Solving complex inverse problems with differentiations

Shuzhe Shi, Tsinghua Univ.

refs:

Li, Han, Lin, Wang, Zhou, ***SS***,	Phys. Rev. D, 111, 074026 + work in progress
SS, Zhou, Zhao, Mukherjee, Zhuang,	Phys. Rev. D **105**, 014017;
Soma, Wang, ***SS***, Stoecker, Zhou,	JCAP08 (2022) 071; 2209.08883;
Wang, ***SS***, Zhou,	Phys. Rev. D **106**, L051502;
SS, Wang, Zhou,	Comput.Phys.Commun. 282 (2023) 108547.

a recent review:

Zhou, Wang, Pang, ***SS*** Prog.Part.Nucl.Phys. 104084(2023)[2303.15136].

Outline

- What (complex) inverse problems are we dealing with?
    - Schroedinger equation
    - spectral function reconstruction
    - neutron star mass-radius

- What are Deep Neural Networks?

- Application of Deep-Learning in solving these problems

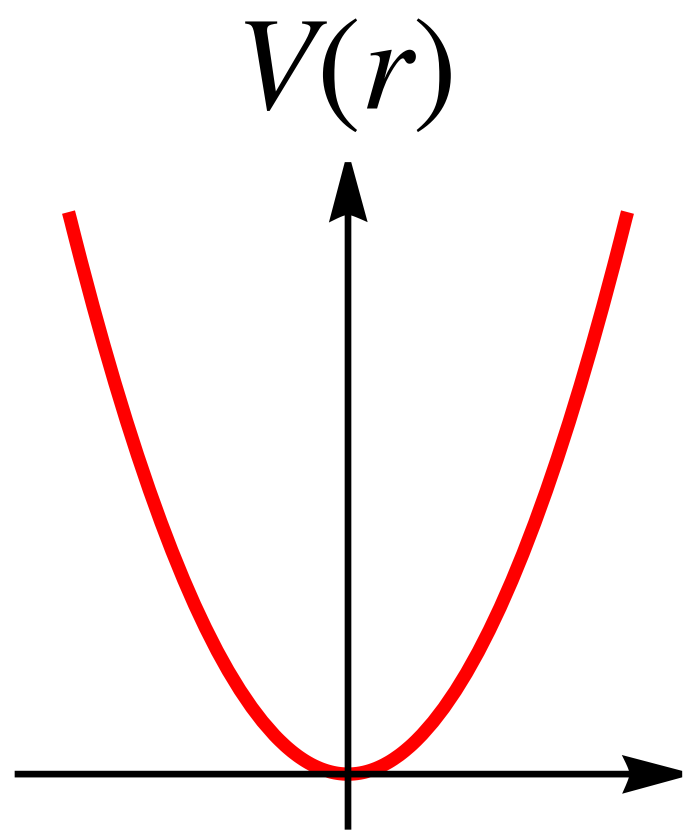
Problem # I:

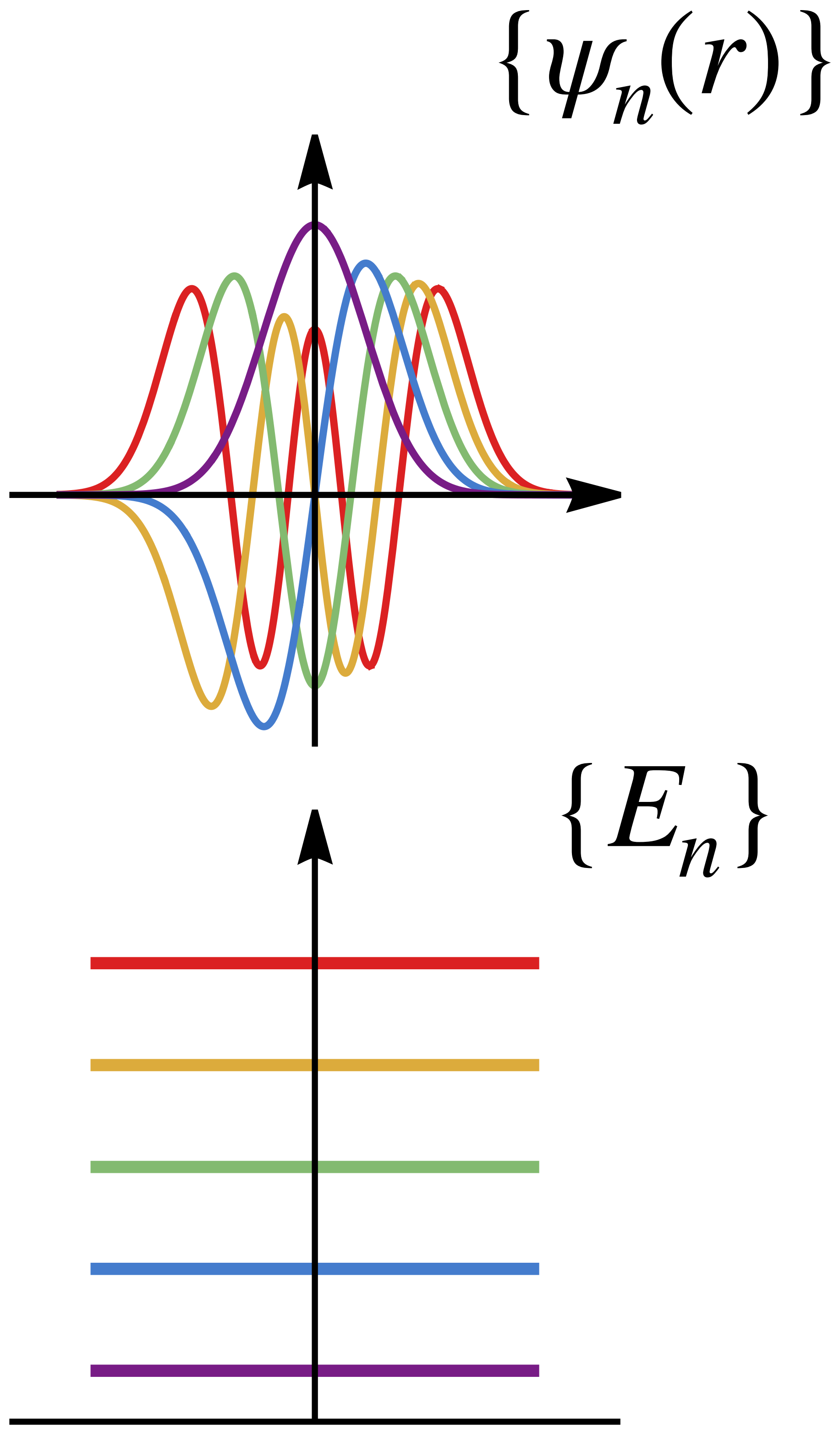
inverse Schroedinger Equation solver

reference: ***SS***, Zhou, Zhao, Mukherjee, Zhuang, PhysRevD.105.014017

1. Schroedinger Equation

$$\hat{H}\psi_n = -\frac{\nabla^2}{2m}\psi_n + V(r)\,\psi_n = E_n\psi_n$$





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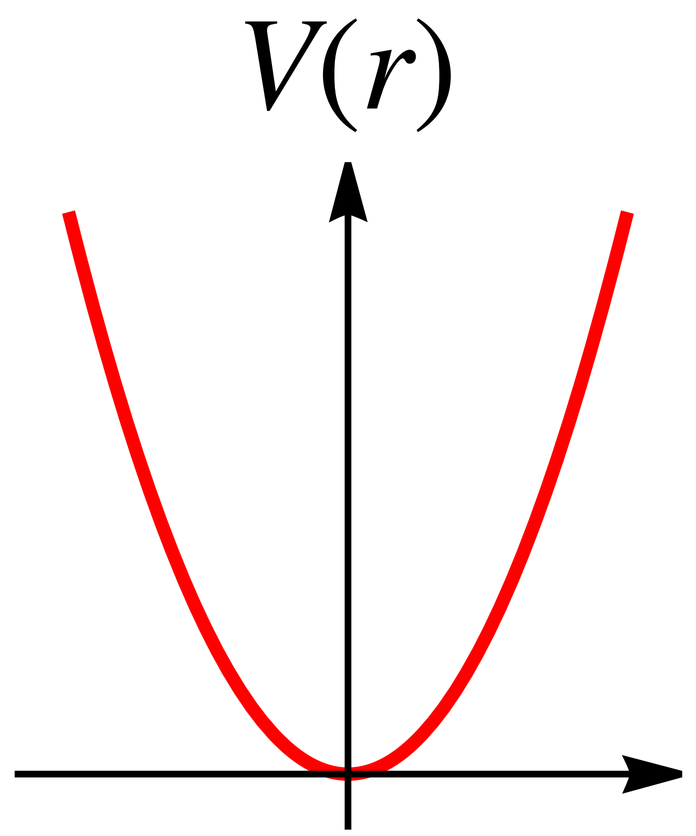
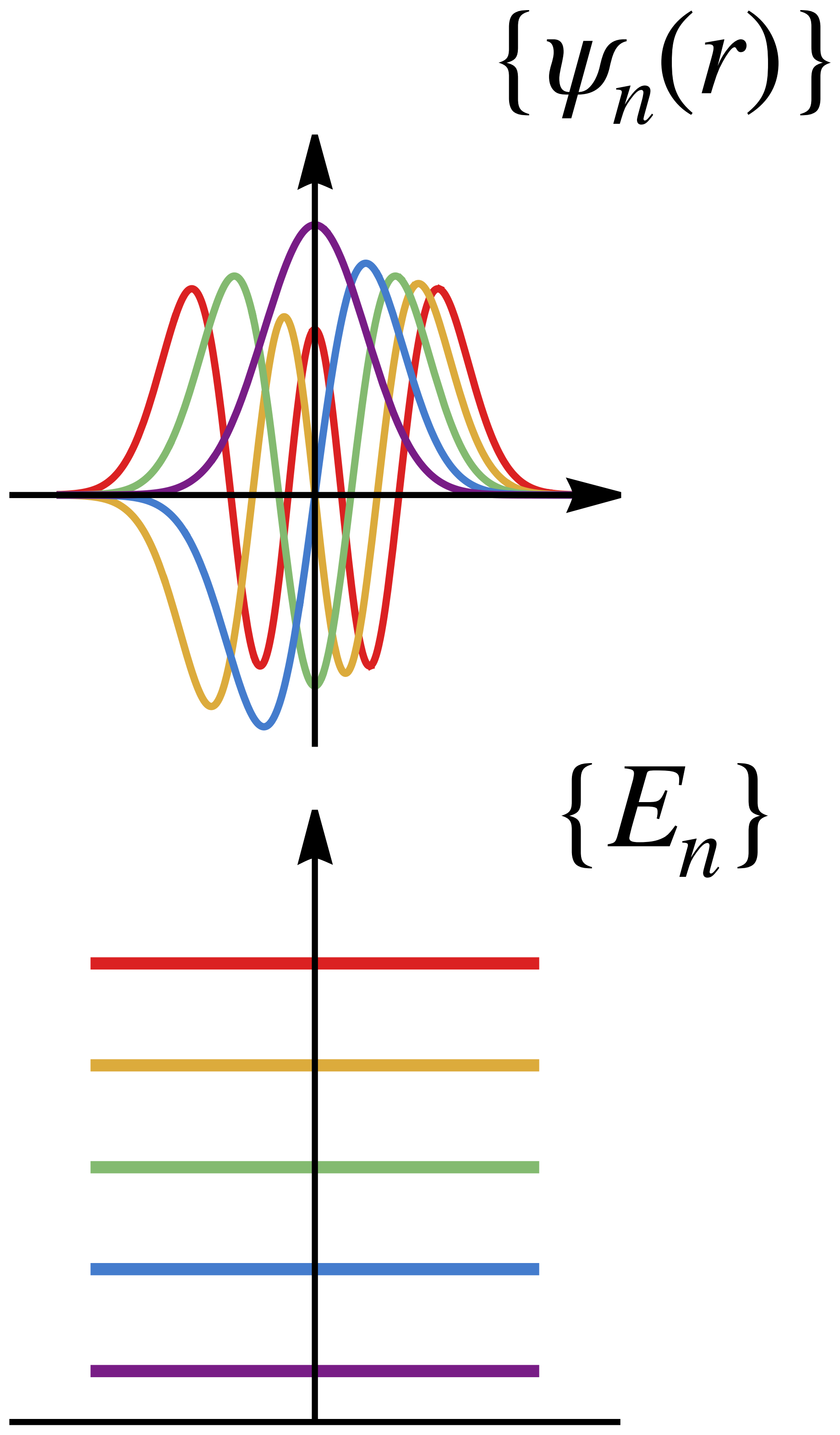


$V(r)$ known $\Longrightarrow \{E_n, \psi_n(r)\}$:
numerical methods established.



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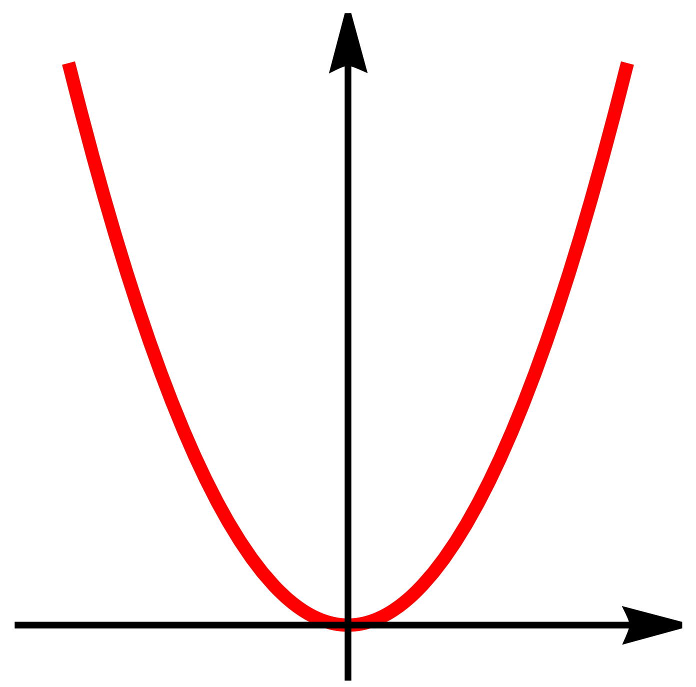

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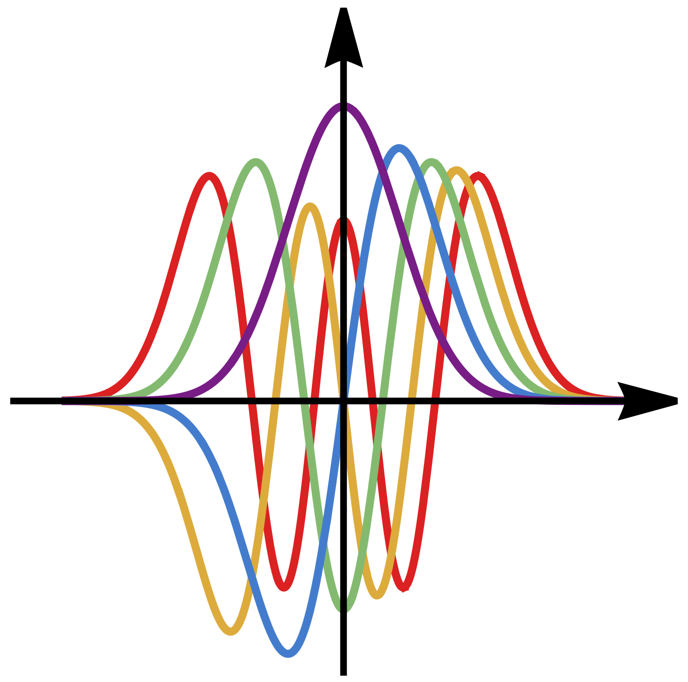
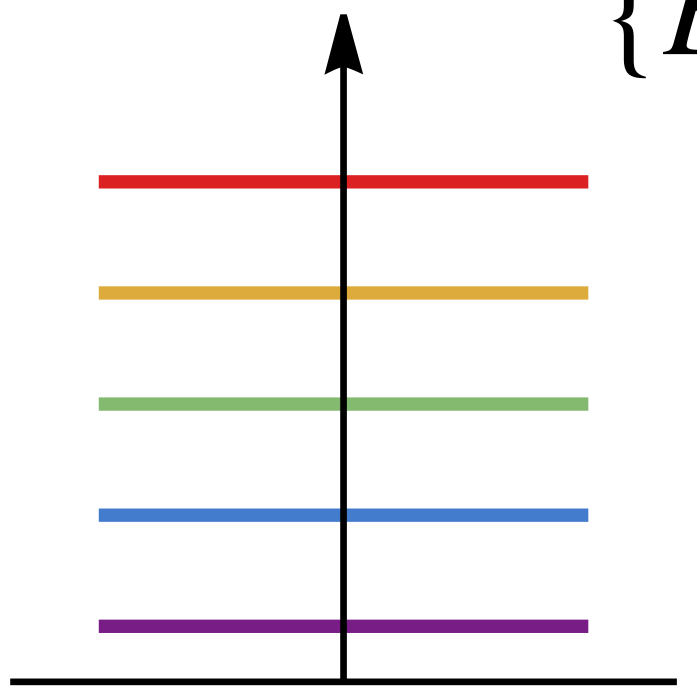




$\psi_n(r)$ known $\Longrightarrow V(r)$:

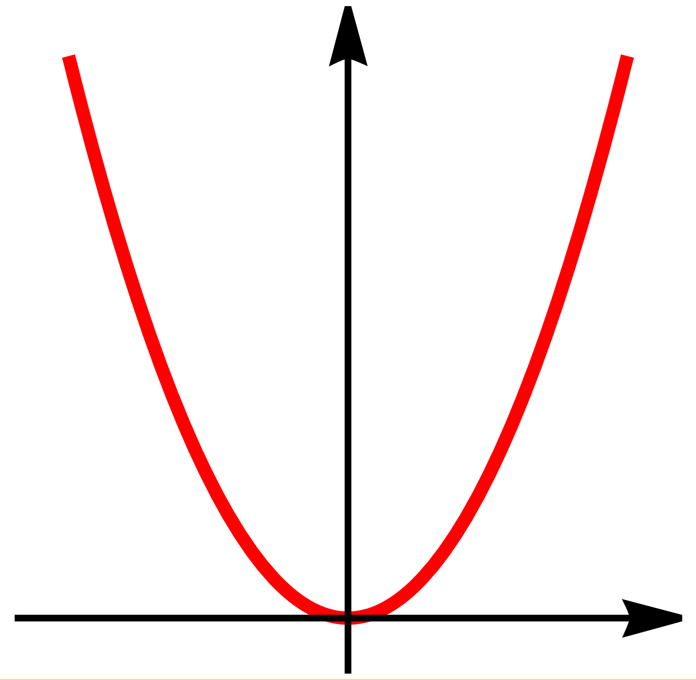
$$\frac{\nabla^2\psi_n}{2m\,\psi_n} = V(r) - E_n$$

1. Schroedinger Equation

$$\hat{H}\psi_n = -\frac{\nabla^2}{2m}\psi_n + V(r)\,\psi_n = E_n\,\psi_n$$

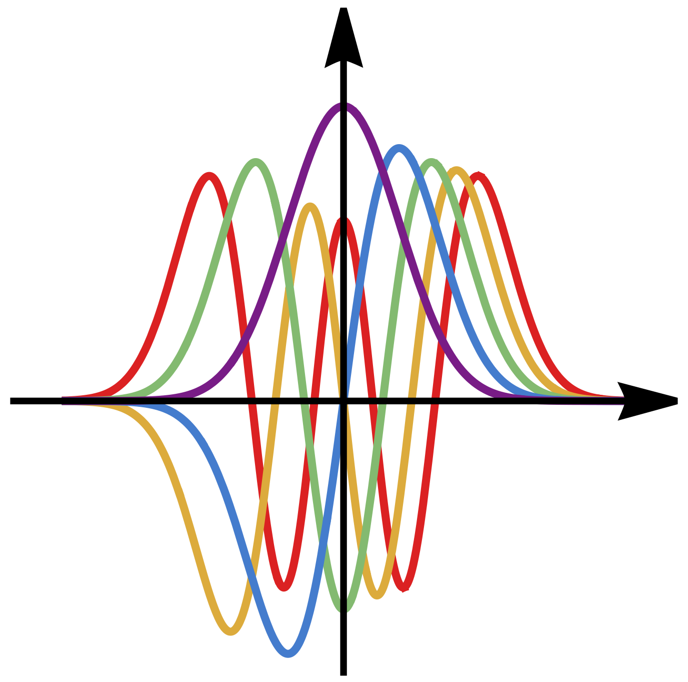
$V(r)$ known $\Longrightarrow \{E_n, \psi_n(r)\}$:
numerical methods established.

$V(r)$

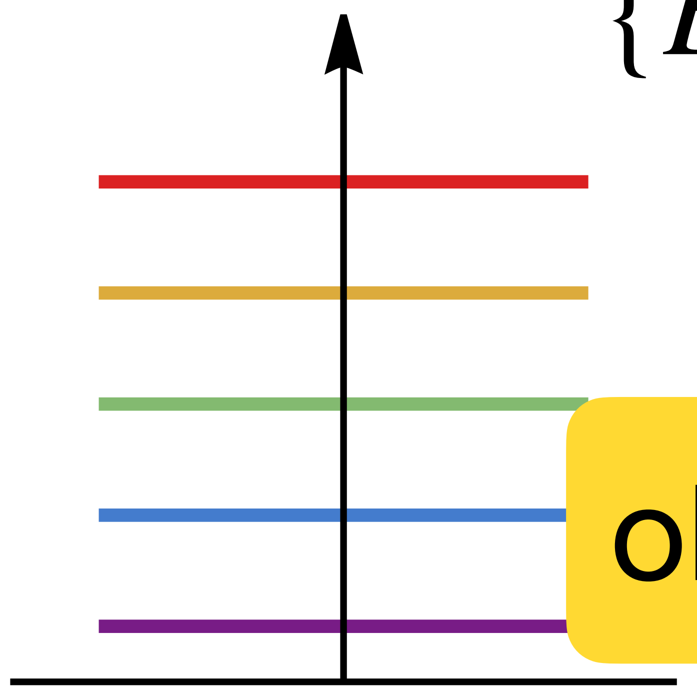


information of interest

$\{\psi_n(r)\}$



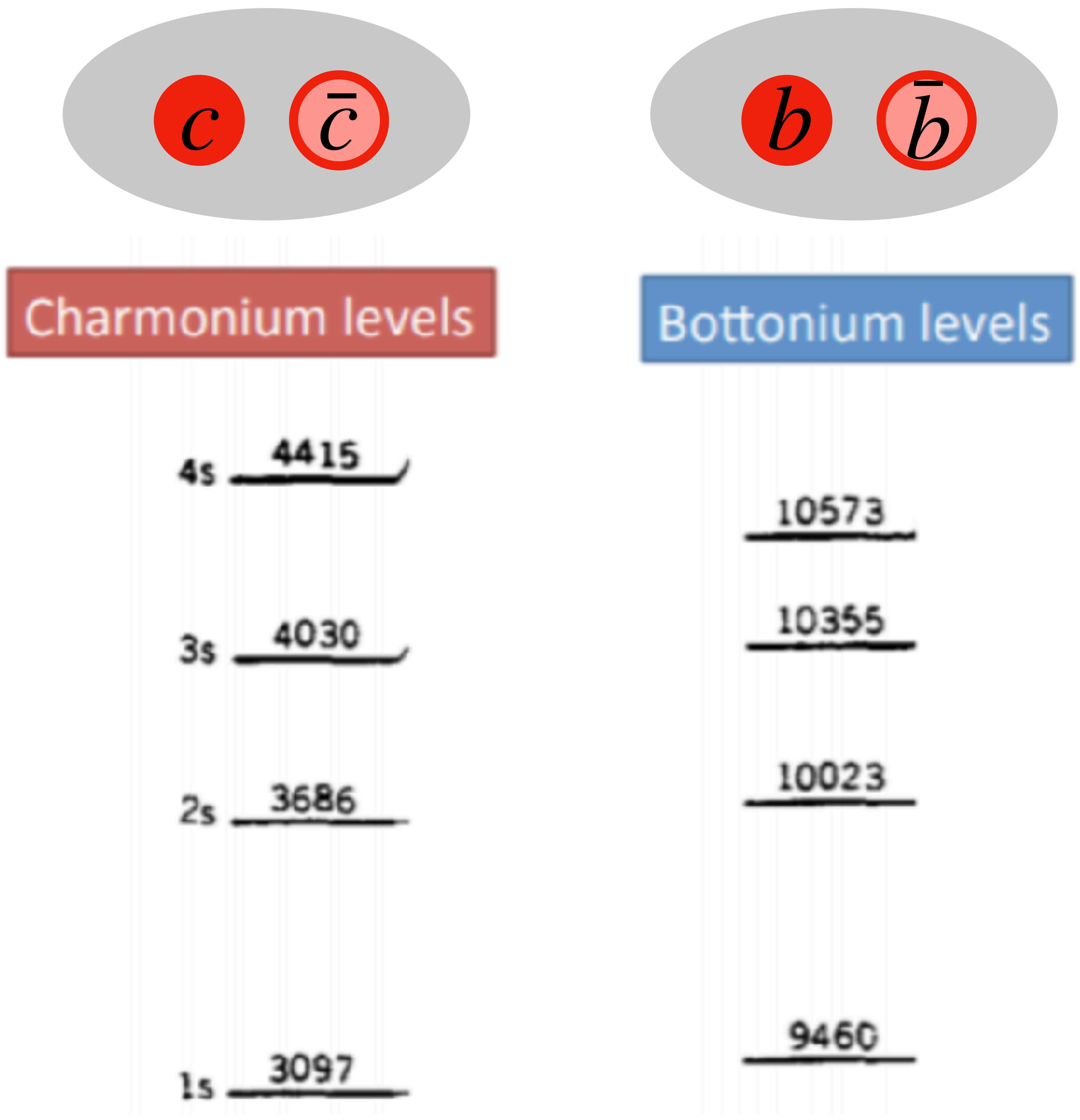
$\{E_n\}$



observations

$\{E_n\}$ known $\Longrightarrow V(r)$: ???

Realistic Example: Quarkonium Spectrum



Cornell Potential

$$V(r) = -\frac{\alpha}{r} + \sigma r$$

How to learn $V(r)$ from $\{E_n\}$?

- parameterize the potential $V(r\,|\,\boldsymbol{\theta})$, ***scan*** the whole $\boldsymbol{\theta}$-space, minimize $\chi^2 \equiv \sum_i \left(\frac{E_{\boldsymbol{\theta},i} - E_i}{\delta E_i}\right)^2$

How to learn $V(r)$ from $\{E_n\}$?

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- a ***gradient-descent*** based method:
    - goal -- find the $\boldsymbol{\theta}$-point that $\nabla_{\boldsymbol{\theta}}\chi^2 = 0$
    - update $\boldsymbol{\theta}$ iteratively according to $\boldsymbol{\Delta\theta} \propto \nabla_{\boldsymbol{\theta}}\chi^2$

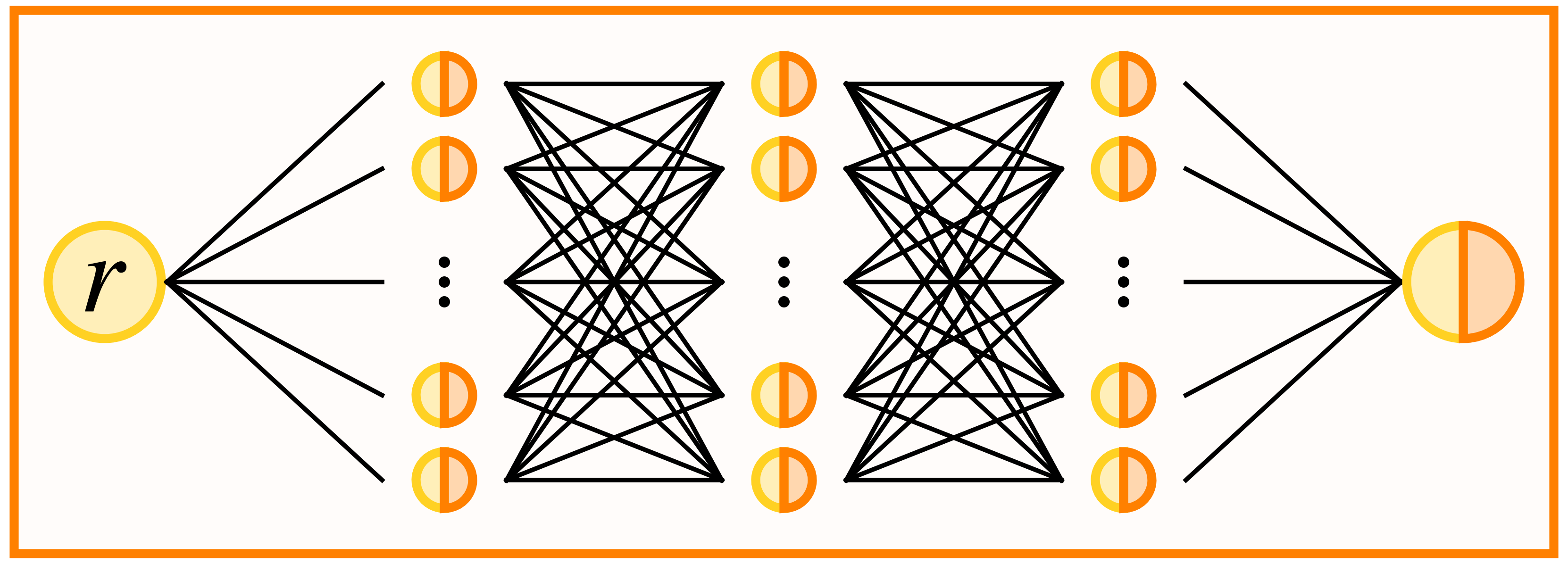
How to learn $V(r)$ from $\{E_n\}$?

- parameterize the potential $V(r\,|\,\boldsymbol{\theta})$, ***scan*** the whole $\boldsymbol{\theta}$-space, minimize $\chi^2 \equiv \sum_i \left(\frac{E_{\boldsymbol{\theta},i} - E_i}{\delta E_i}\right)^2$

- general unbiased parameterization scheme? Deep Neural Network!

How to learn $V(r)$ from $\{E_n\}$ using DNN?

