvalue λ, χ^2 rapidly worsens away from minimum, the fit places a stringent constraint on this particular linear combination of parameters.

Soft direction ⟹ small eigenvalue λ, little deterioration in χ^2. The corresponding eigenvector ξ involves a particular linear combination of model parameters that is not constrained by the observables included in the fit.

Model manifolds of nonlinear sloppy models have boundaries that can be analysed using geodesics. The geodesic curve in parameter space corresponds to a curve on the model manifold. The arc length of geodesics on the manifold are a measure of the manifold width in each direction.

The parameters corresponding to a geodesic path can be found as the solution of the differential equation:

$$\ddot{p}_\mu + \sum_{\alpha\beta} \Gamma^{\mu}_{\alpha\beta} \dot{p}_\alpha \dot{p}_\beta = 0$$

➔ initial value problem in the parameter space.

connection coefficients: $$\Gamma^{\alpha}_{\mu\nu} = \sum_{\beta} (g^{-1})_{\alpha\beta} \sum_{m} \frac{\partial r_m}{\partial p_\beta} \frac{\partial^2 r_m}{\partial p_\mu \partial p_\nu}$$

metric tensor: $$g_{\mu\nu} = \sum_{m} \frac{\partial r_m}{\partial p_\mu} \frac{\partial r_m}{\partial p_\nu}$$

Derivatives with respect to the model parameters →if possible use the automatic differentiation packages (for self-consistent models this is not possible)

The boundary of the manifold is identified by the metric tensor becoming singular.

Manifold Boundary Approximation Method

Transtrum et al., PRL **104**, 060201 (2010)

PRL **113**, 098701 (2014)

J. Chem. Phys. **143**, 010901 (2015)

1. Given a model and a set of parameters, determine the best-fit model, calculate the Hessian and identify the eigendirection with smallest eigenvalue.

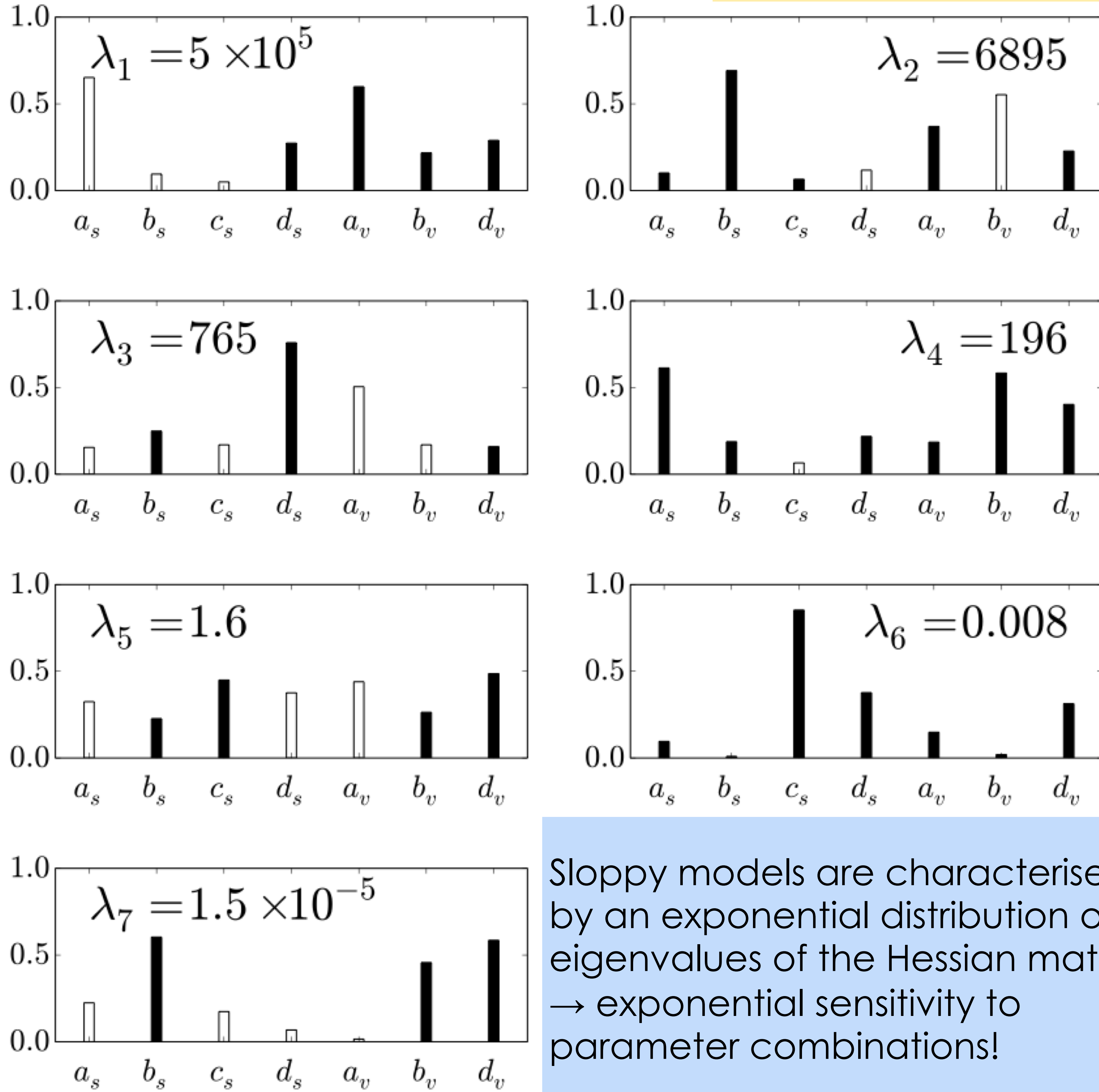
2. Integrate the geodesic equation using the best-fit parameter values and the eigendirection with smallest eigenvalue as initial conditions, until the boundary of the model manifold is reached.

