Sloppy Nuclear Energy Density Functionals: effective model optimisation

T. Nikšić and D. Vretenar

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 chart of nuclides.

Kohn-Sham DFT

For any interacting system, there exists a local single-particle (Kohn-Sham) potential, such that the exact ground-state density equals the ground-state density of a non-interacting system:

$$n(\mathbf{r}) = n_s(\mathbf{r}) \equiv \sum_{i}^{occ} |\phi_i(\mathbf{r})|^2$$

The single-particle orbitals are solutions of the Kohn-Sham equations:

$$\left[-\nabla^2/2 + v_s(\mathbf{r})\right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

⇒ local Kohn-Sham potential:

$$v_s[n(\mathbf{r})] = v_{ext}(\mathbf{r}) + v_{\mathrm{Hartree}}[n(\mathbf{r})] + v_{xc}[n(\mathbf{r})]$$

…the ***exchange-correlation potential*** is defined by:

$$v_{xc}[n(\mathbf{r})] = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}$$

self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the Hartree-Fock. It has the advantage of being a ***local scheme***.

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{XC} can be found!

Microscopic NEDFs

... universal exchange-correlation functional $E_{xc}[\varrho]$ from a microscopic many-body calculation of the nuclear matter EoS.

1st step: Local Density Approximation

$$E_{xc}^{LDA} \equiv \int \varepsilon^{micro}[\rho(\mathbf{r})]\rho(\mathbf{r})d^3r$$

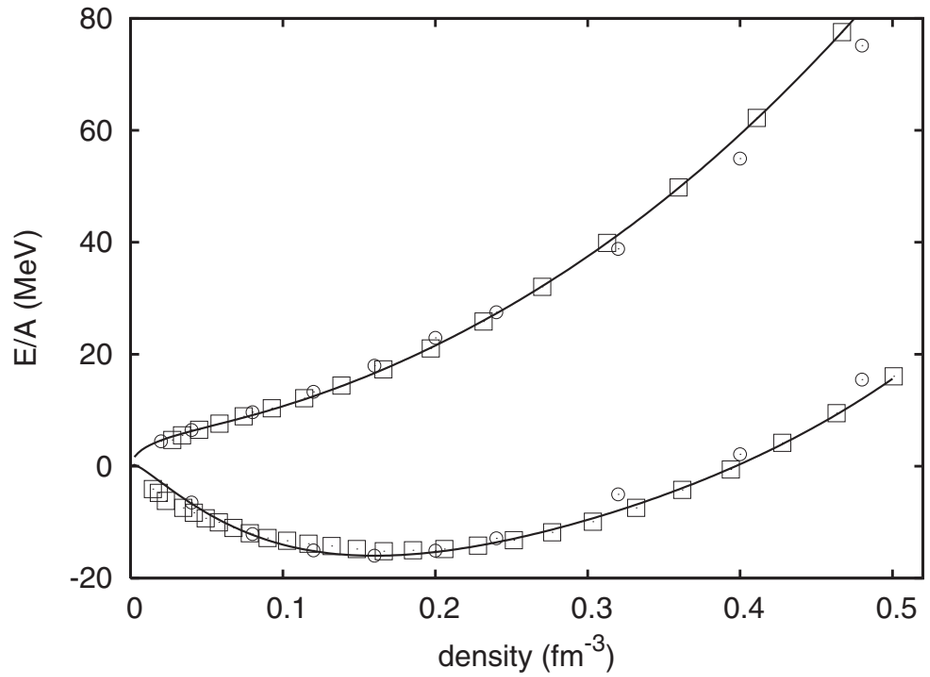
2nd step: second-order gradient correction to the LDA

Microscopic calculations for inhomogeneous nuclear matter ⇒ $E_{xc}^{GGA}[\rho, \nabla\rho]$

… ladder of higher order approximations → functionals of τ, $\Delta\varrho$, explicit exchange, …

Semi-phenomenological functionals

M. BALDO, L. M. ROBLEDO, P. SCHUCK, AND X. VIÑAS



$$E^{\infty}_{\text{int}}[\rho_p, \rho_n] = \int d^3r \left[P_s(\rho)\left(1-\beta^2\right) + P_n(\rho)\beta^2\right]\rho$$

$$\beta = (\rho_n - \rho_p)/\rho$$

$$P_s(\rho) = \sum_{n=1}^{5} a_n \left(\frac{\rho}{\rho_0}\right)^n, \qquad P_n(\rho) = \sum_{n=1}^{5} b_n \left(\frac{\rho}{\rho_{0n}}\right)^n$$

PHYSICAL REVIEW C **87**, 064305 (2013)

Aurel Bulgac, Michael McNeil Forbes, Shi Jin

arXiv:1506.09195

$$\mathscr{E}_{\text{int}}(\rho_n,\rho_p) = (\eta - \tfrac{1}{9}) \sum_{\tau=n,p} \frac{\hbar^2}{2m_\tau} \left|\boldsymbol{\nabla}\rho_\tau^{1/2}\right|^2$$

$$+ \sum_{j=0}^{2} \mathscr{E}_j(\rho)\beta^{2j} + \mathscr{E}_{\text{entrain}}(\rho_n,\rho_p),$$

$$\mathscr{E}_j(\rho) = a_j\rho^{5/3} + b_j\rho^2 + c_j\rho^{7/3},$$

$$\rho = \rho_n + \rho_p, \qquad \beta = \frac{\rho_n - \rho_p}{\rho_n + \rho_p}.$$

Semi-phenomenological functionals

S. Typel and H. H. Wolter, Nucl. Phys. **A656**

$$g_i(\rho) = g_i(\rho_{\rm sat}) f_i(x) \quad \text{for} \quad i = \sigma, \omega, \qquad f_i(x) = a_i \frac{1 + b_i(x + d_i)^2}{1 + c_i(x + d_i)^2} \qquad x = \rho/\rho_{\rm sat}$$

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

P. Finelli et al. / Nuclear Physics A 770 (2006) 1–31

$$G_i(\hat{\rho}) = G_i^{(0)} + G_i^{(\pi)}(\hat{\rho}) \qquad (\text{for } i = \text{S, V}),$$
$$G_i(\hat{\rho}) = G_i^{(\pi)}(\hat{\rho}) \qquad (\text{for } i = \text{TS, TV}),$$

$$G_i^{(\pi)}(\rho) = c_{i1} + c_{i2}\rho^{1/3} + c_{i3}\rho^{2/3} + c_{i4}\rho + \cdots \qquad (i = \text{S, V, TS, TV}).$$

$$\mathcal{E}(\rho, \boldsymbol{\nabla}\rho) = \rho \bar{E}(k_f) + (\boldsymbol{\nabla}\rho)^2 F_\nabla(k_f) + \cdots.$$

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.

⇒ effective Lagrangian:

$$
\begin{aligned}
\mathcal{L} \quad = \quad & \bar{\psi}(i\gamma\cdot\partial - m)\psi \\
& -\frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\
& -\frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\
& -\frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma\cdot A\frac{(1-\tau_3)}{2}\psi
\end{aligned}
$$

$$
\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} \quad (i \equiv S, V, TV) \quad x = \rho/\rho_{sat}
$$

Hartree

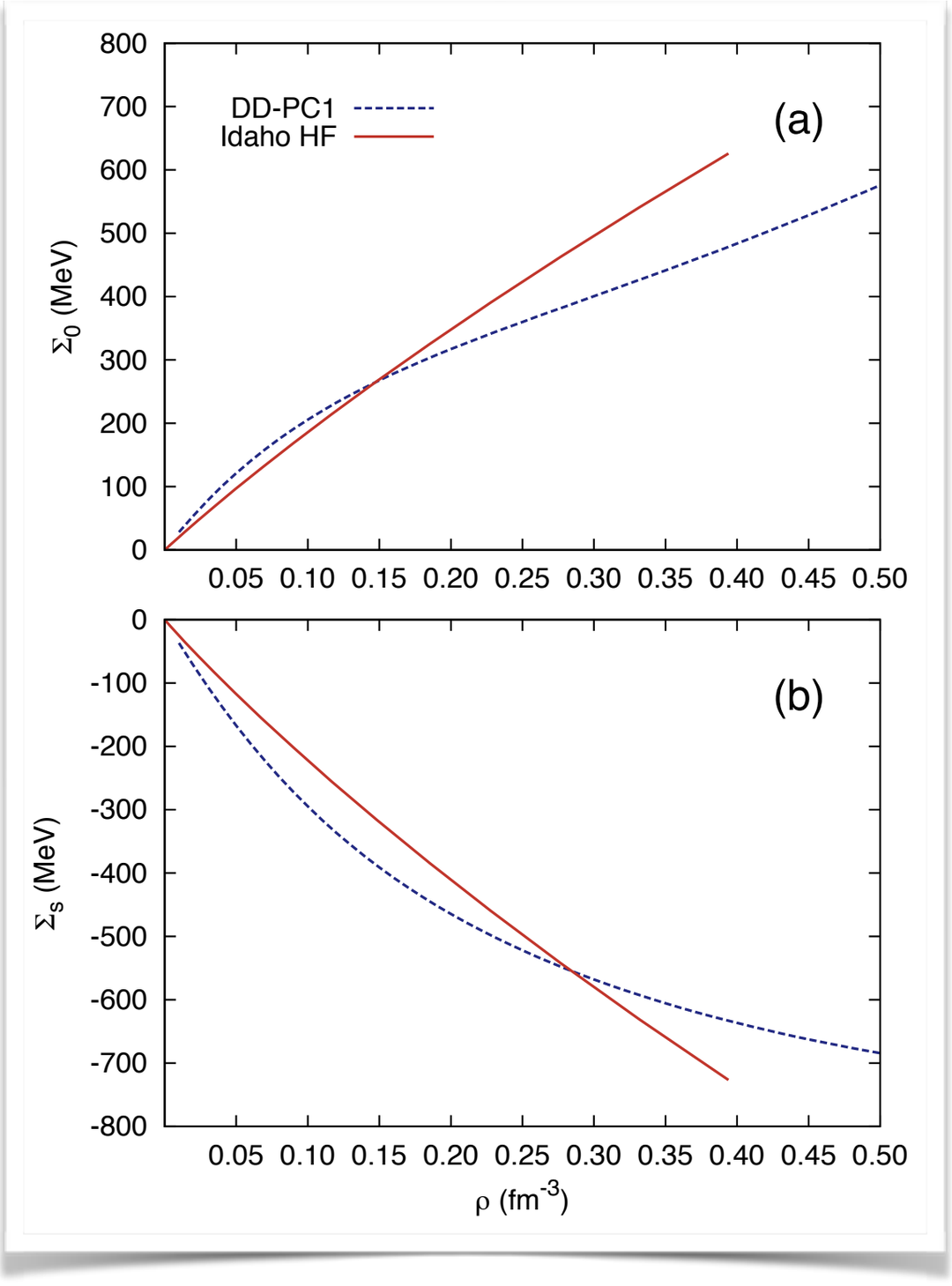
correlations

DD-PC1

... starts from microscopic nucleon self-energies in nuclear matter.

... parameters adjusted in self-consistent mean-field calculations of masses of *64* axially deformed nuclei in the mass regions A ~ 150-180 and A ~ 230-250.

Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter.



… energy density functional DD-PC1⇒ is it "predictive" ? Agreement with experiment?
… functional form of the density dependence ⇒ is it "sloppy"? Large parameter uncertainties when fit to data?

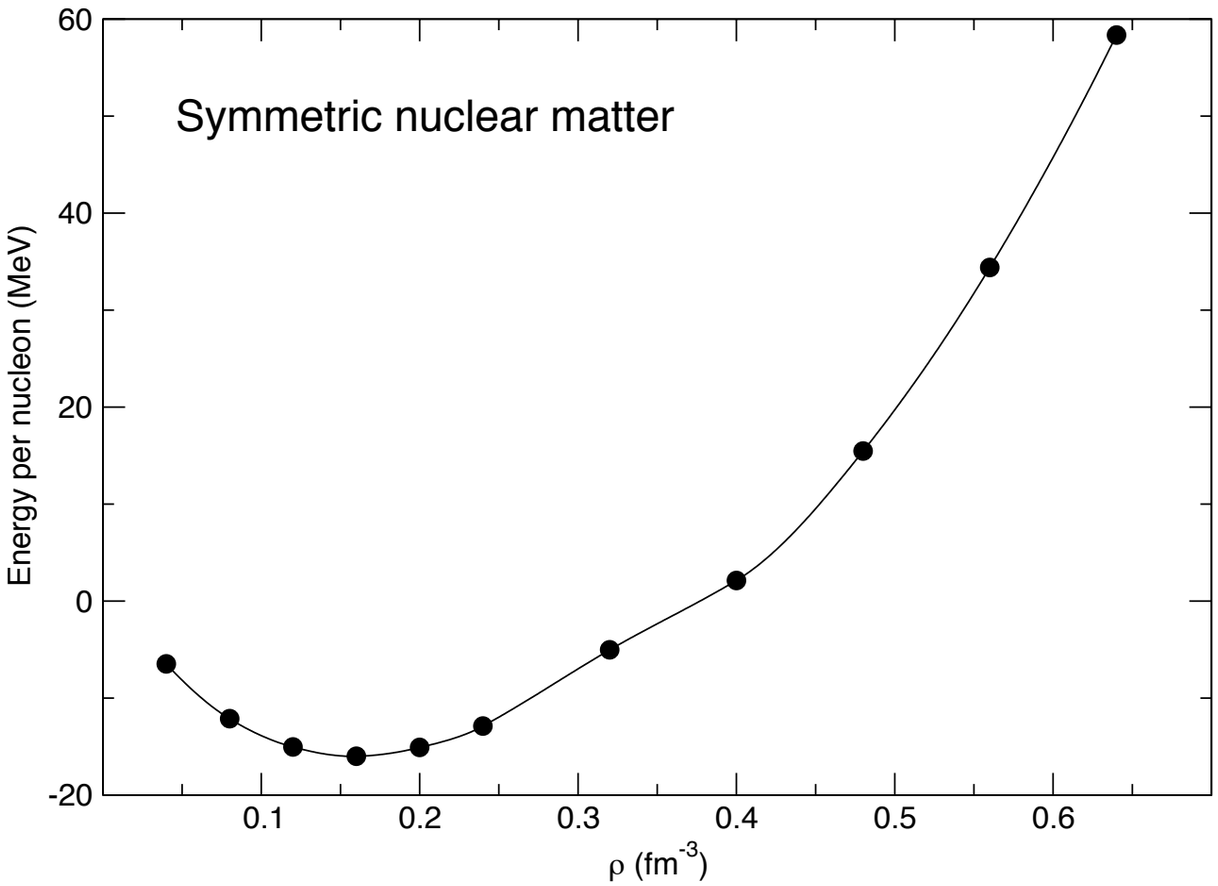
$$\alpha_s(\rho) = a_s + (b_s + c_s x)e^{-d_s x}$$
$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$
$$\alpha_{tv}(\rho) = b_{tv} e^{-d_{tv} x}$$

$$x = \rho/\rho_{\rm sat}$$

PARAMETER	
a_s (fm^2)	-10.0462
b_s (fm^2)	-9.1504
c_s (fm^2)	-6.4273
d_s	1.3724
a_v (fm^2)	5.9195
b_v (fm^2)	8.8637
d_v	0.6584
b_{tv} (fm^2)	1.8360
d_{tv}	0.6403
δ_s (fm^4)	-0.8149

Can the parameters of such a density functional form be determined by a microscopic nuclear matter EoS?