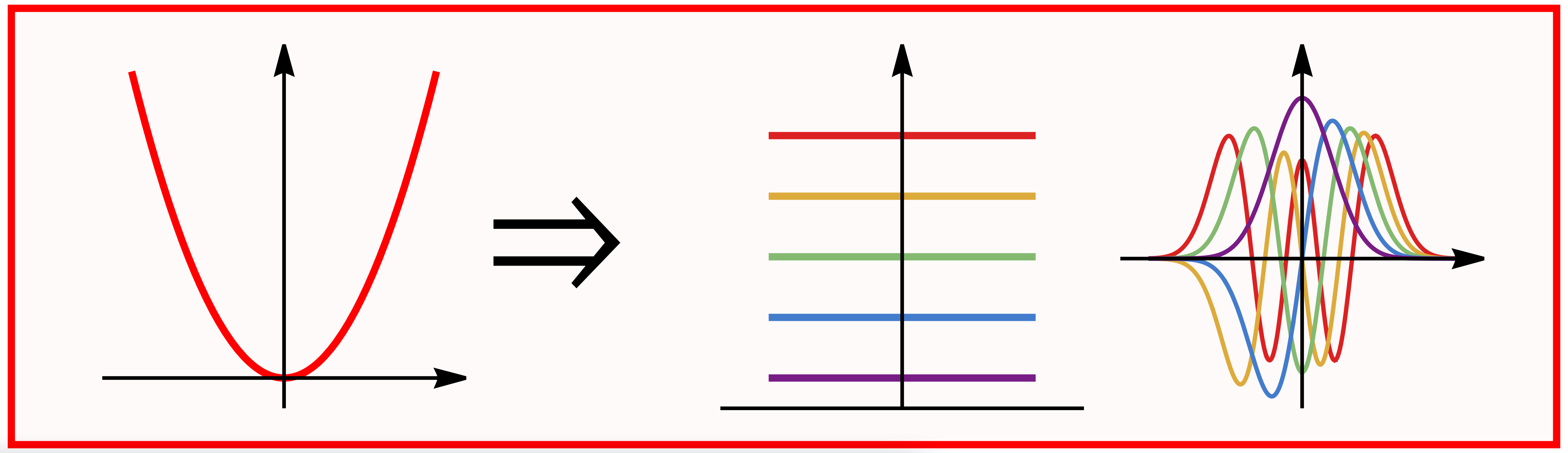
DNN potential



$W^{(l)}_{i,j}, b^{(l)}_i$

$V(r)$

Schrödinger equation



$$\hat{H}\psi_n = -\frac{\nabla^2}{2m}\psi_n + V(r)\,\psi_n = E_n\,\psi_n$$

$E_n, \psi_n(r)$

$$\chi^2 = \sum_n \frac{(E_n - E_n^{\mathrm{tgt}})^2}{\Delta_n^2}$$

$$\delta E_n = \langle \psi_n \,|\, \delta V(r) \,|\, \psi_n \rangle$$

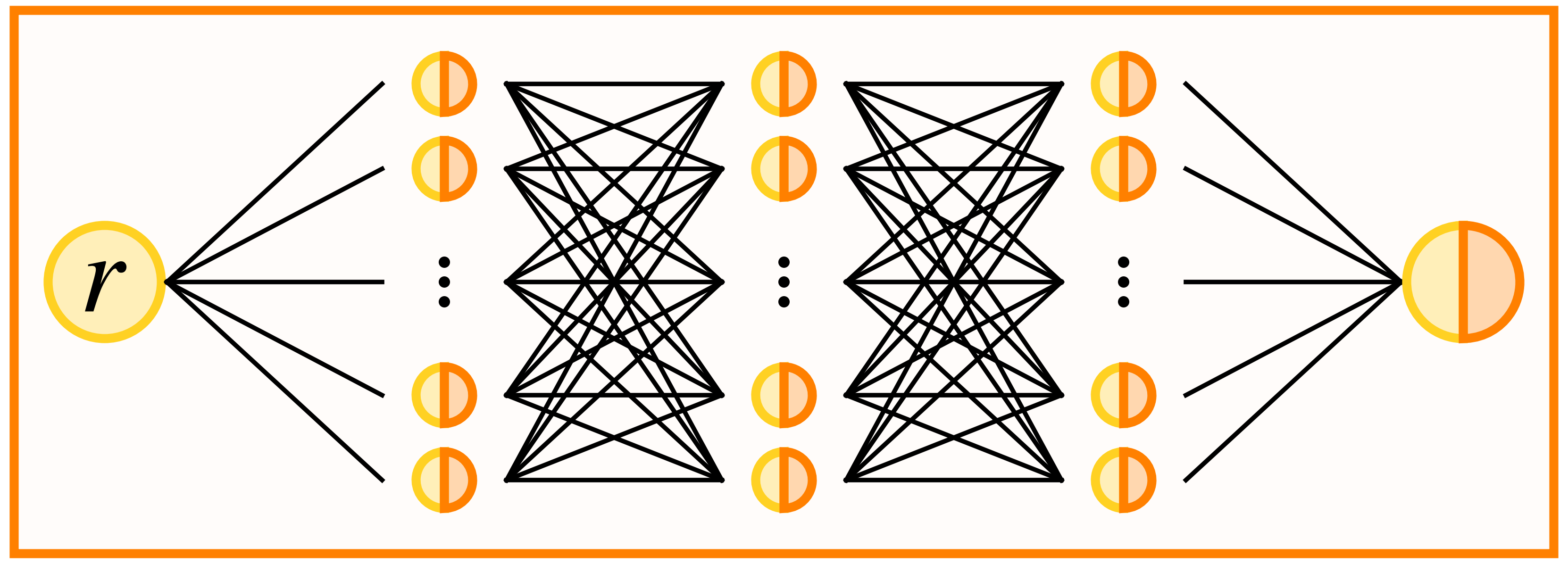
$$\frac{\delta \chi^2}{\delta V(r)}$$

$$\Delta W^{(l)}_{i,j} \sim -\frac{\partial \chi^2}{\partial W^{(l)}_{i,j}}, \quad \Delta b^{(l)}_i \sim -\frac{\partial \chi^2}{\partial b^{(l)}_i}$$

update

How to learn $V(r)$ from $\{E_n\}$ using DNN?

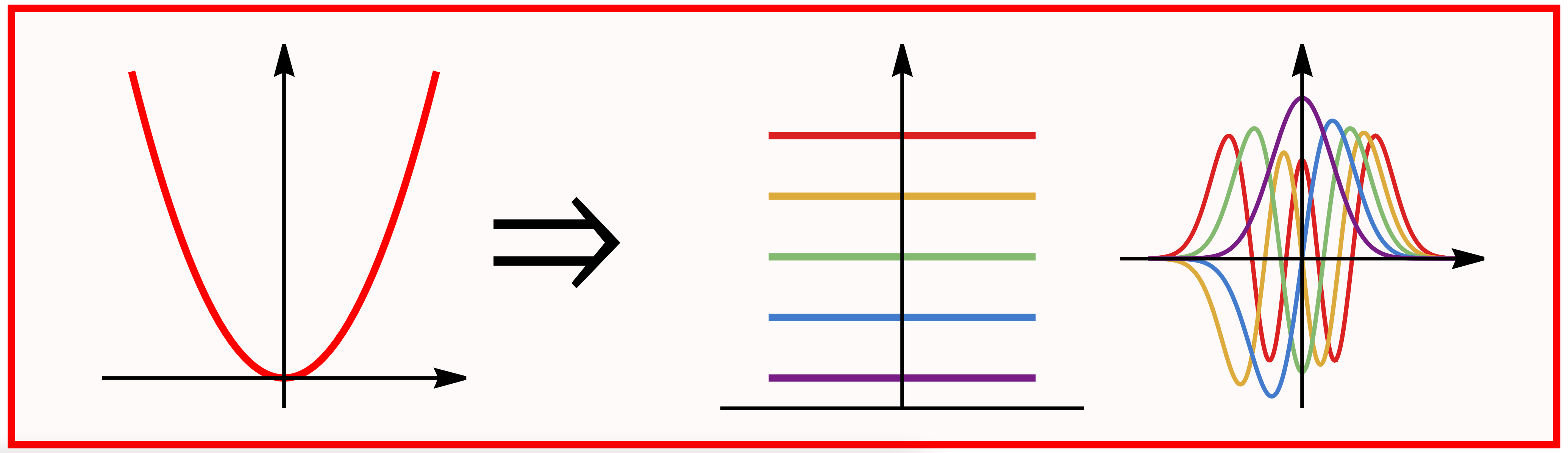
DNN potential



$W_{i,j}^{(l)}, b_i^{(l)}$

$V(r)$

Schrödinger equation



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update

uncertainty: $P(V_{\boldsymbol{\theta}})\mathrm{d}V = \text{Posterior}(\boldsymbol{\theta}\,|\,\text{data})\mathrm{d}^N\boldsymbol{\theta}$

Can we really learn $V(r)$ from $\{E_n\}$?

continuous

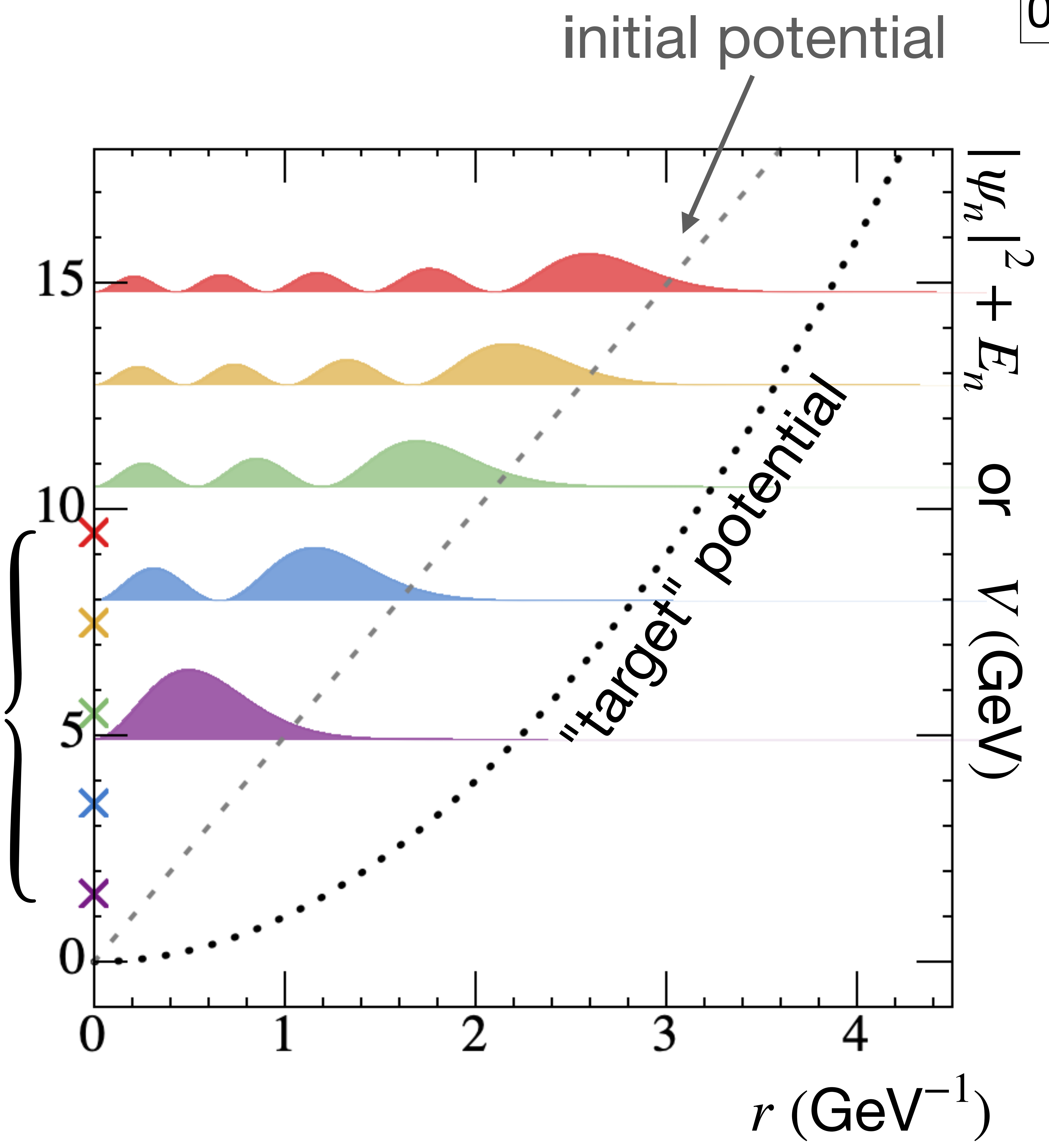
discrete, finite

Can we really learn $V(r)$ from $\{E_n\}$?

learn $V(r)$ according to

$$\{E_n\} = \left\{\frac{3}{2},\frac{7}{2},\frac{11}{2},\frac{15}{2},\frac{19}{2}\right\} \text{ GeV}$$

target spectrum



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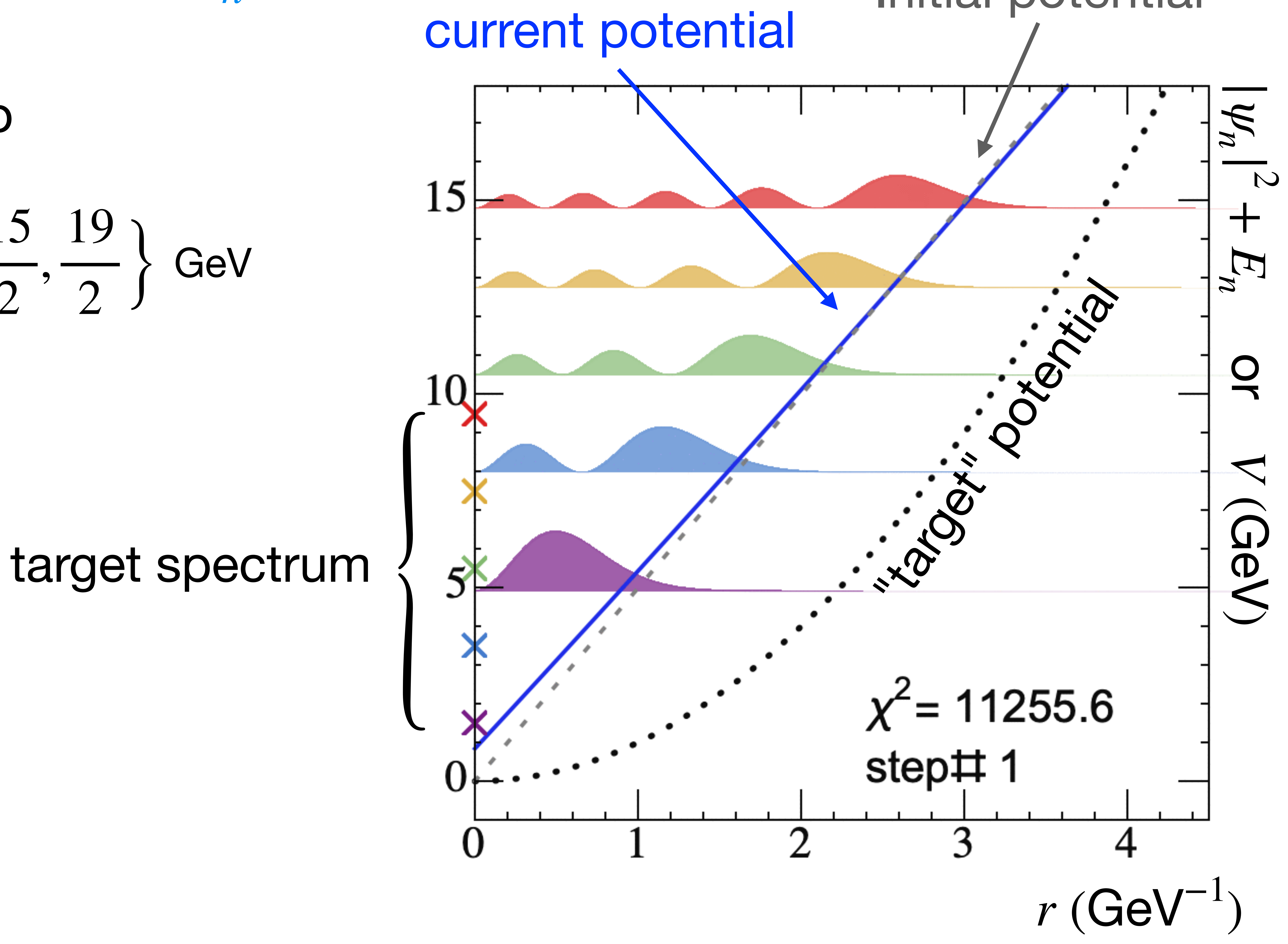


Can we really learn $V(r)$ from $\{E_n\}$?

-- Yes! (for a certain r range)

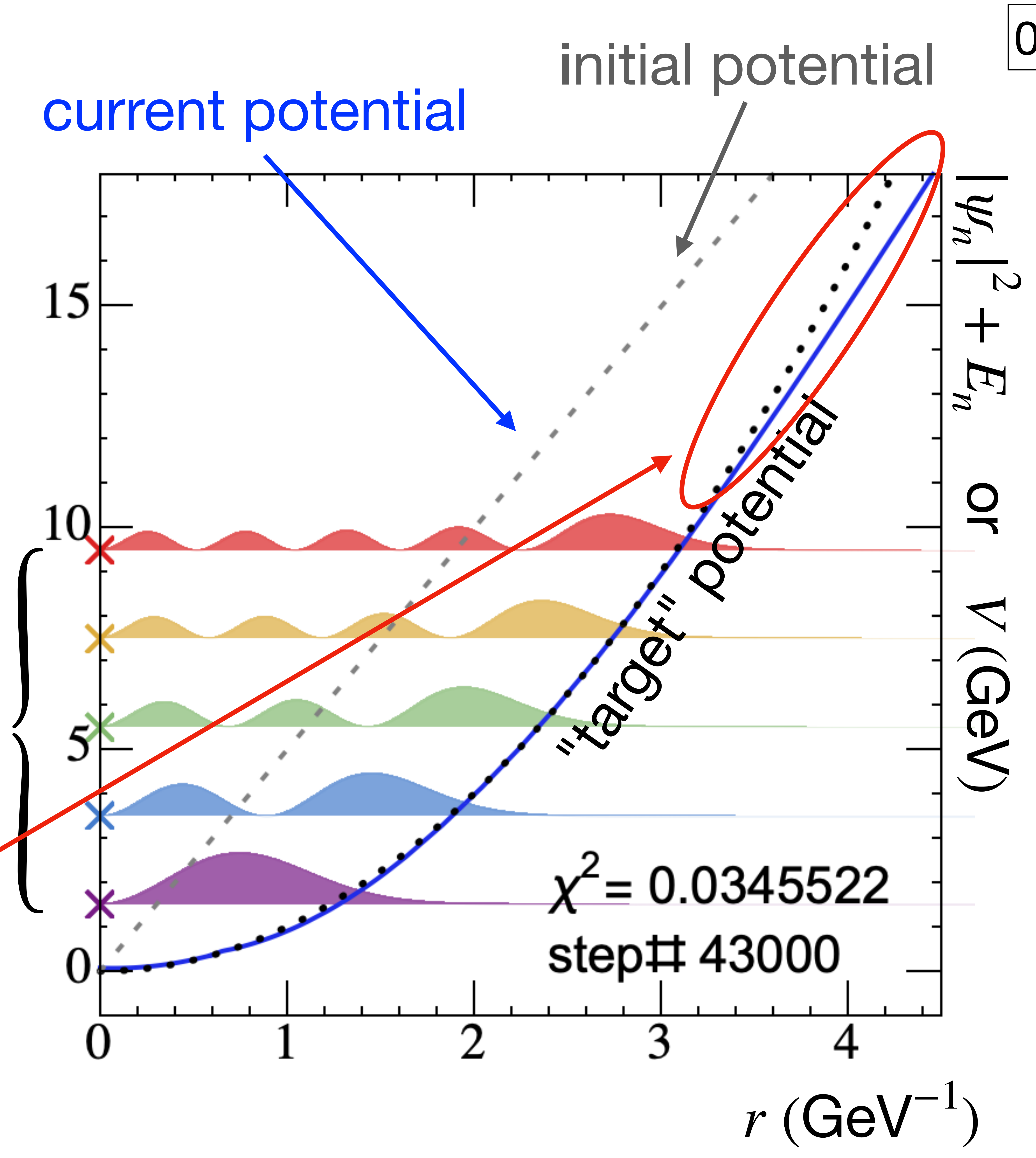
learn $V(r)$ according to

$$\{E_n\} = \left\{\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \frac{15}{2}, \frac{19}{2}\right\} \text{ GeV}$$

target spectrum

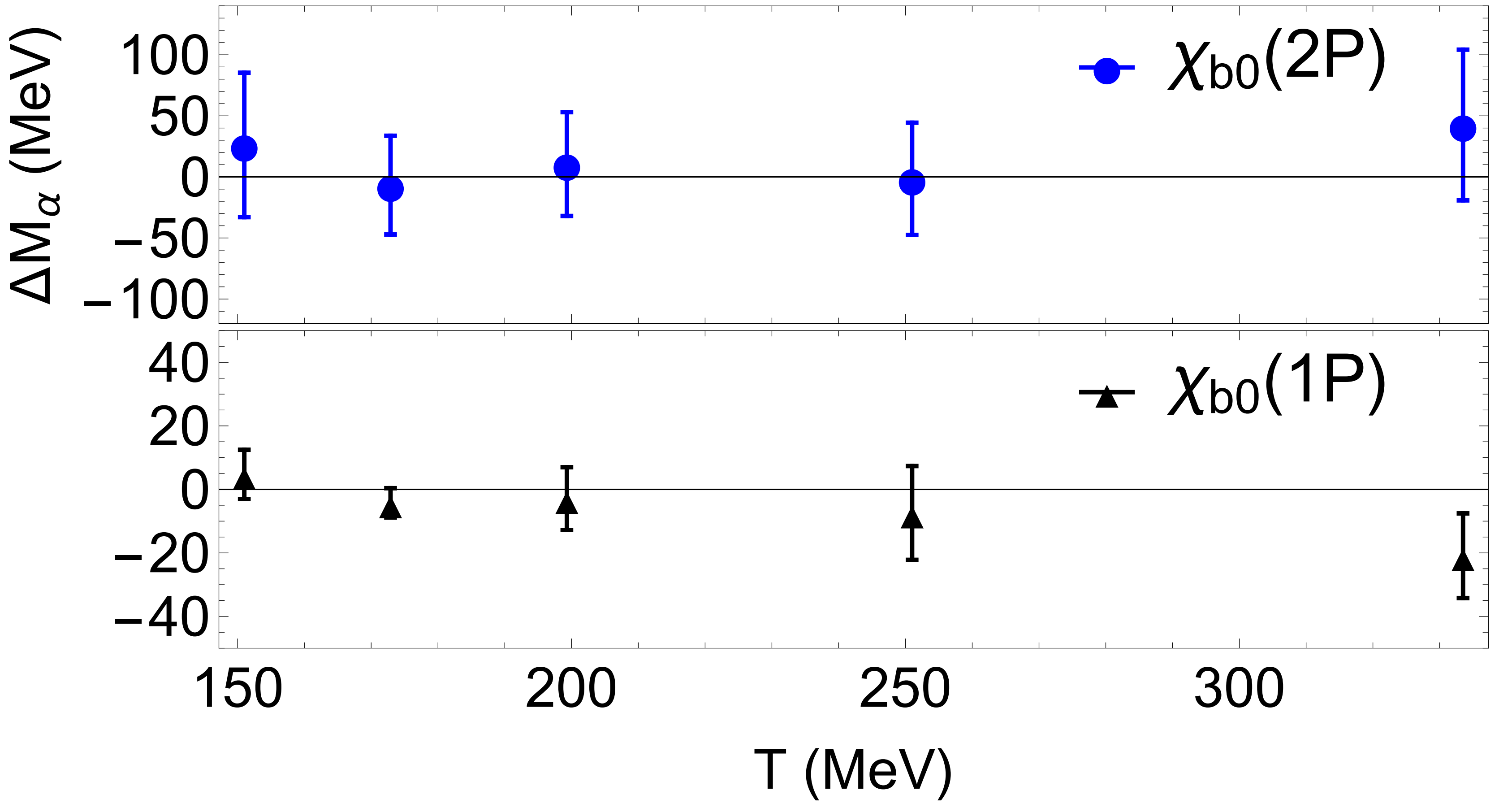
Deviate from the exact potential where all $\psi_n \to 0$,

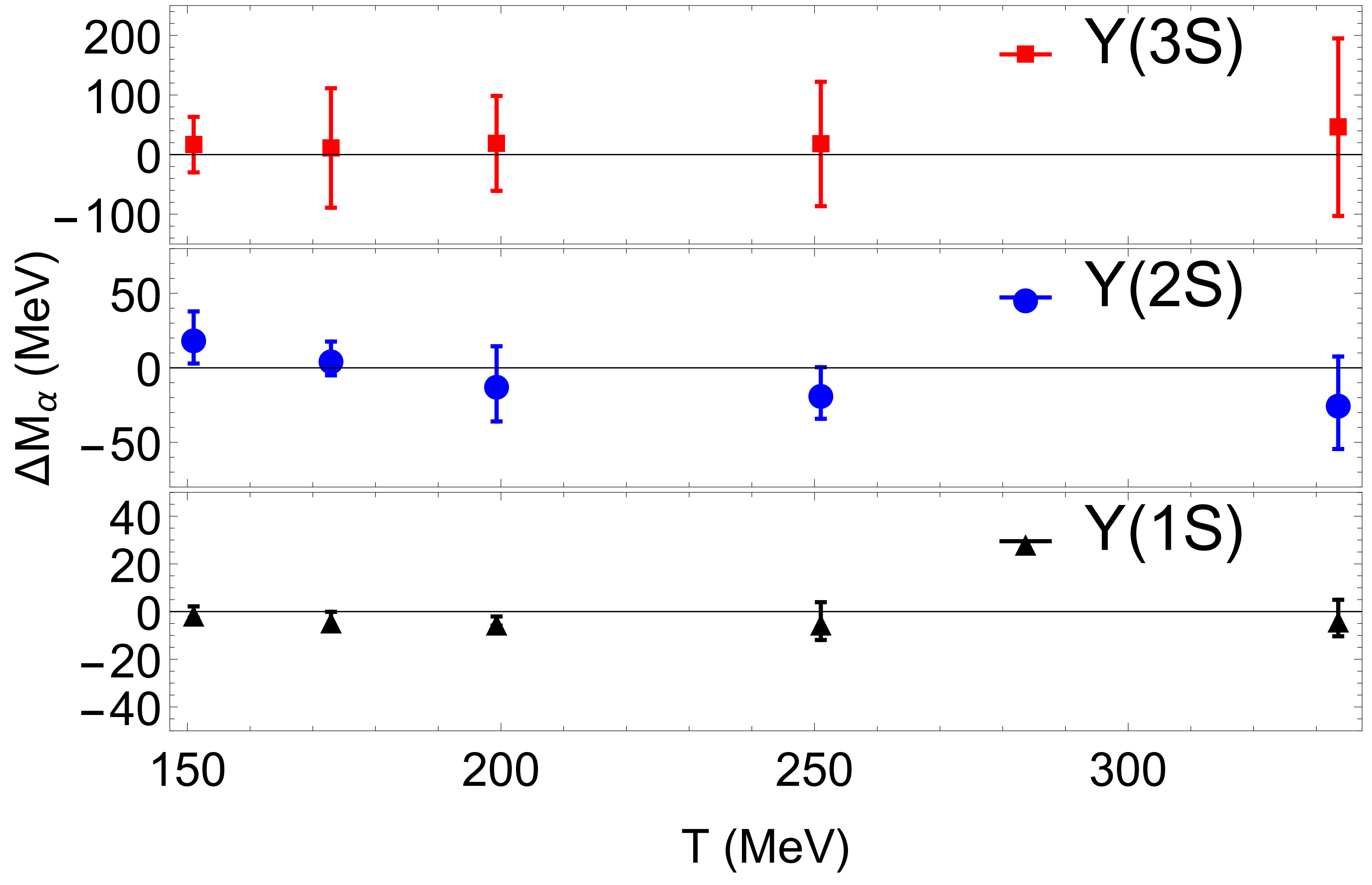
$$\delta E_n = \langle \psi_n | \delta V(r) | \psi_n \rangle$$



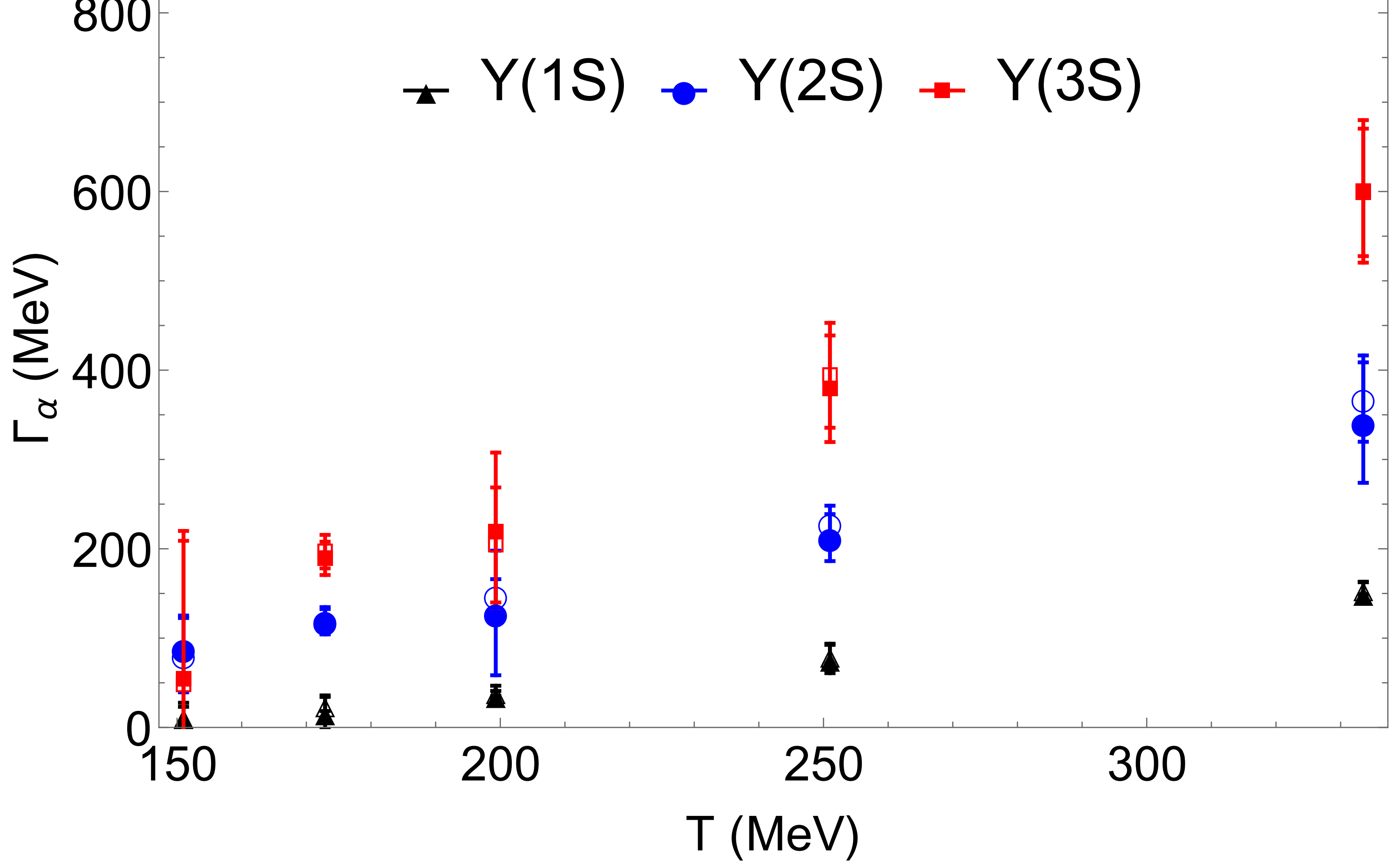
Bottomonium mass and thermal width, lattice QCD with finite m_Q