3. Evaluate the limit associated with this boundary to produce a new model with one less parameters.

4. Optimise the new model by a least-square fit to the data, and use it as a starting point for the next iteration.

Phys. Rev. C 95, 054304 (2017)
Phys. Rev. C 94, 024333 (2016)

Least-squares fit of the EDF parameters to the APR microscopic EoS of symmetric nuclear matter.



Eigenvectors and eigenvalues of the Hessian matrix $\mathcal{M}$ of second derivatives of $\chi^2(p)$ ➟

...empty and filled bars ⇒ the corresponding amplitudes contribute with opposite signs.

Sloppy models are characterised by an exponential distribution of eigenvalues of the Hessian matrix → exponential sensitivity to parameter combinations!

Phys. Rev. C 95, 054304 (2017)
Phys. Rev. C 94, 024333 (2016)

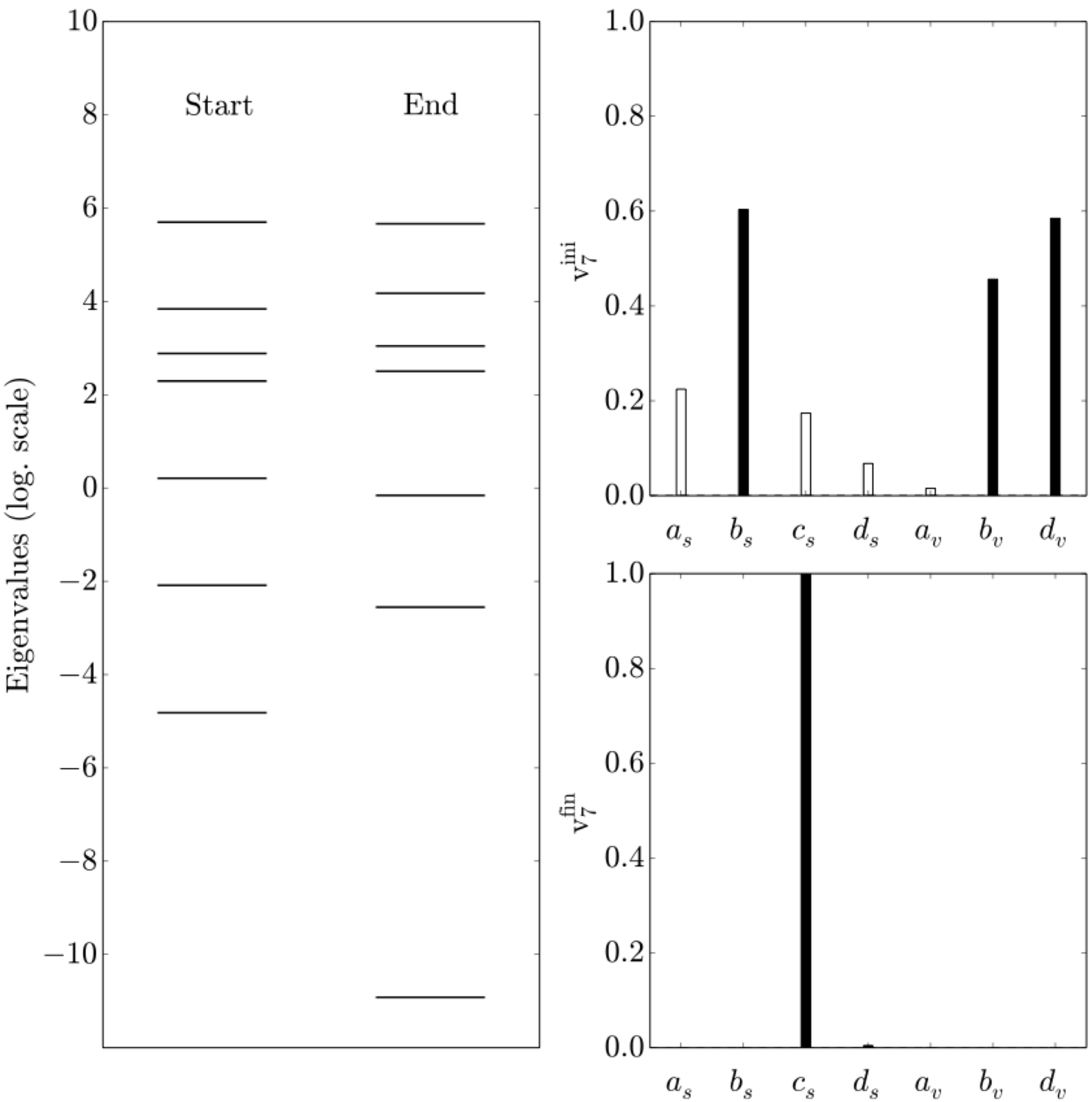
First iteration:

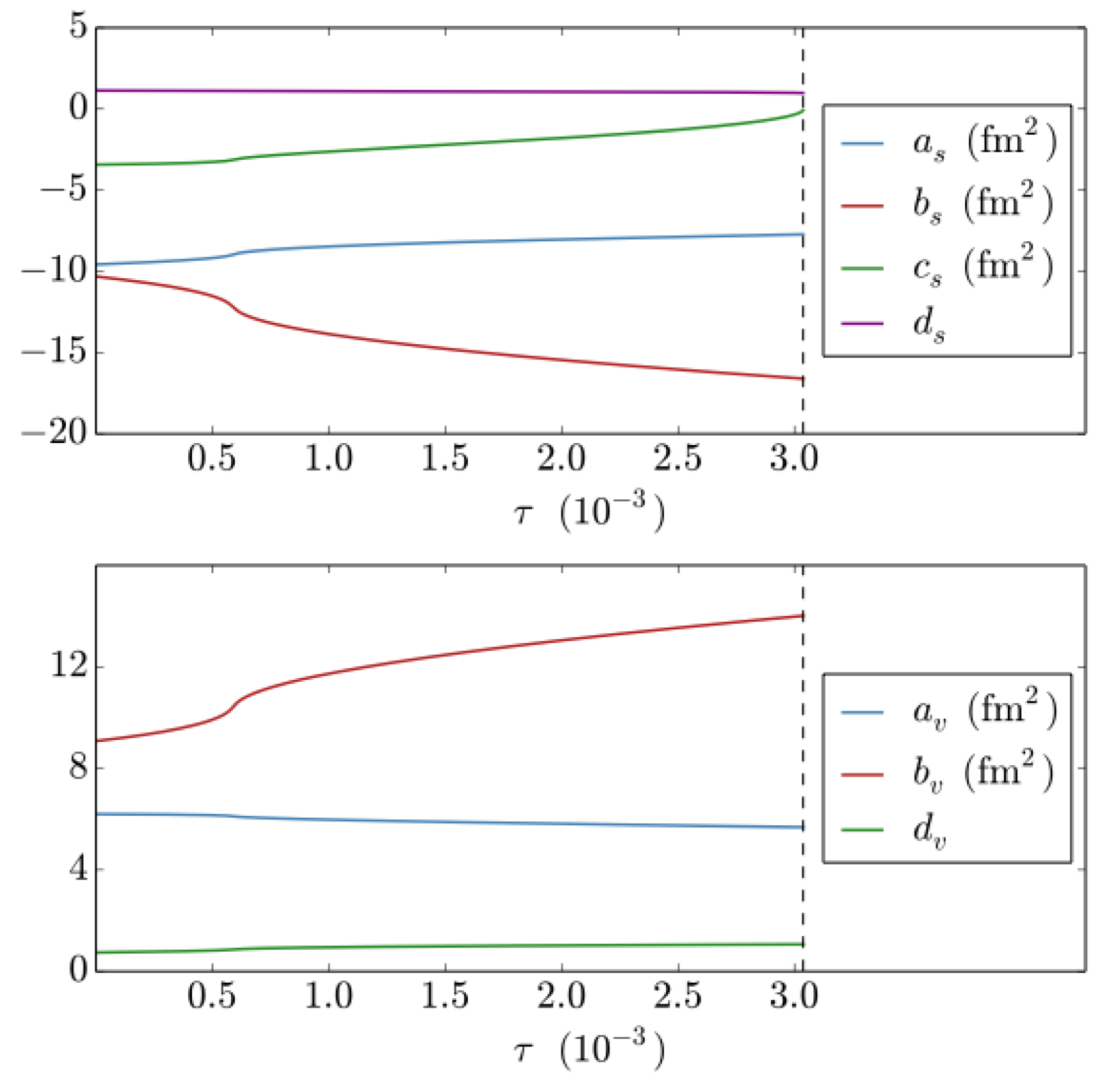
$$\alpha_s(\rho) = a_s + (b_s + c_s x)e^{-d_s x}$$
$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$

$$c_s \longrightarrow 0$$

$$\alpha_s(\rho_v) = a_s + b_s e^{-d_s x}$$

The initial (best-fit point) and final (at the boundary of the model manifold) eigenspectrum of the FIM, and the initial and final eigenvectors that correspond to the smallest eigenvalues.