Symmetric nuclear matter EoS: Akmal, Pandharipande & Ravenhall, Phys. Rev. C 58



Density dependence of the couplings:

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

$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$

PSEUDO-OBSERVABLE	
$\epsilon(0.04\ fm^{-3})$	-6.48 MeV
$\epsilon(0.08\ fm^{-3})$	-12.43 MeV
$\epsilon(0.12\ fm^{-3})$	-15.43 MeV
$\epsilon(0.16\ fm^{-3})$	-16.03 MeV
$\epsilon(0.20\ fm^{-3})$	-14.99MeV
$\epsilon(0.24\ fm^{-3})$	-12.88 MeV
$\epsilon(0.32\ fm^{-3})$	-6.49 MeV
$M_D(0.152\ fm^{-3})$	0.58 m

Dirac mass

$$M_D = m_N + \alpha_s(p_1, \ldots, p_n; \rho_B)\rho_s$$

Least-squares fit to the pseudo-data:

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

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

$$\chi^2(\mathbf{p}) = \sum_{n=1}^{N} r_n(\mathbf{p})^2 \qquad \text{➟ the residuals:} \qquad r_n(\mathbf{p}) = \frac{\mathcal{O}_n^{(mod)}(\mathbf{p}) - \mathcal{O}_n}{\Delta\mathcal{O}_n}$$

➟ 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:

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

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

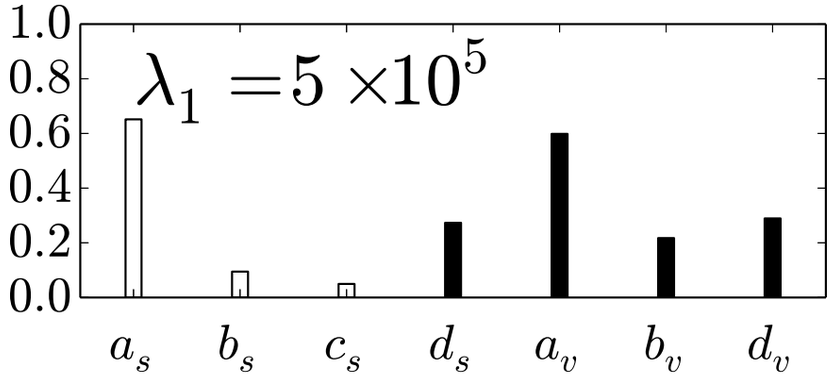
The symmetric Hessian matrix of second derivatives: $$\mathcal{M}_{\mu\nu} = \left.\frac{\partial^2 \chi^2}{\partial p_\mu \partial p_\nu}\right|_{\mathbf{p}=\mathbf{p}_0}$$

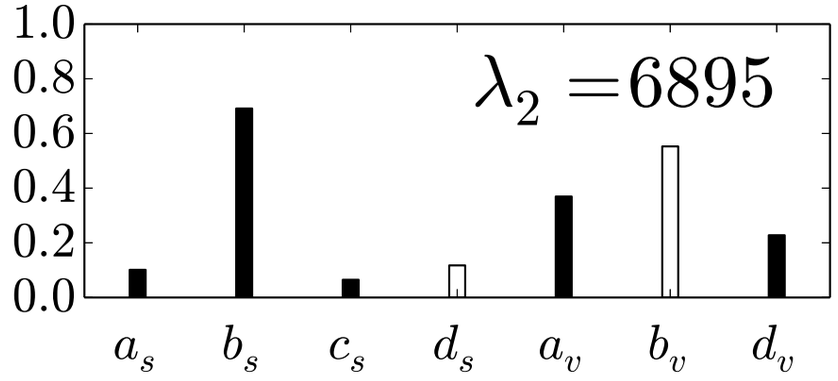
Diagonalization $\Rightarrow$ $$\Delta\chi^2(\mathbf{p}) = \frac{1}{2}\Delta\mathbf{p}^T\left(\mathcal{A}\mathcal{D}\mathcal{A}^T\right)\Delta\mathbf{p} = \frac{1}{2}\xi^T\mathcal{D}\xi = \frac{1}{2}\sum_{\alpha=1}^{F}\lambda_\alpha\xi_\alpha^2$$

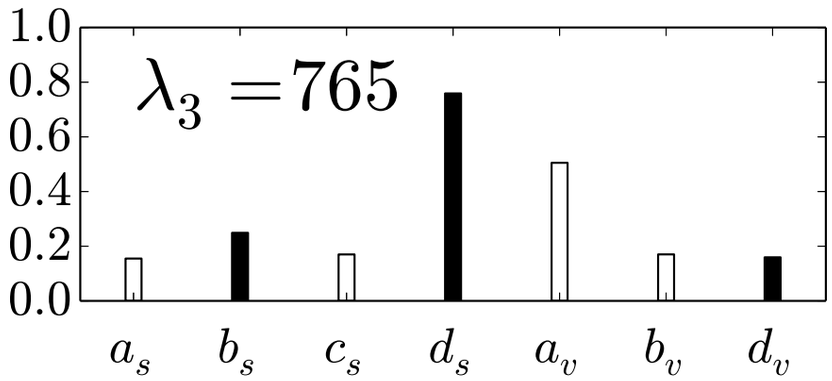
Stiff direction $\Longrightarrow$ large eigenvalue λ, χ^2 rapidly worsens away from minimum, the fit places a stringent constraint on this particular linear combination of parameters.

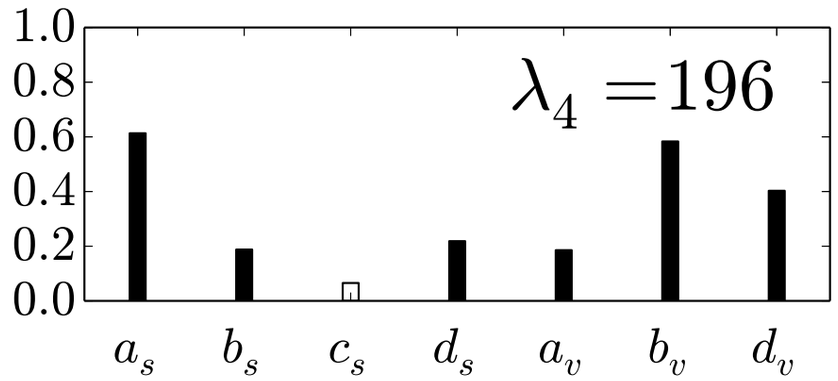
Soft direction $\Longrightarrow$ small eigenvalue λ, little deterioration in χ^2. The corresponding eigenvector ξ involves a particular linear combination of model parameters that is not constrained by the observables included in the fit.

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

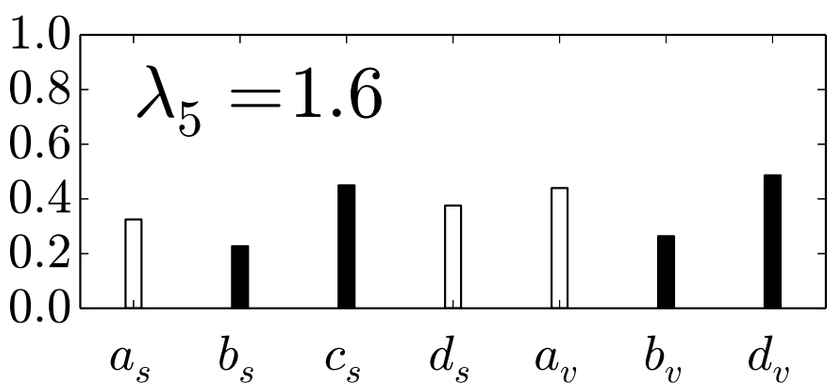


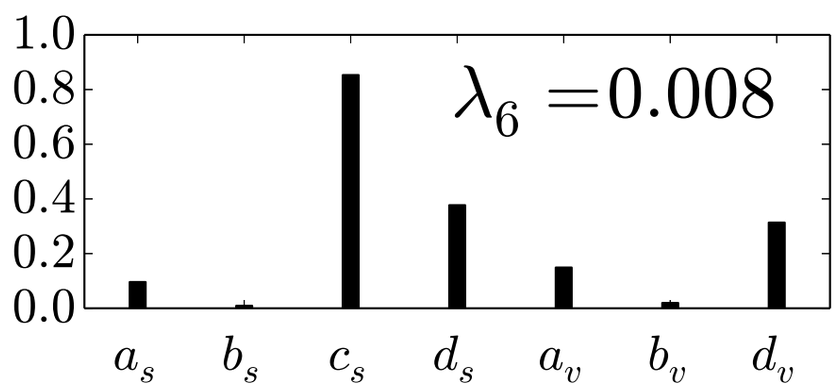


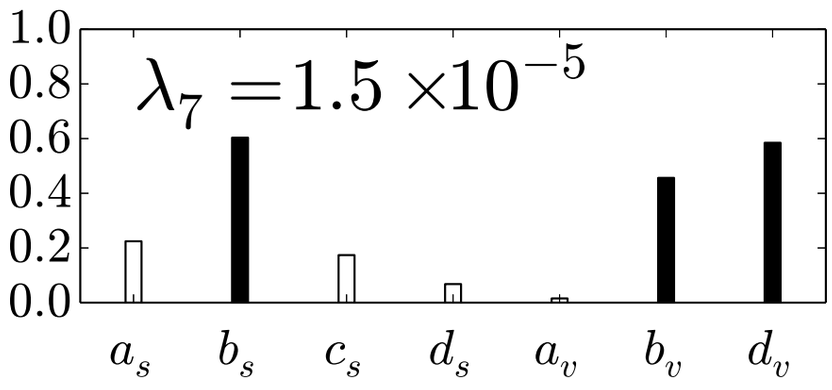




Eigenvectors and eigenvalues of the Hessian matrix $\mathcal{M}$ of second derivatives of $\chi^2(p)$ ➟







The empty and filled bars indicate that 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!

Model parameters define an F-dimensional Riemann manifold embedded in the N-dimensional data space (Euclidian metric for the data space):

$$dr^2 = \sum_m {dr_m}^2$$

The Jacobian matrix that relates changes in the parameters **p** to changes in the residuals:

$$dr_m = \sum_\mu \frac{\partial r_m}{\partial p_\mu} dp_\mu = \sum_\mu J_{m\mu} dp_\mu$$

$$dr^2 = \sum dr_m^2 = \sum (J^T J)_{\mu\nu} dp_\mu dp_\nu = \sum g_{\mu\nu} dp_\mu dp_\nu$$

The Euclidean metric of data space induces a metric on the model manifold $g = J^T J$.