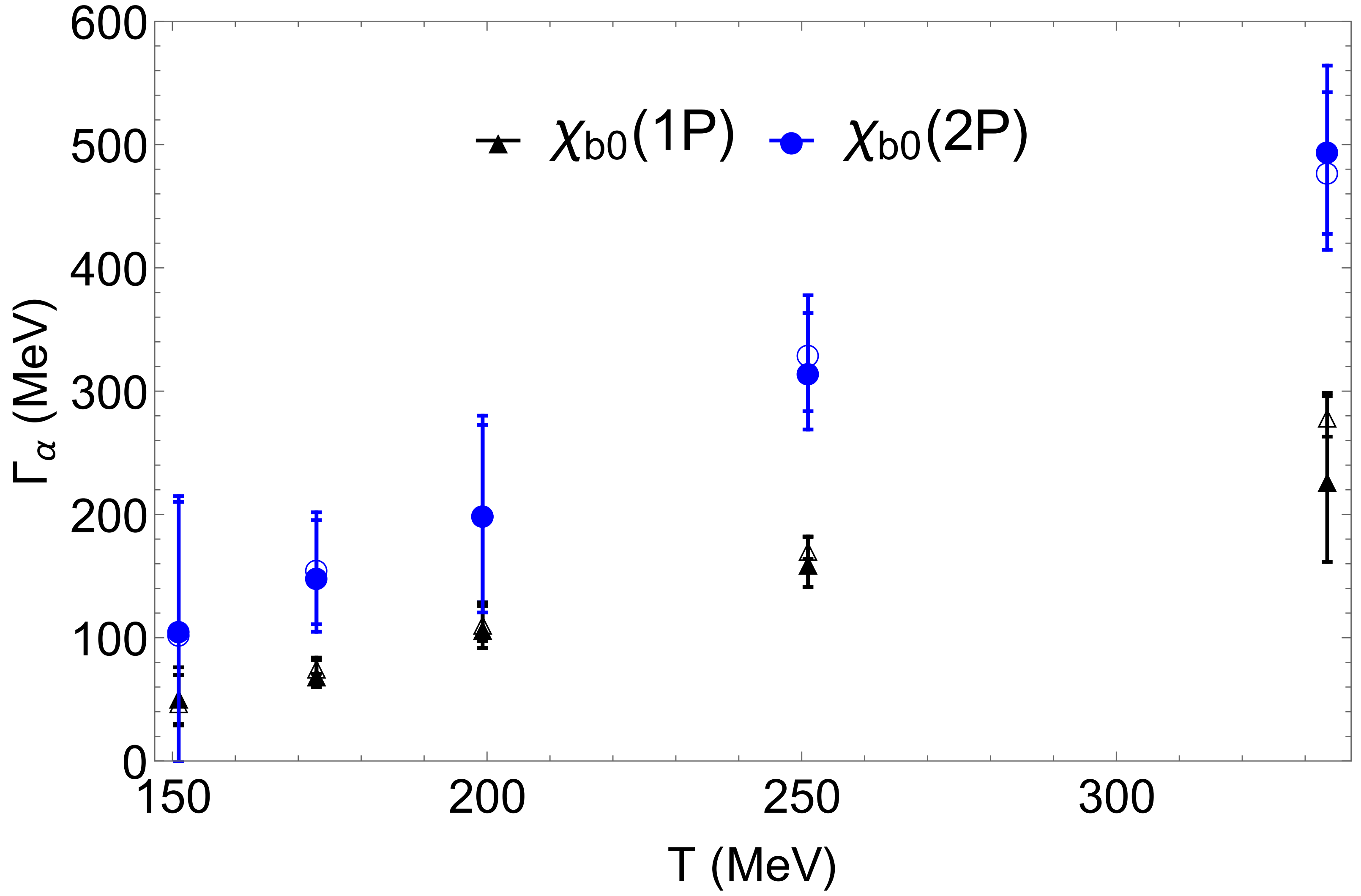
Mass





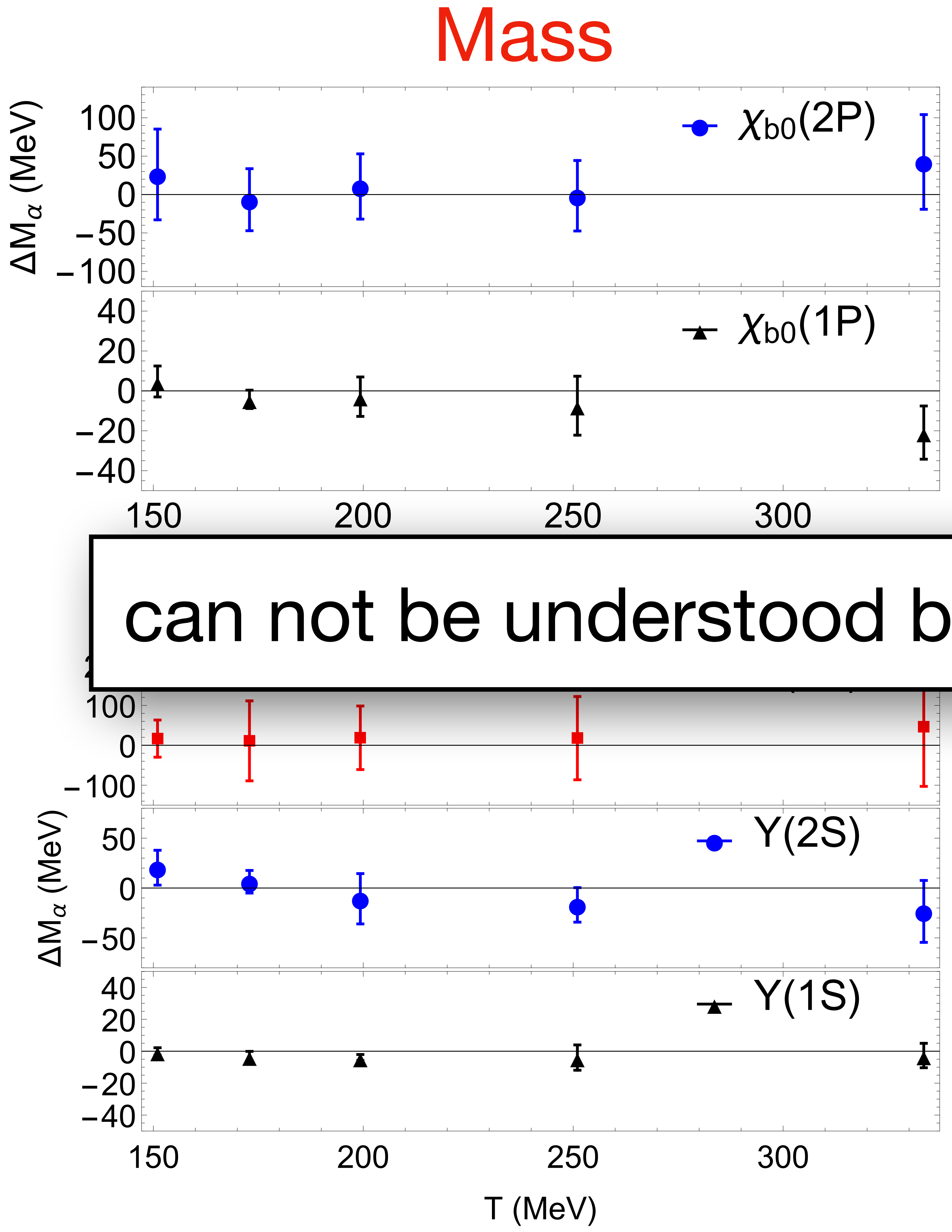
Thermal Width

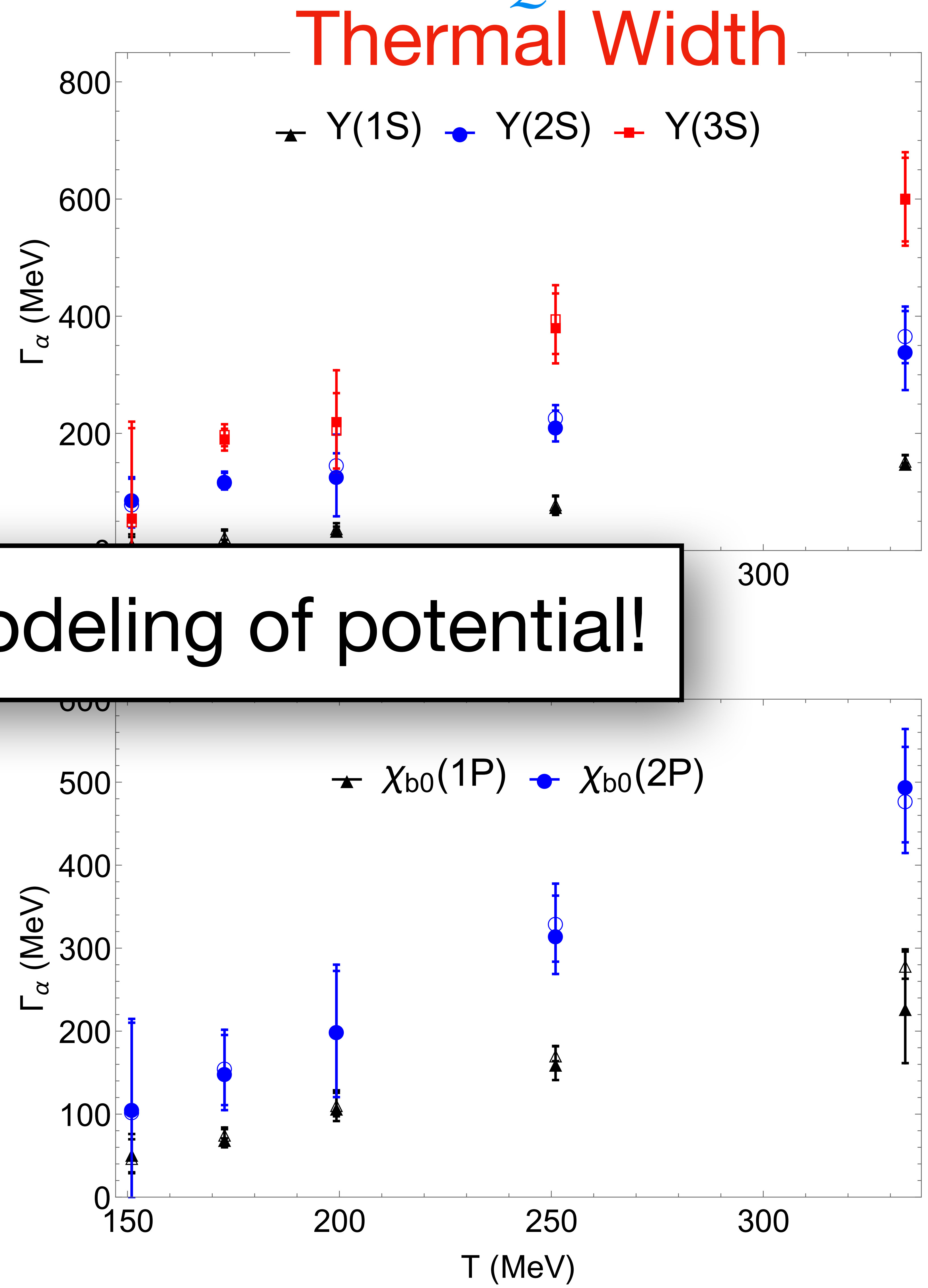




Lattice QCD: Phys.Rev.D100,074506(2019),Phys.Lett.B800,135119(2020),Phys.Rev.D102,114508(2020)

Bottomonium mass and thermal width, lattice QCD with finite m_Q

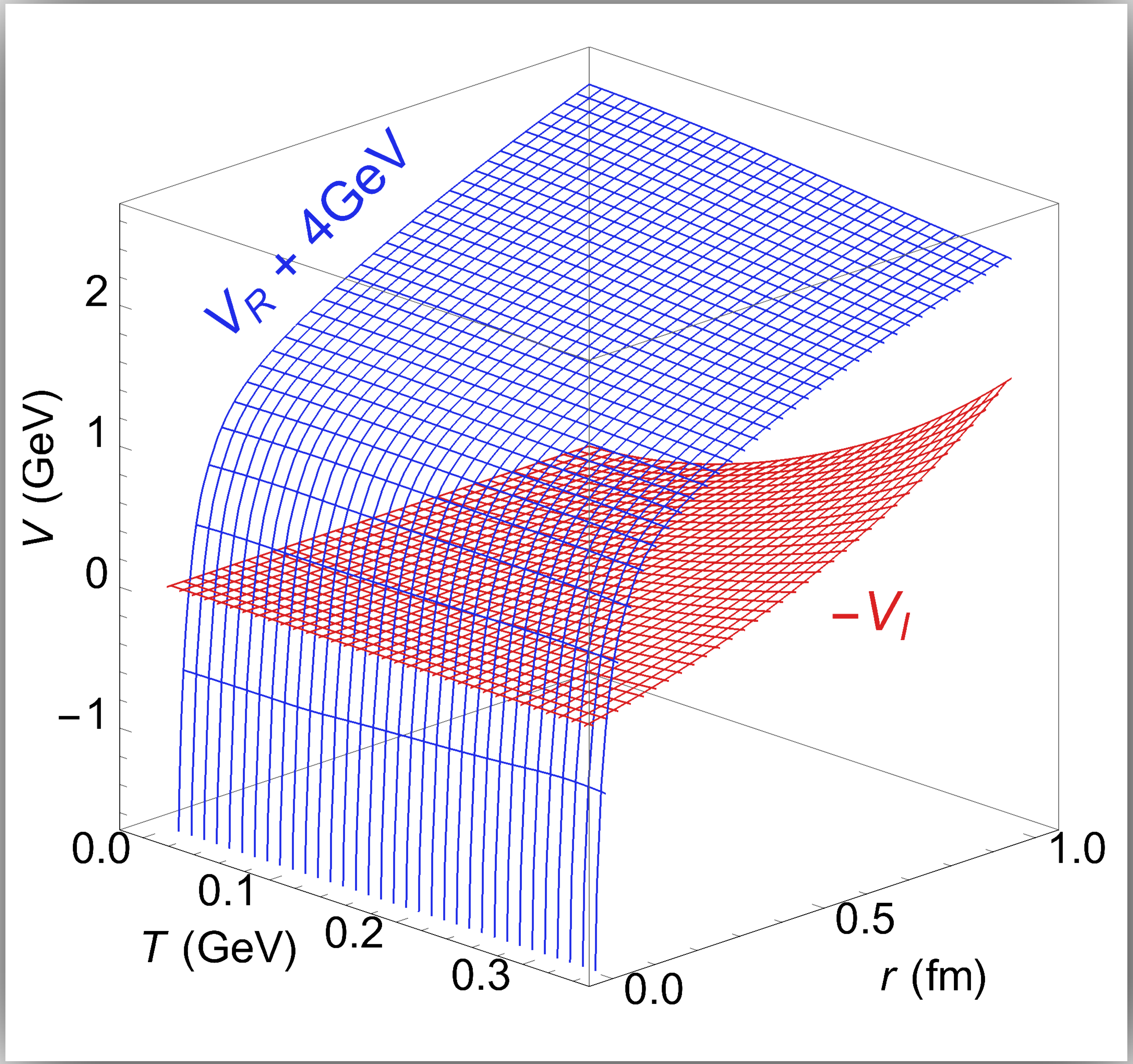




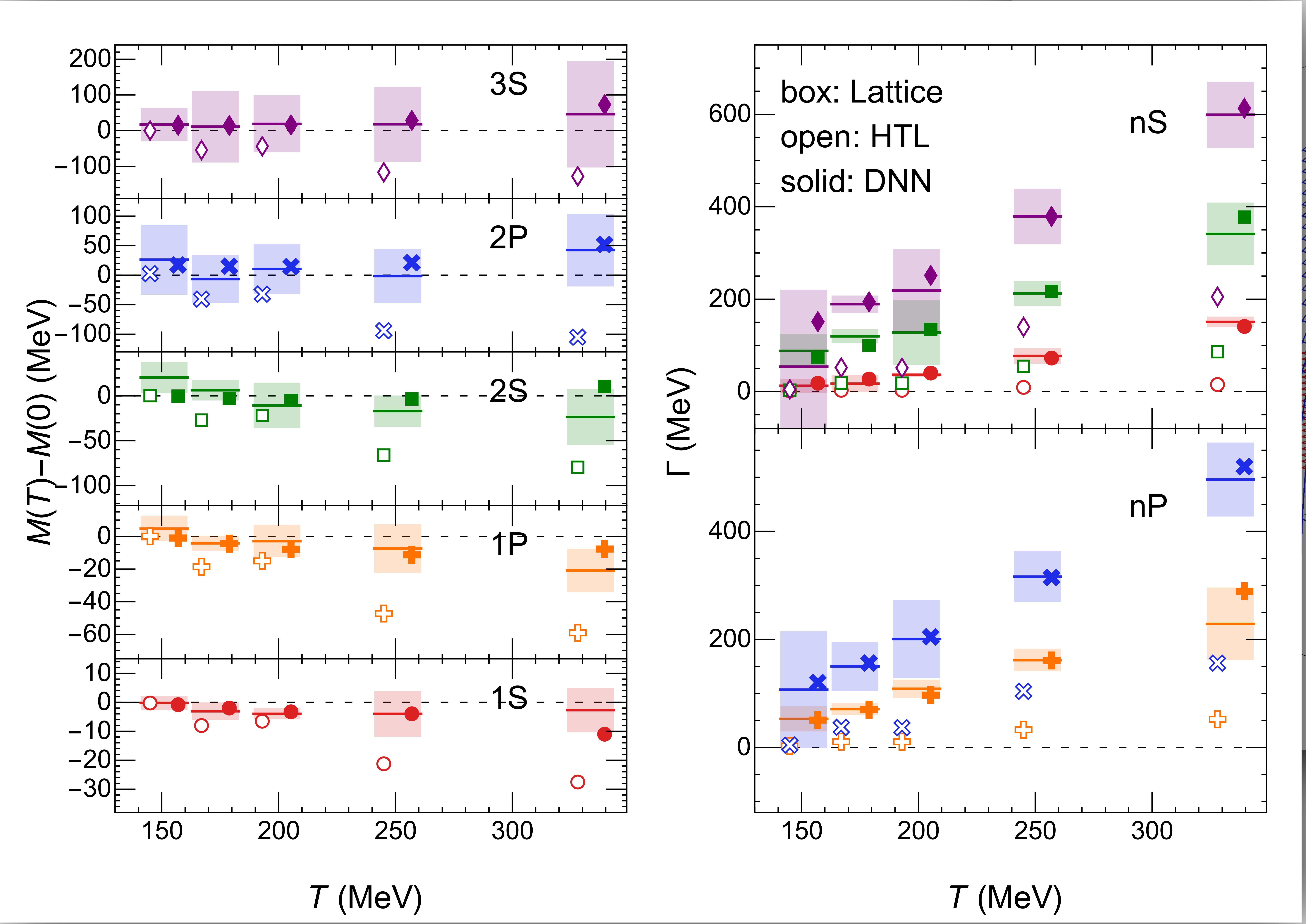
can not be understood by existing modeling of potential!

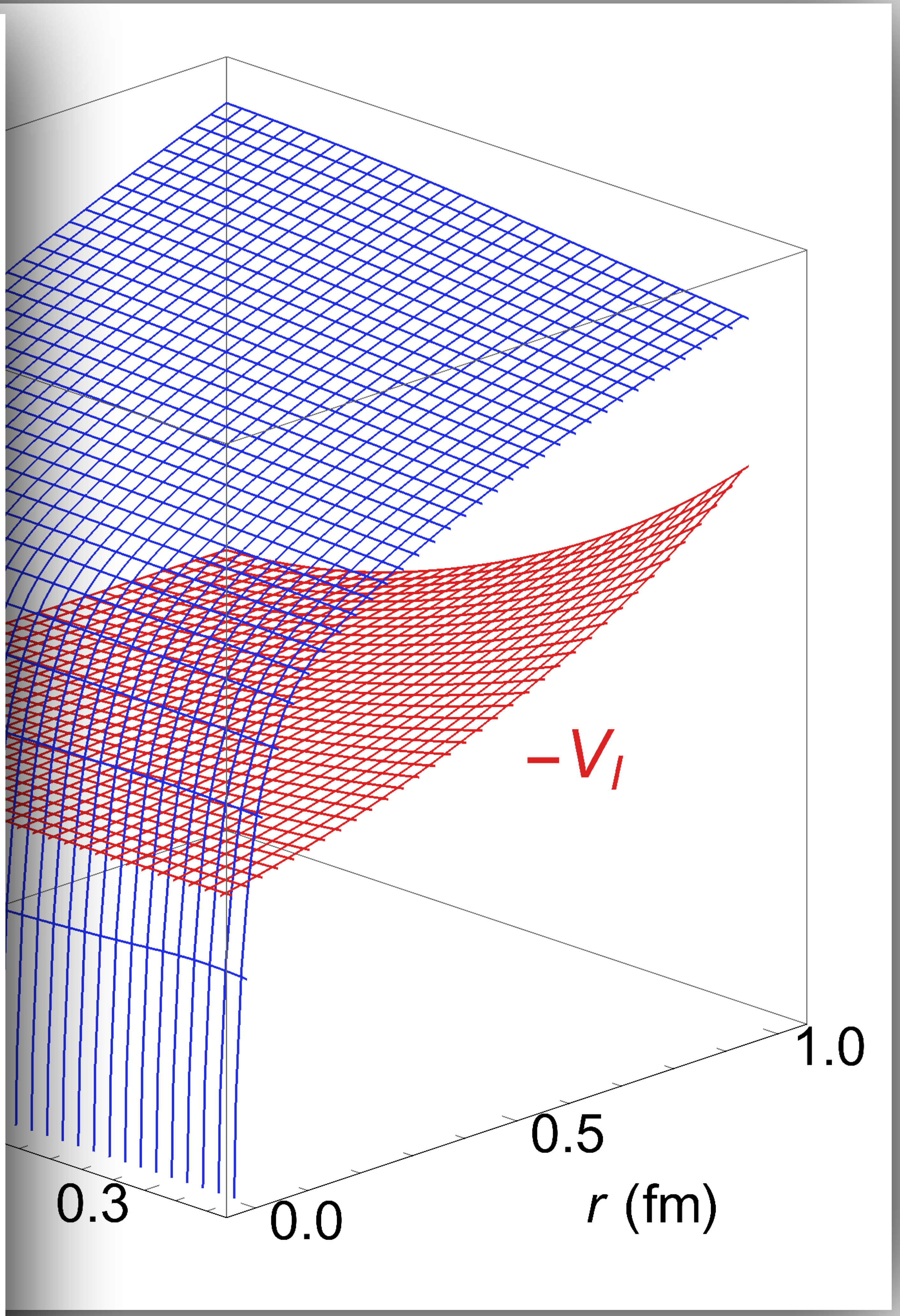
Lattice QCD: Phys.Rev.D100,074506(2019),Phys.Lett.B800,135119(2020),Phys.Rev.D102,114508(2020)

Finite Temperature Heavy-Quark Potential

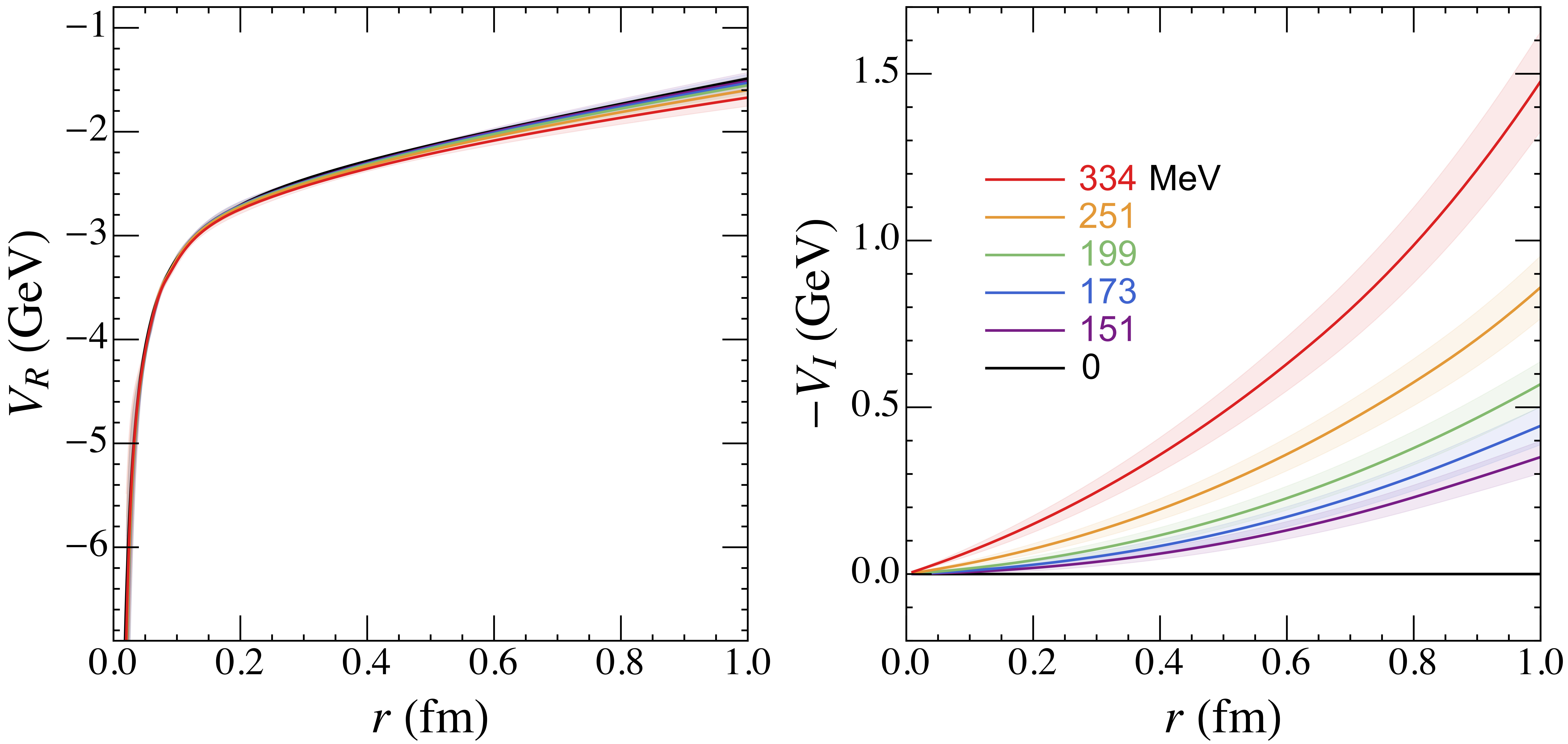


Finite Temperature Heavy-Quark Potential



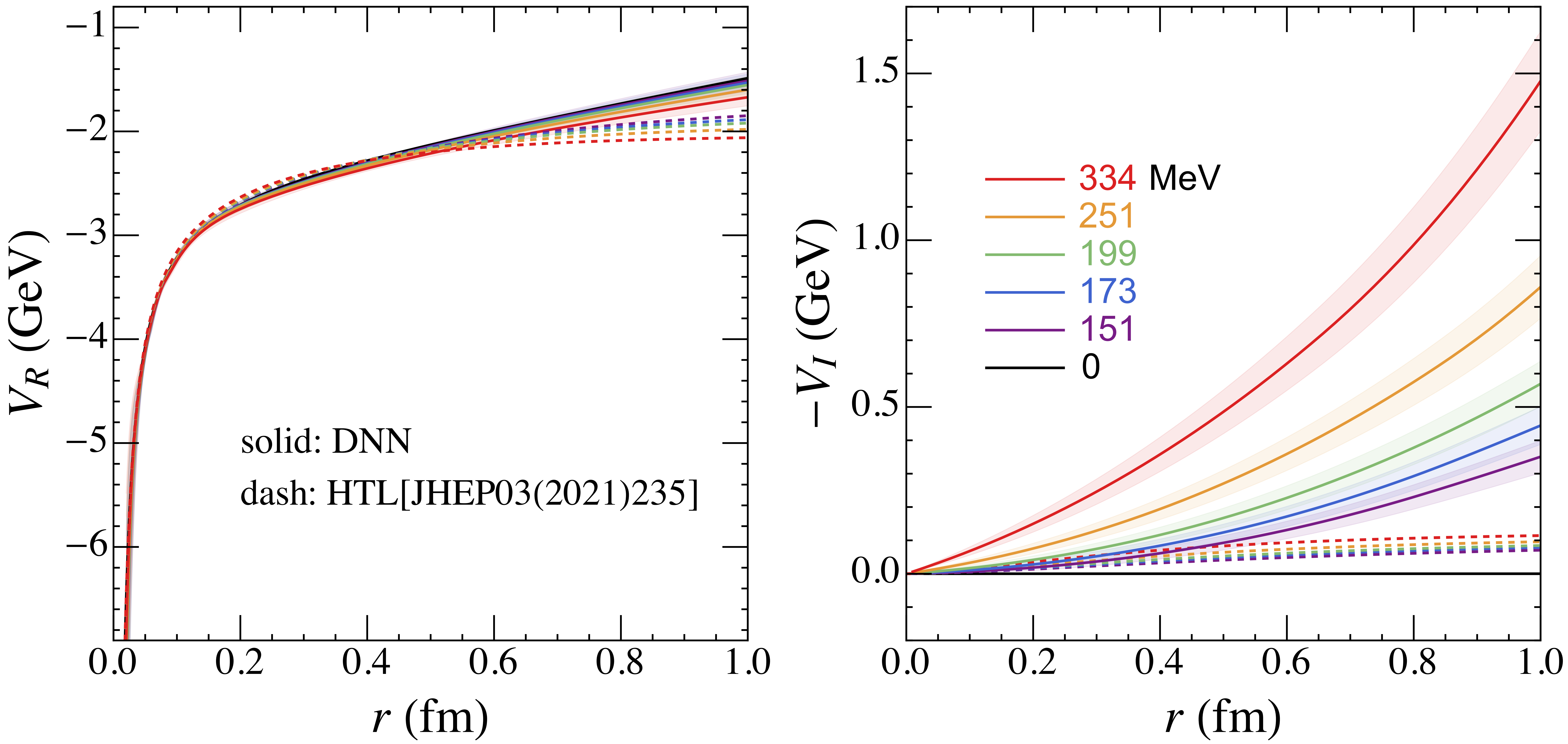


What physics we have learned from $V_{\text{DNN}}(T, r)$?



What physics we have learned from $V_{\text{DNN}}(T, r)$?

--- compare with HTL potential model



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PHYSICAL REVIEW D **105**, 054513 (2022)

Static quark-antiquark interactions at nonzero temperature from lattice QCD

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PHYSICAL REVIEW D **105**, 014017 (2022)

Heavy quark potential in the quark-gluon plasma: Deep neural network meets lattice quantum chromodynamics

Shuzhe Shi,[1,*] Kai Zhou,[2,†] Jiaxing Zhao,[3] Swagato Mukherjee,[4] and Pengfei Zhuang[3]
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[2]*Frankfurt Institute for Advanced Studies, Ruth Moufang Strasse 1, D-60438, Frankfurt am Main, Germany*
[3]*Department of Physics, Tsinghua University, Beijing 100084, China*
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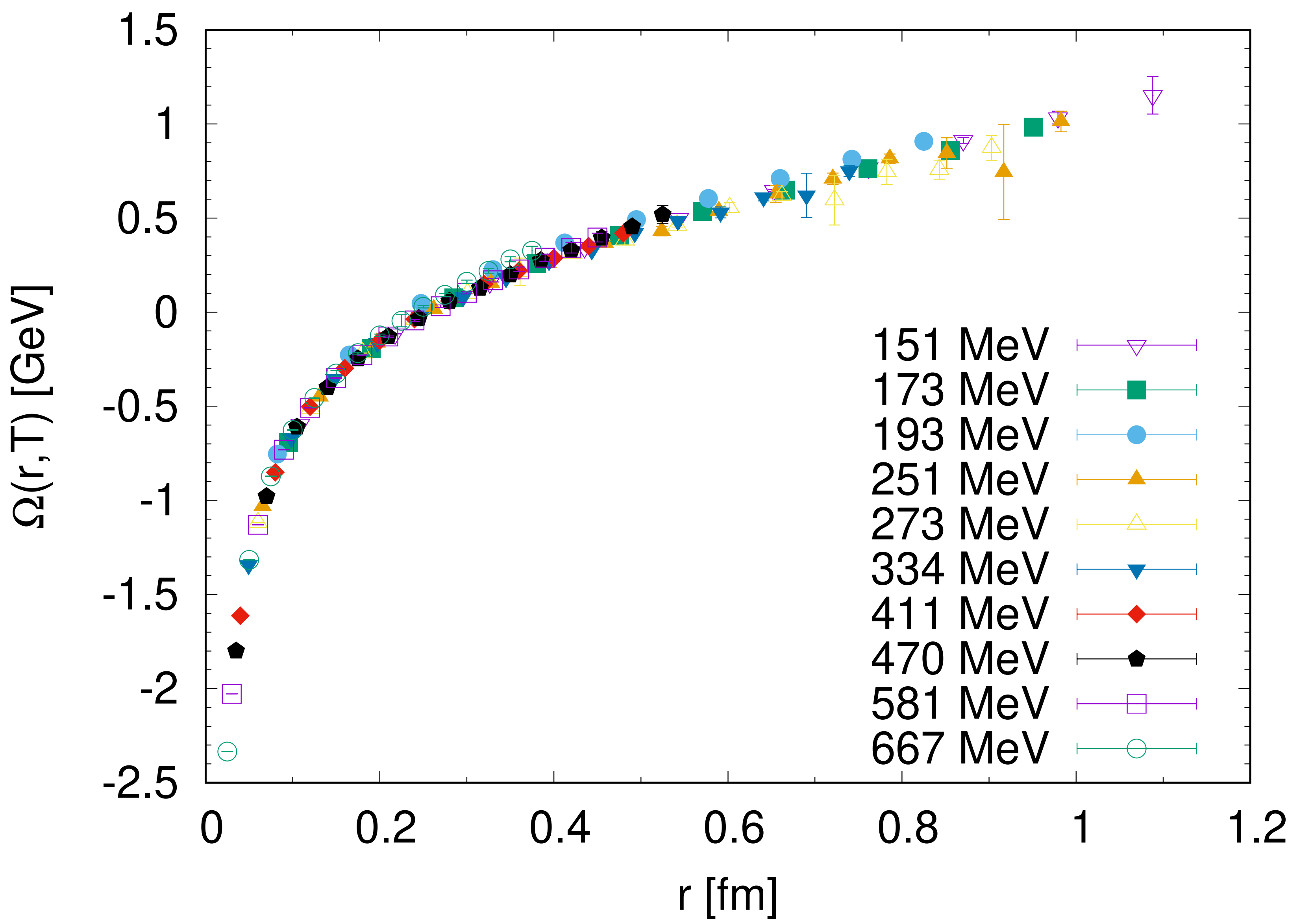