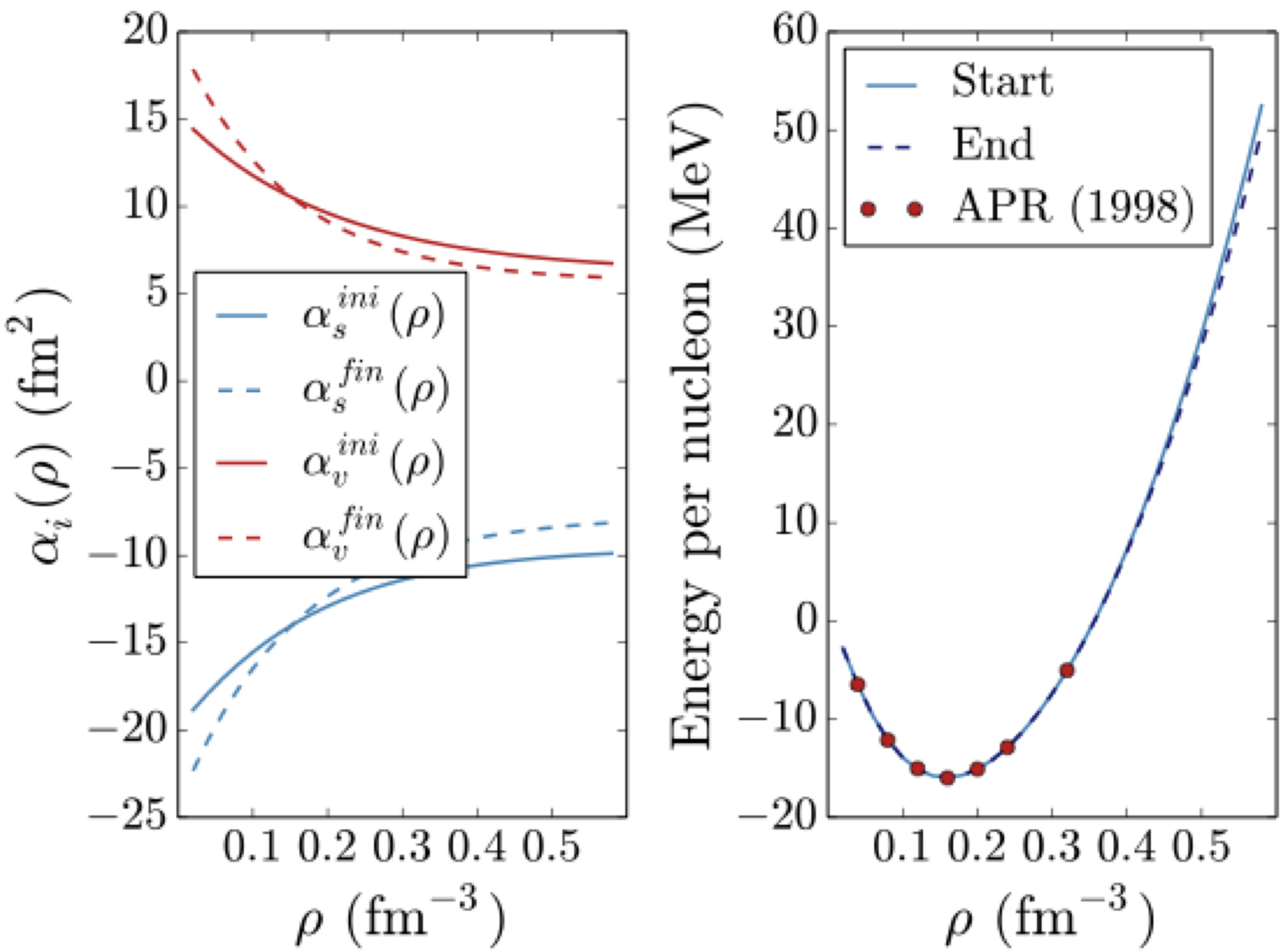




Evolution of the seven parameters of the isoscalar part of the functional defined as functions of the affine parametrisation, along the geodesic path determined by the eigenvector of the Hessian matrix that corresponds to the smallest eigenvalue.