Close to the best-fit point the Hessian matrix can be approximated by the metric tensor:

$$\mathcal{M}_{\mu\nu} = \left.\frac{\partial^2 \chi^2}{\partial p_\mu \partial p_\nu}\right|_{\mathbf{p}=\mathbf{p}_0} = \left.\sum_m \frac{\partial r_m}{\partial p_\mu}\frac{\partial r_m}{\partial p_\nu}\right|_{\mathbf{p}=\mathbf{p}_0} + \left.\sum_m r_m \frac{\partial^2 r_m}{\partial p_\nu^2}\right|_{\mathbf{p}=\mathbf{p}_0}$$

$$\mathcal{M}_{\mu\nu} \approx \left.\sum_m \frac{\partial r_m}{\partial p_\mu}\frac{\partial r_m}{\partial p_\nu}\right|_{\mathbf{p}=\mathbf{p}_0}$$

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:

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

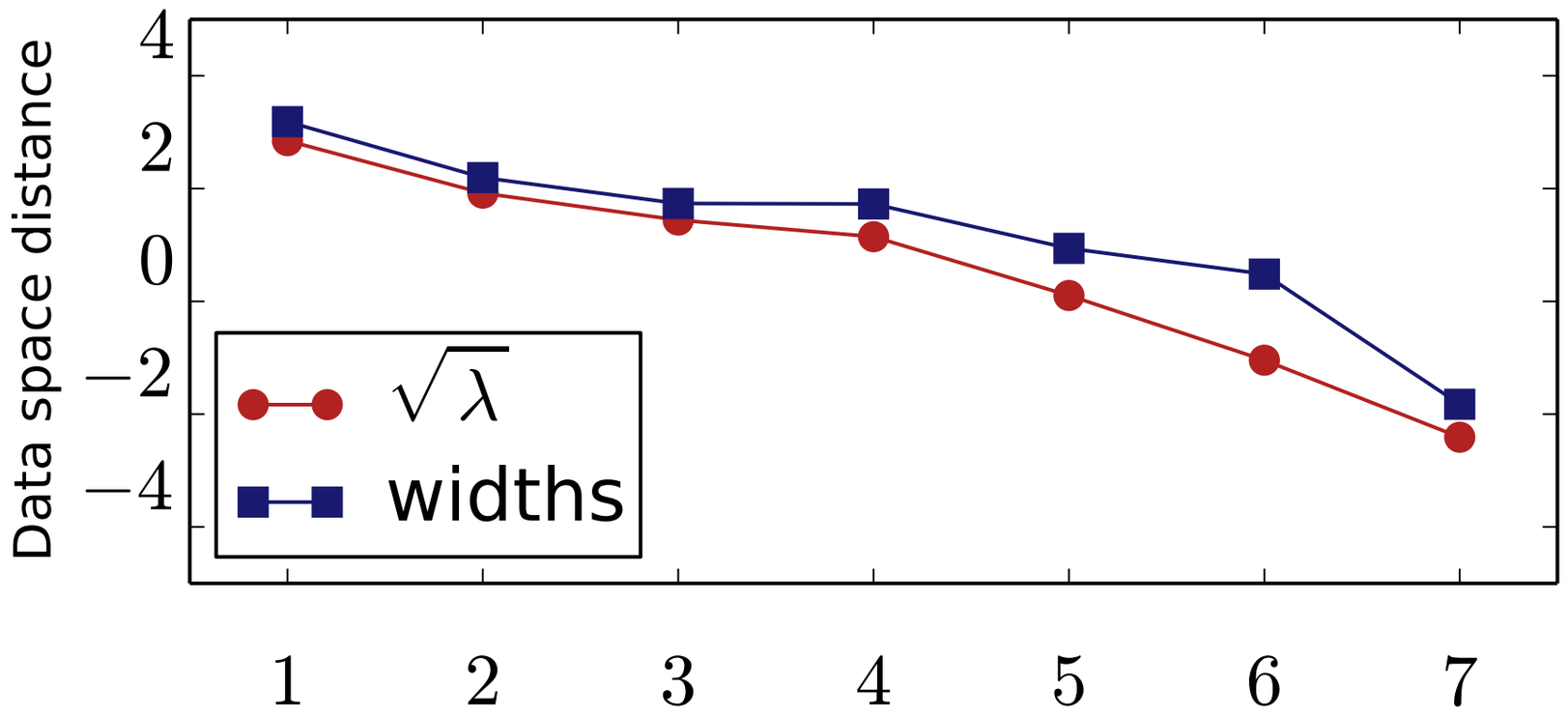
➔ initial value problem in the parameter space.

with the connection coefficients:

$$\Gamma^\alpha_{\mu\nu} = \sum_\beta (g^{-1})_{\alpha\beta} \sum_m \frac{\partial r_m}{\partial p_\beta} \frac{\partial^2 r_m}{\partial p_\mu \partial p_\nu}$$

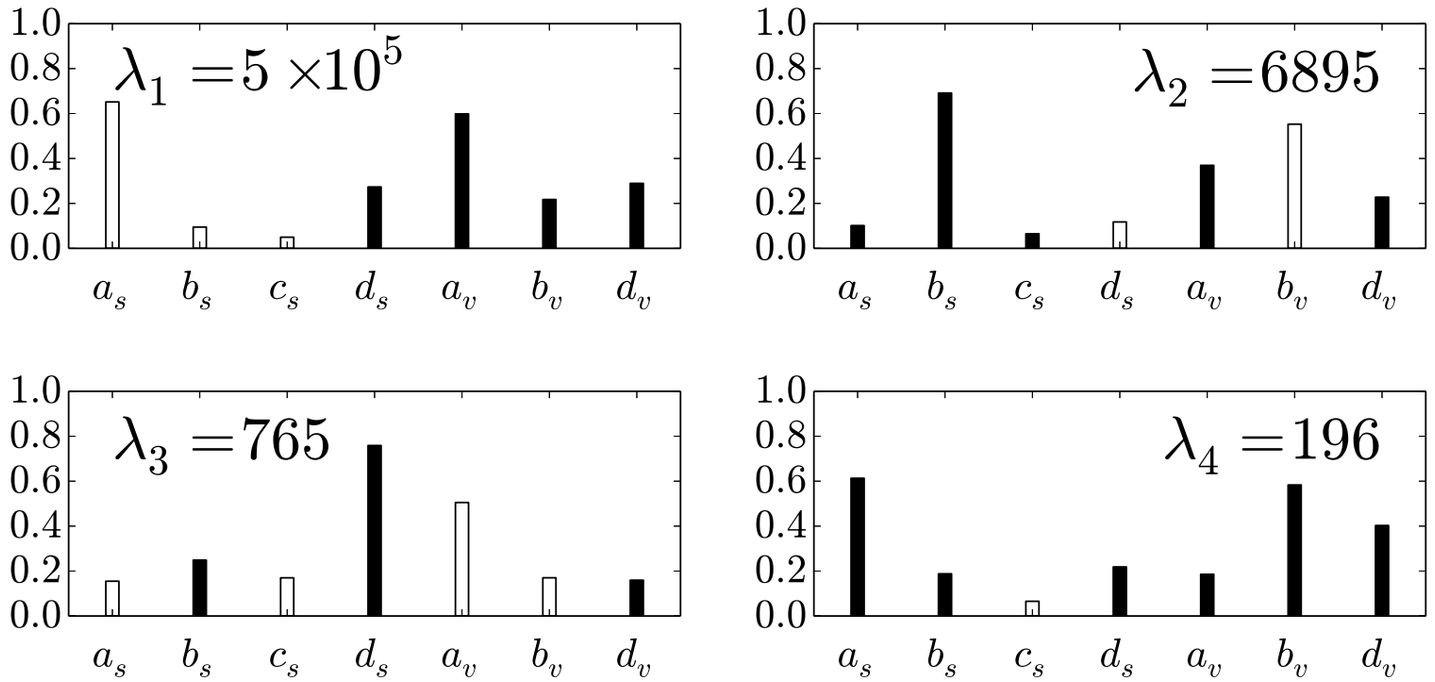
The boundary of the manifold is identified by the metric tensor becoming singular.

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.

The characteristic eigenvalue spectrum of the Hessian and the hierarchy of widths of the model manifold suggest a *lower effective dimensionality* of the model.



How can a simpler effective model of lower dimension be constructed from a sloppy representation of the system?

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.

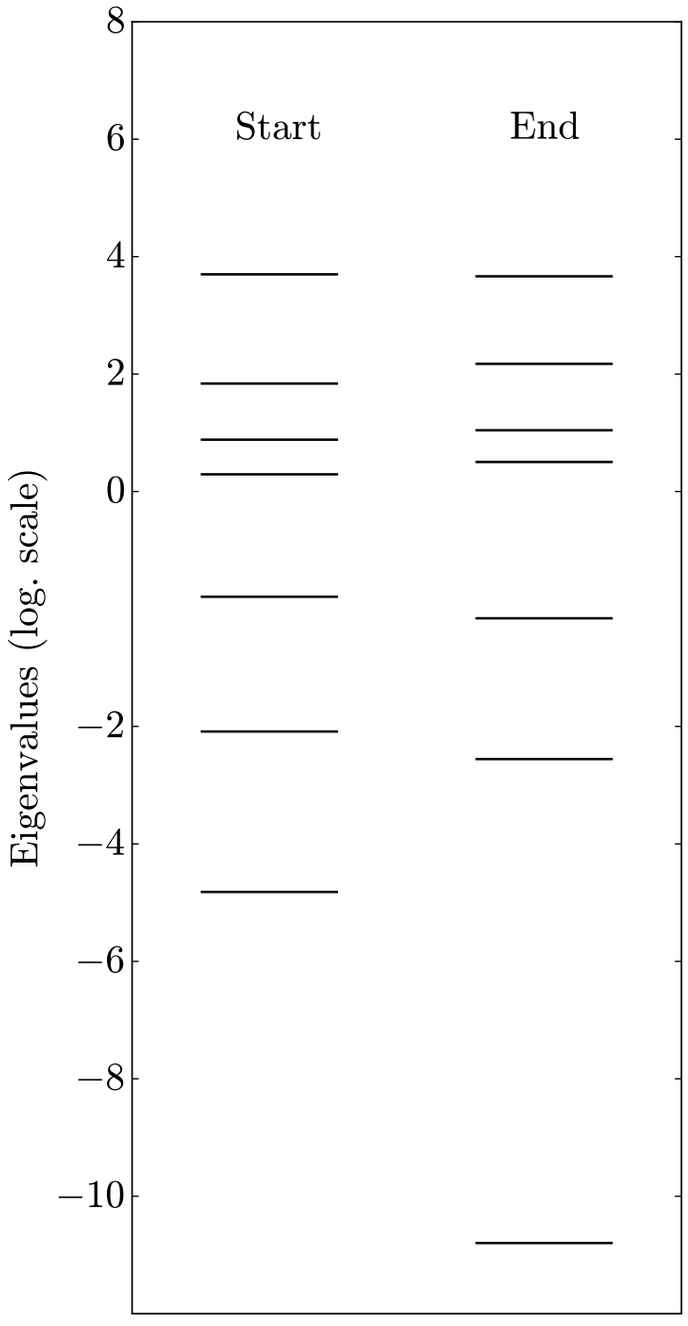
4. Optimise the new model by a least-square fit to the data, and use it as a starting point for the next iteration.

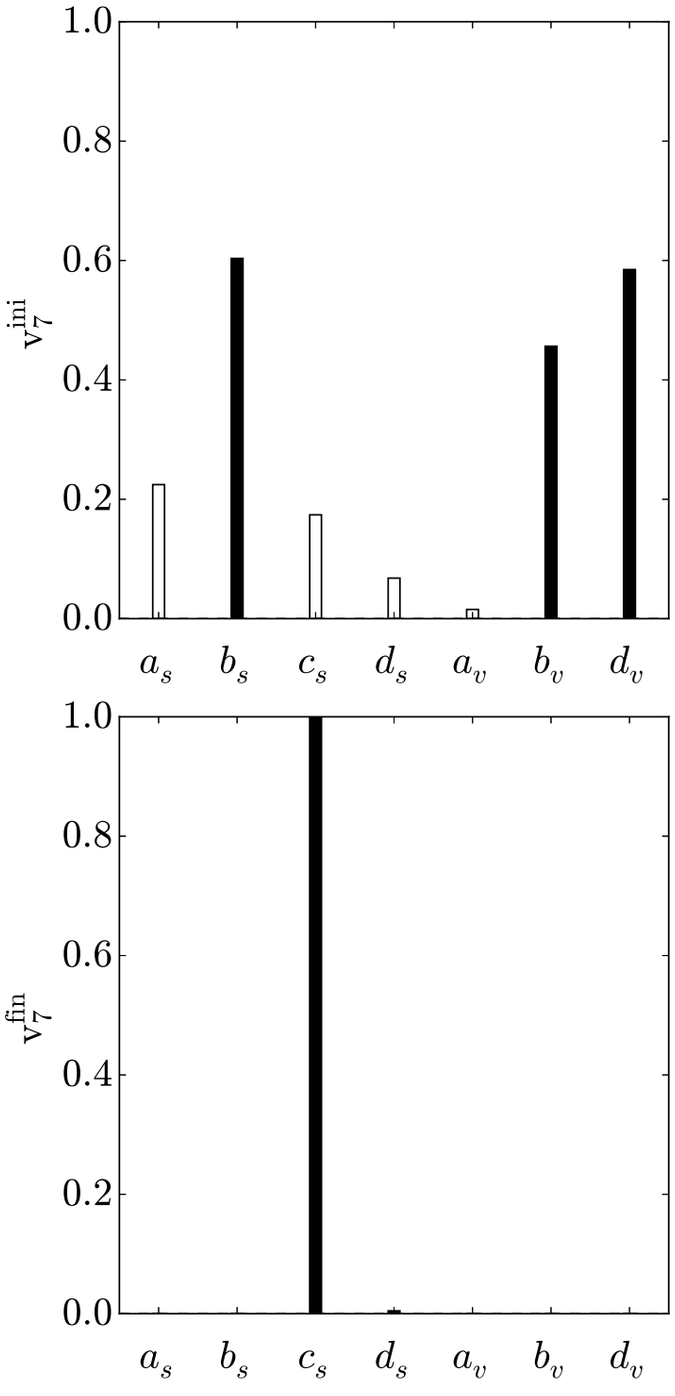
$$\alpha_s(\rho) = a_s + (b_s + c_s x)e^{-d_s x}$$
$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$

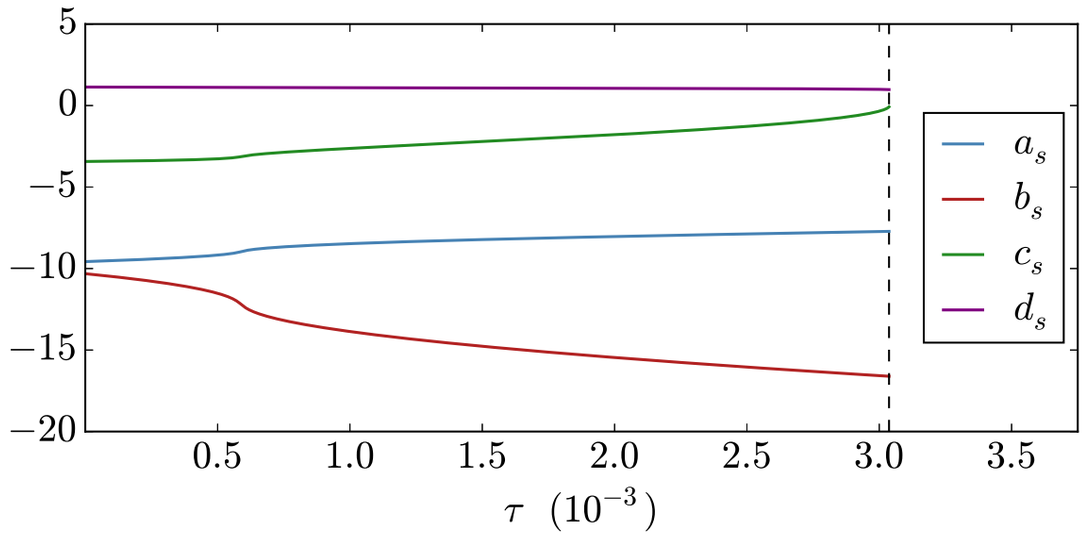
$$\longrightarrow \quad c_s \longrightarrow 0 \quad \longrightarrow$$