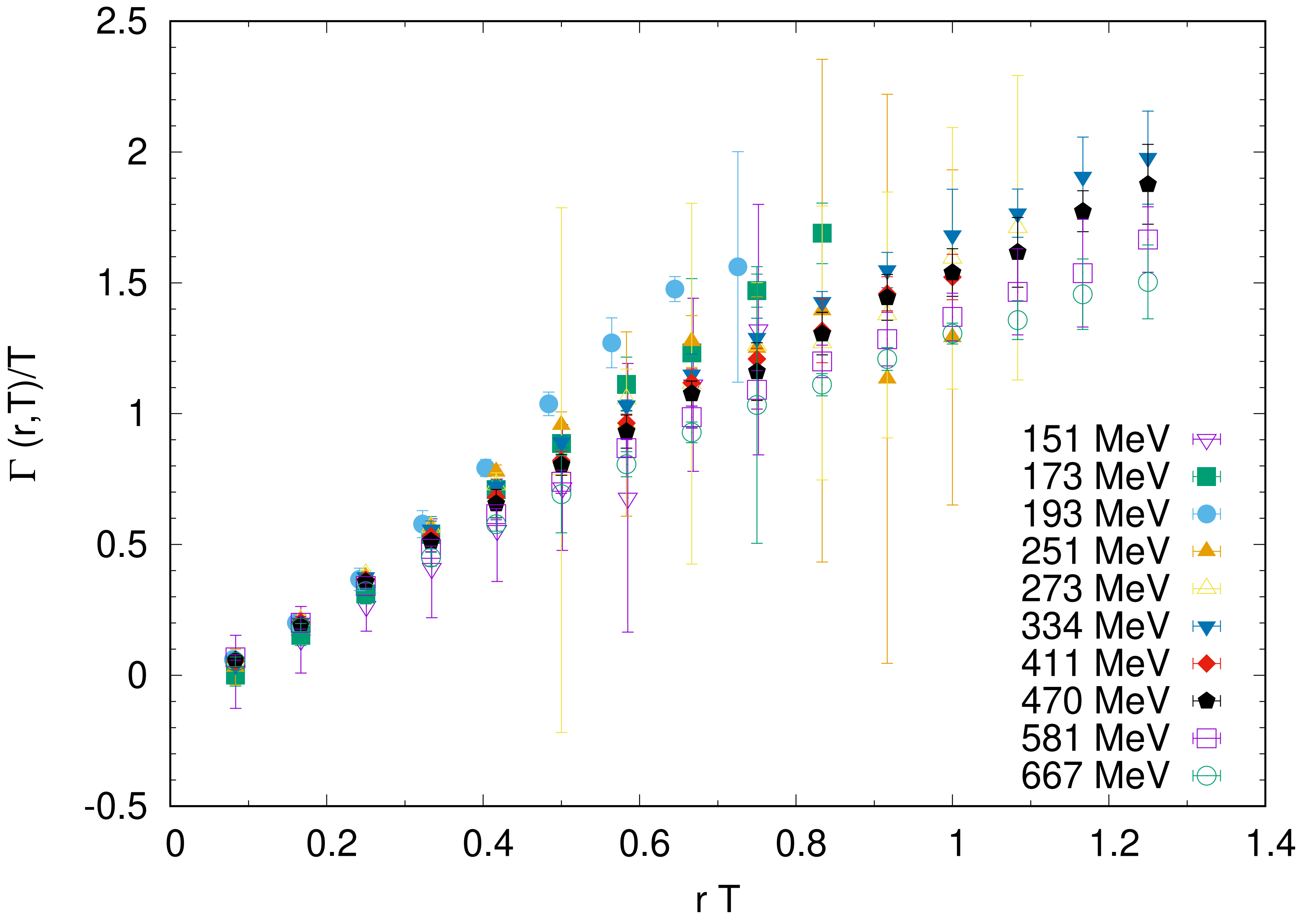

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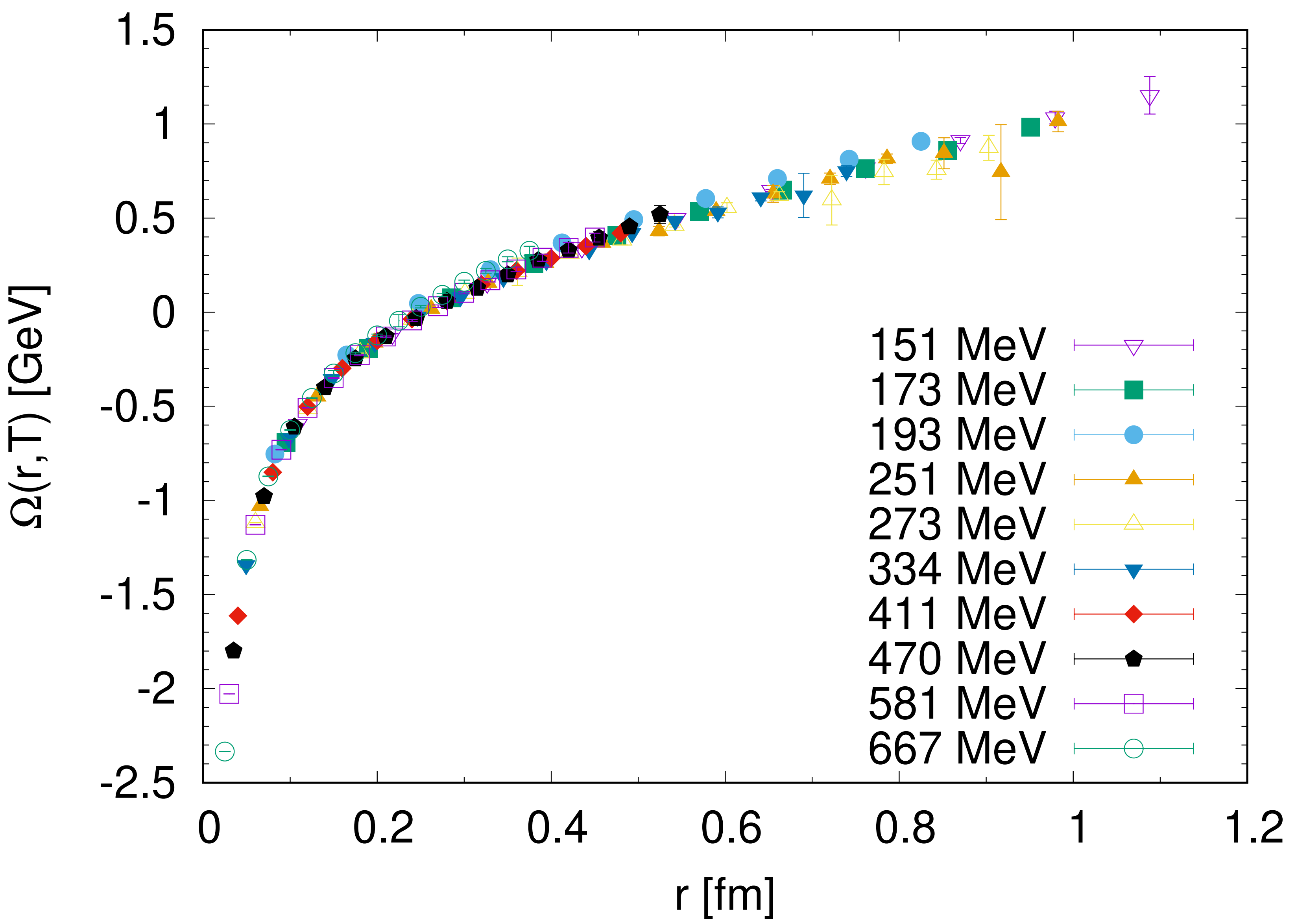

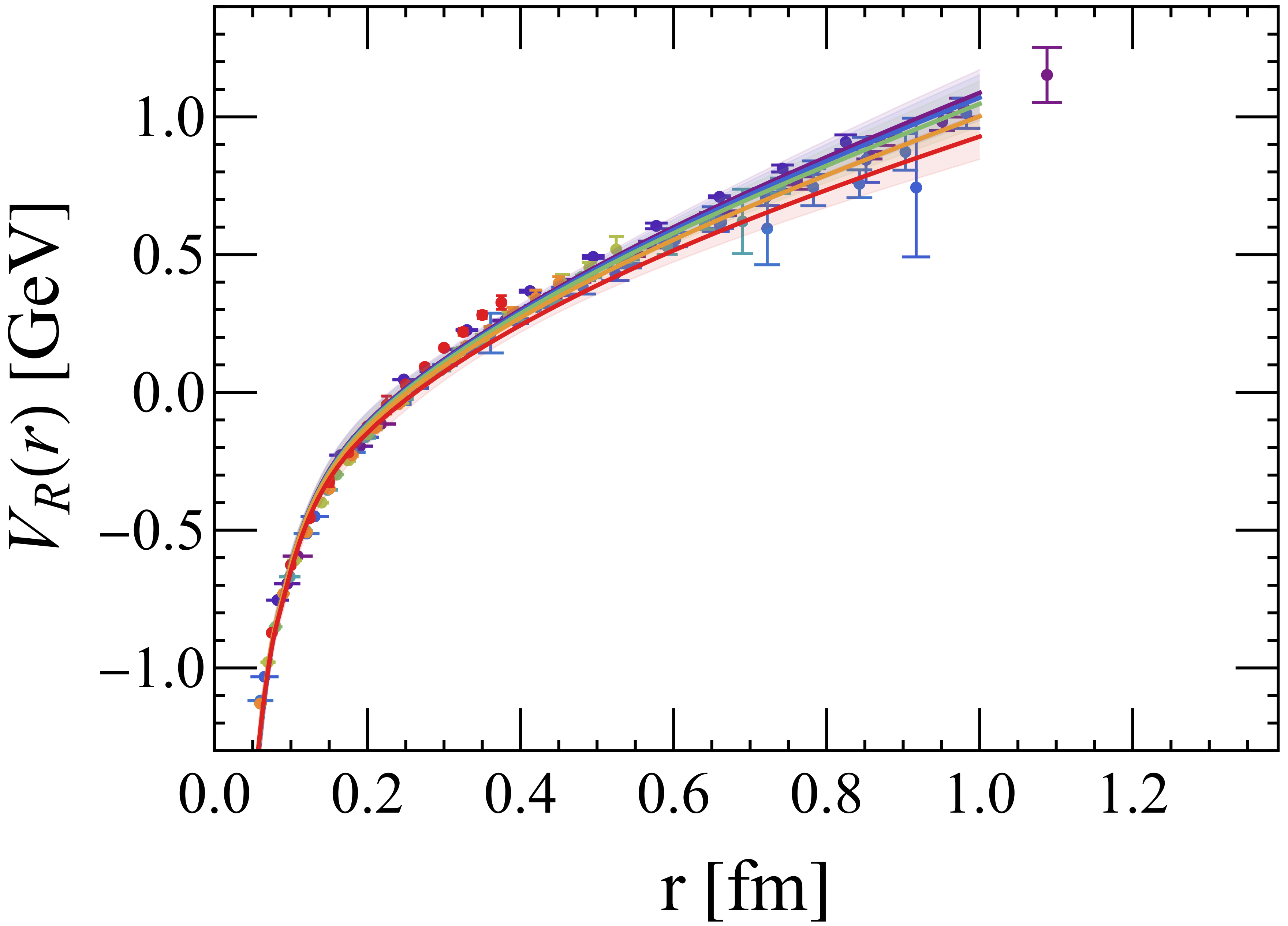

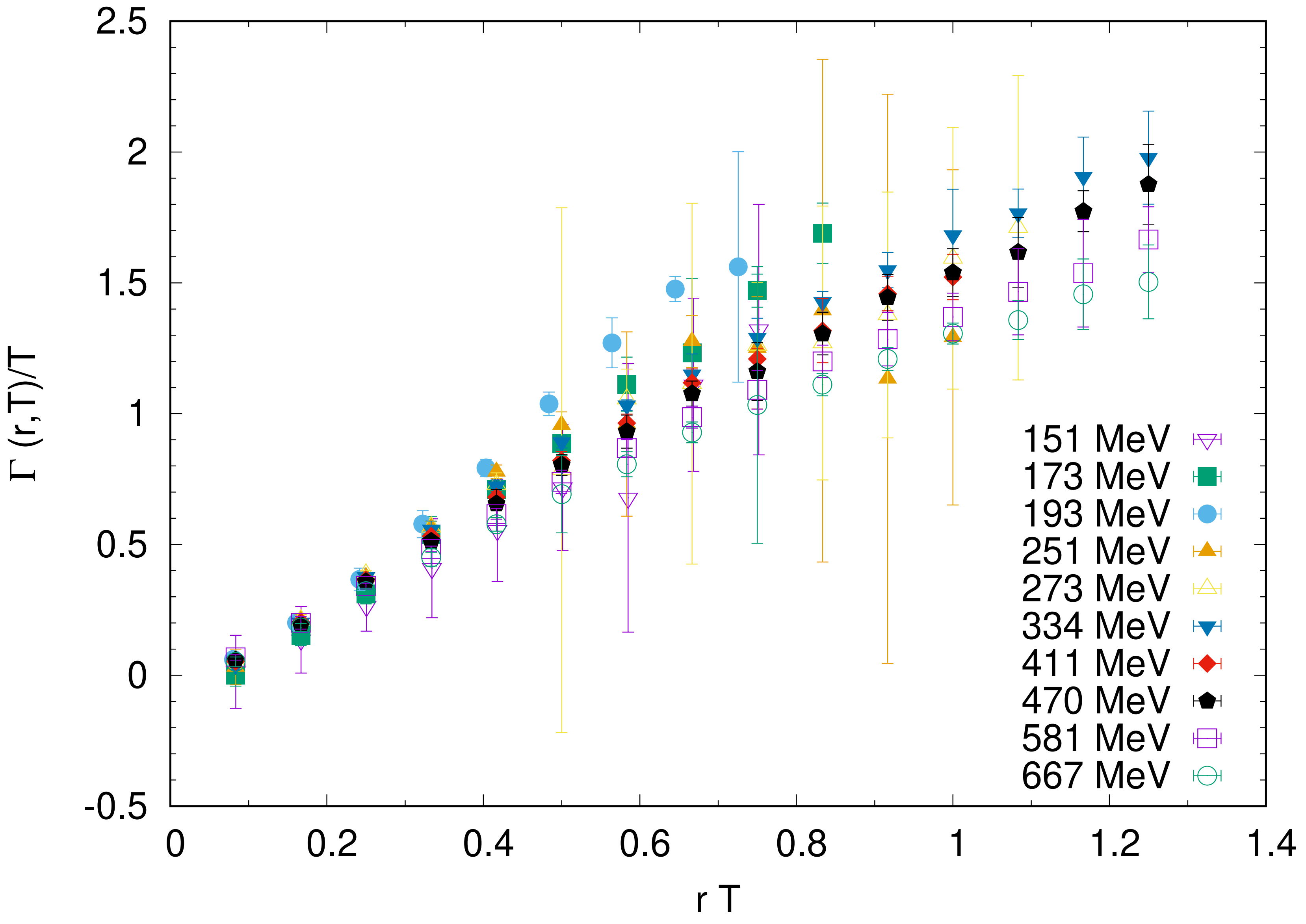

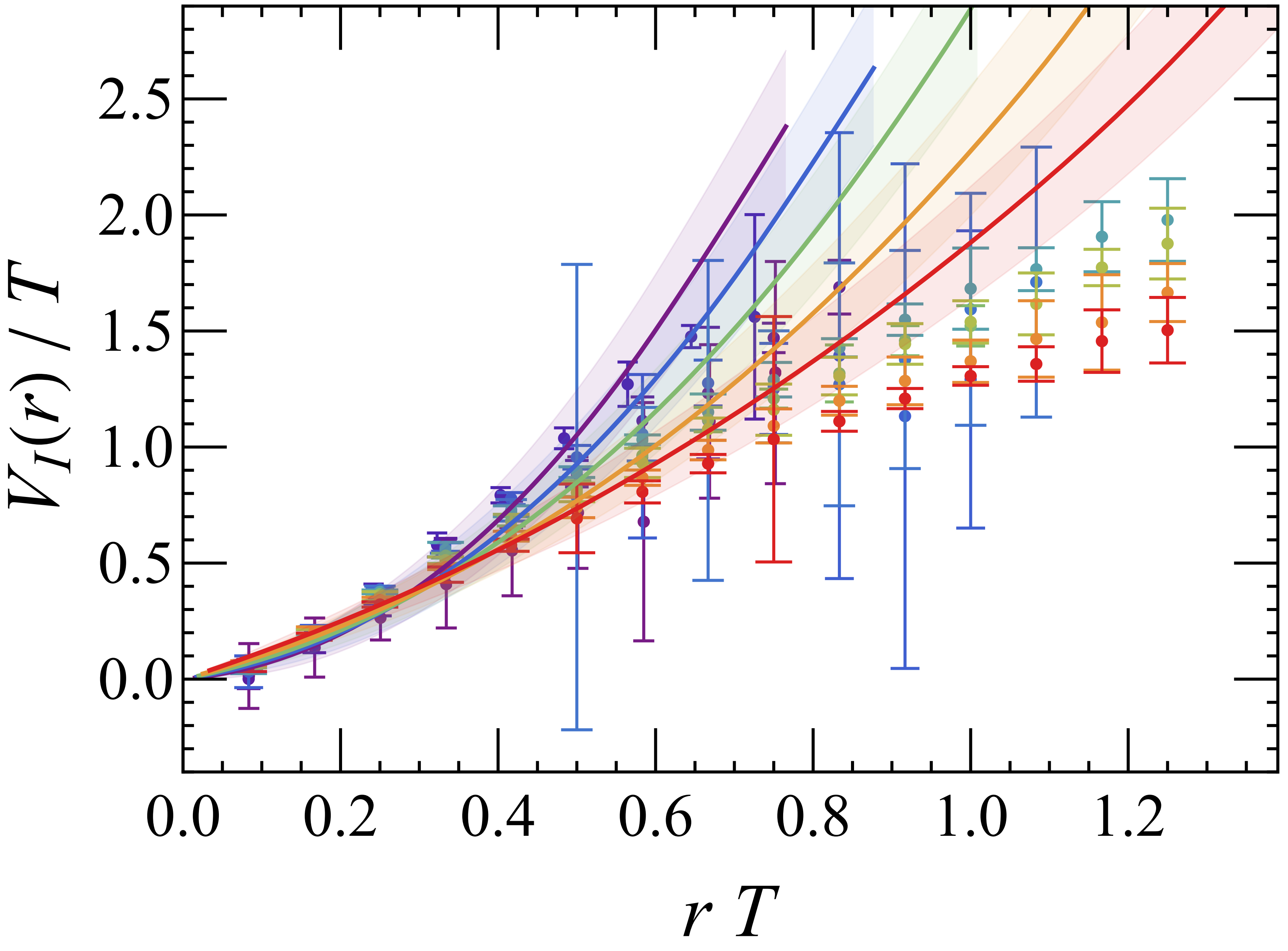

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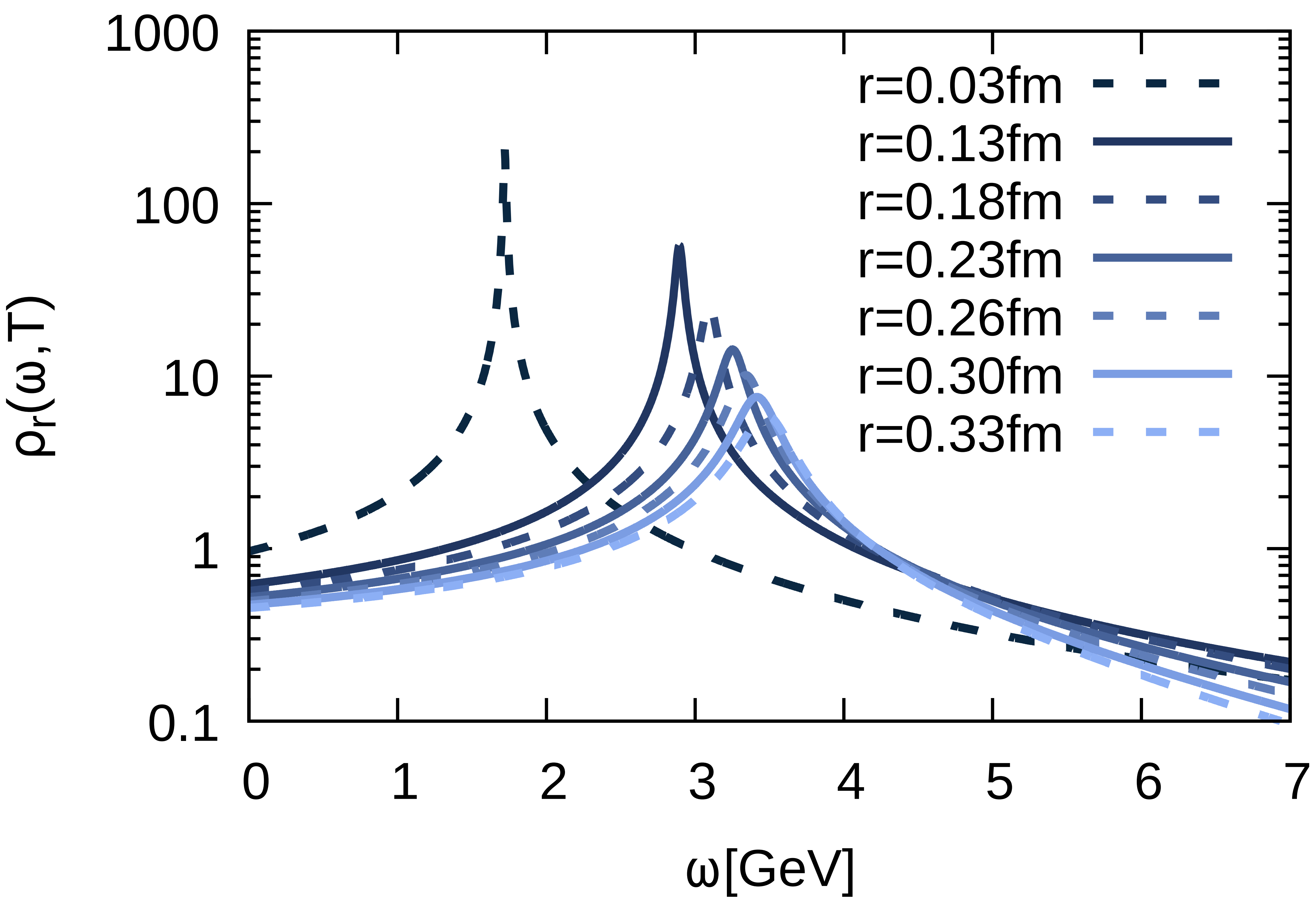

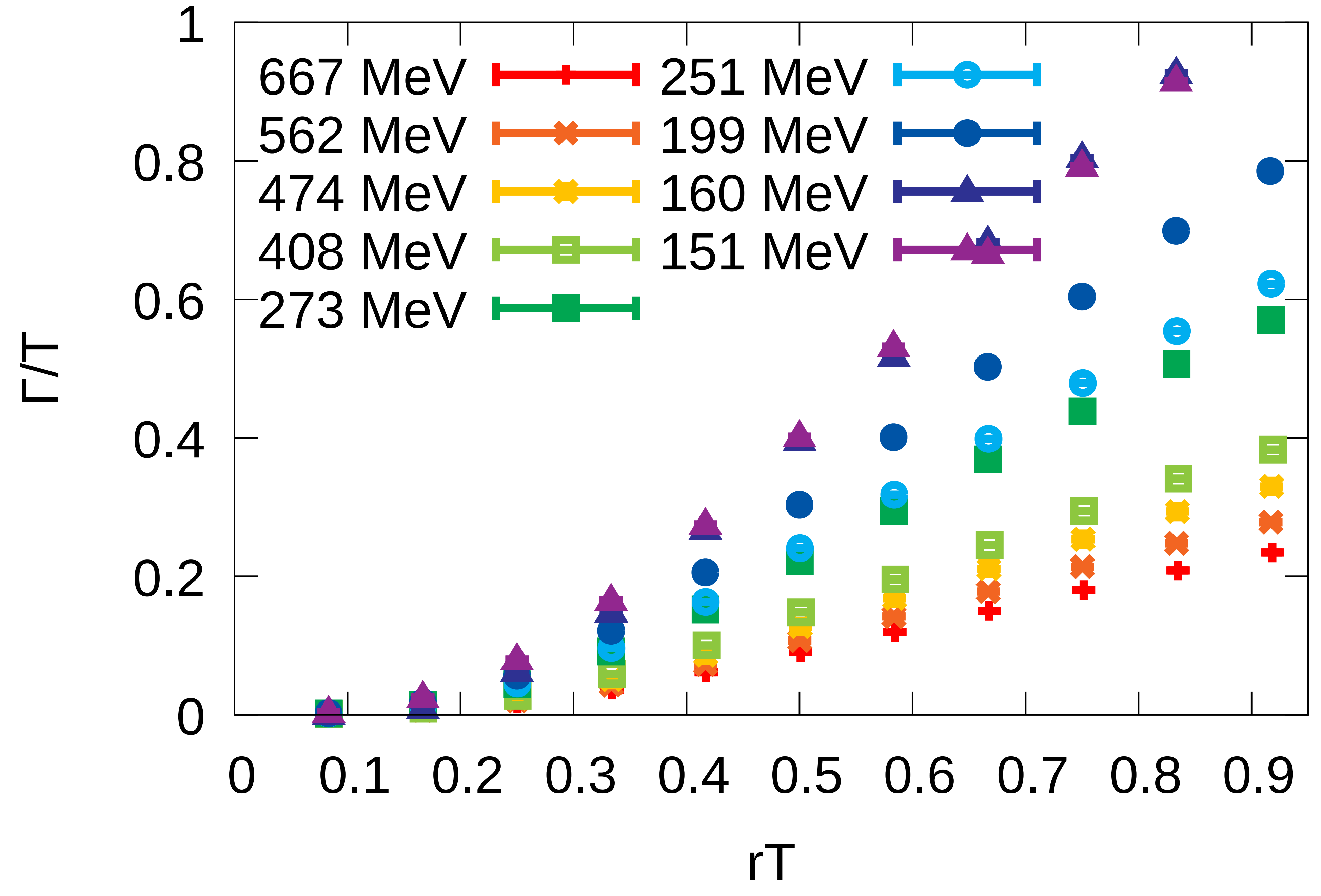

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Problem # II:

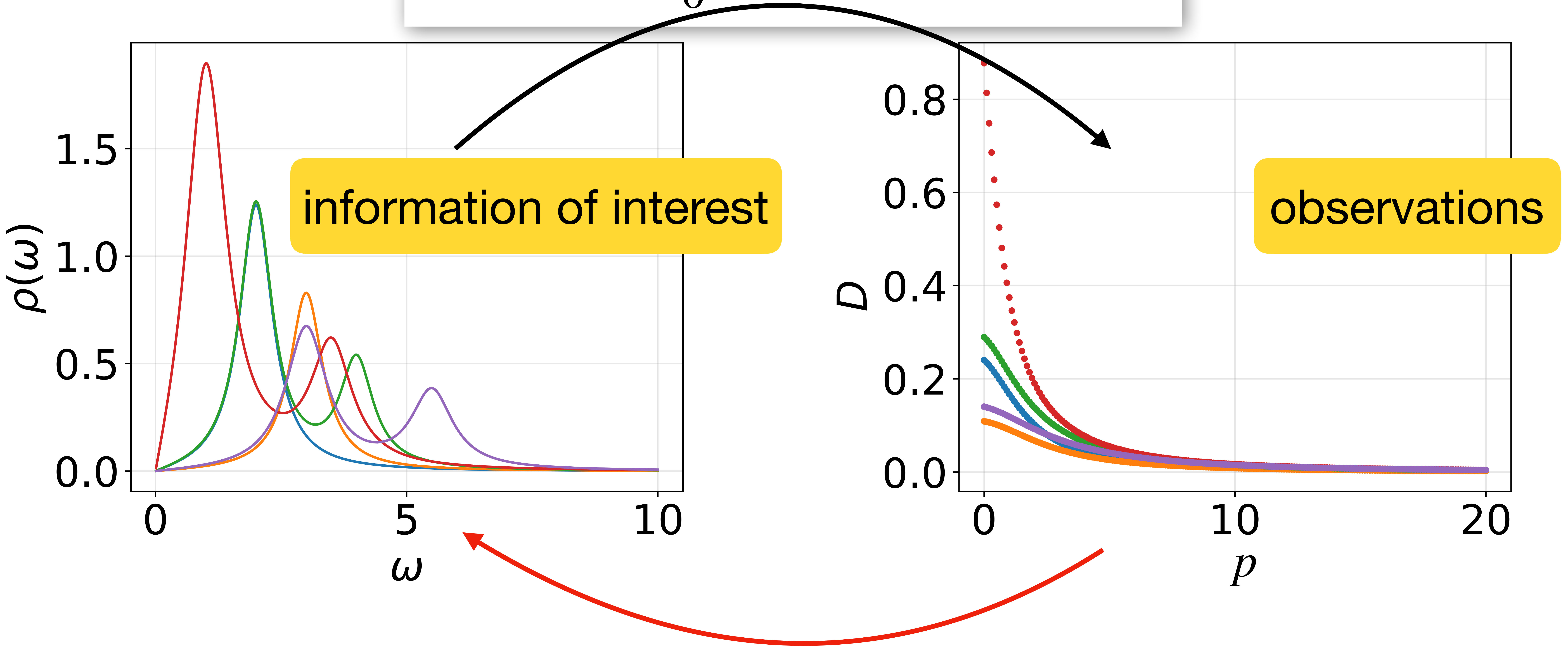
spectral function reconstruction

refs:

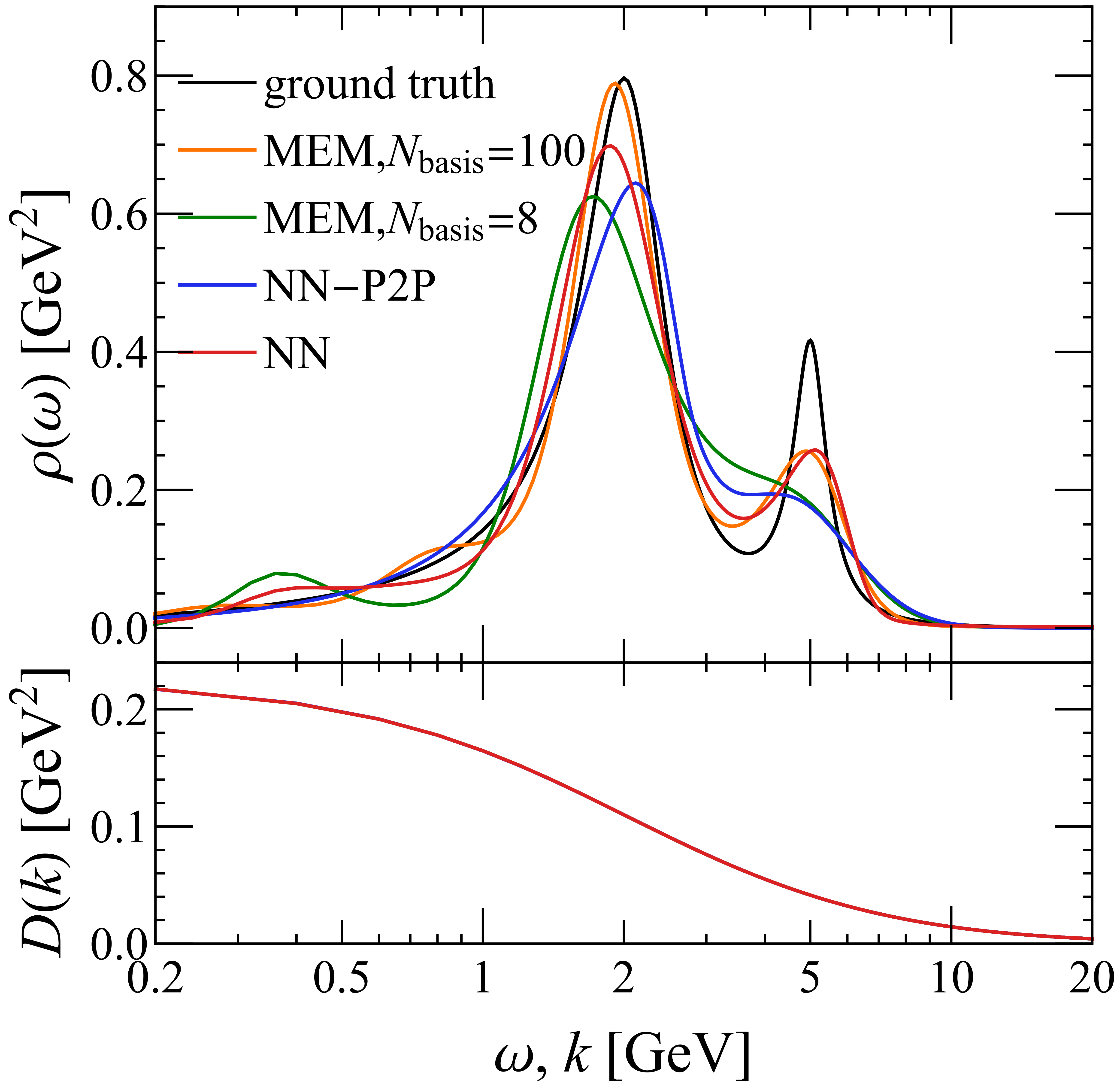
SS, Wang, Zhou, Comput.Phys.Commun. 282 (2023) 108547;
Wang, ***SS***, Zhou, Phys. Rev. D **106**, L051502;

3. spectral function <=> correlation

$$D(p) = \int_0^\infty K(p,\omega)\,\rho(\omega)\,d\omega \qquad K(p,\omega) \equiv \frac{\pi^{-1}\,\omega}{\omega^2 + p^2}$$



Can one learn the spectral function from correlation?