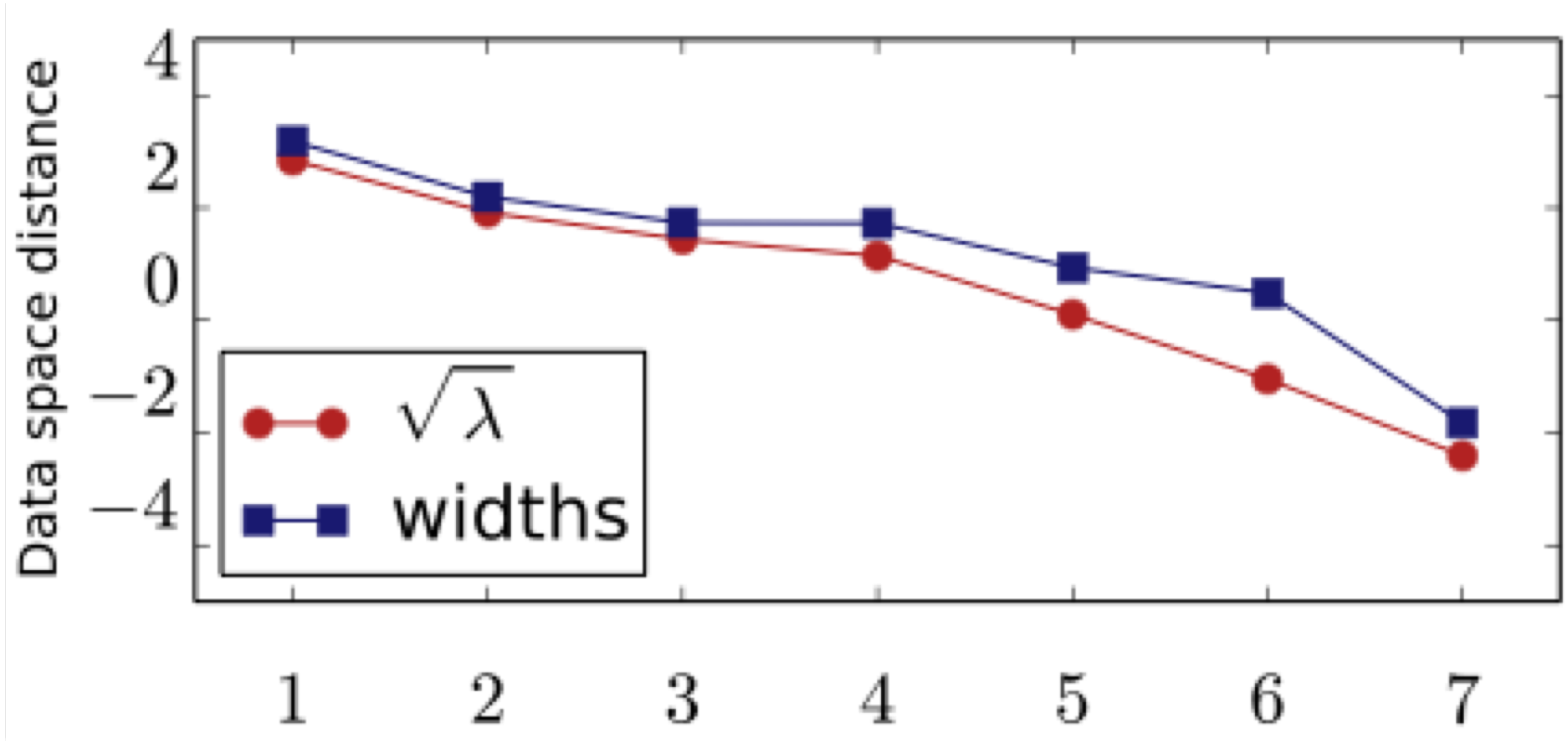
Phys. Rev. C 95, 054304 (2017)
Phys. Rev. C 94, 024333 (2016)

The initial (best-fit point) and final (at the boundary of the model manifold) density-dependent isoscalar coupling functions, and the corresponding initial and final EoS curves.