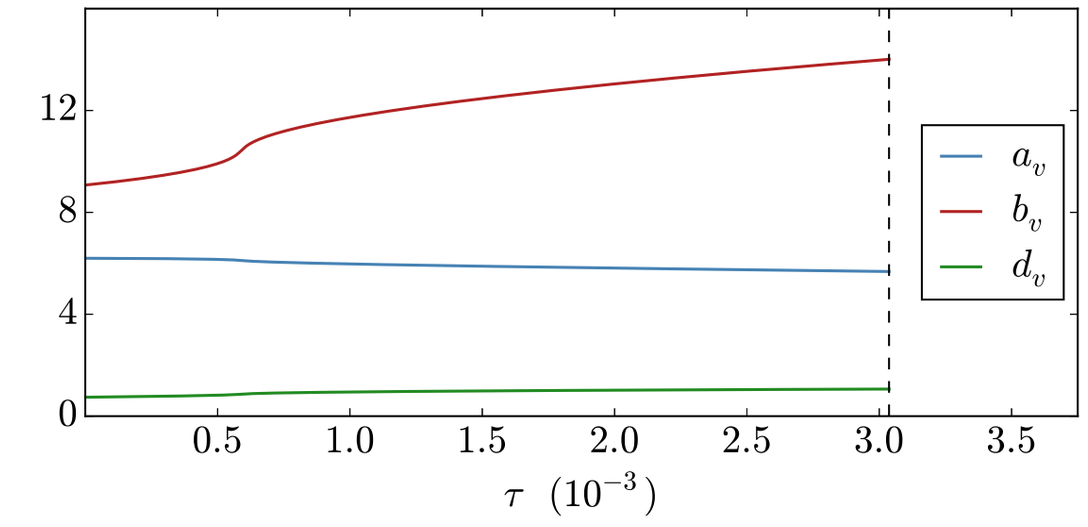
$$\alpha_s(\rho_v) = a_s + b_s e^{-d_s x}$$

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.



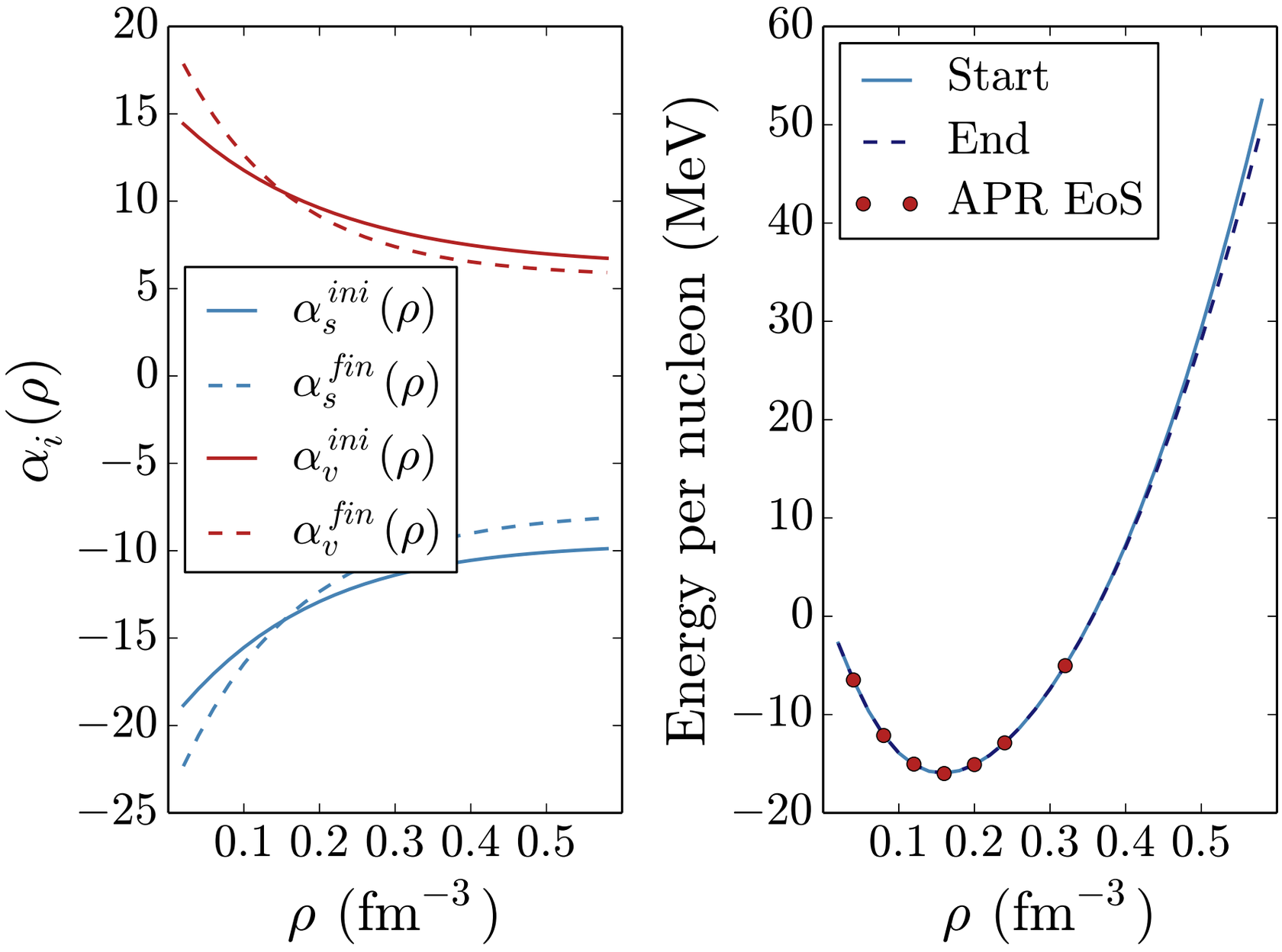






Evolution of the seven parameters of the isoscalar part of the functional defined as functions of the affine parametrisation, along the geodesic path determined by the eigenvector of the Hessian matrix that corresponds to the smallest eigenvalue.

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.



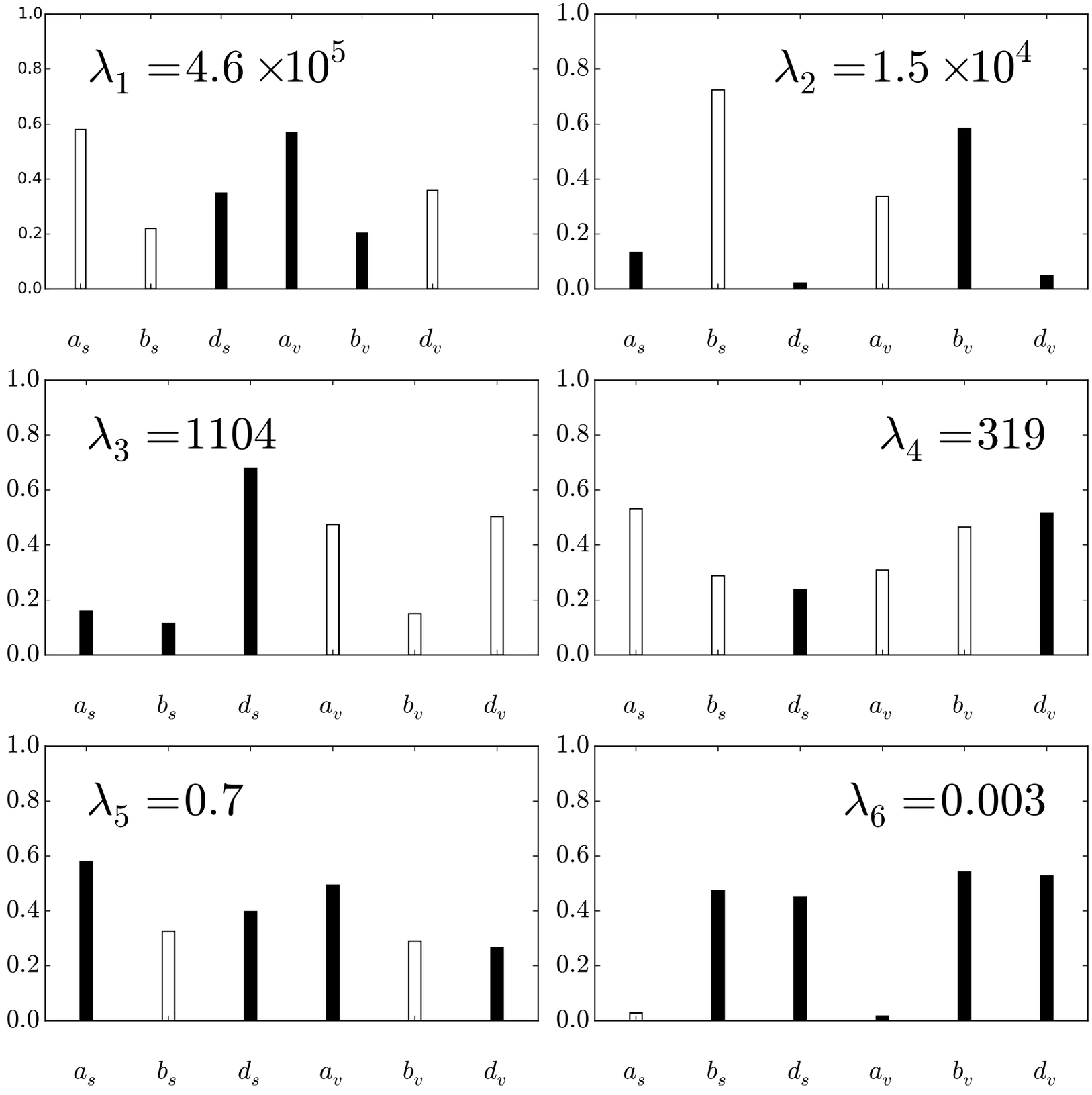
Second iteration:

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

$$\alpha_v(\rho_v) = a_v + b_v e^{-d_v x}$$

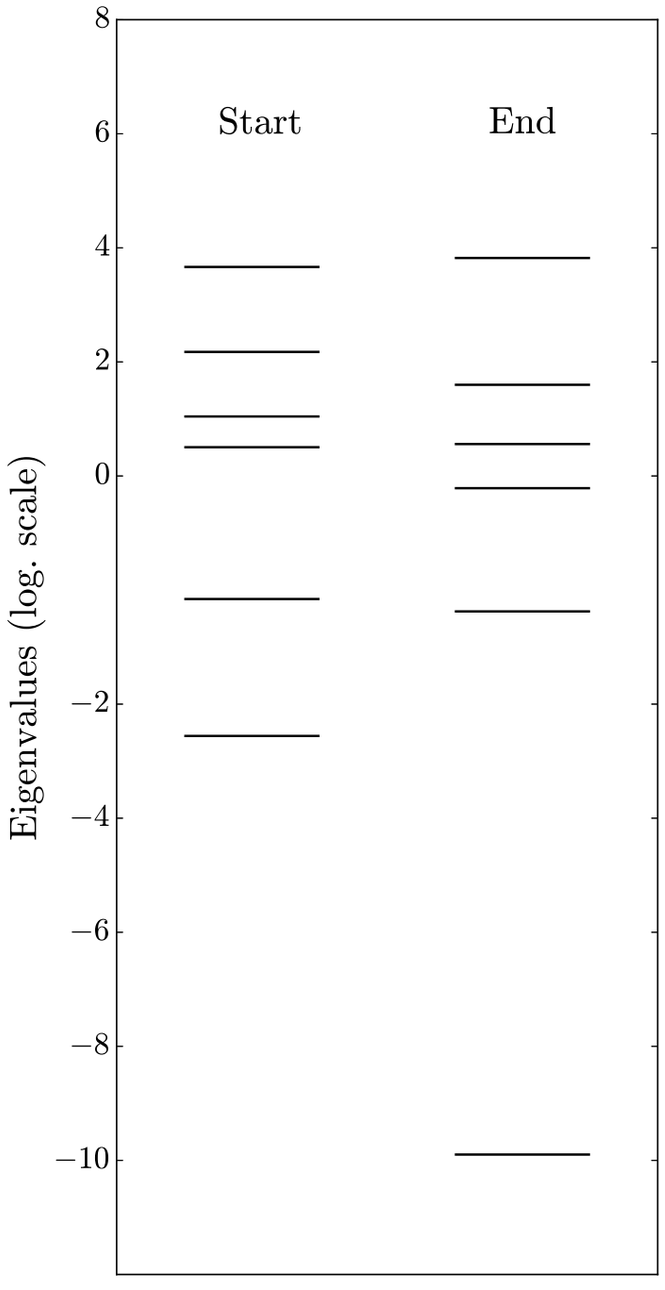
The parameters are refitted to data!