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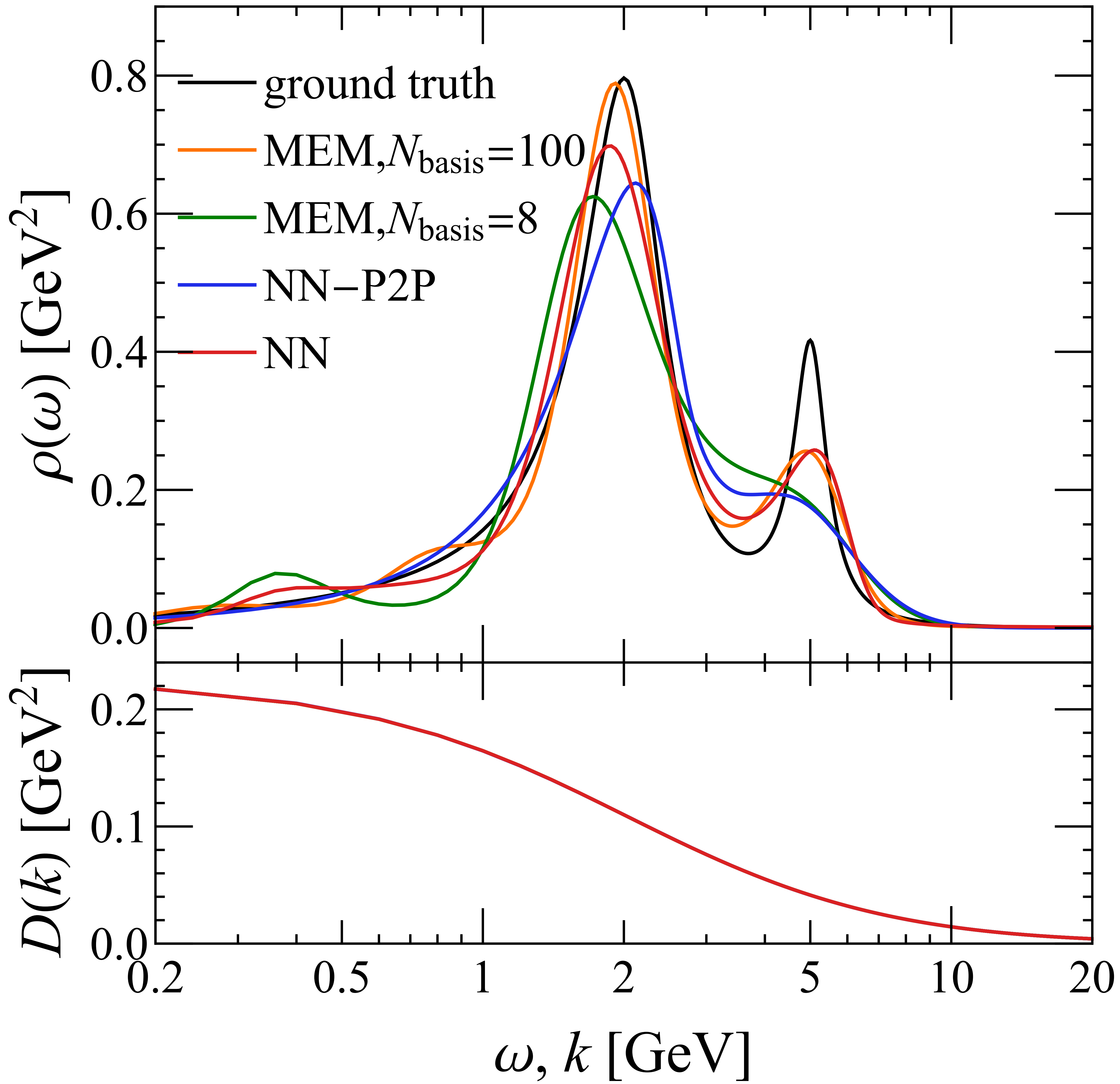
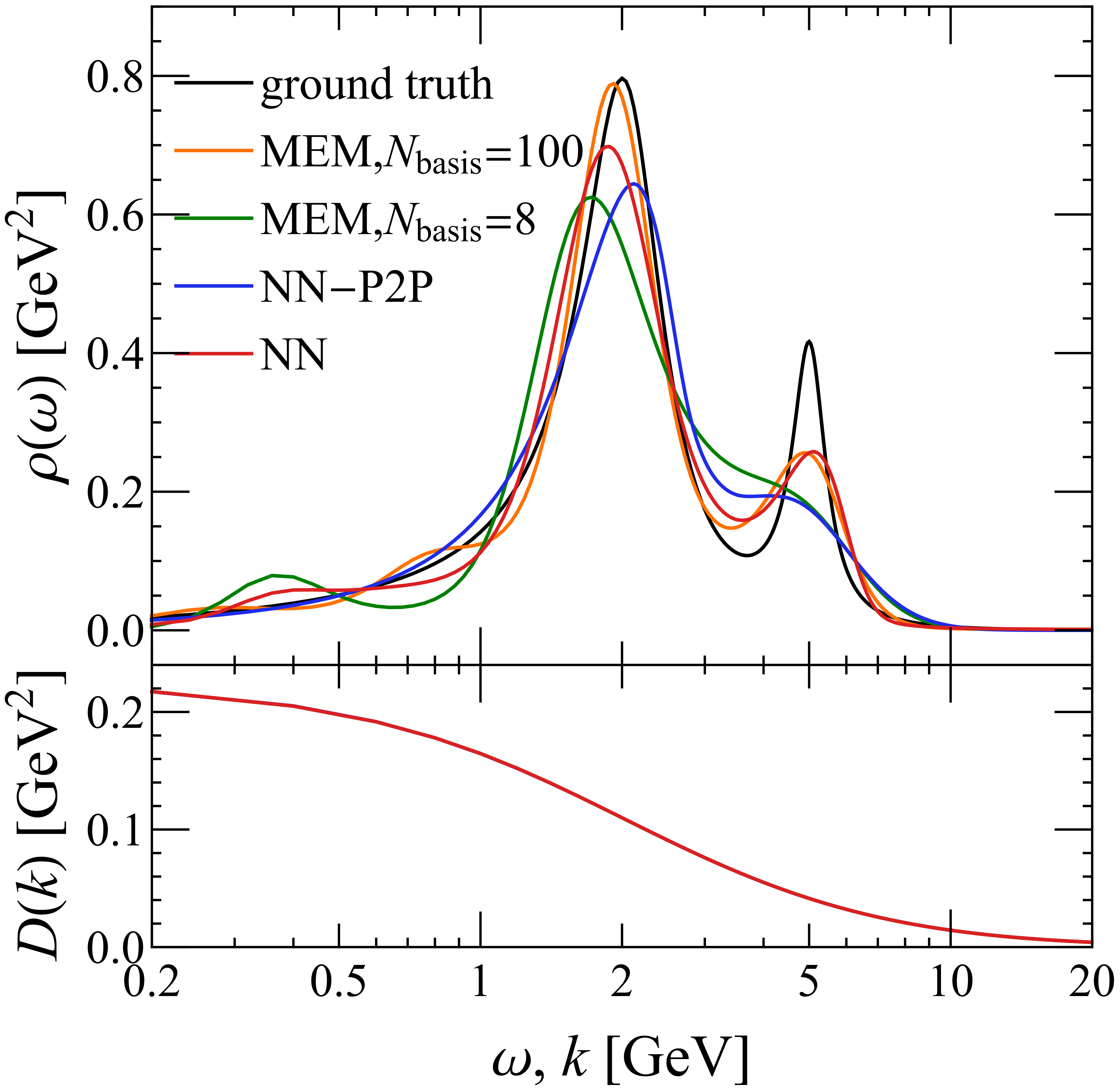


- ill-conditioned?
  - one needs more points in ω than that were given in k

Can one learn the spectral function from correlation?



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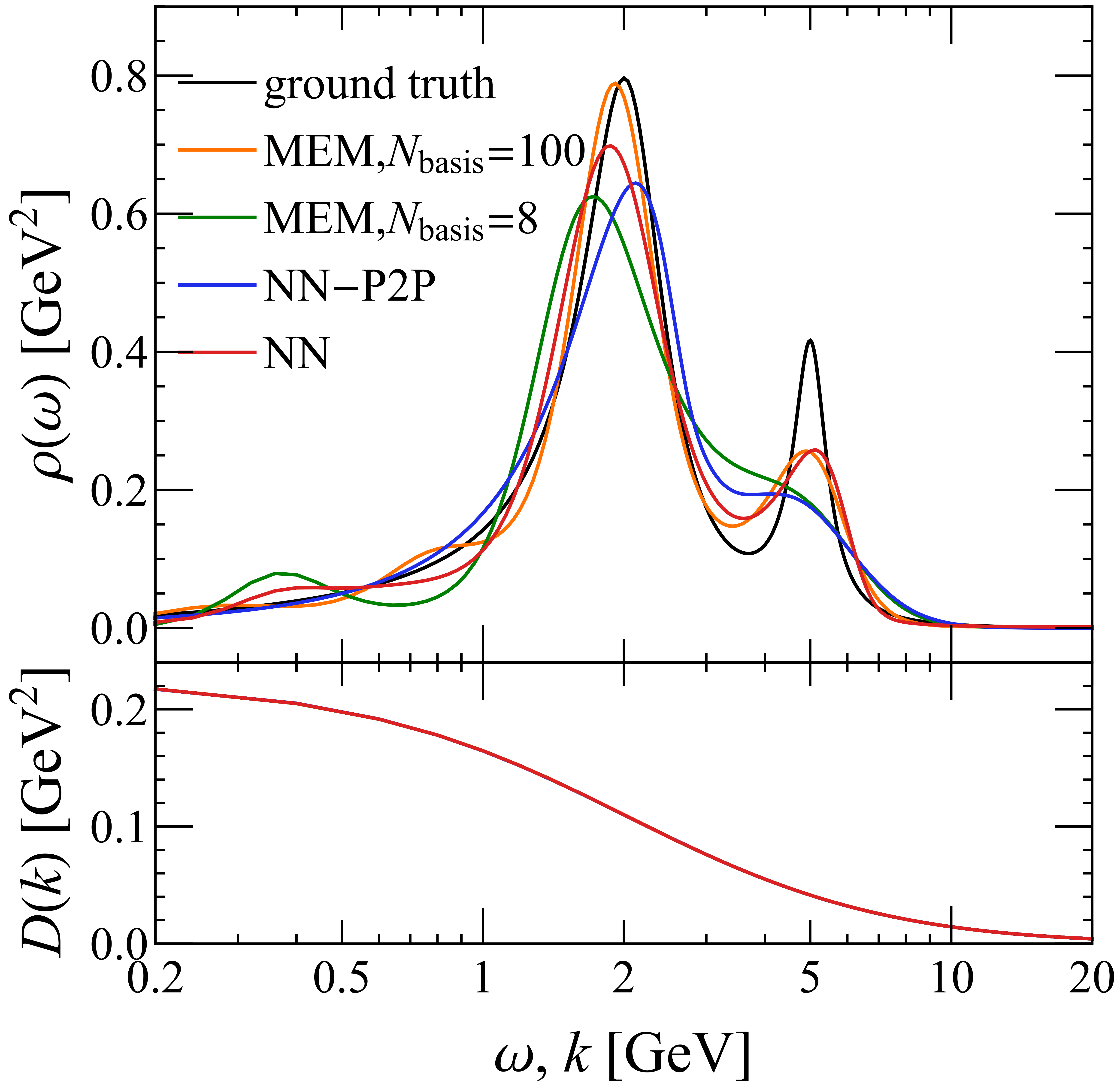
resolved by increasing # of k-points?

Can one learn the spectral function from correlation?



- ill-conditioned?
  - one needs more points in ω than that were given in k

resolved by increasing # of k-points?

- No!!! The problem is ill-posed!!!

ill-posedness of inverse KL convolution

$$D(k) = \frac{1}{\pi}\int_0^\infty \frac{\omega\,\mathrm{d}\omega}{\omega^2 + k^2}\rho(\omega)$$

Linear operator in continuous space,
maps $\mathbb{R}_{[0,+\infty)}$ to $\mathbb{R}_{[0,+\infty)}$.

$\mathbb{R}_{[0,+\infty)}$: Real function defined in the domain $[0, +\infty)$.

ill-posedness of inverse KL convolution

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Linear operator in continuous space,

maps $\mathbb{R}_{[0,+\infty)}$ to $\mathbb{R}_{[0,+\infty)}$.

One can define its eigenfunctions and eigenvalues:

$$\boxed{\frac{1}{\pi} \int_0^\infty \frac{\omega \, \mathrm{d}\omega}{\omega^2 + k^2} \psi(\omega) = \lambda \, \psi(k) \, ,}$$

$\mathbb{R}_{[0,+\infty)}$: Real function defined in the domain $[0, +\infty)$.

eigenfunctions and eigenvalues of KL convolution:

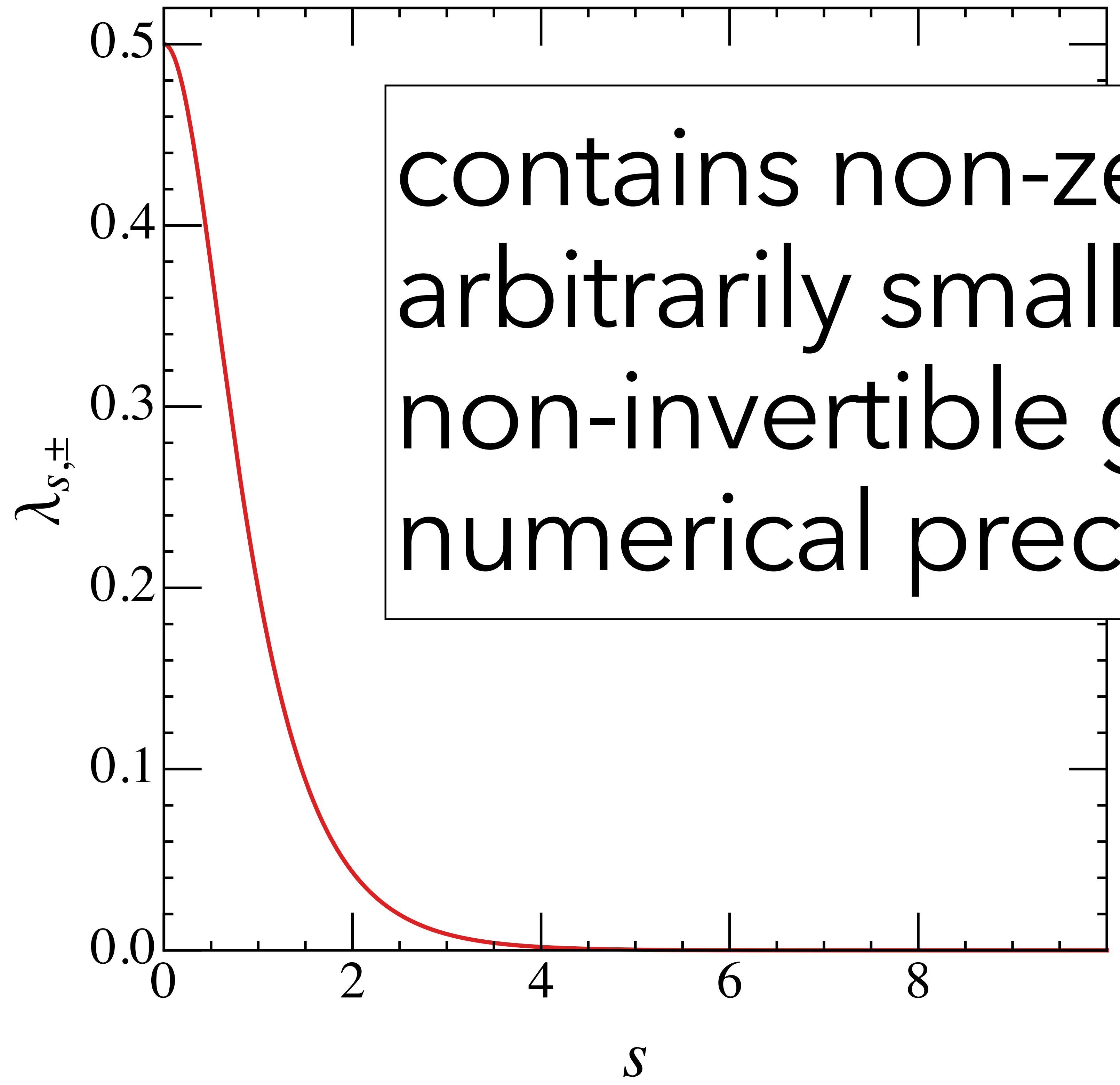
$$\frac{1}{\pi}\int_0^\infty \frac{\omega\, \mathrm{d}\omega}{\omega^2+k^2}\psi(\omega) = \lambda\, \psi(k)\,,$$

infinite amount of solutions, labeled by (continuous) s:

$$\psi_{s,+}(x) = \frac{\cos\big(s\ln(x/a)\big)}{\sqrt{\pi\, x/a}}\,,$$

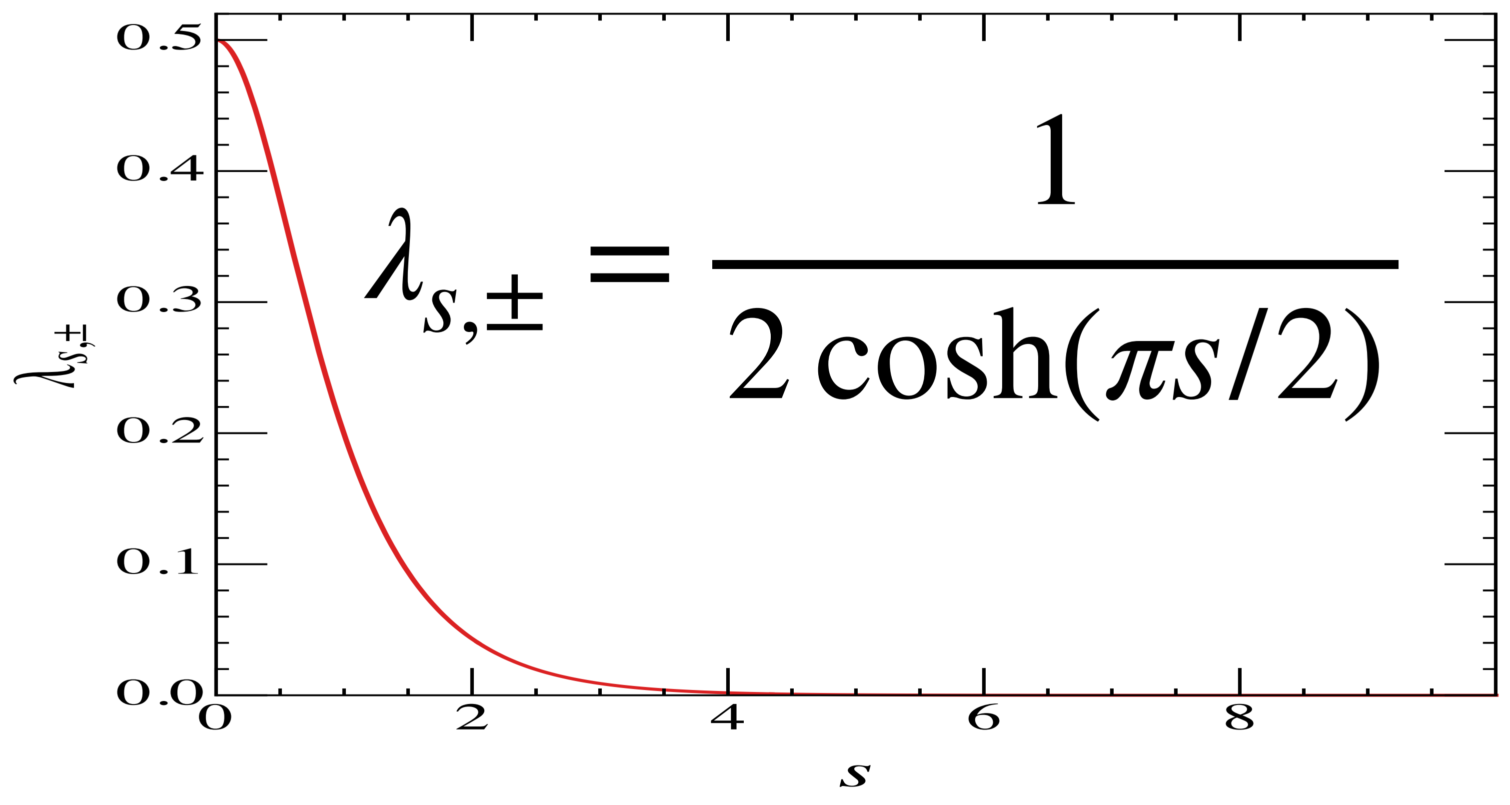
$$\psi_{s,-}(x) = \frac{\sin\big(s\ln(x/a)\big)}{\sqrt{\pi\, x/a}}\,,$$

$$\lambda_{s,\pm} = \frac{1}{2\cosh(\pi s/2)}\,.$$



contains non-zero but arbitrarily small eigenvalues, non-invertible given finite numerical precision.

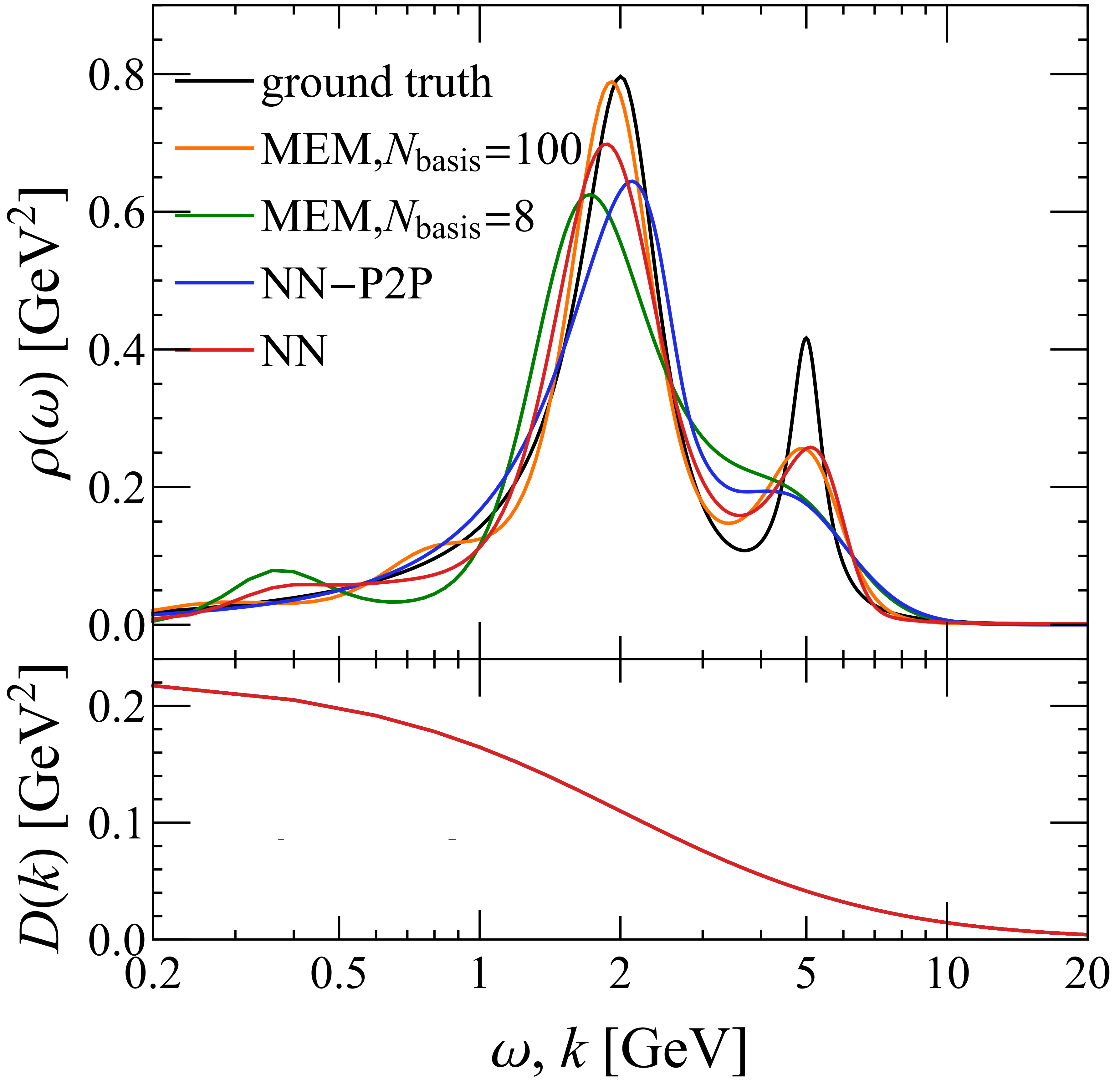
relook at the discrepancy

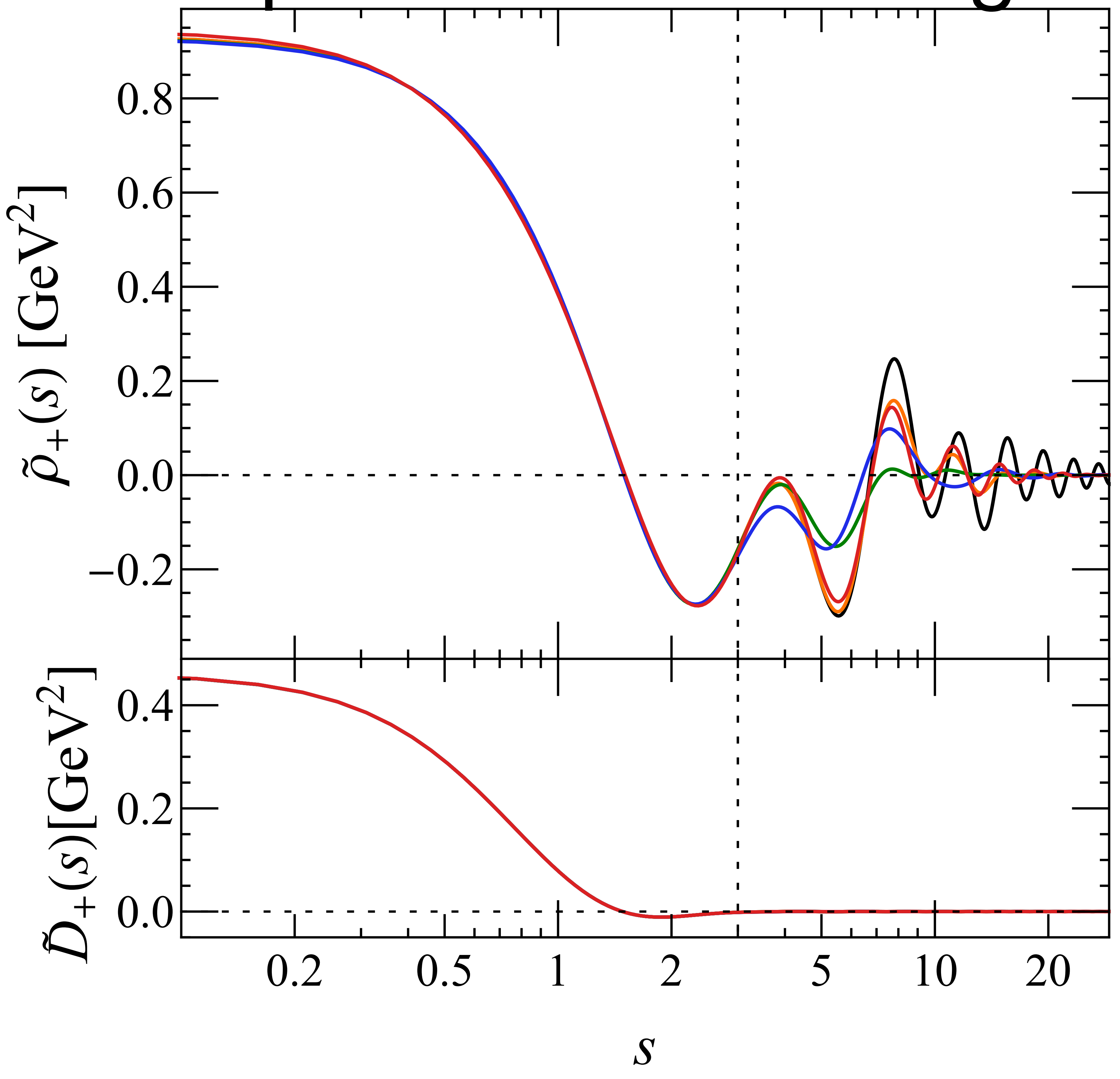


$$\lambda_{s,\pm} = \frac{1}{2\cosh(\pi s/2)}$$

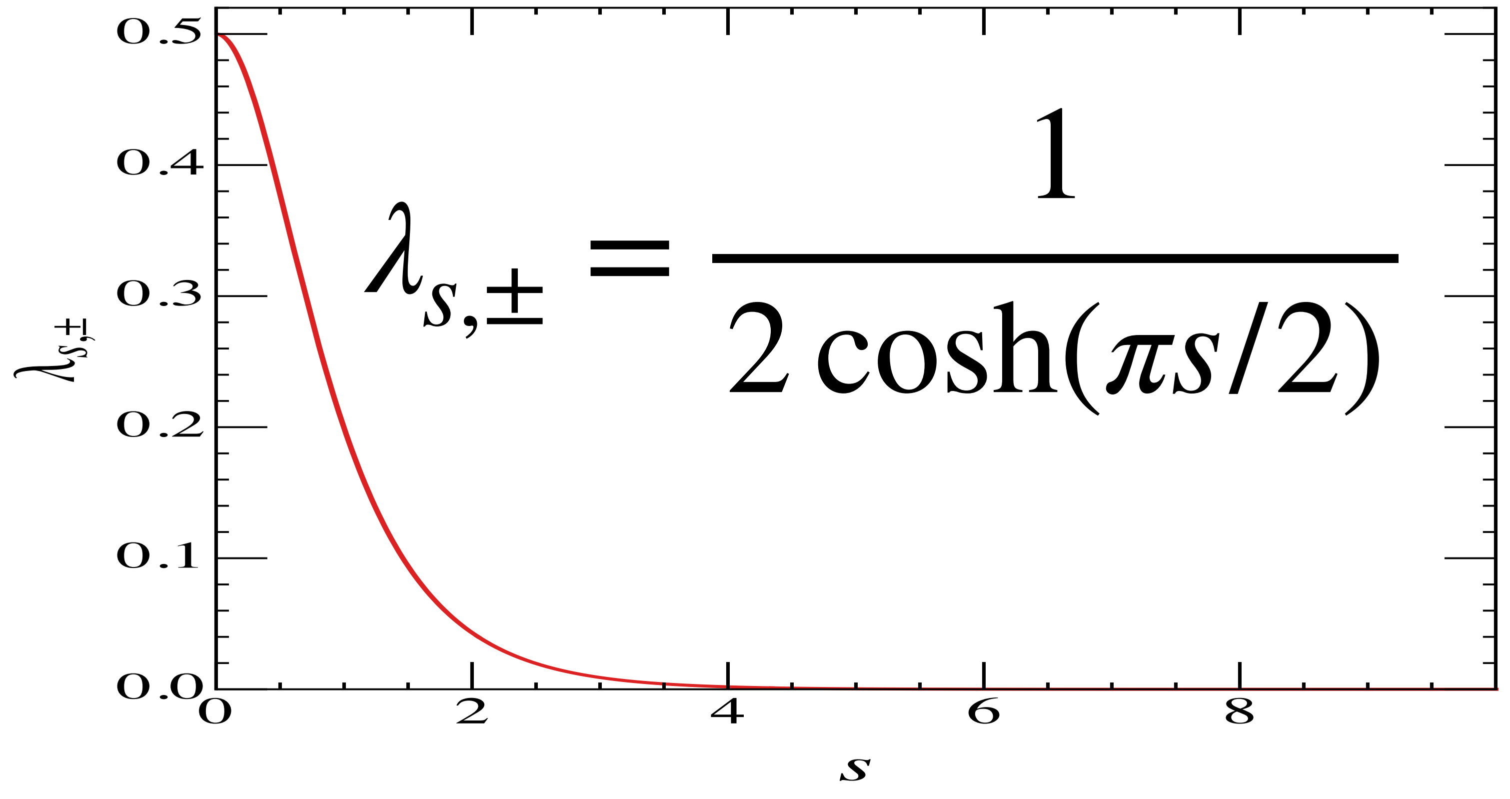
$$\psi_{s,+}(x) = \frac{\cos\left(s \ln(x/a)\right)}{\sqrt{\pi}\, x/a}$$