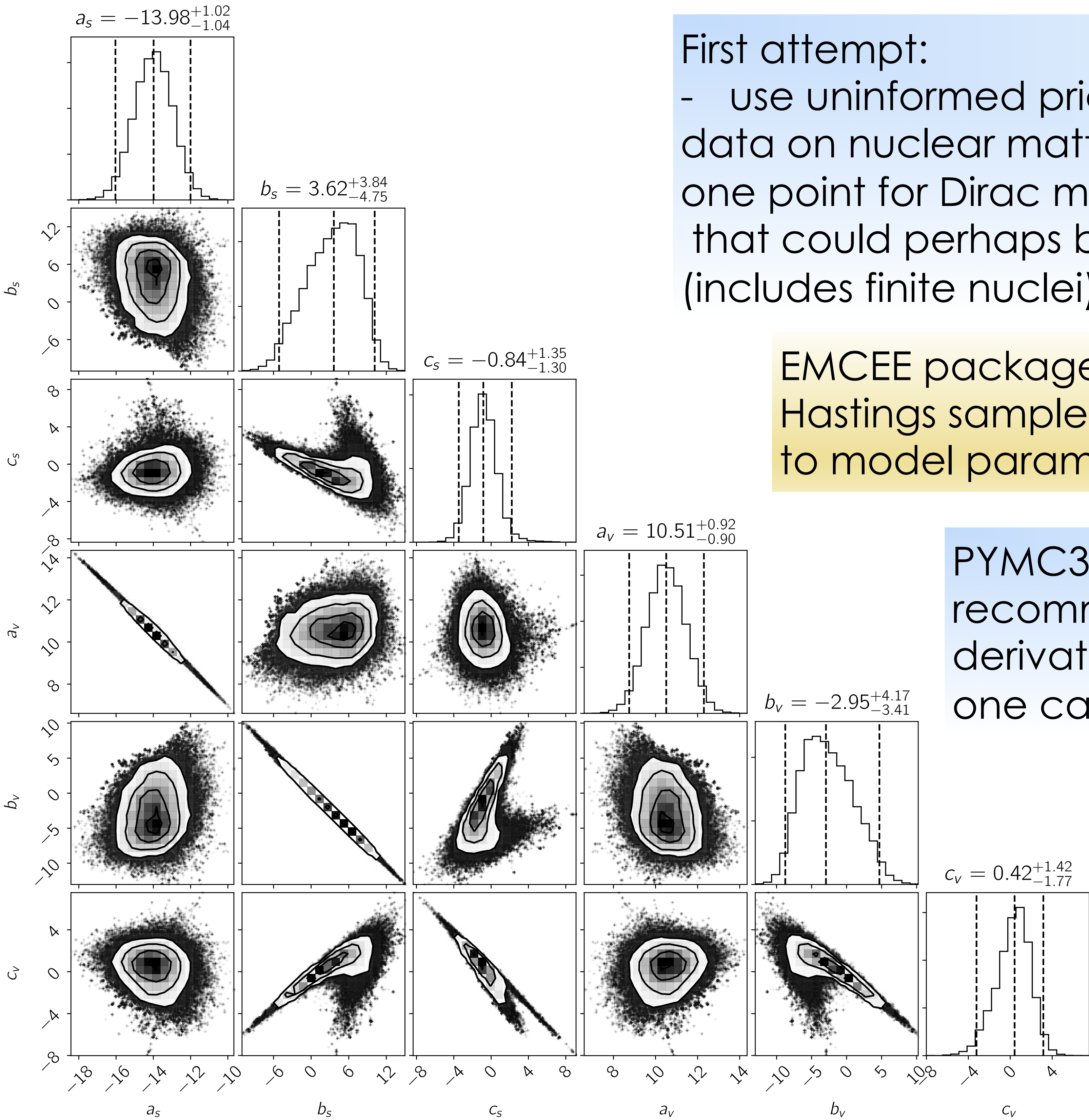
Phys. Rev. C 95, 054304 (2017)
Phys. Rev. C 94, 024333 (2016)

Widths of the model manifold of the EDF in the directions of the eigenvectors of the Hessian matrix at $\mathbf{p}_0$, compared to the square-roots of the corresponding eigenvalues.



The widths of sloppy model manifolds are exponentially distributed ➔ hyperribbon.