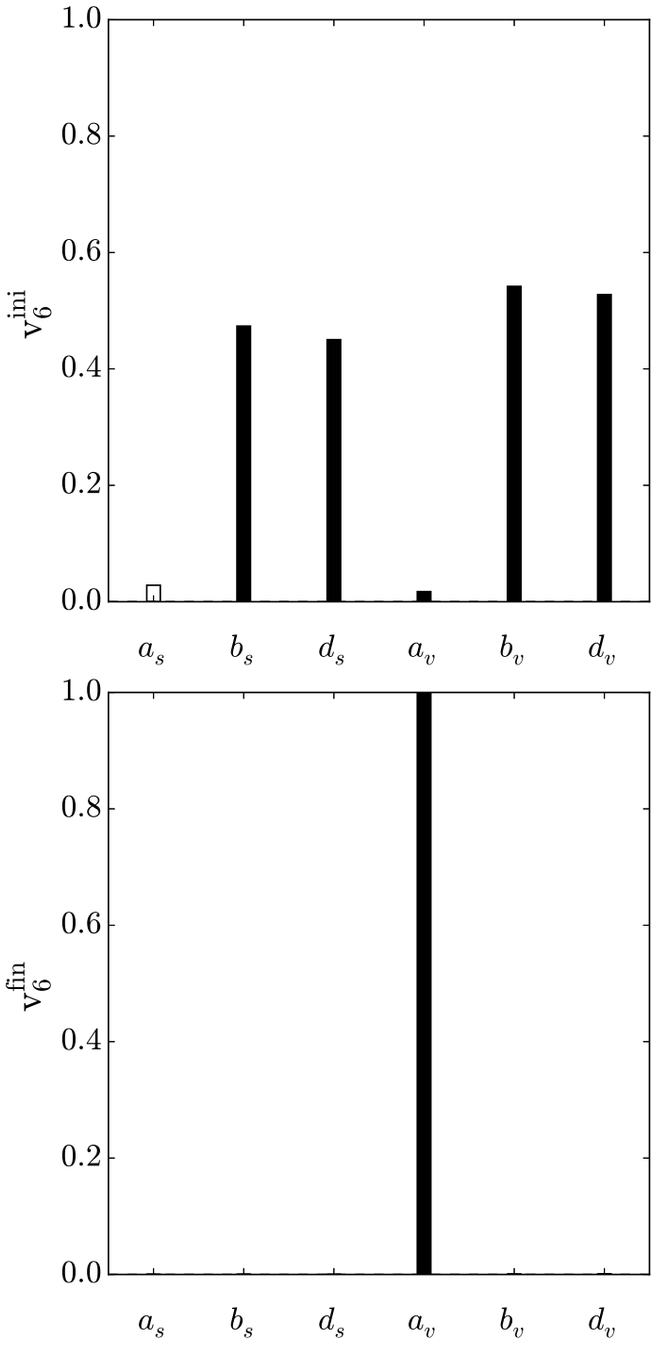
Eigenvectors and eigenvalues of the Hessian matrix $\mathscr{M}$ at the best-fit point ➟

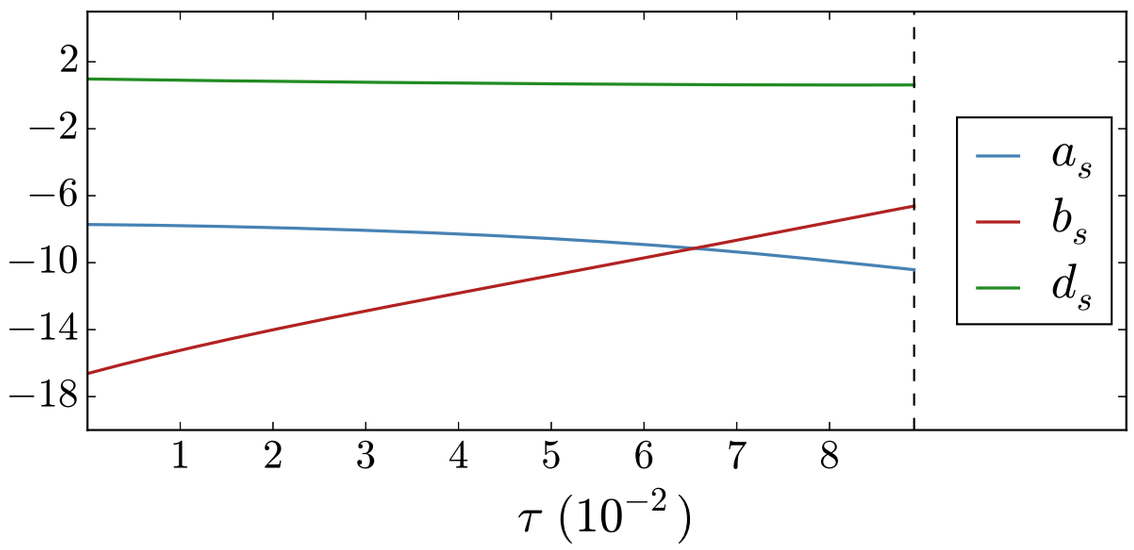


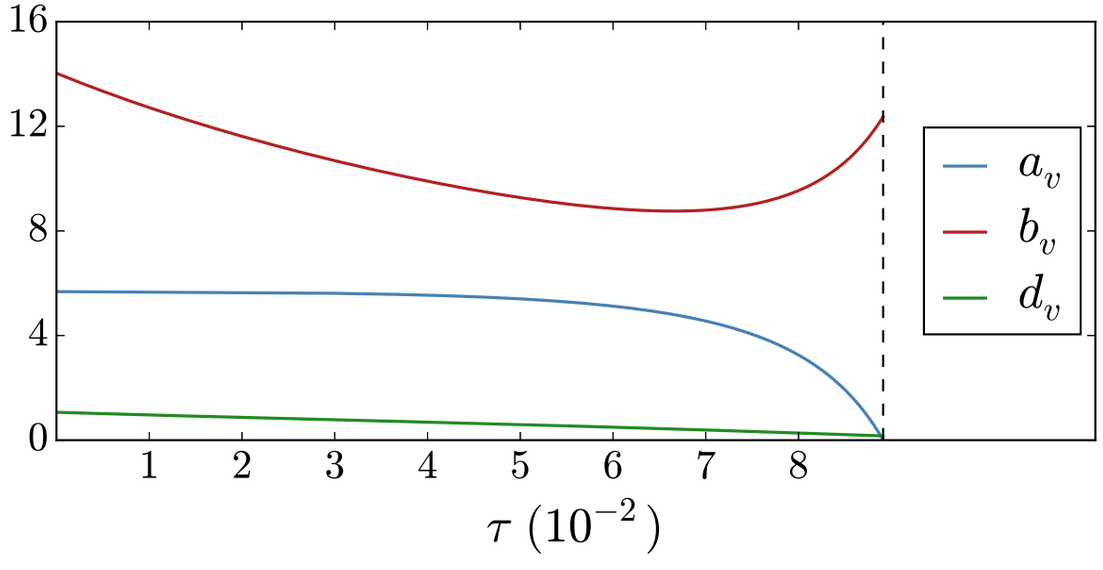
$$\alpha_s(\rho_v) = a_s + b_s e^{-d_s x}$$
$$\alpha_v(\rho_v) = a_v + b_v e^{-d_v x}$$

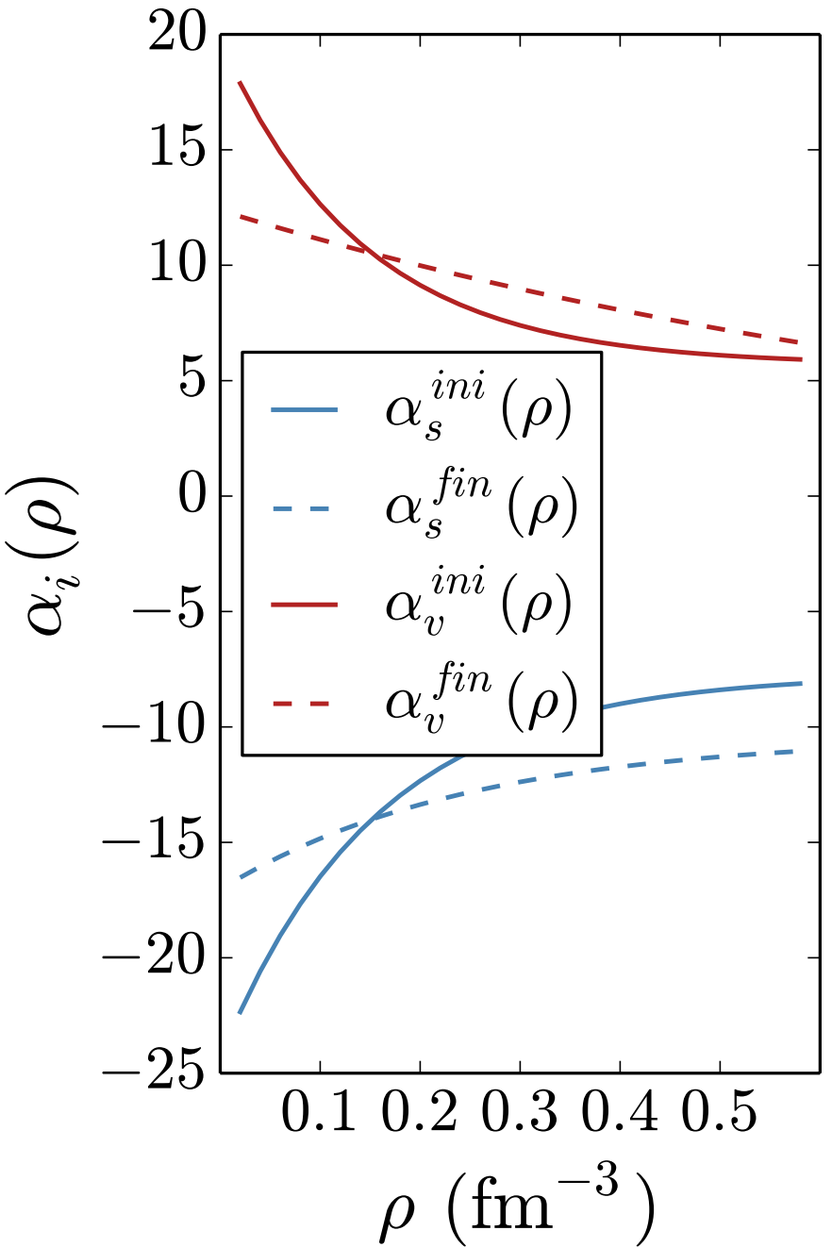
$$\alpha_v(\rho) \approx a_v + b_v(1 - d_v x)$$
$$= a_v + b_v - b_v d_v x = \tilde{a}_v + \tilde{b}_v x$$

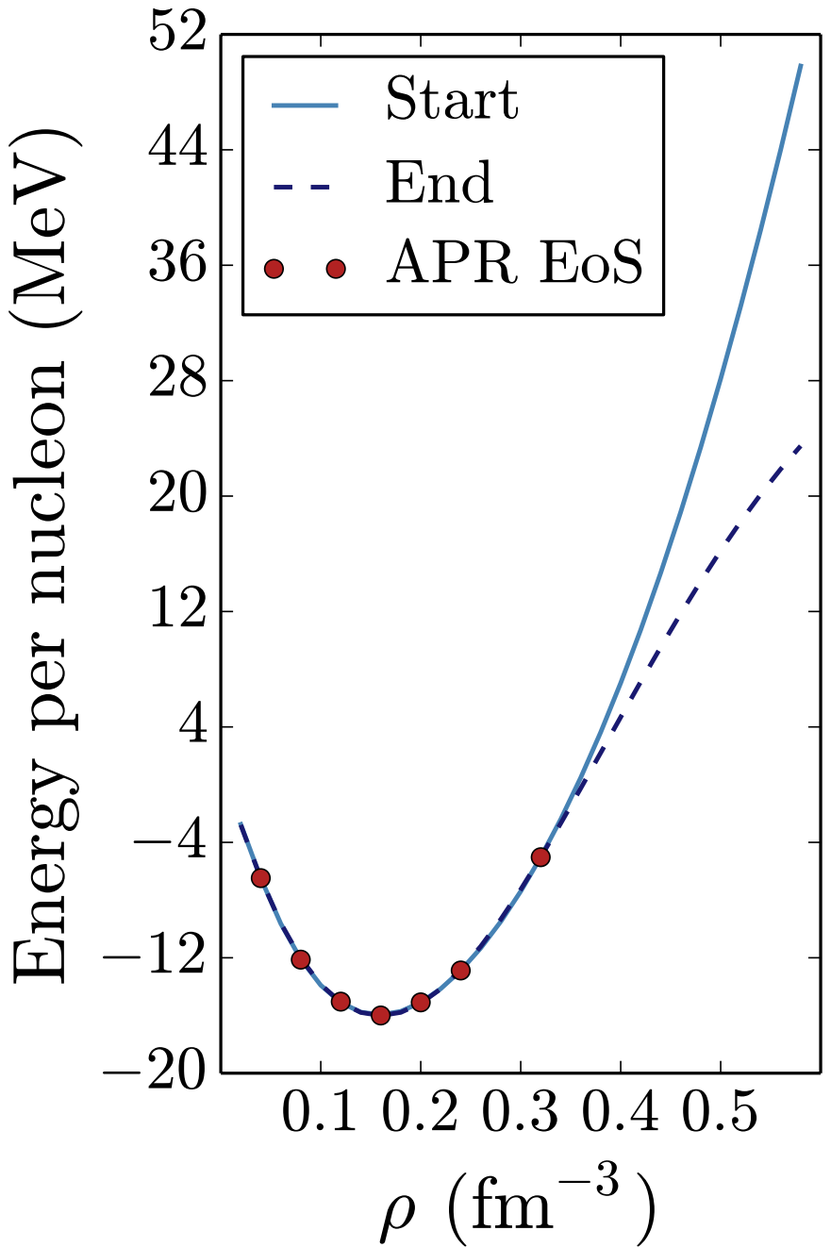









20
15
10
5
0
−5
−10
−15
−20
−25
$\alpha_i(\rho)$
$\alpha_s^{ini}(\rho)$
$\alpha_s^{fin}(\rho)$
$\alpha_v^{ini}(\rho)$
$\alpha_v^{fin}(\rho)$
0.1 0.2 0.3 0.4 0.5
ρ (fm^{-3})