decomposition into the eigen-space

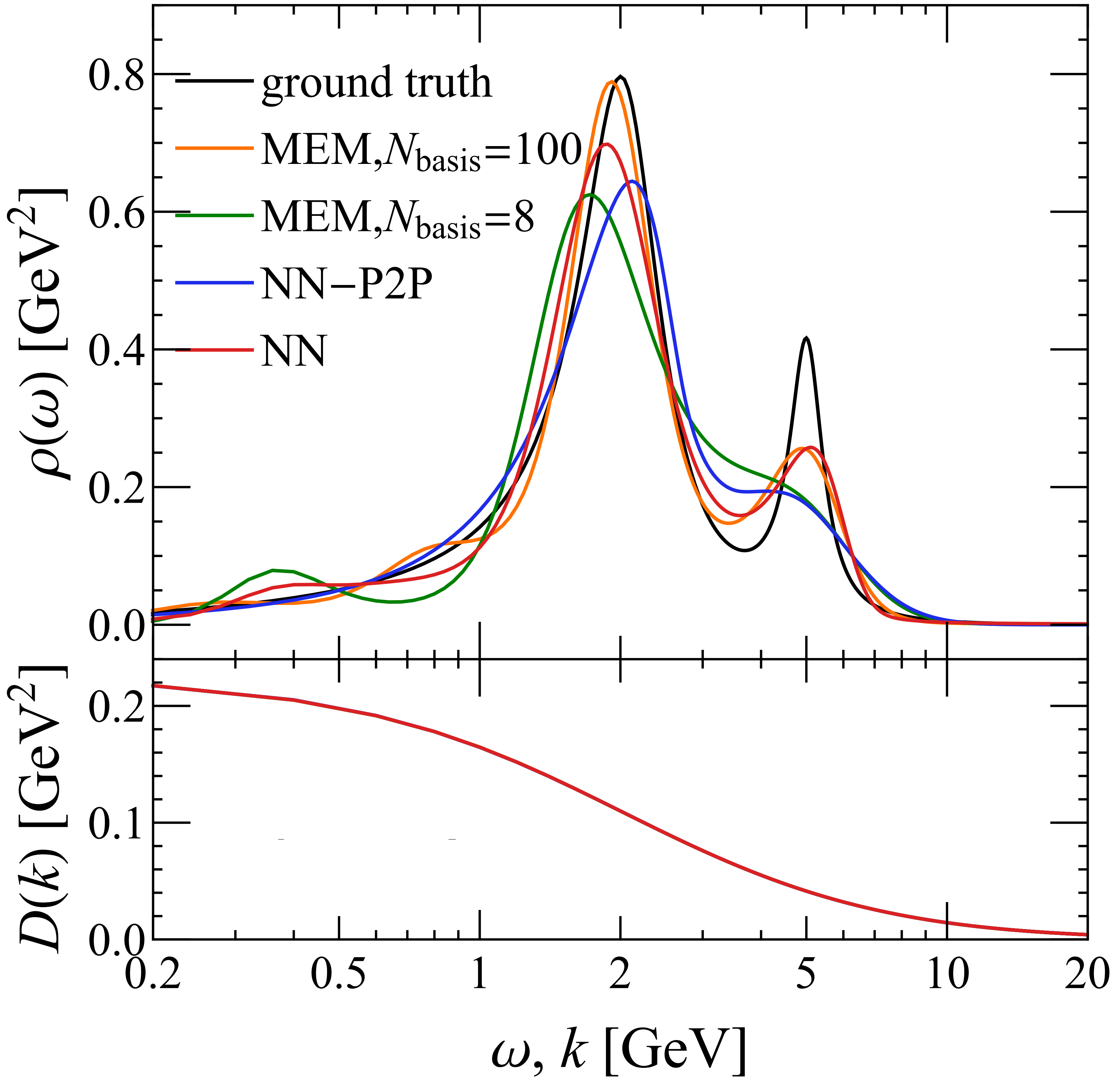




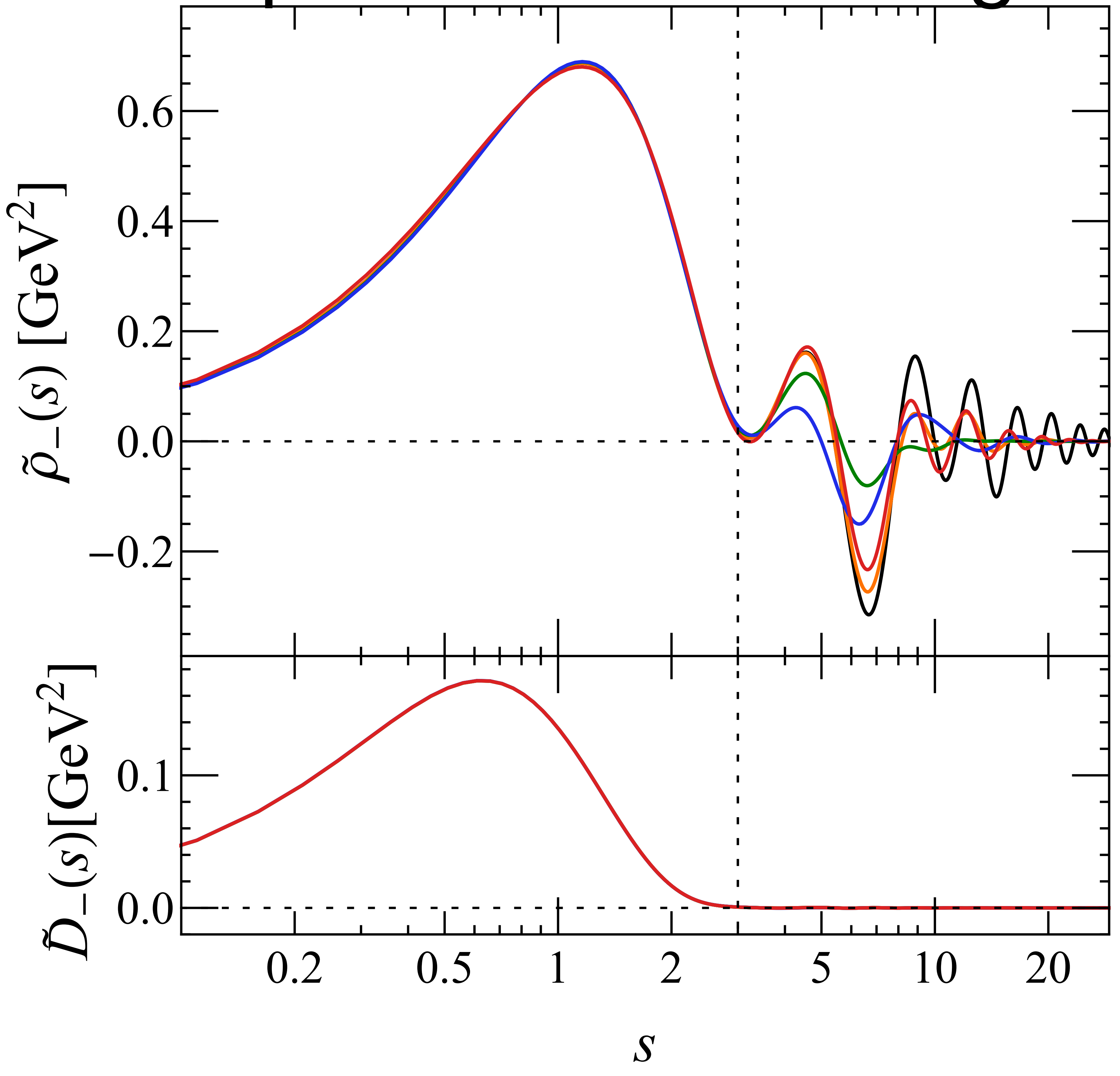
relook at the discrepancy



$$\psi_{s,-}(x) = \frac{\sin\left(s \ln(x/a)\right)}{\sqrt{\pi}\, x/a}$$

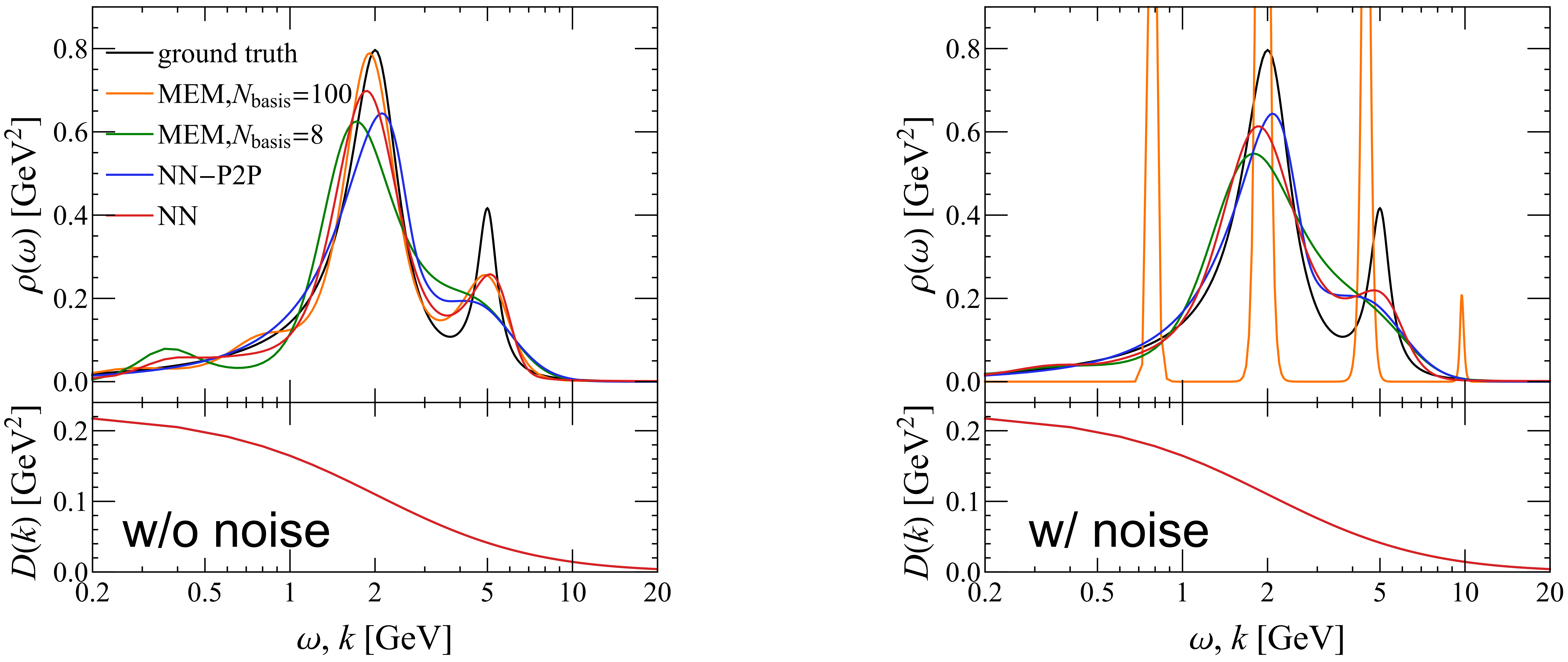


decomposition into the eigen-space



Then, why Deep Learning?

DNN is a natural implementation of smoothness regularization!



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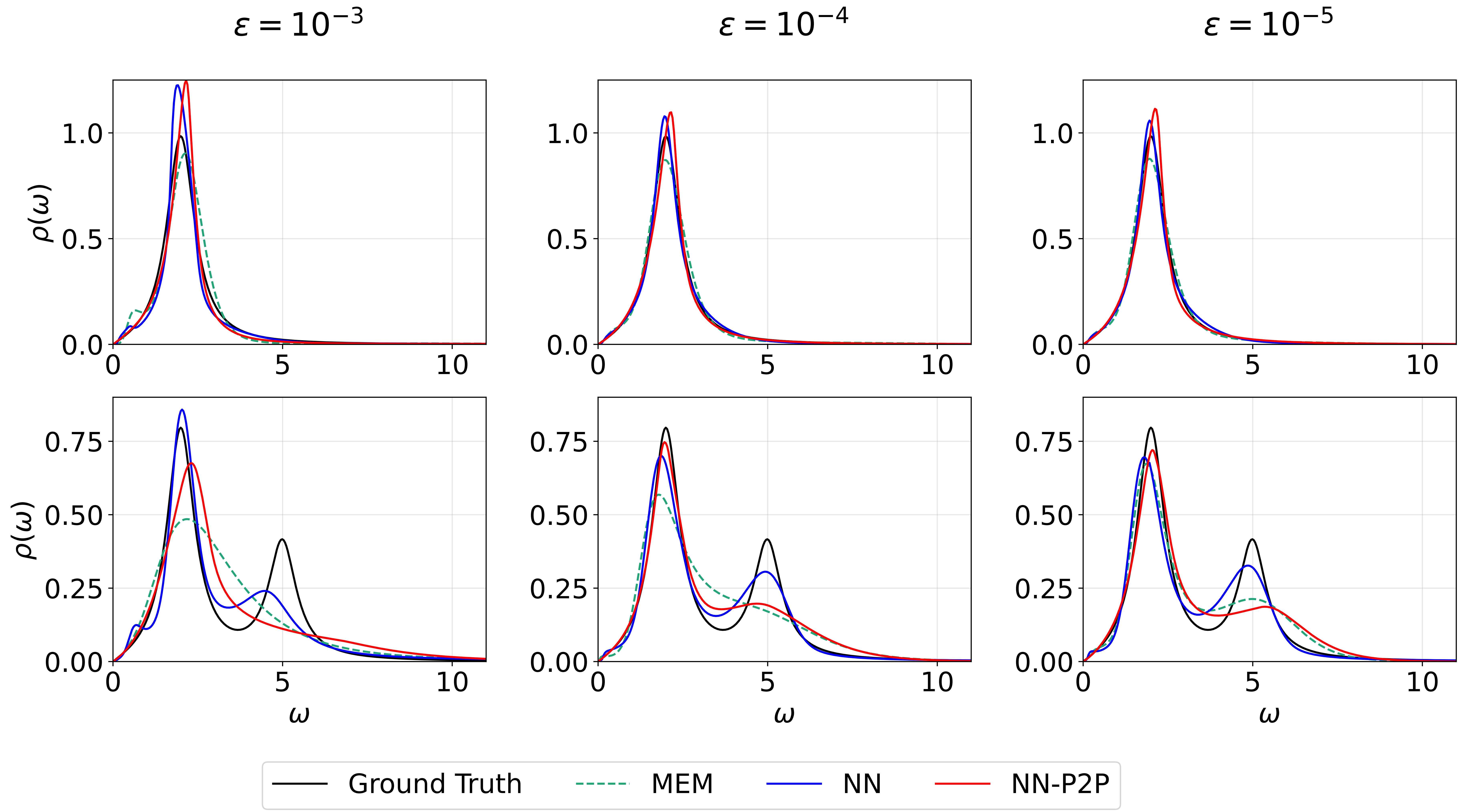
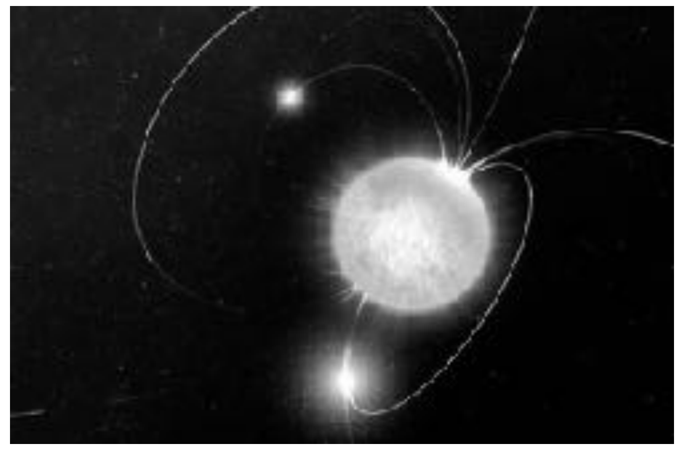
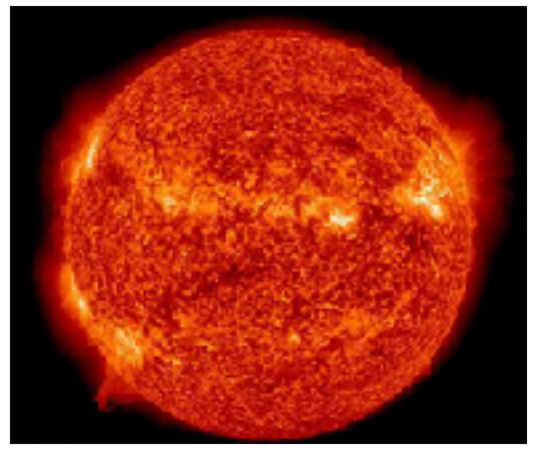
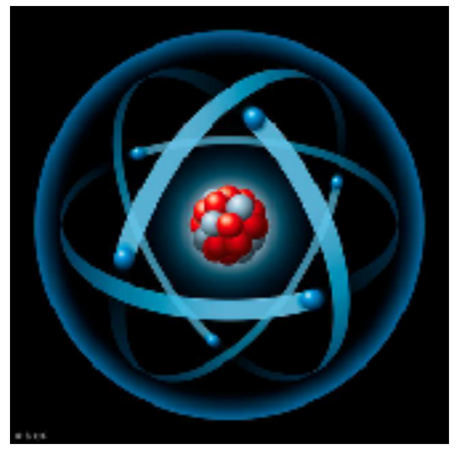


Problem # III:

Neutron Star: EoS <=> {M,R}

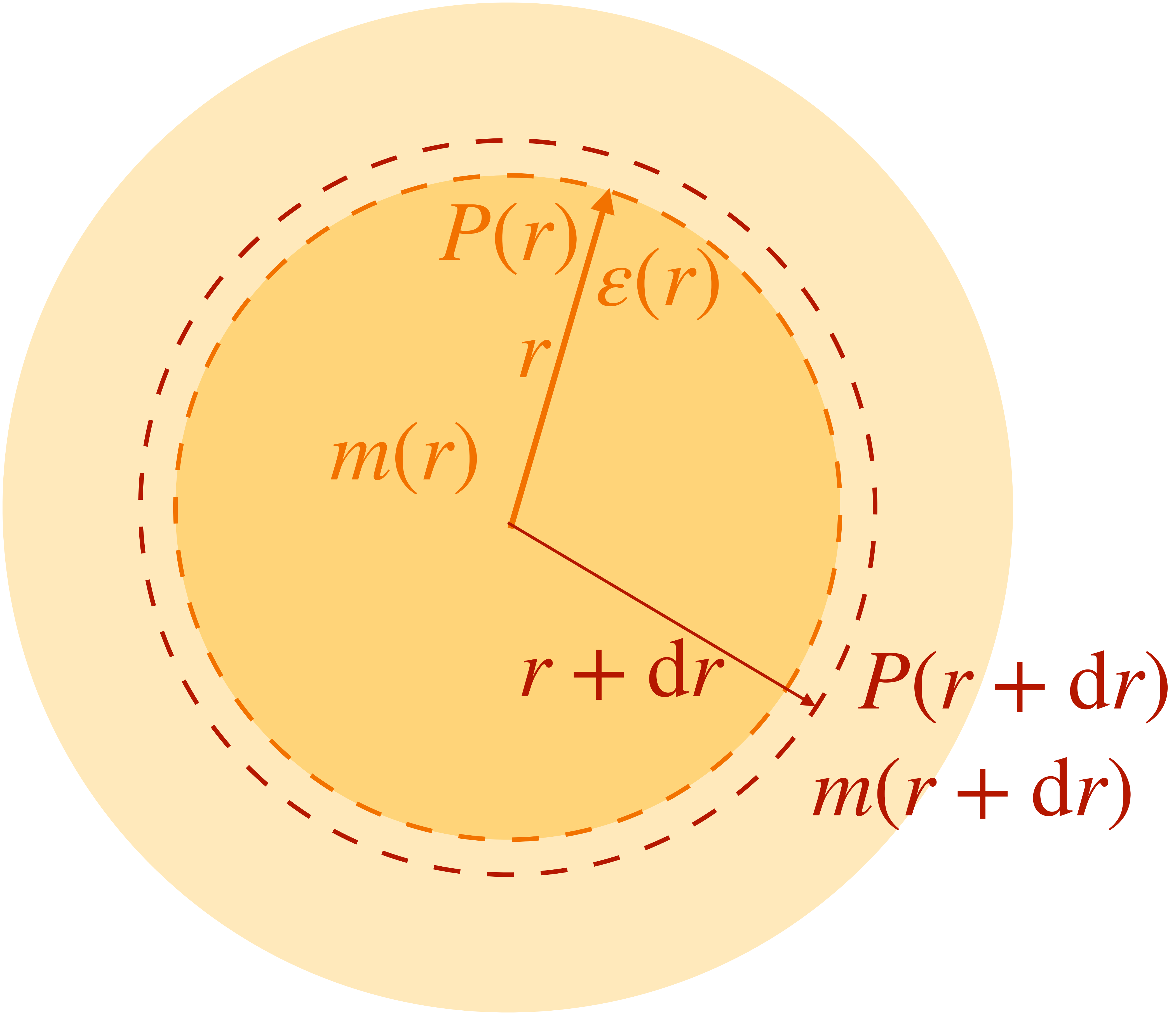
Ronghao Li, Sophia Han, Zidu Lin, Lingxiao Wang, Kai Zhou, ***SS***,
Phys. Rev. D, 111, 074026 + work in progress

Neutron Star

	Neutron Star	Sun	Nucleus
Mass ($M_\odot$)	$0.5 \sim 2$	1	$\sim 10^{0\sim 2} \times 10^{-57}$
Radius (km)	~ 10	7×10^5	$\sim 10^{-18}$
Density ($M_\odot$/km^3)	$\sim 5 \times 10^{-3}$	$\sim 7 \times 10^{-19}$	$\sim 3 \times 10^{-3}$

Tolman-Oppenheimer-Volkoff equations



Pressure at radius r: $P(r)$

Mass density at r: $\varepsilon(r)$

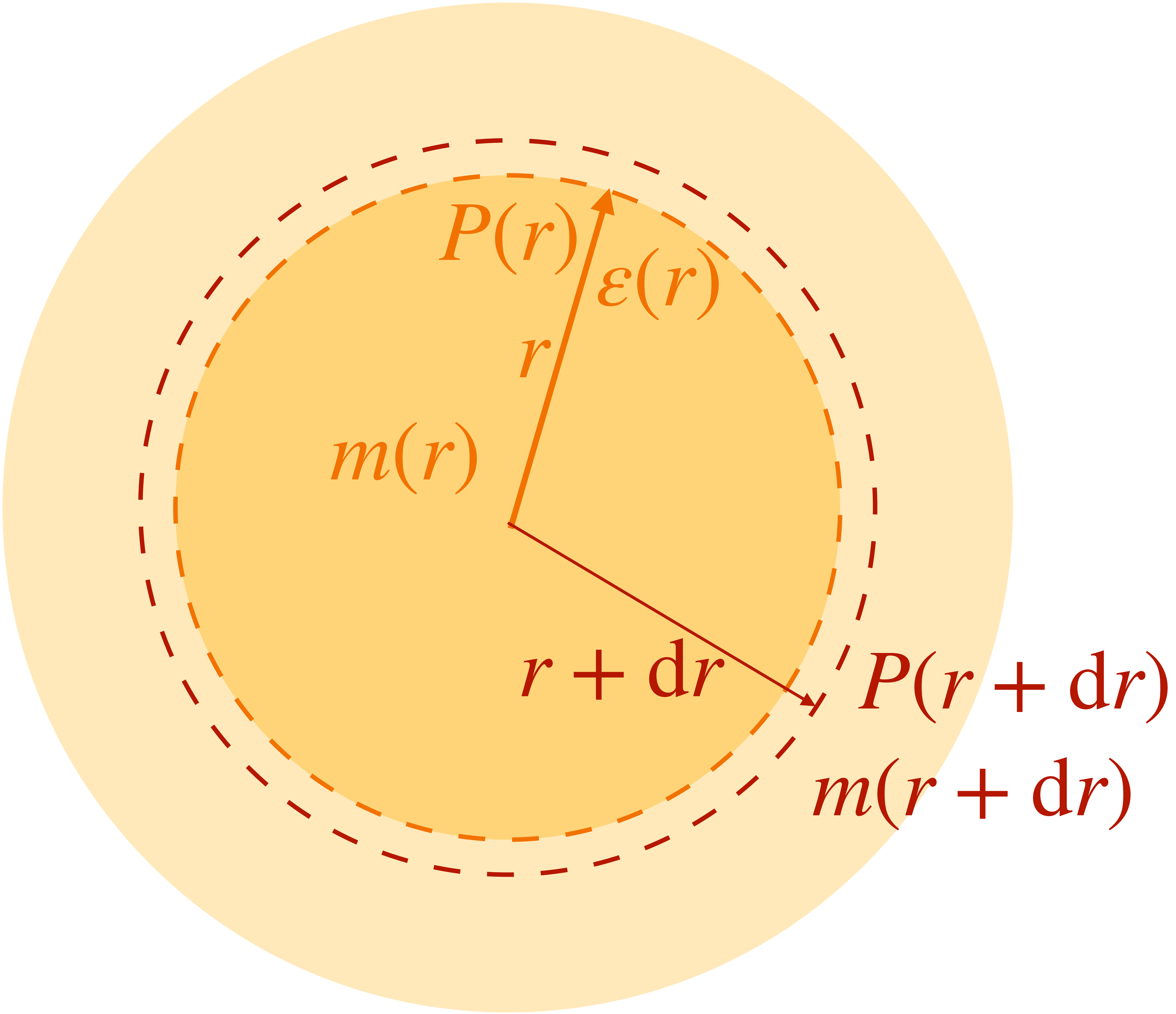
Mass enclosed within shell: $m(r)$

Continuation equation:

$$m(r + \mathrm{d}r) = m(r) + \underbrace{4\pi r^2}_{\text{area}} \overbrace{\varepsilon(r)}^{\text{density}} \underbrace{\mathrm{d}r}_{\text{thickness}},$$

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon \,,$$

Tolman-Oppenheimer-Volkoff equations



Pressure at radius r: $P(r)$

Mass density at r: $\varepsilon(r)$

Mass enclosed within shell: $m(r)$

Balance of force:

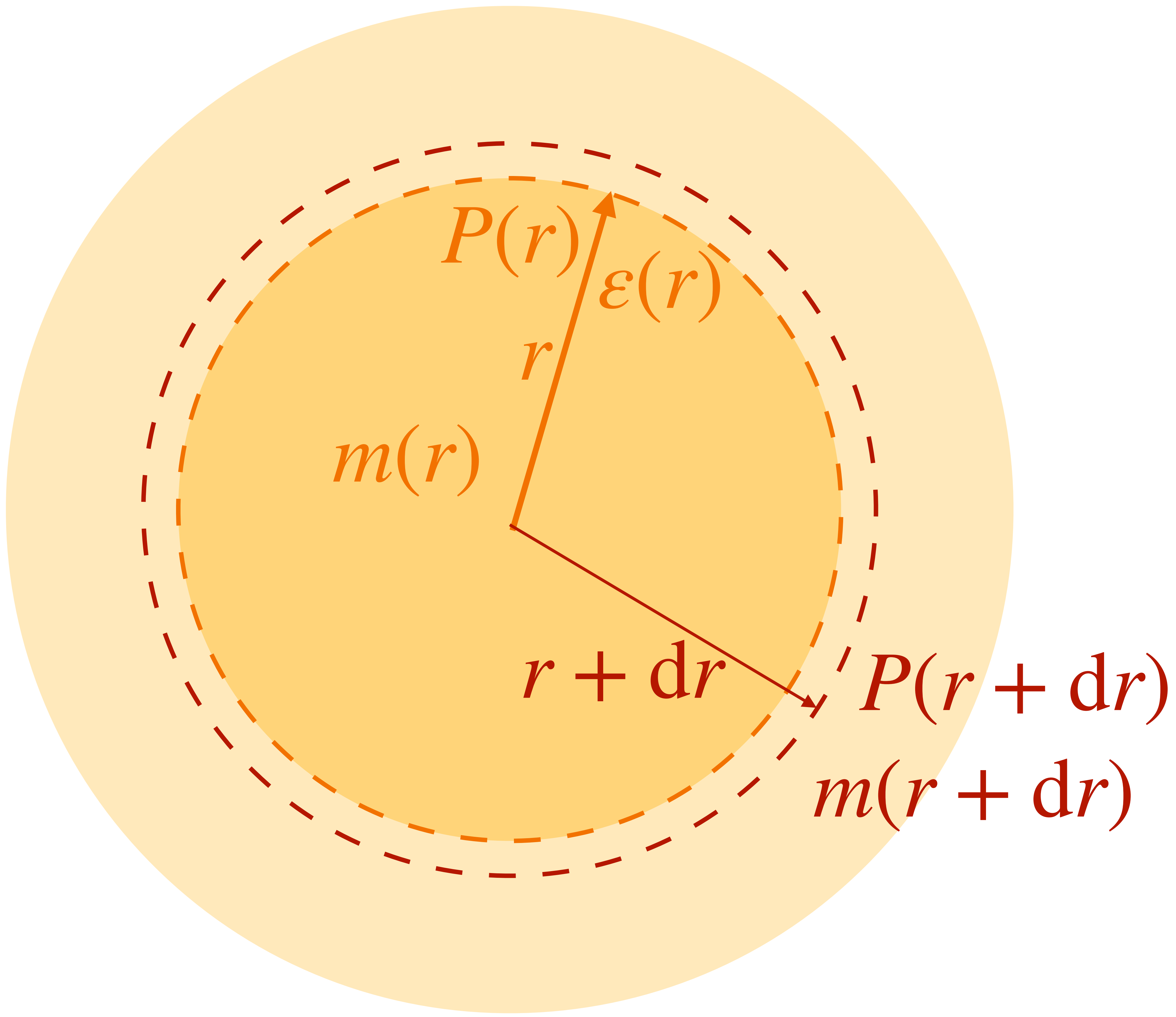
$$4\pi r^2 P(r) = 4\pi(r + \mathrm{d}r)^2 P(r + \mathrm{d}r) + F_G(r)\,,$$

$$F_G = \frac{G\,\overbrace{m(r)}^{m_1}\,\overbrace{4\pi r^2 \varepsilon \mathrm{d}r}^{m_2}}{r^2}$$

distance-squared

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,,$$

Tolman-Oppenheimer-Volkoff equations



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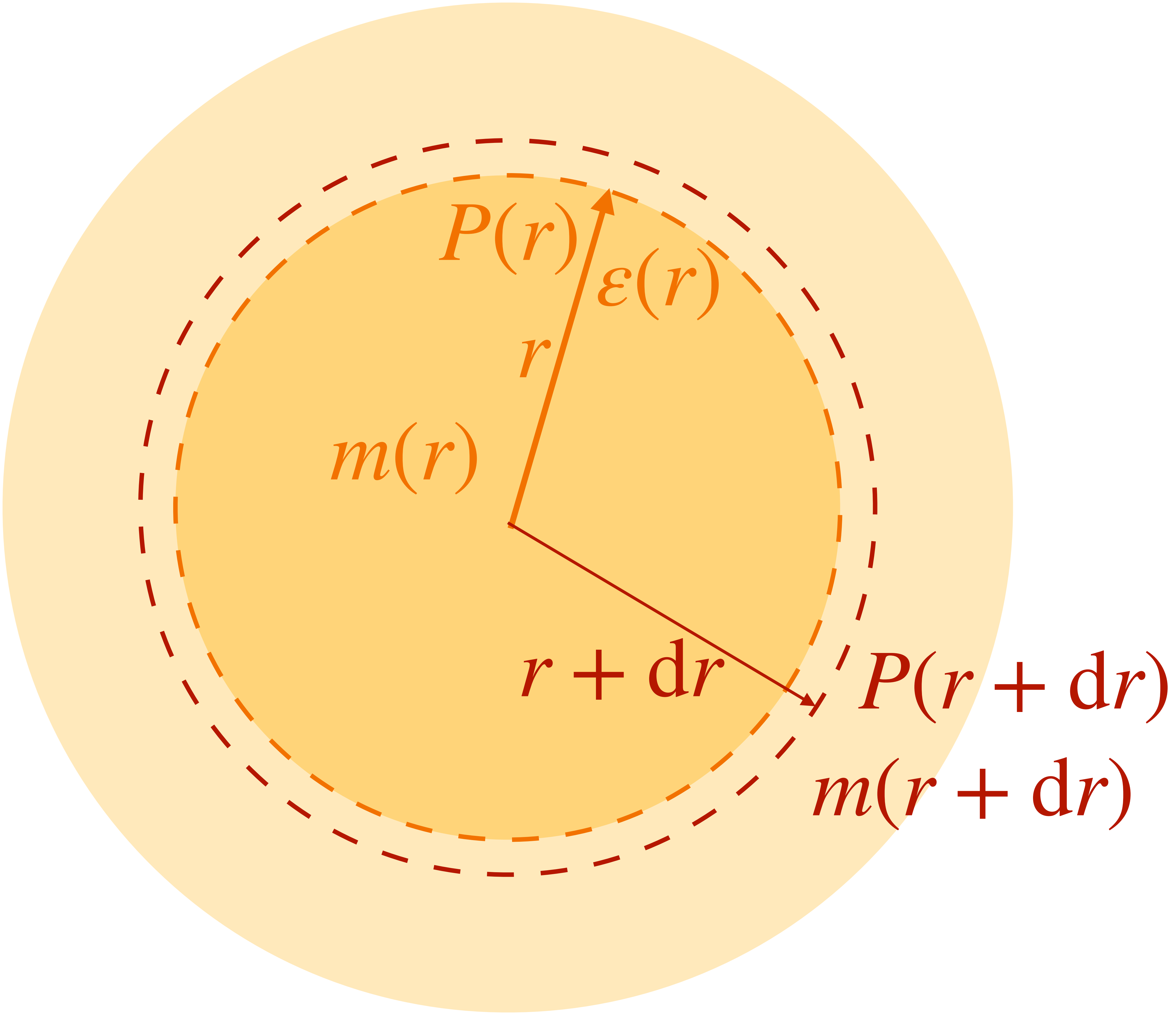
$$F_G = \frac{G\,\overbrace{m(r)}^{m_1}\,\overbrace{4\pi r^2 \varepsilon \mathrm{d}r}^{m_2}}{\underbrace{r^2}_{\text{distance-squared}}}$$

+GR effect

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,, \qquad \frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r}\,,$$