Bayesian parameter estimation - preliminary calculations



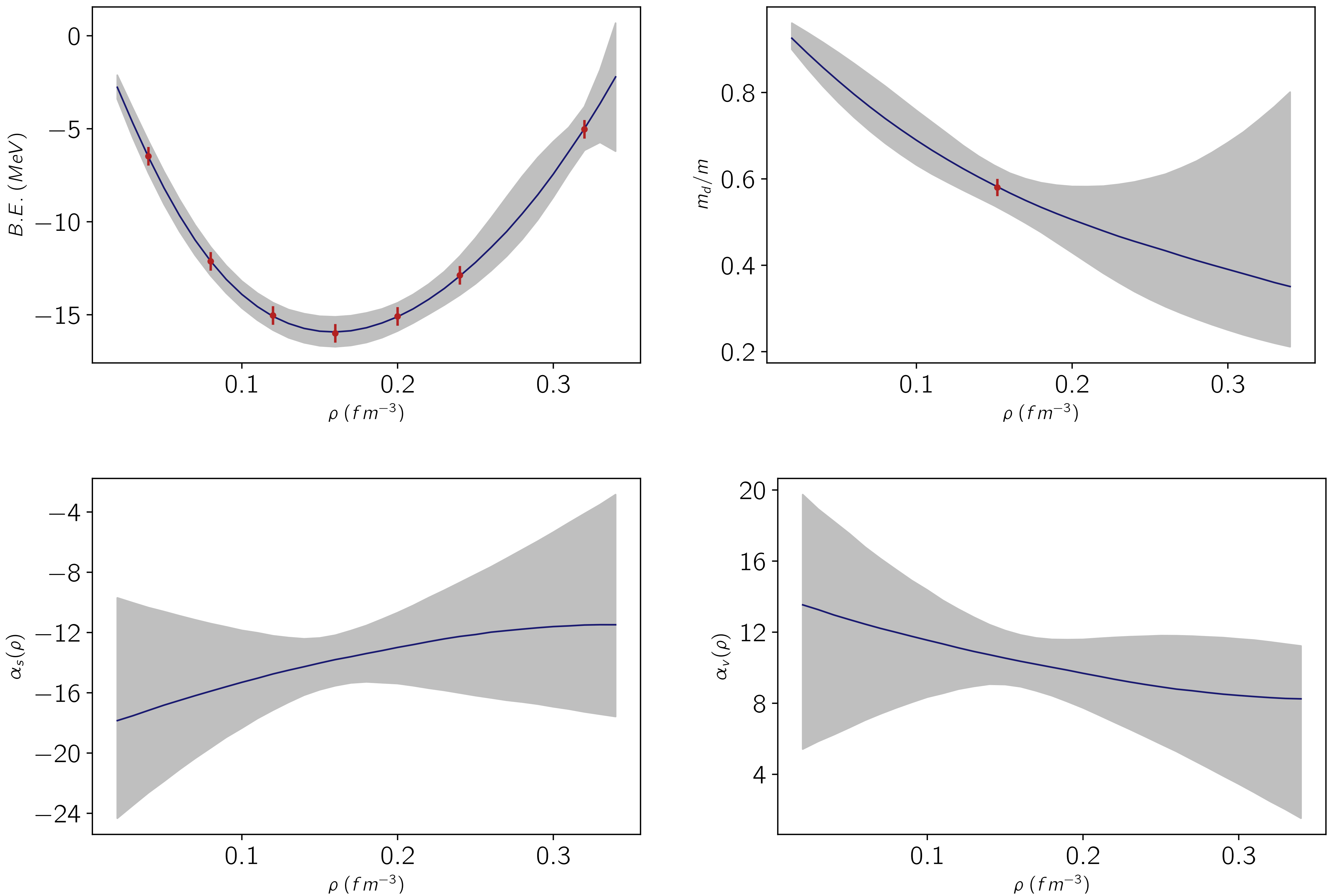
First attempt:
- use uninformed priors for model parameters and data on nuclear matter (several points for B.E. and one point for Dirac mass) to obtain posterior distributions that could perhaps be used as priors in the next step (includes finite nuclei)

EMCEE package: MCMC with Metropolis-Hastings sampler – no derivatives with respect to model parameters required

PYMC3 package: NUTS sampler recommended for continuous variables - derivatives are required (again, if possible one can use automatic differentiation)

Finite nuclei: computationally expensive model → emulators

Bayesian parameter estimation - preliminary calculations



Summary and outlook

Sloppy models: complex models that can be adjusted to data but are only sensitive to a few stiff parameter combinations, while displaying an exponential decrease of sensitivity to variations of soft parameter combinations.

The exponential distribution of model manifold widths in the directions of the eigen-vectors of the Hessian is nearly identical to the distribution of the square roots of the corresponding eigenvalues (sensitivity).

The Manifold Boundary Approximation Method (MBAM) can be used to remove the irrelevant parameters and construct a simpler, non-sloppy functional of lower dimension.

Technical point: MBAM is particularly suitable when implemented together with the automatic differentiation packages (although finite differences are also acceptable in practice)

Next step: a Bayesian approach for NEDF parameter estimation

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For more information please visit:
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https://strukturnifondovi.hr/

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