52
44
36
28
20
12
4
−4
−12
−20
Energy per nucleon (MeV)
Start
End
APR EoS
0.1 0.2 0.3 0.4 0.5
ρ (fm^{-3})

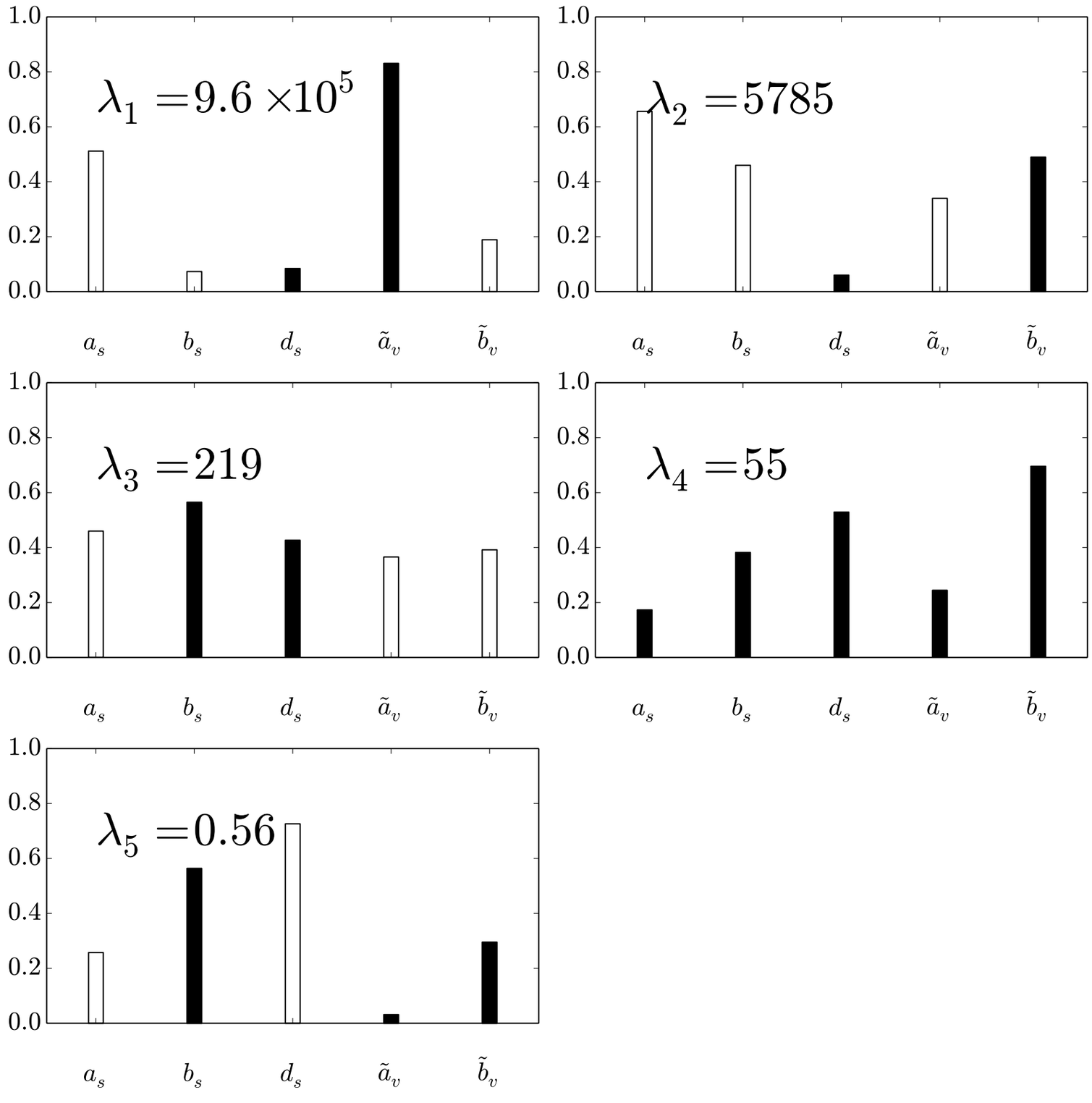
Third iteration:

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

$$\alpha_v(\rho_v) = \tilde{a}_v + \tilde{b}_v x$$

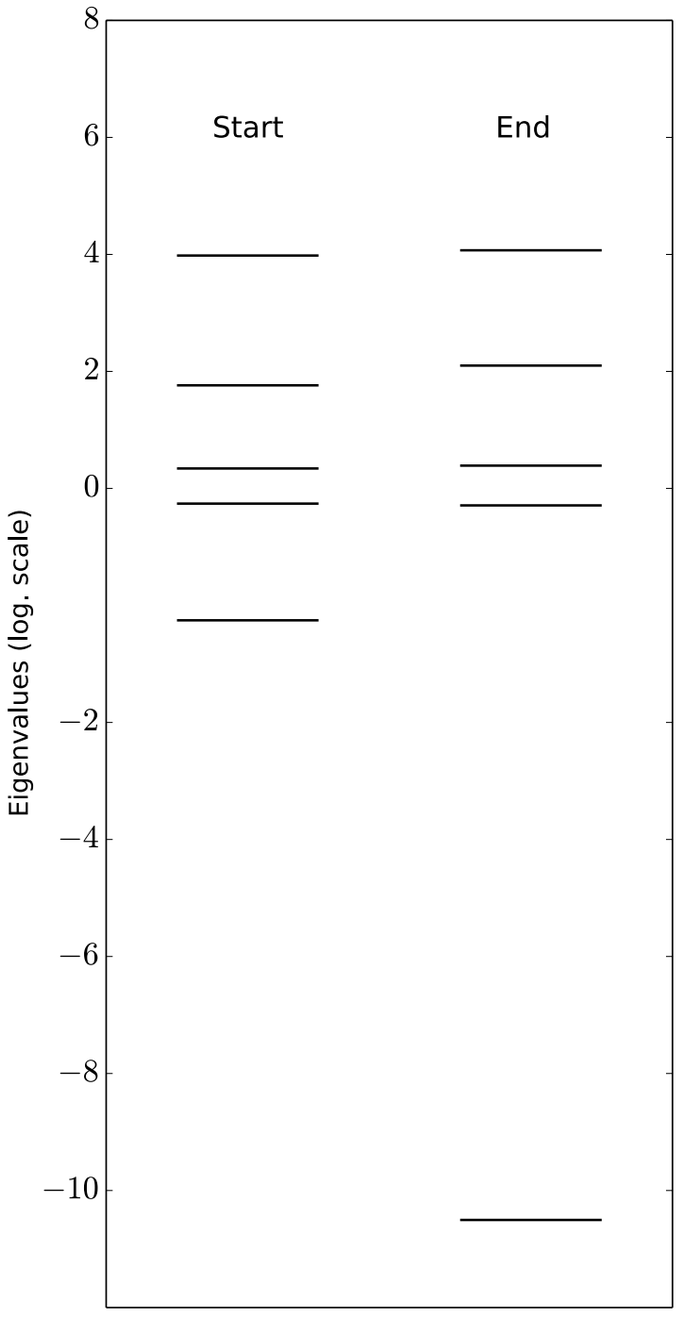
The parameters are refitted to data!

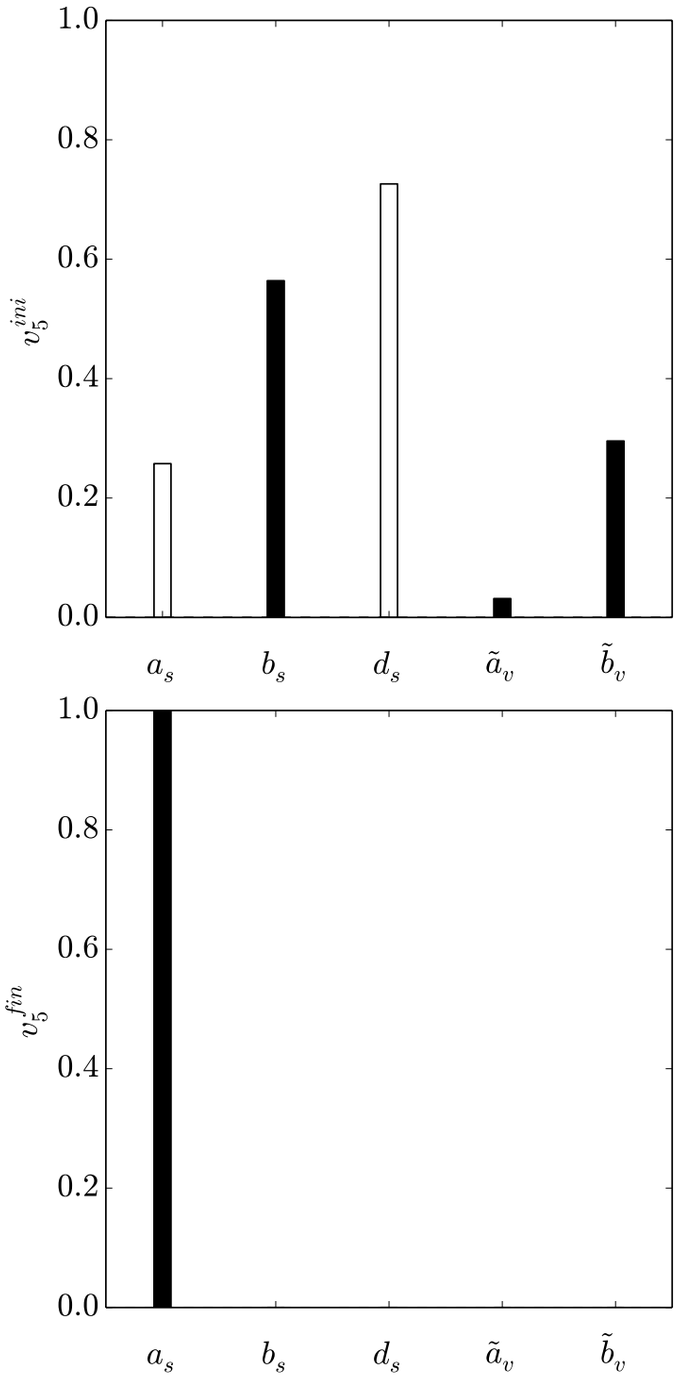
Eigenvectors and eigenvalues of the Hessian matrix $\mathscr{M}$ at the best-fit point ➡

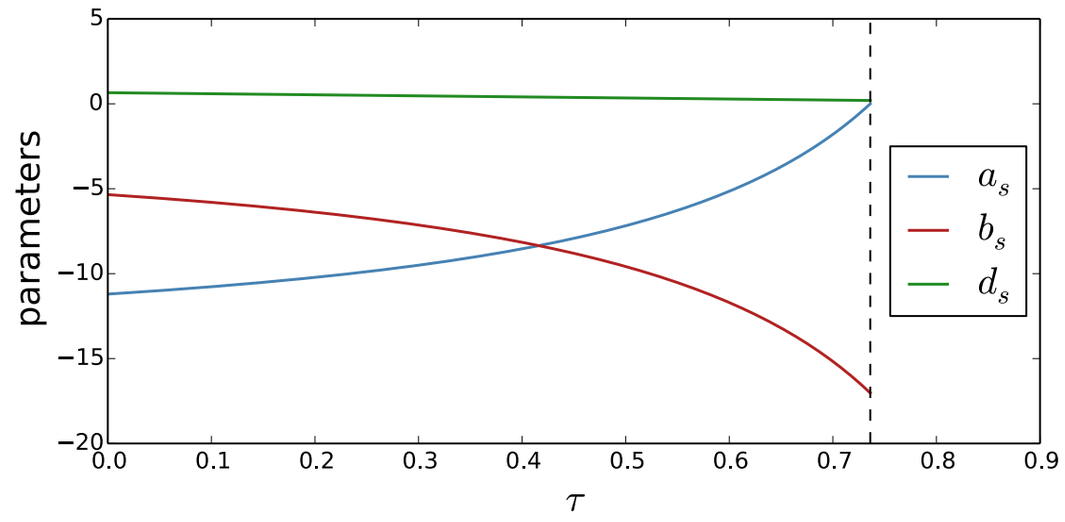


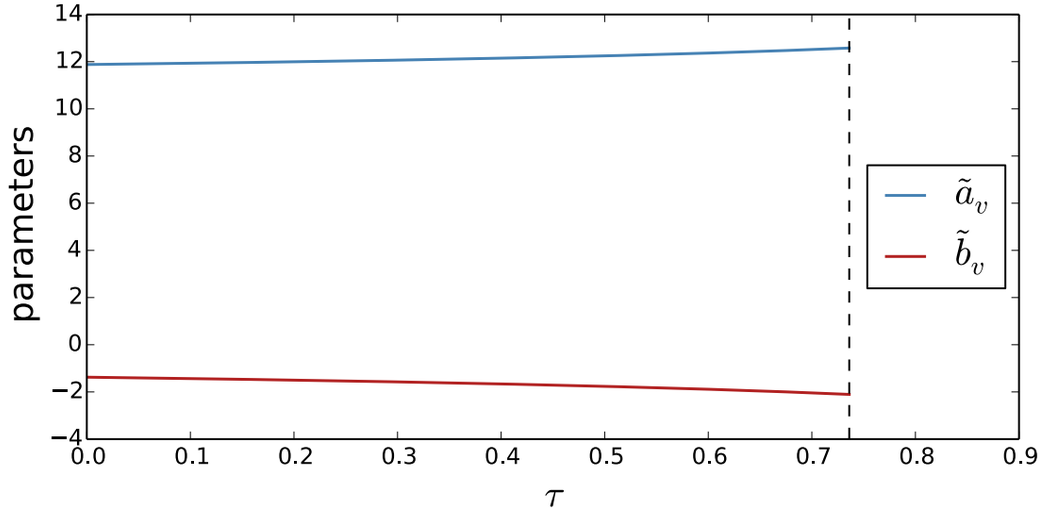
$$\alpha_s(\rho_v) = a_s + b_s e^{-d_s x}$$
$$\alpha_v(\rho_v) = \tilde{a}_v + \tilde{b}_v x$$

$$\alpha_s(\rho) \approx a_s + b_s(1 - d_s x)$$
$$= a_s + b_s - b_s d_s x = \tilde{a}_s + \tilde{b}_s x$$