Tolman-Oppenheimer-Volkoff equations



Pressure at radius r: $P(r)$

Mass density at r: $\varepsilon(r)$

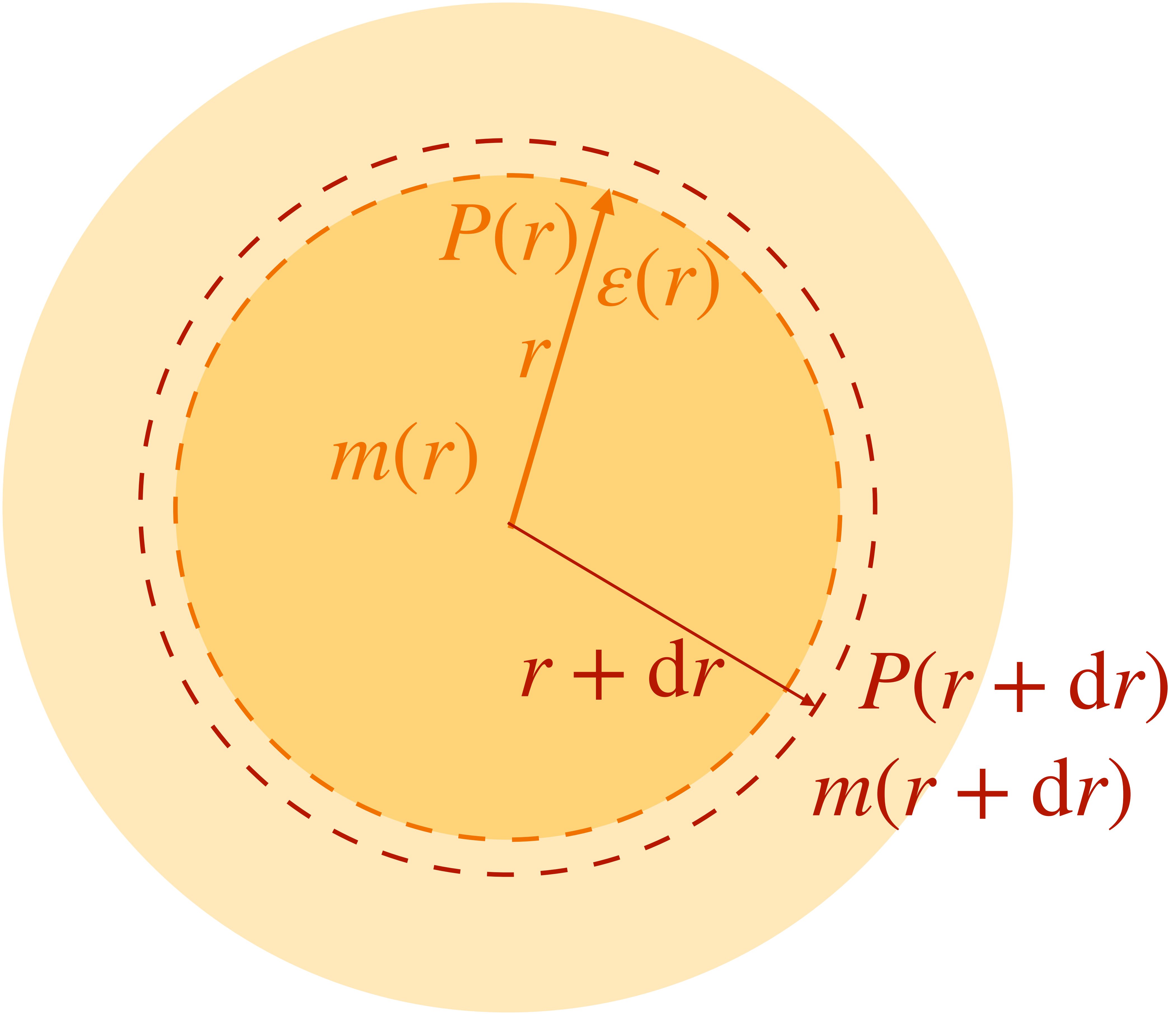
Mass enclosed within shell: $m(r)$

Equation of state:

$$\varepsilon = \varepsilon_{\mathrm{EoS}}(P)\,,$$
$$\varepsilon(r) = \varepsilon_{\mathrm{EoS}}(P(r))\,,$$

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,, \qquad \frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r}\,, \qquad \varepsilon = \varepsilon(P)\,,$$

Tolman-Oppenheimer-Volkoff equations



Pressure at radius r: $P(r)$

Mass density at r: $\varepsilon(r)$

Mass enclosed within shell: $m(r)$

boundary conditions:

$$m(r = 0) = 0, \qquad m(r = R) = M,$$
$$P(r = 0) = P_{\mathrm{cen}}, \qquad P(r = R) = 0.$$

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,, \qquad \frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r}\,, \qquad \varepsilon = \varepsilon(P)\,,$$

Tolman-Oppenheimer-Volkoff equations

Tolman-Oppenheimer-Volkoff equations:

Tolman, Phys.Rev. 55 (1939) 364-373

Oppenheimer, Volkoff, Phys.Rev. 55 (1939) 374-381

$$m(r=0)=0, \qquad m(r=R)=M,$$

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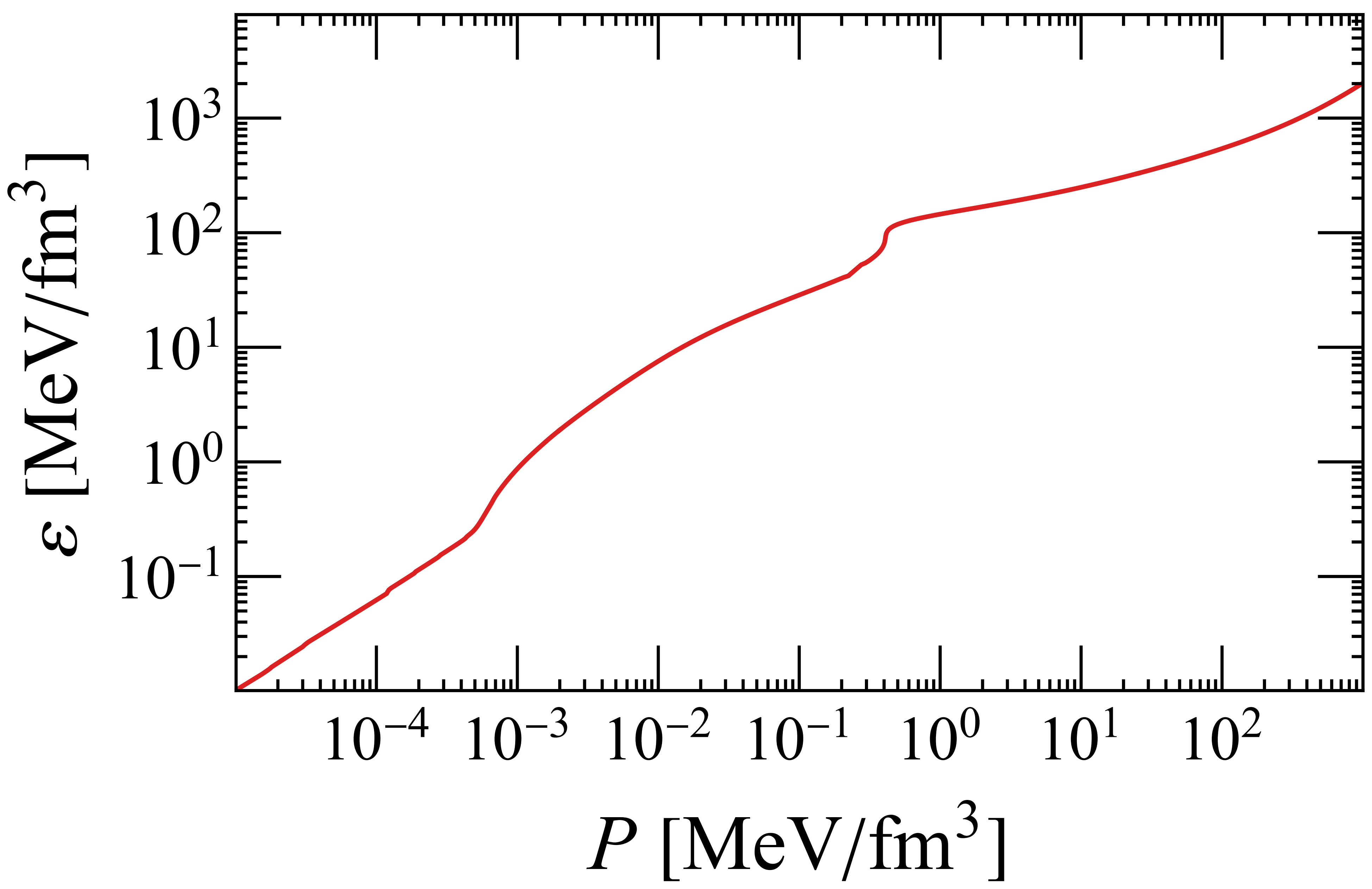
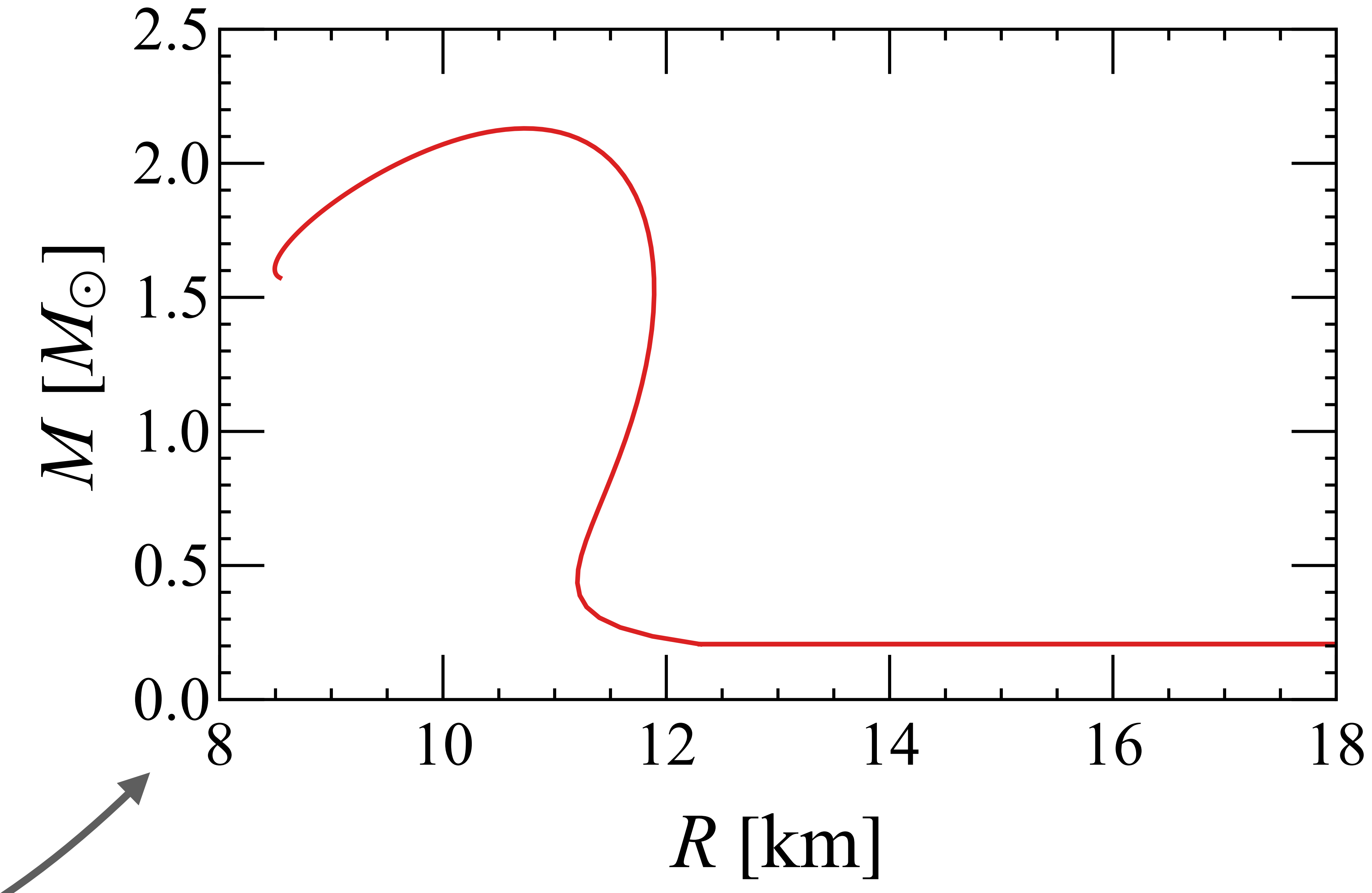
Tolman-Oppenheimer-Volkoff equations





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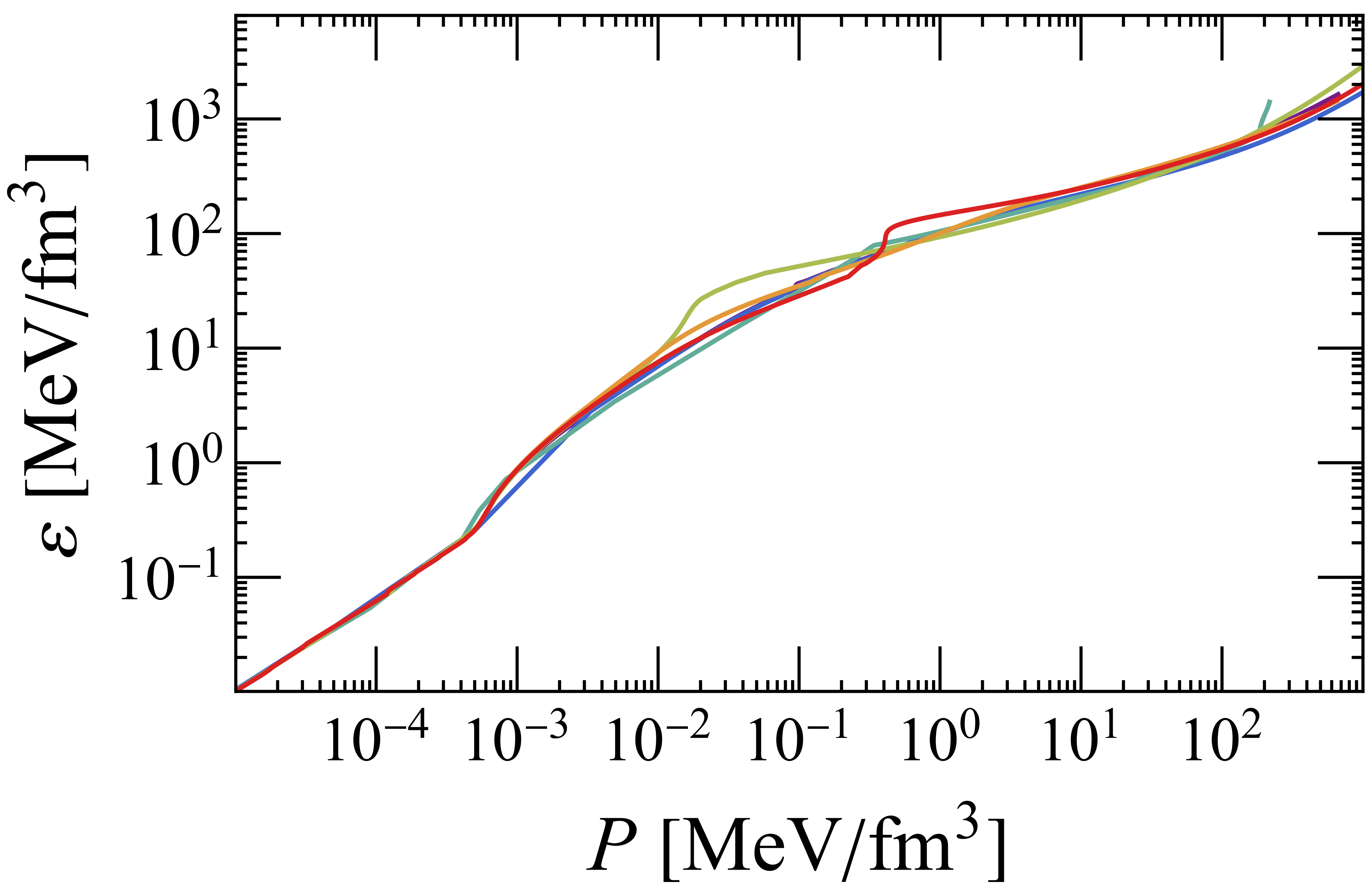
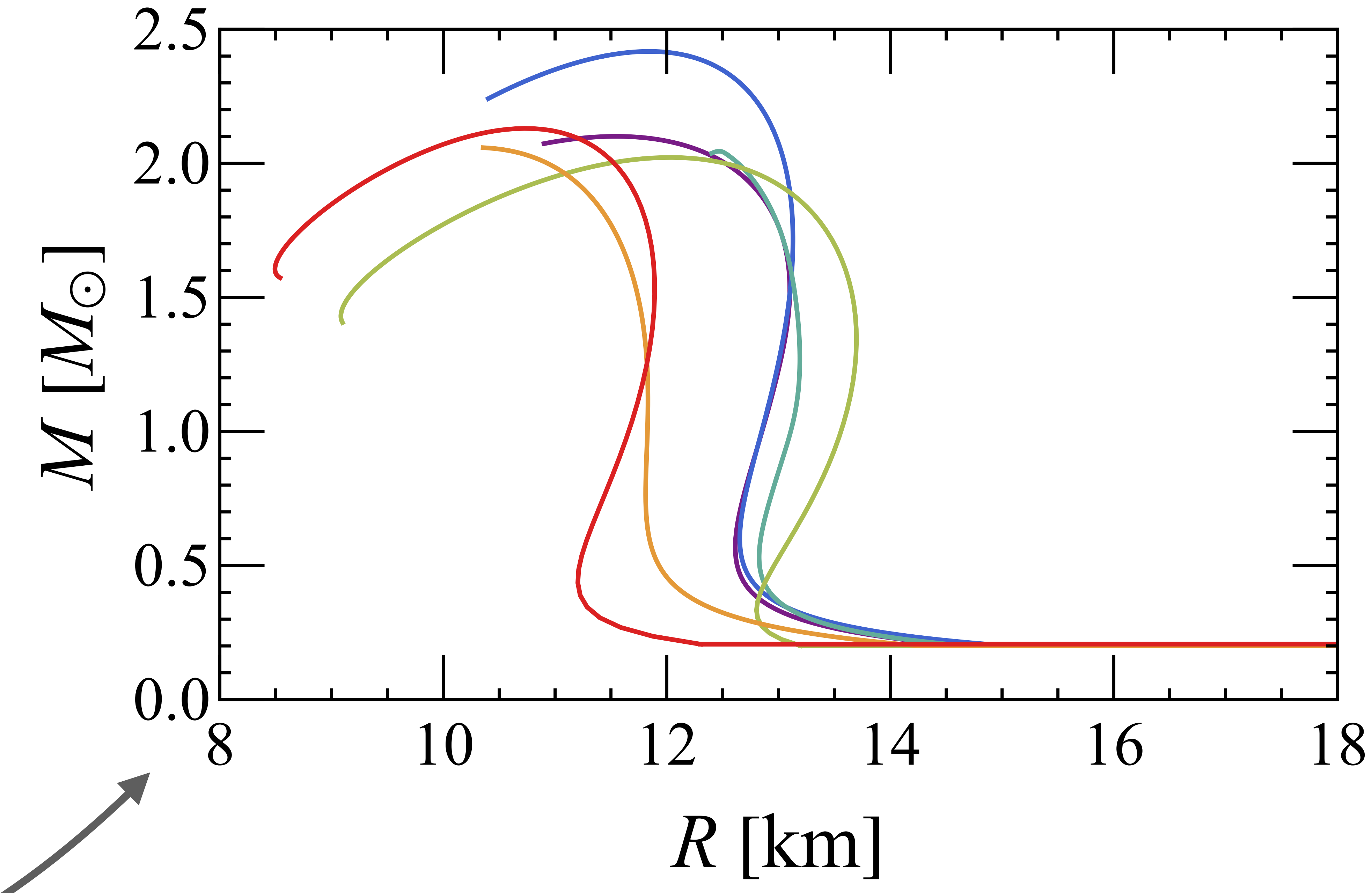
Tolman-Oppenheimer-Volkoff equations





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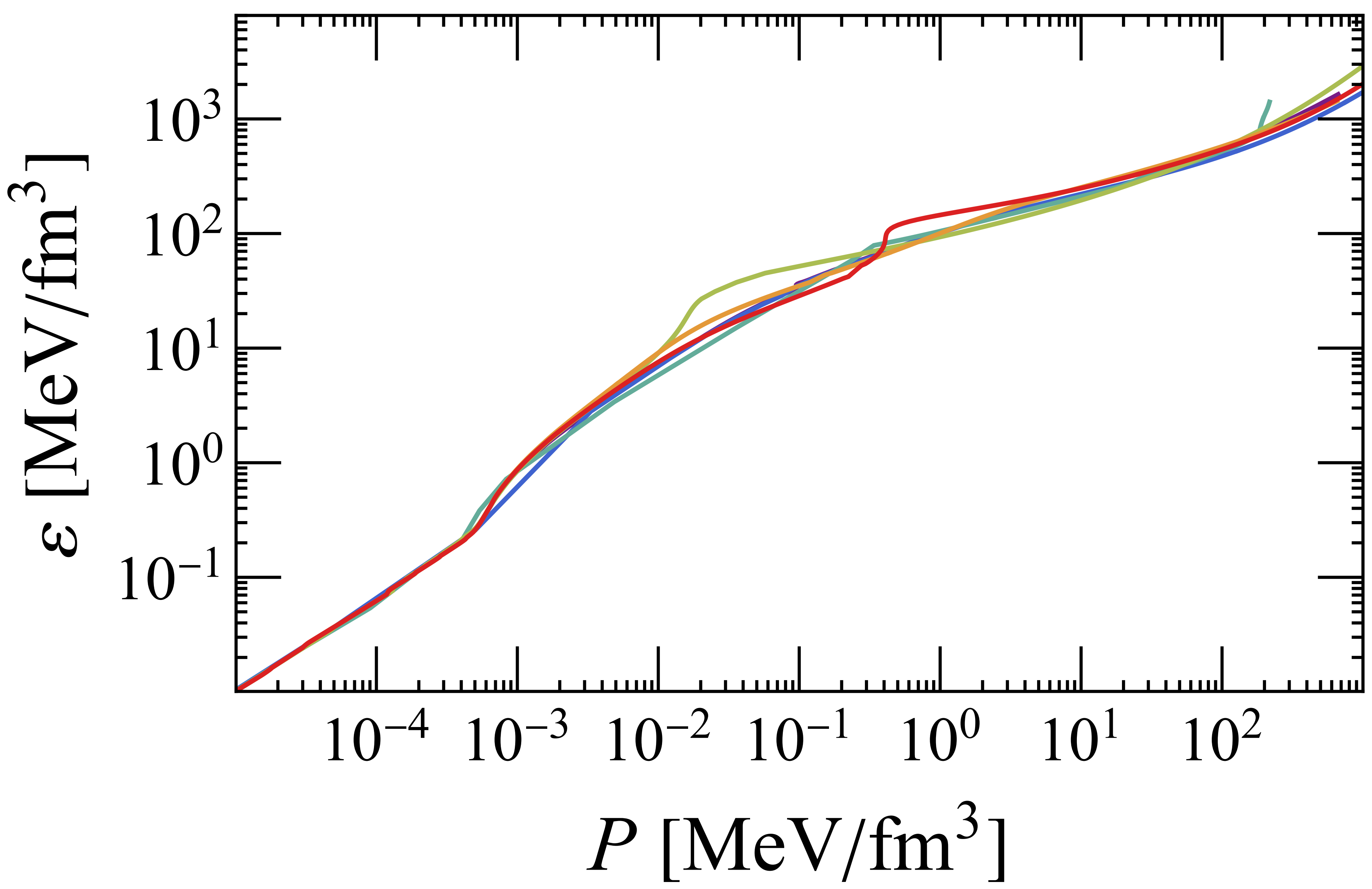
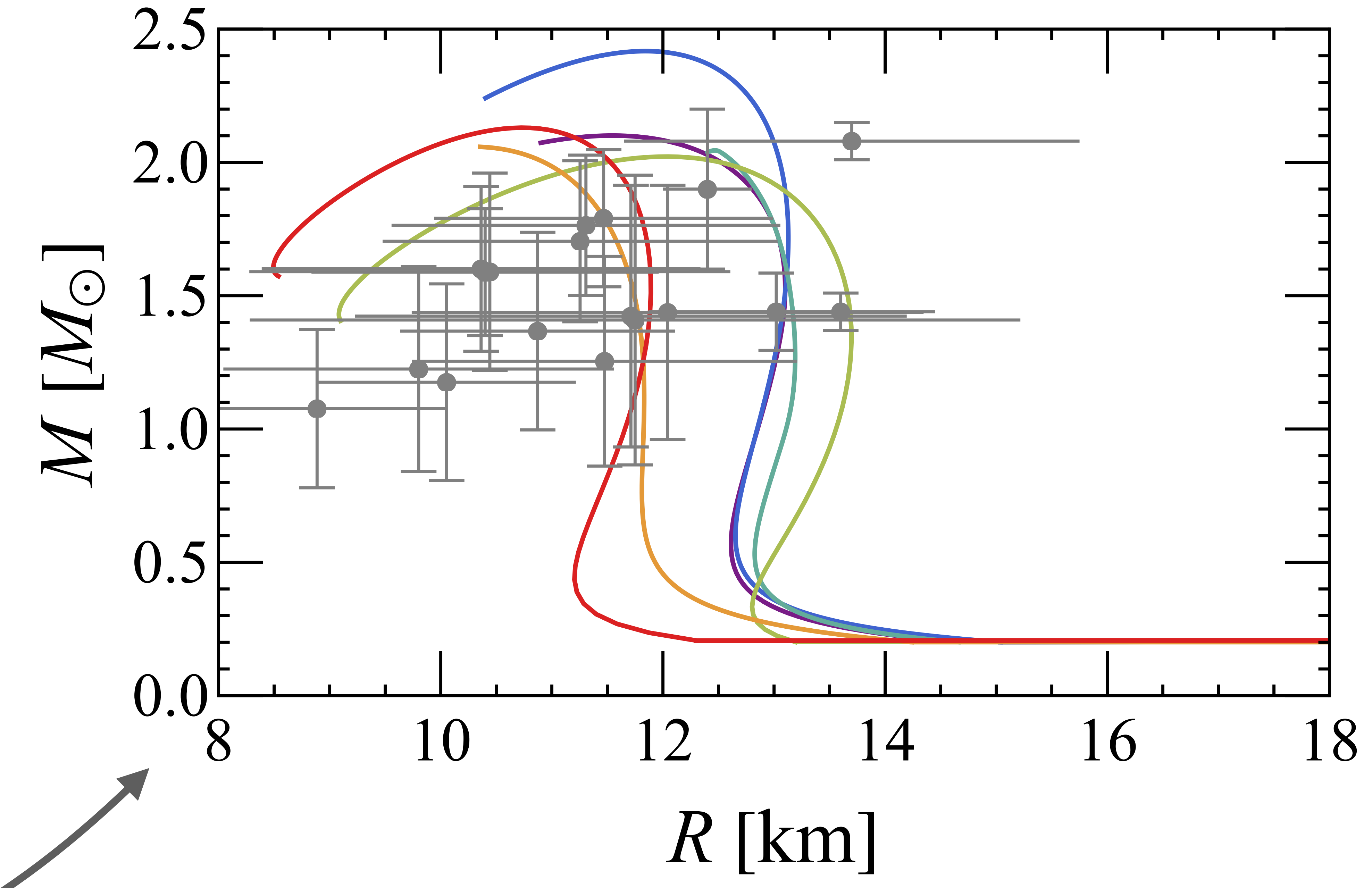
Tolman-Oppenheimer-Volkoff equations



18 observations



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gradient: linear response of TOV

input:
EoS

$$\frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r}\,,$$

$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,,$$

$$\varepsilon = \varepsilon(P)\,,$$

output:
M-*R* curve

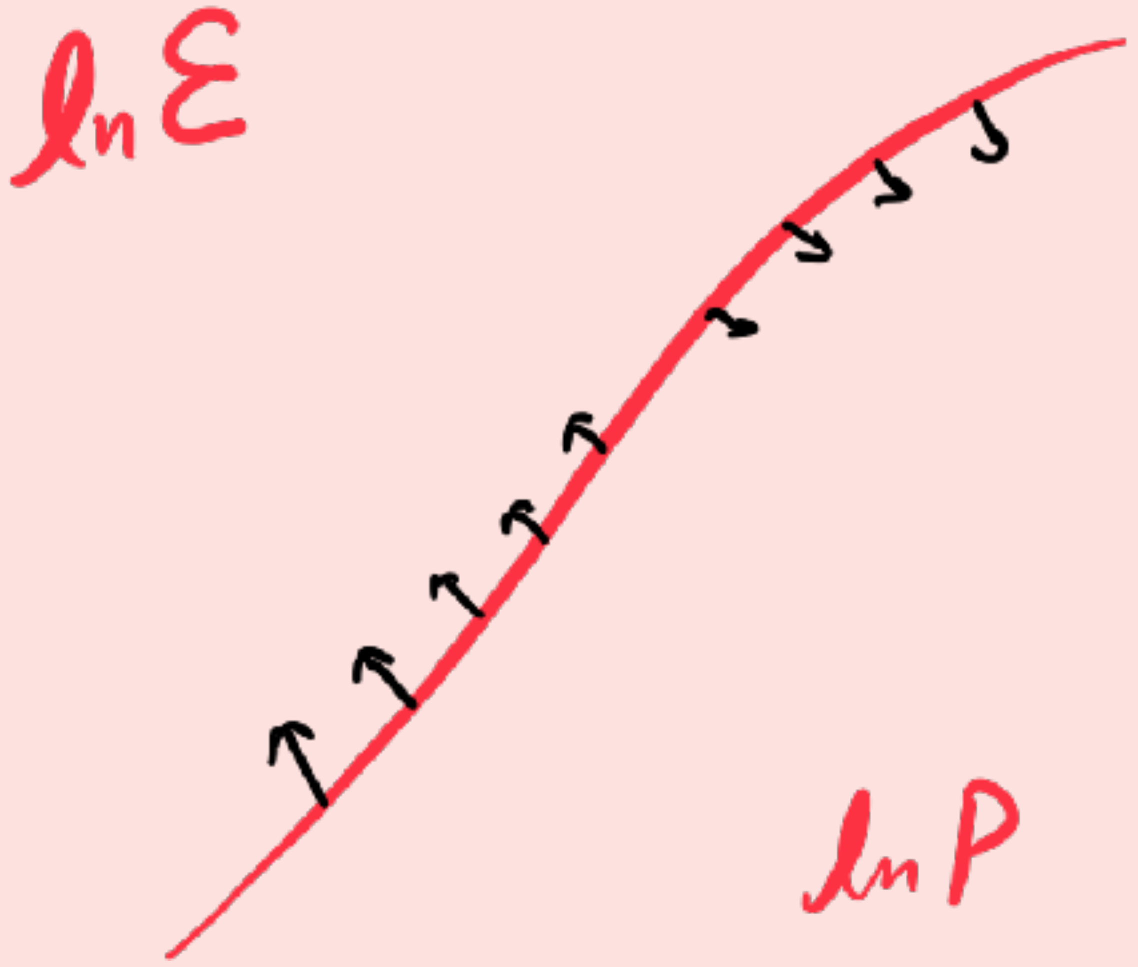
gradient: linear response of TOV

input:
EoS

$$\frac{\mathrm{d}P}{\mathrm{d}r} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2\,m\,r}\,,$$
$$\frac{\mathrm{d}m}{\mathrm{d}r} = 4\pi r^2 \varepsilon\,,$$

output:
M-R curve

TOV equation: functional mapping EoS to M-R;
Inverse TOV: functional derivatives!