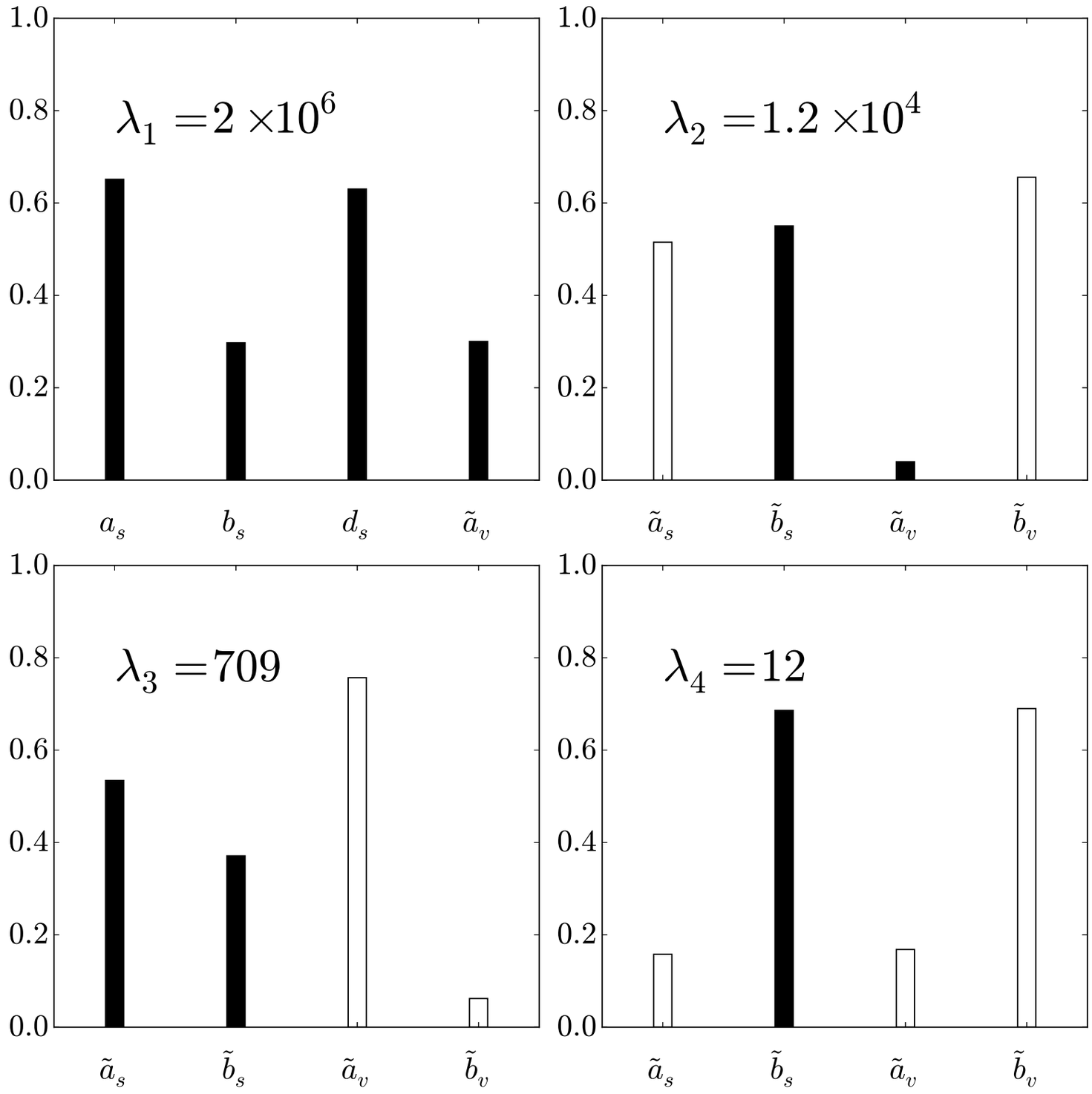
Fourth iteration:

$$\alpha_s(\rho_v) = \tilde{a}_s + \tilde{b}_s x$$

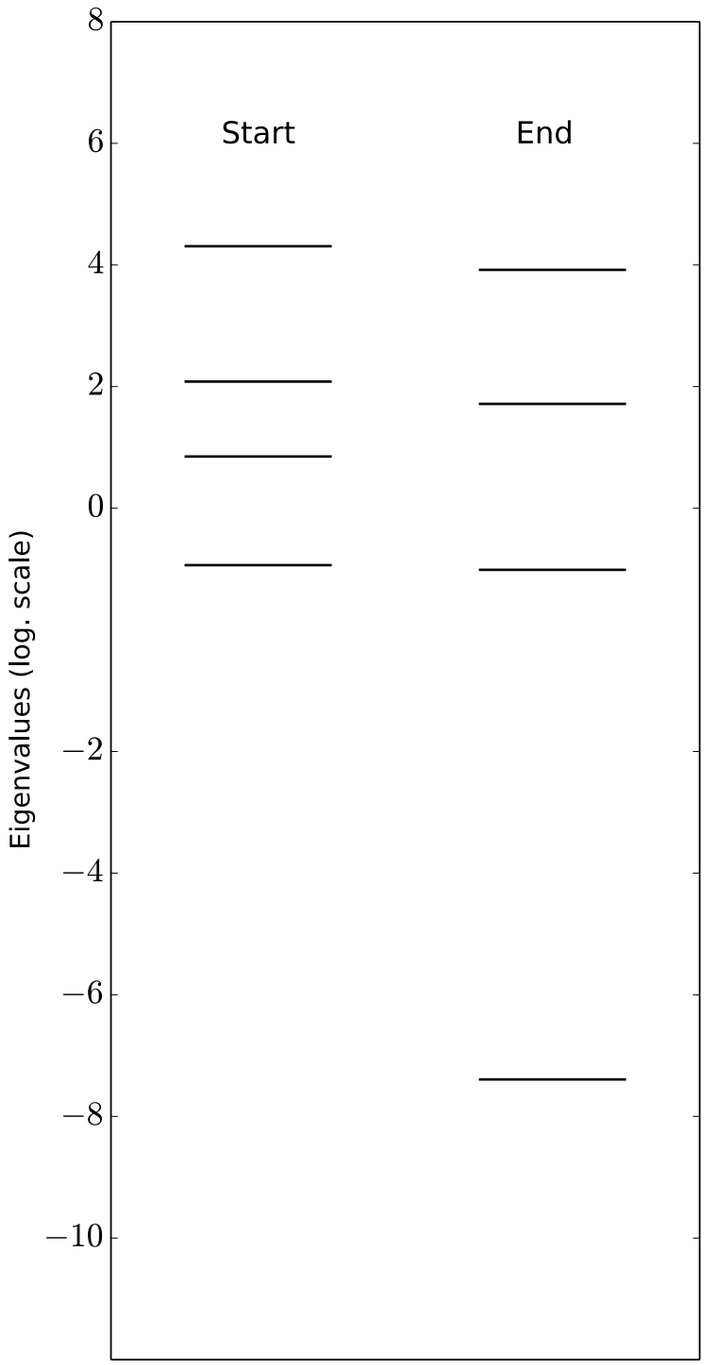
$$\alpha_v(\rho_v) = \tilde{a}_v + \tilde{b}_v x$$

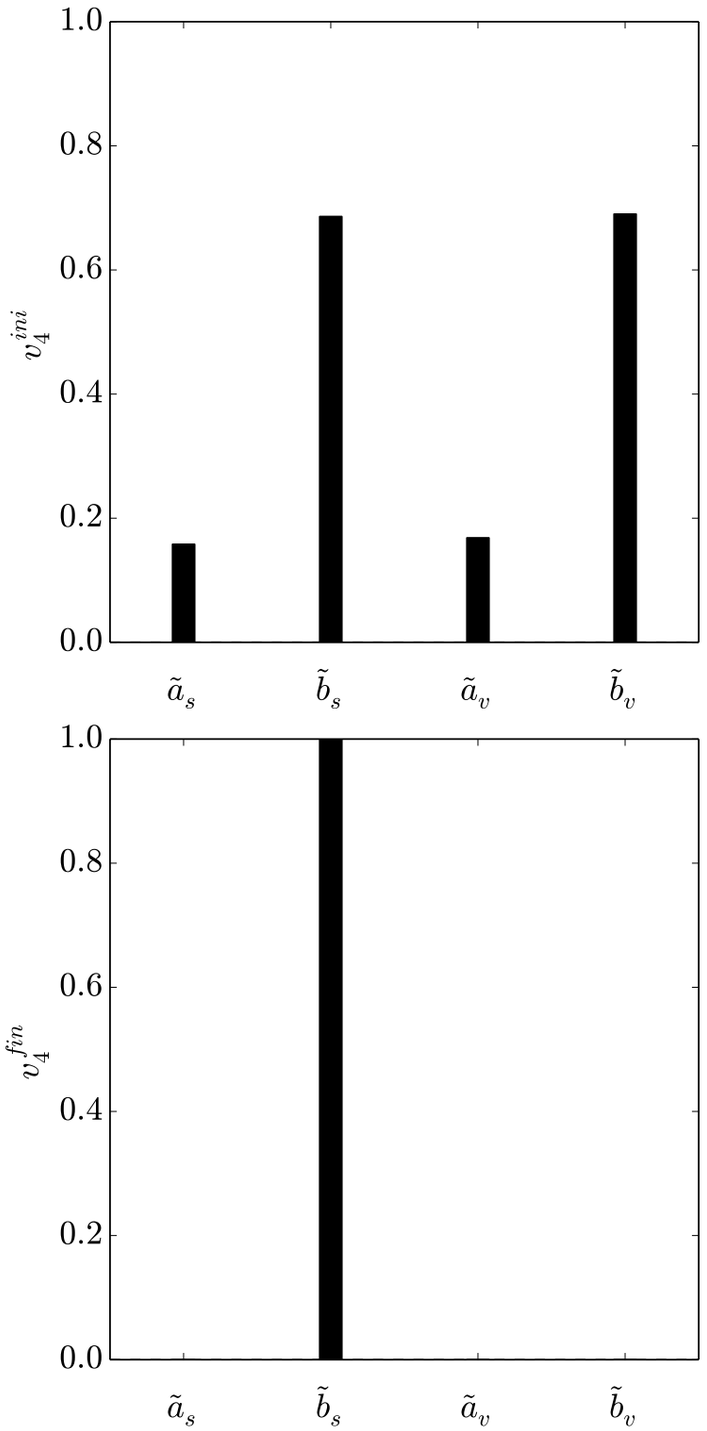
The parameters are refitted to data!

Eigenvectors and eigenvalues of the Hessian matrix $\mathscr{M}$ at the best-fit point ➡

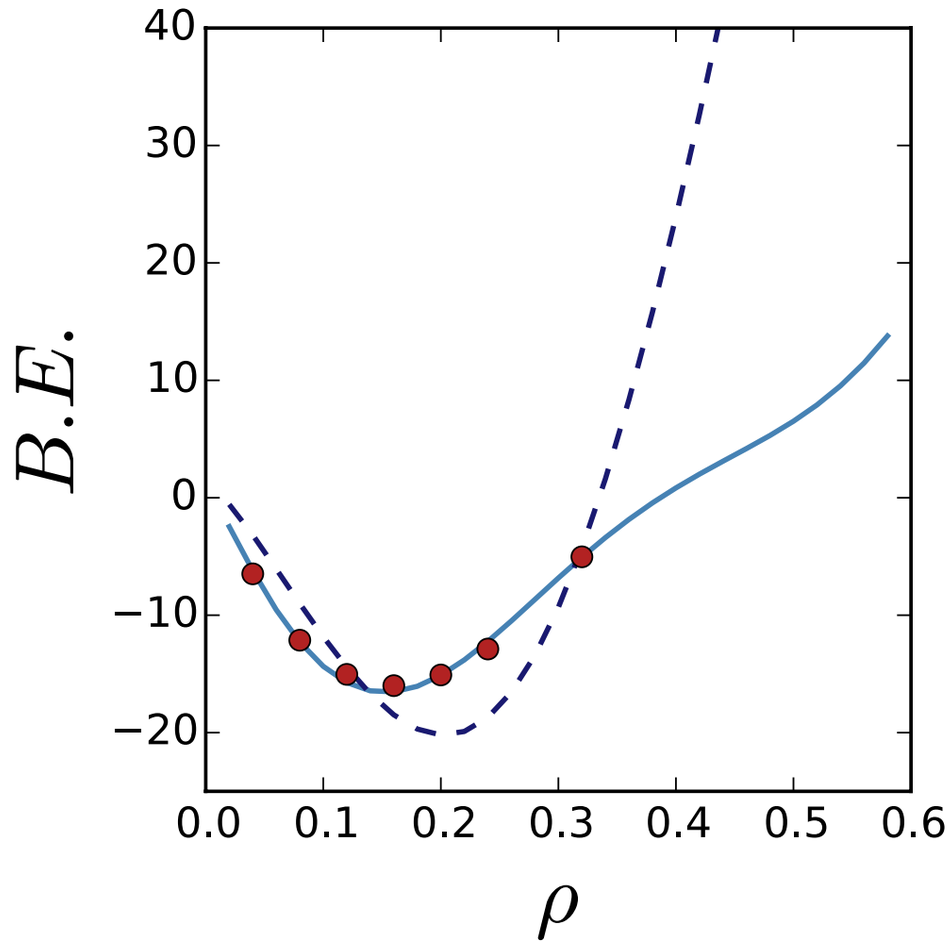


$$\alpha_s(\rho_v) = \tilde{a}_s + \tilde{b}_s x$$
$$\alpha_v(\rho_v) = \tilde{a}_v + \tilde{b}_v x$$





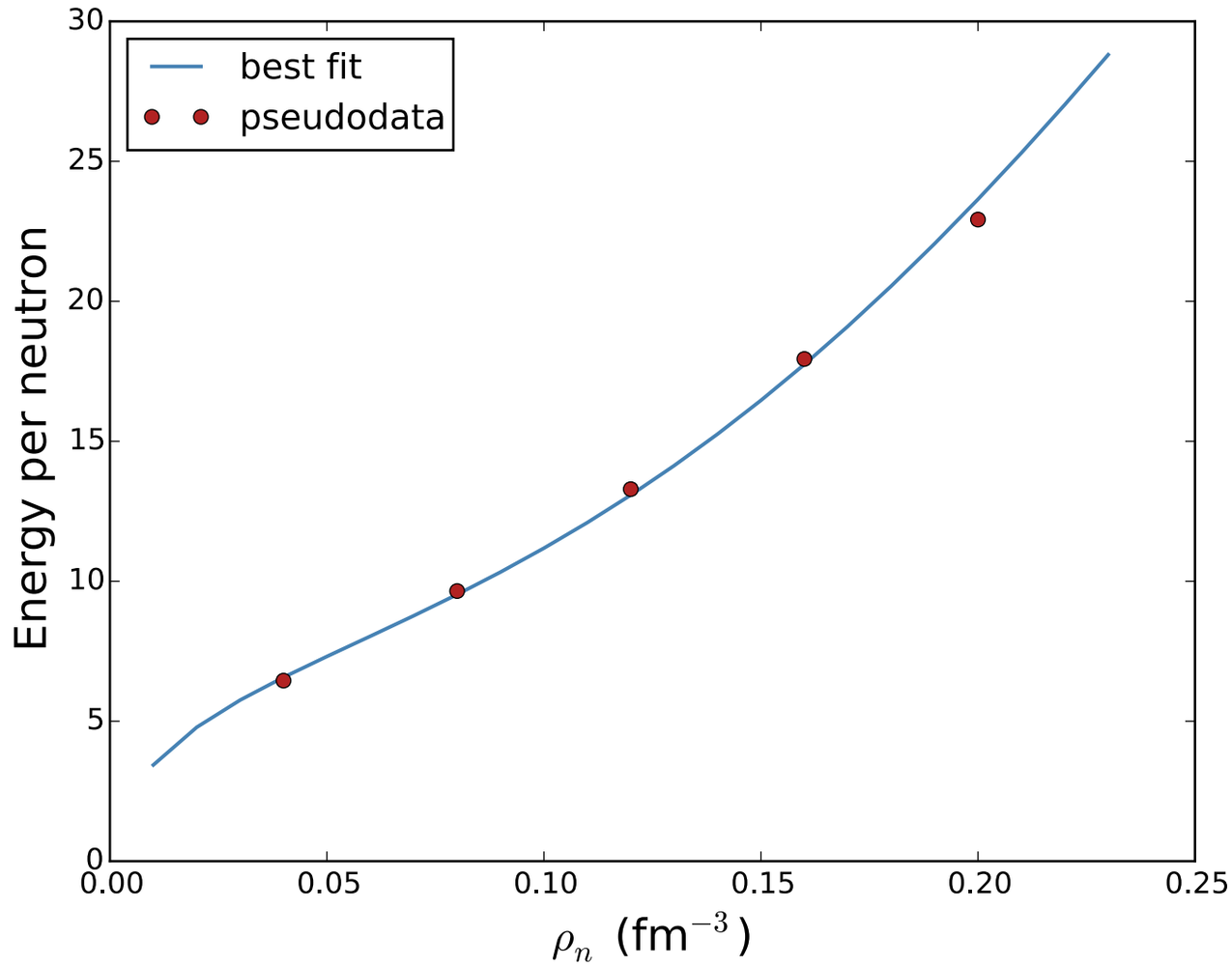
etc. ⇒ Walecka model, but not possible to get any agreement with experimental binding energies of finite nuclei!



With only two parameters, the model is not sloppy in the isovector channel!

$$\alpha_{tv}(\rho) = b_{tv} e^{-d_{tv} x}$$

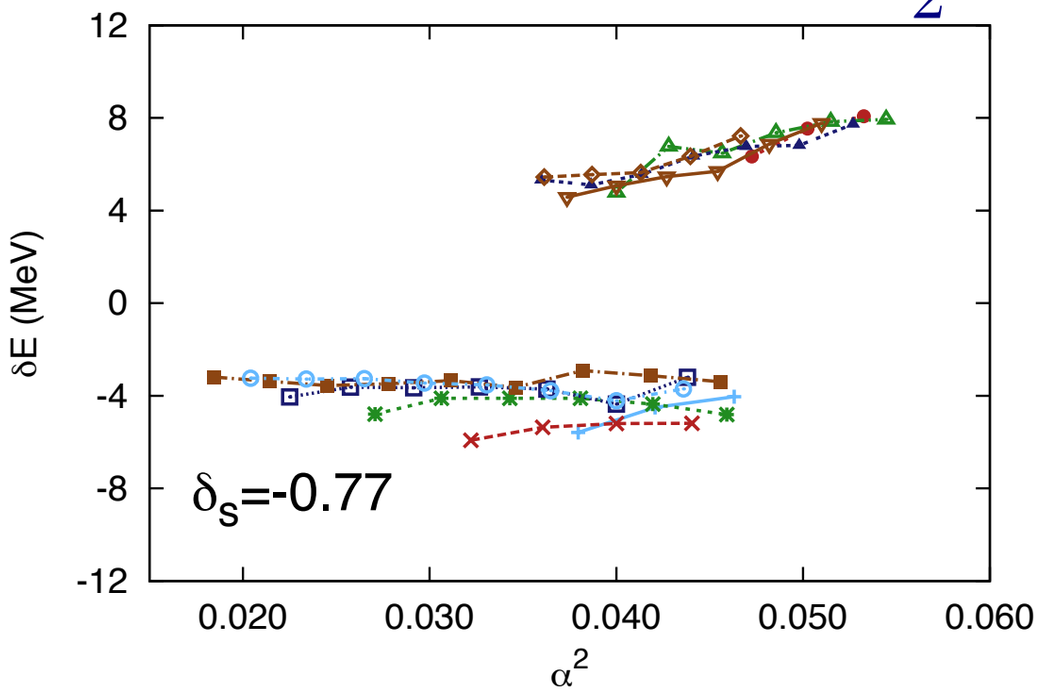
Neutron matter EoS.

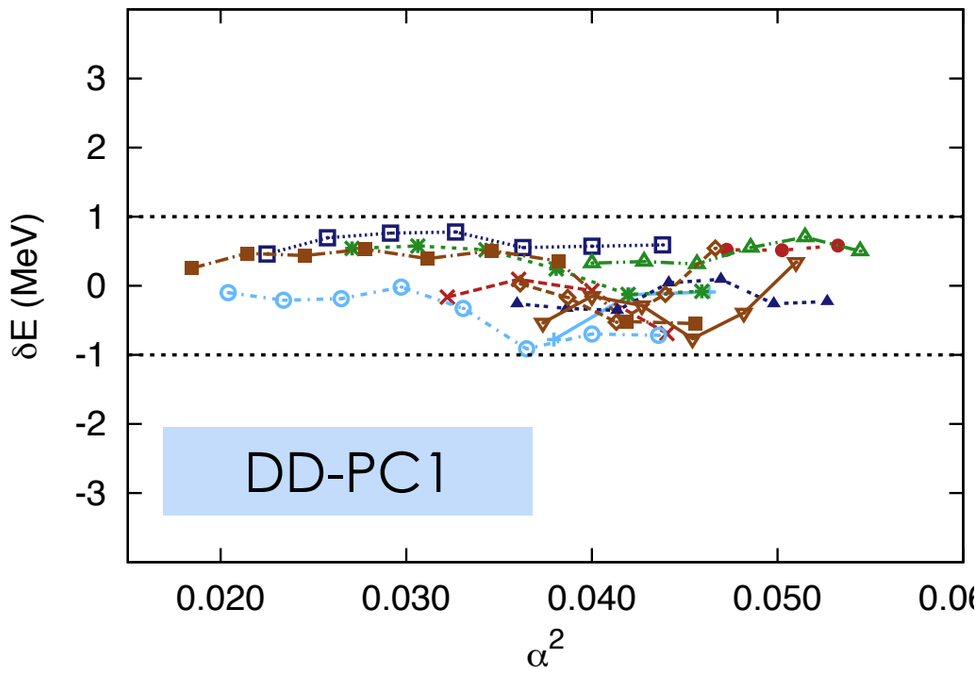


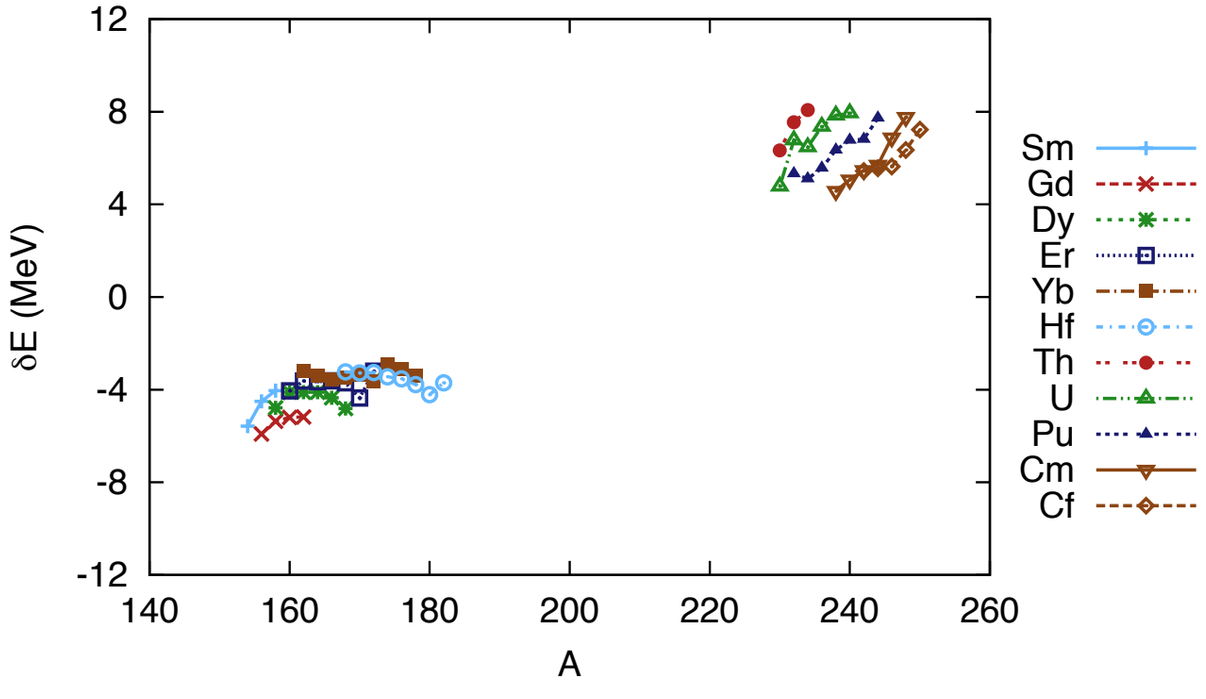
Model with five parameters

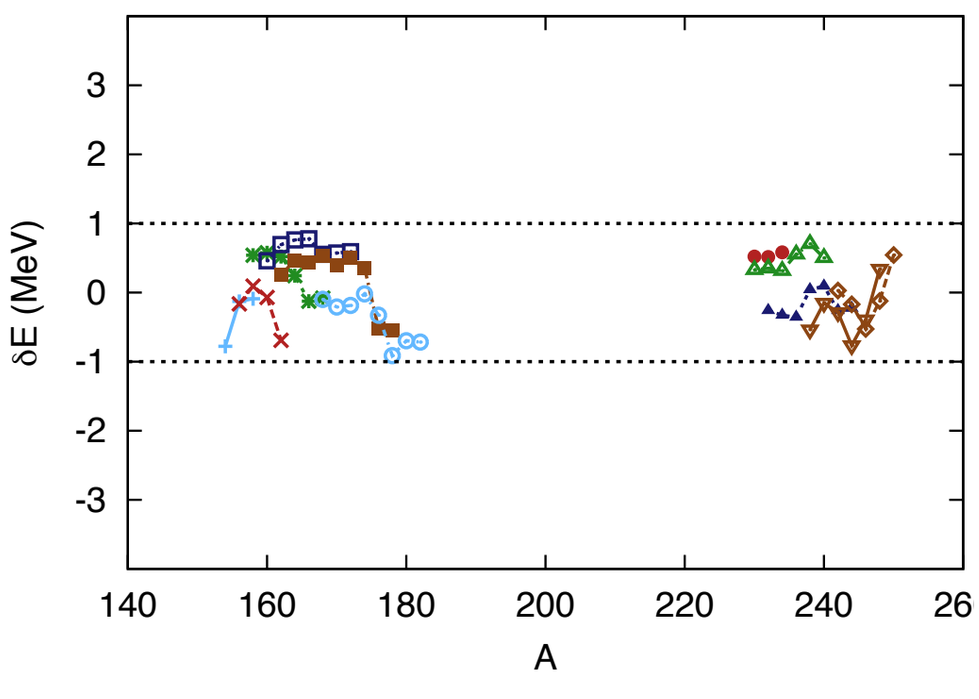
Binding energies of finite nuclei: all the parameters are determined by the nuclear matter EoS, except for the parameter of the derivative term which is directly fitted to masses.

$$-\frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi)$$









Nuclear energy density functionals are *sloppy*: 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).

A sloppy multi-parameter model can still be used to make predictions, but its sloppiness really points to an underlying model of lower effective dimension associated with the stiff parameters.

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