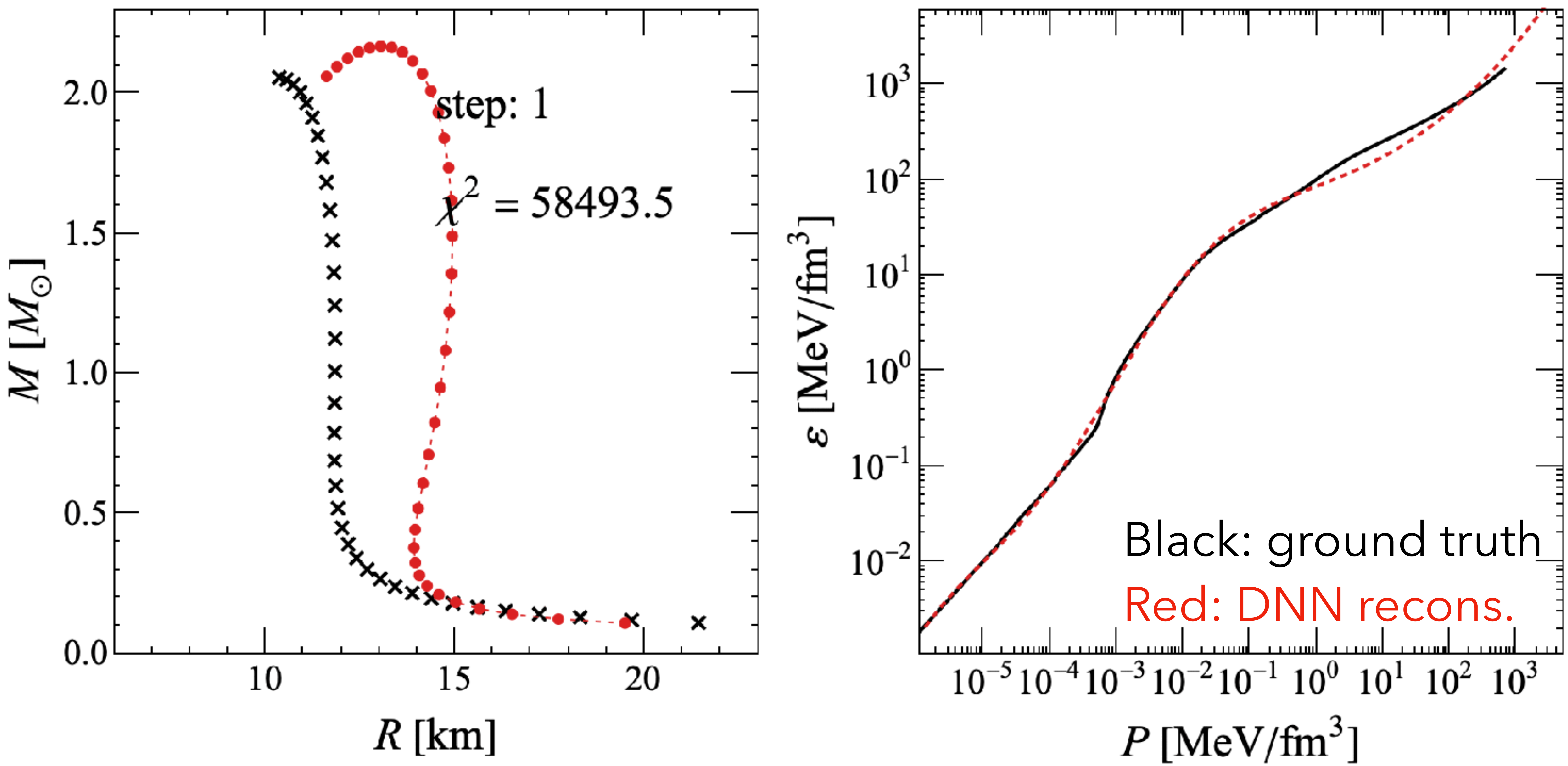


change in EoS

$$\xleftarrow{\quad \dfrac{\delta\,(M\text{-}R)}{\delta\,(\mathrm{EoS})} \quad}$$

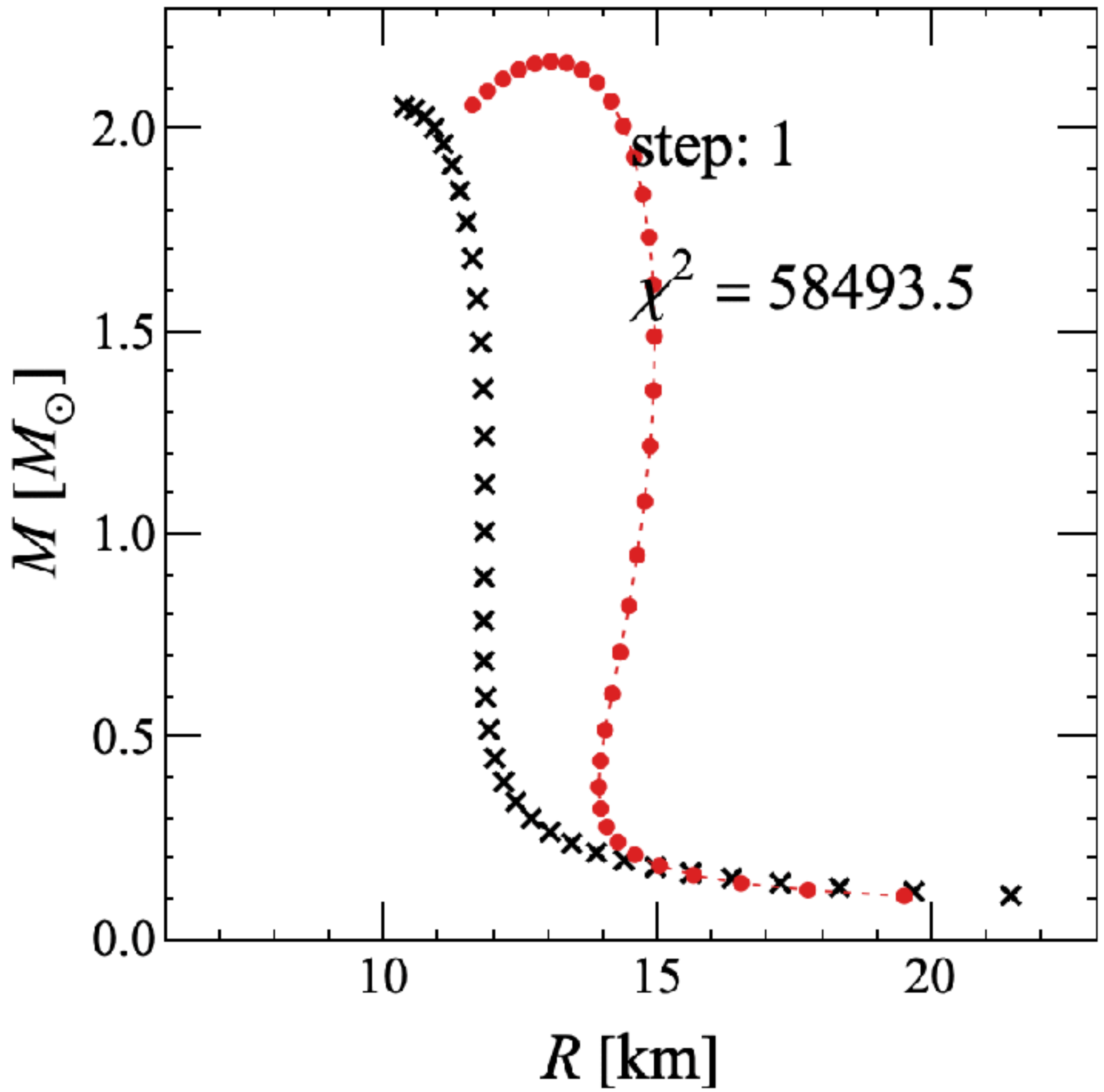
$(M\text{-}R)_{\mathrm{desired}}$ - $(M\text{-}R)_{\mathrm{curr.}}$

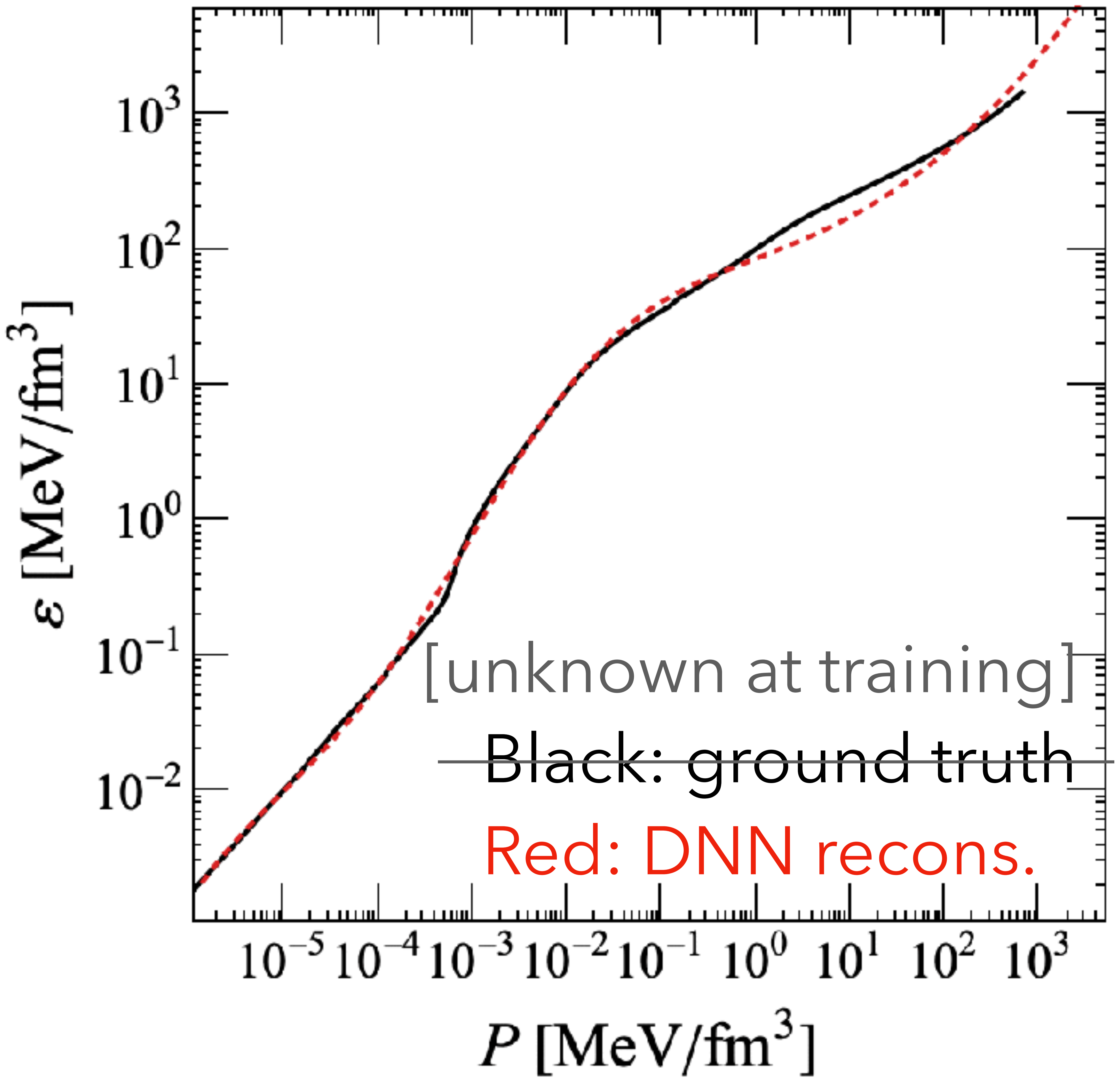
closure test



$$\chi^2 = \sum_i \left(\frac{m_i - m_i^{\mathrm{obs}}}{\Delta m_i}\right)^2 + \left(\frac{R_i - R_i^{\mathrm{obs}}}{\Delta R_i}\right)^2$$

closure test





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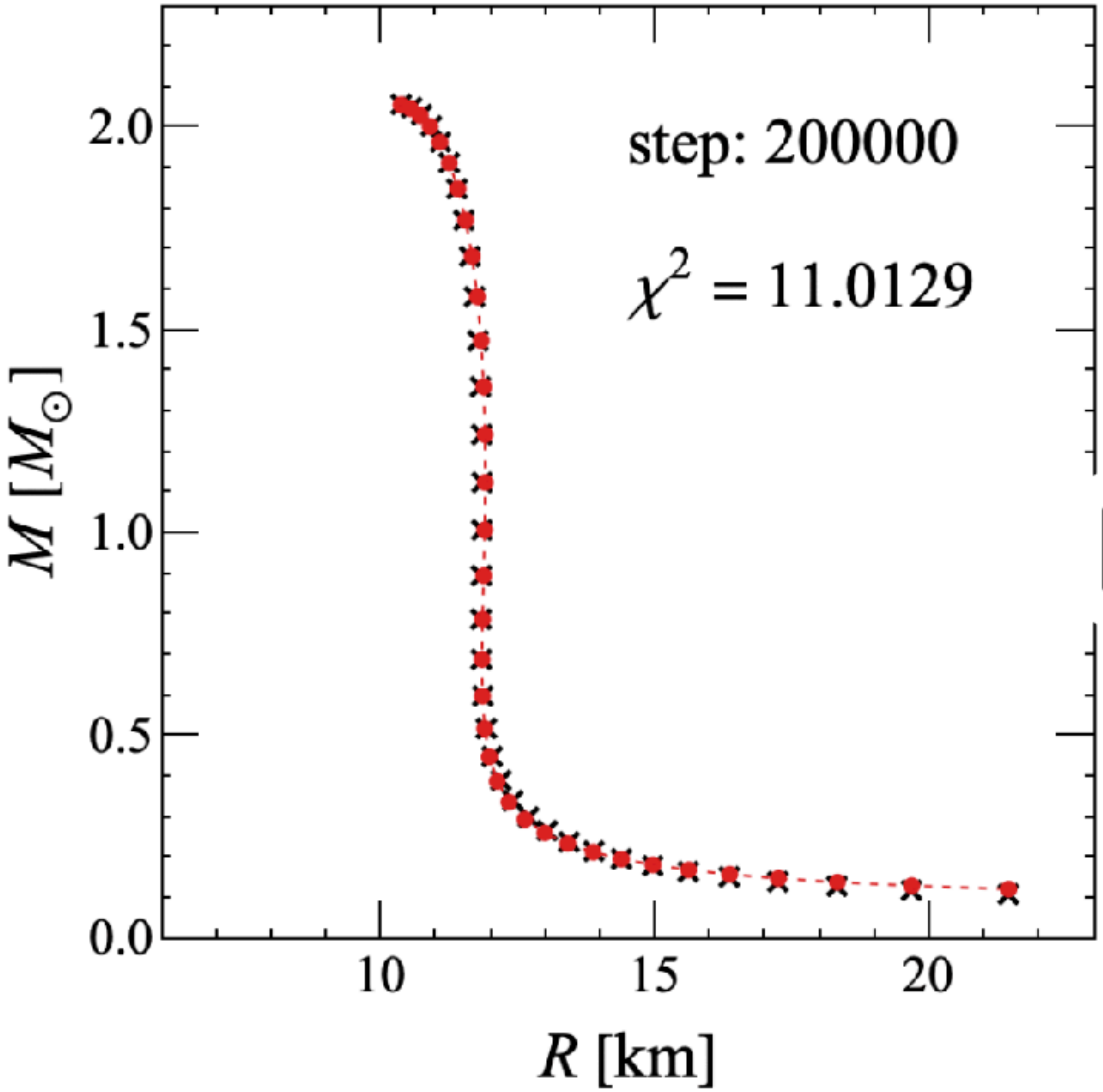

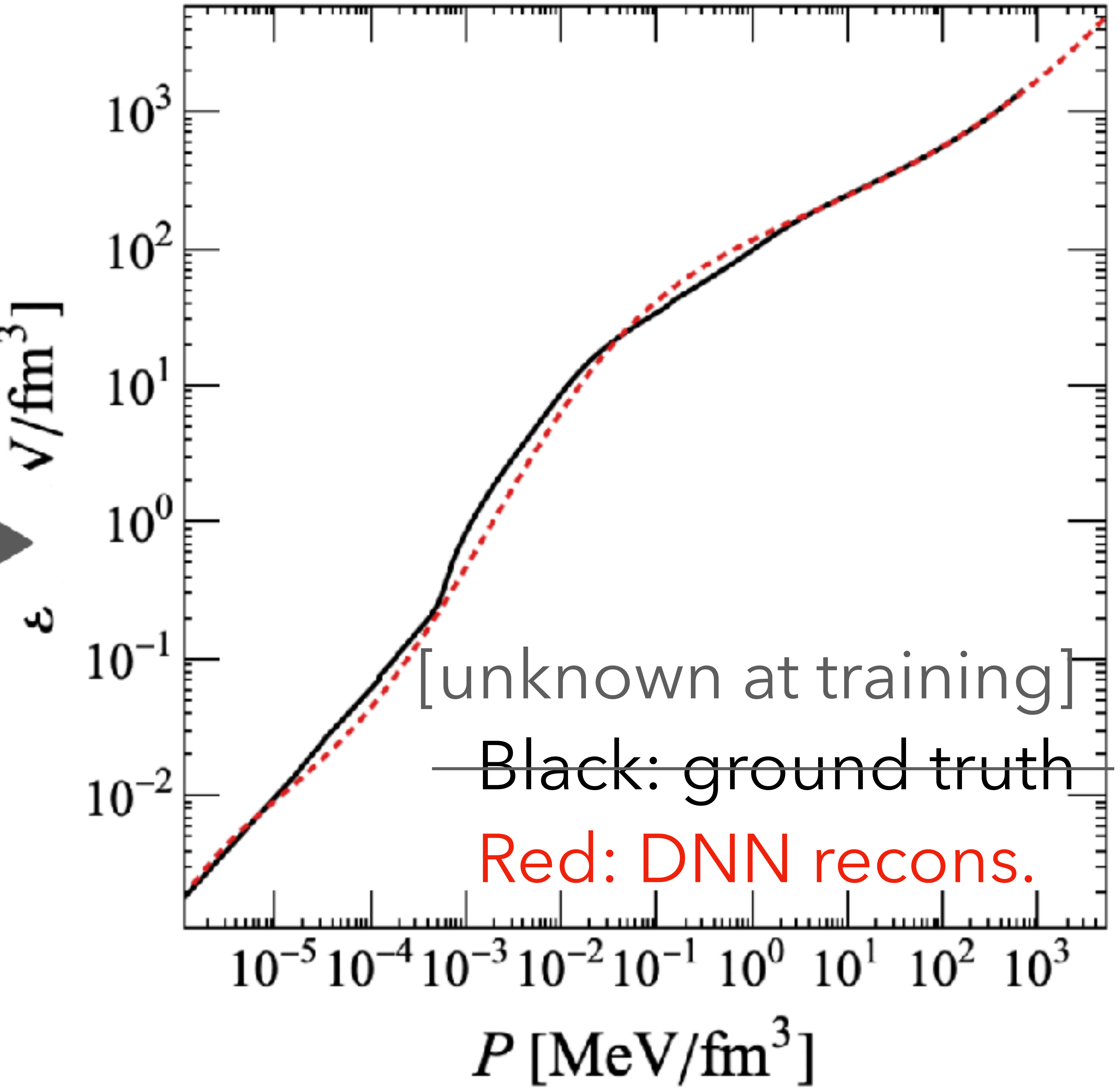

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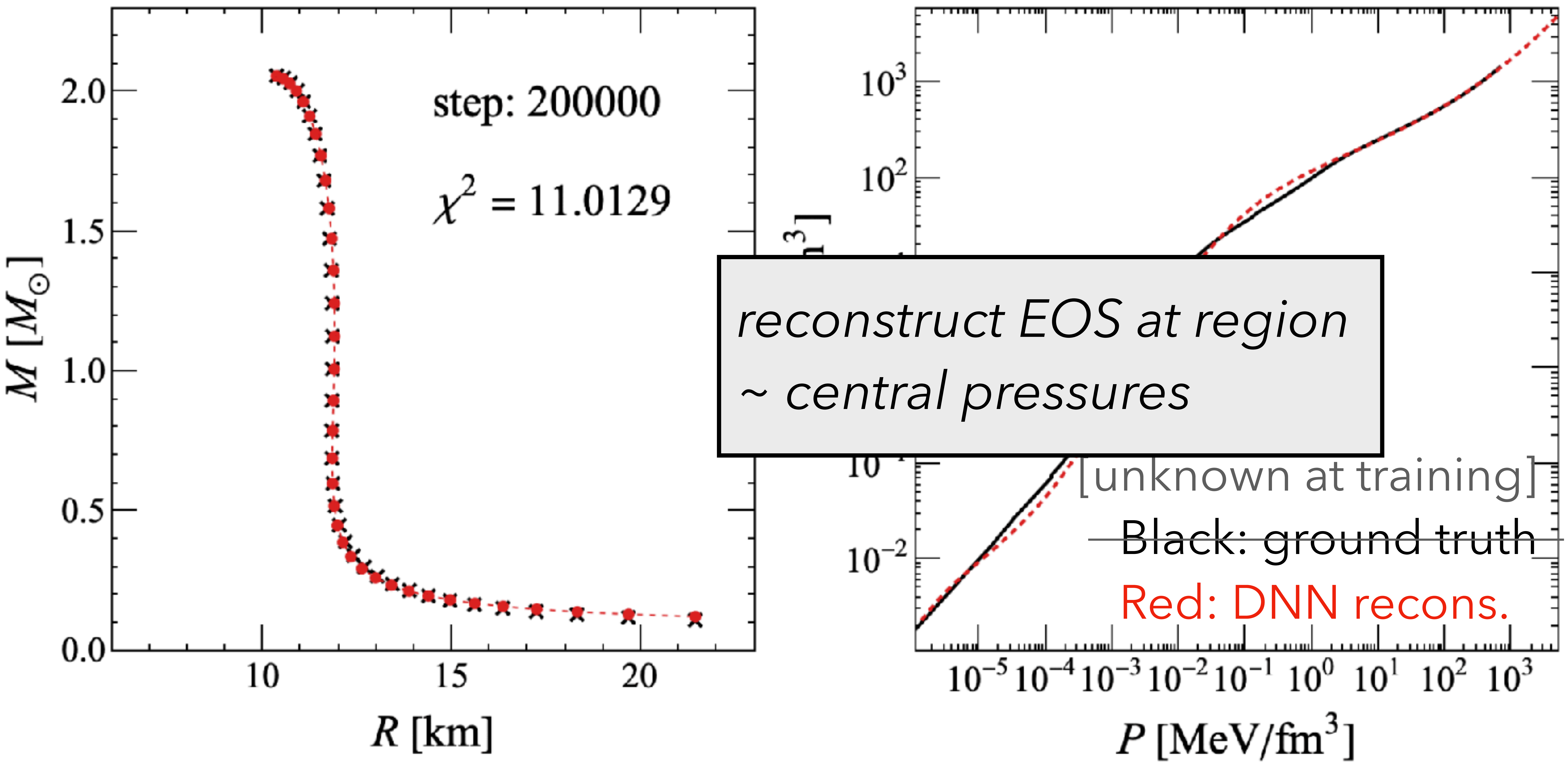
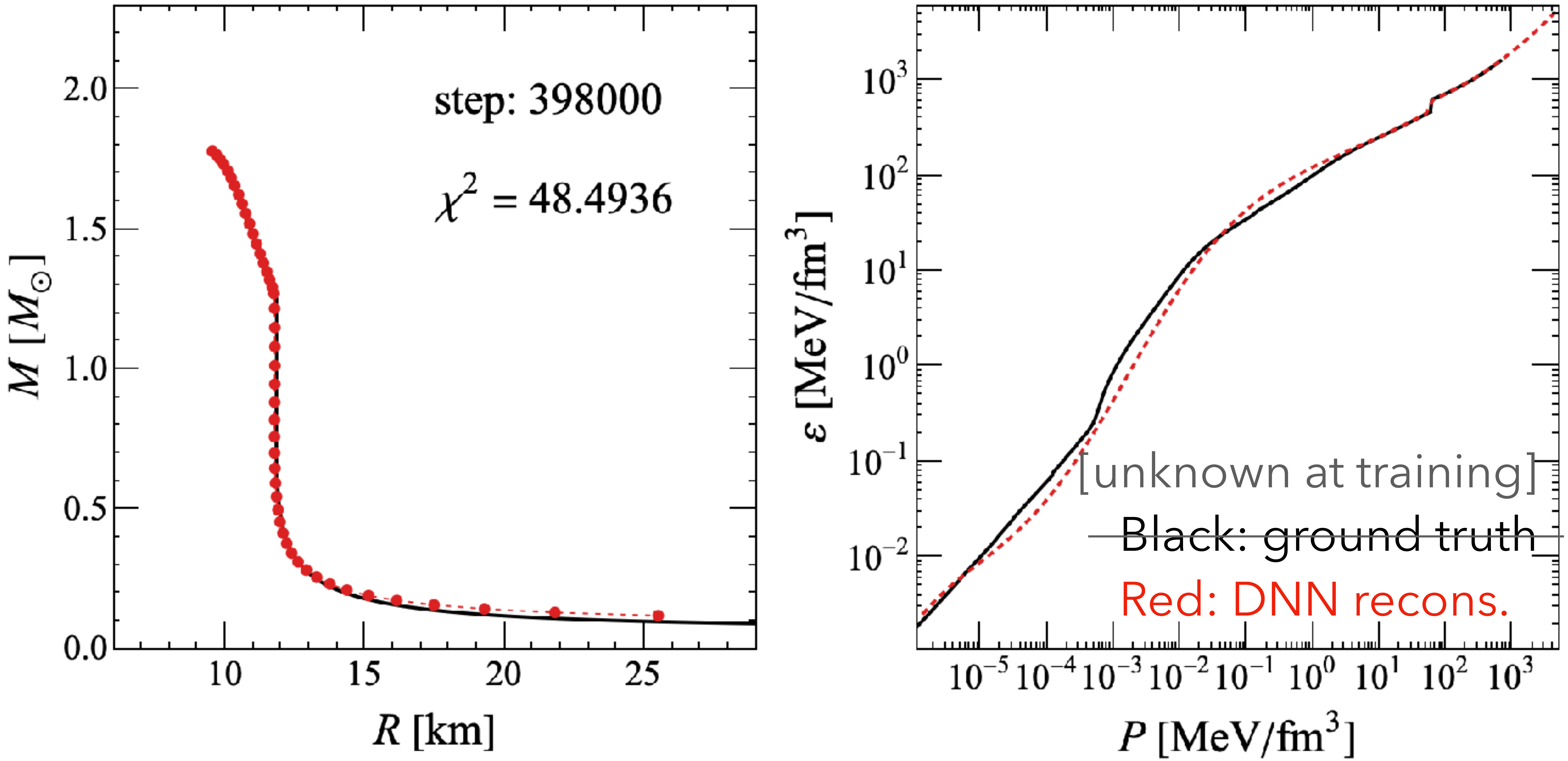
closure test



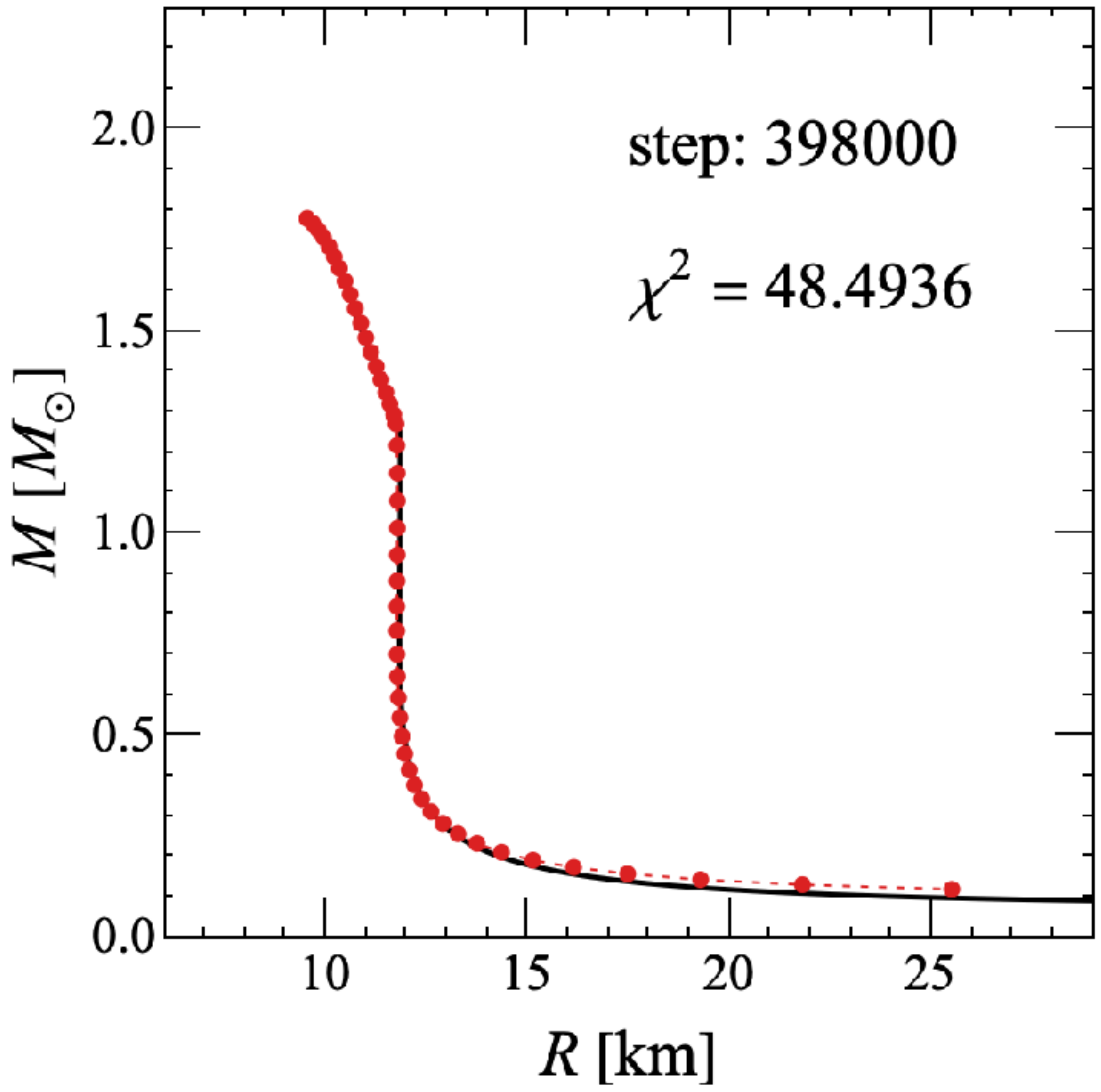
reconstruct EOS at region
~ central pressures

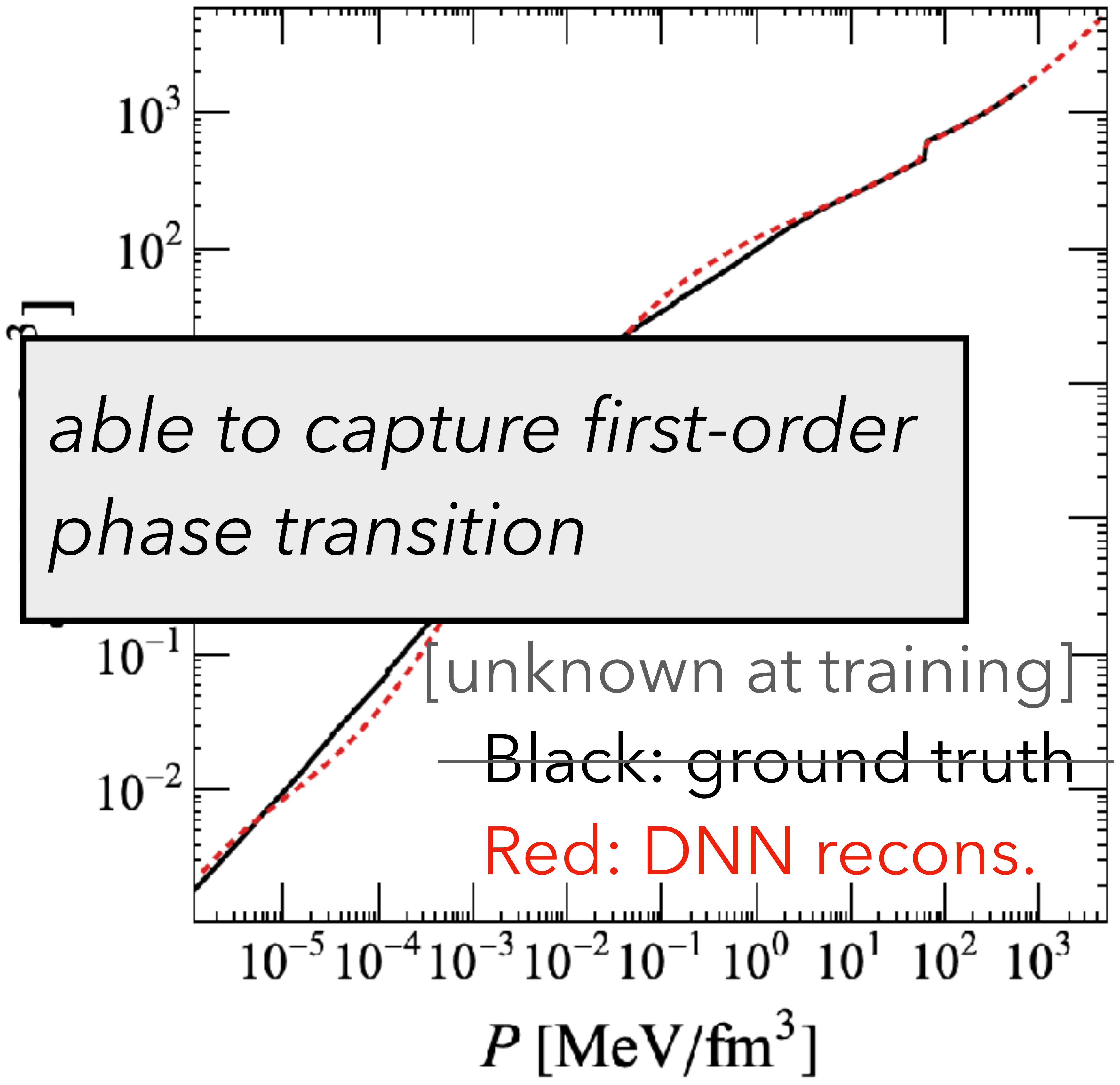
$$\chi^2 = \sum_i \left(\frac{m_i - m_i^{\rm obs}}{\Delta m_i}\right)^2 + \left(\frac{R_i - R_i^{\rm obs}}{\Delta R_i}\right)^2$$

closure test: with phase transition



closure test: with phase transition





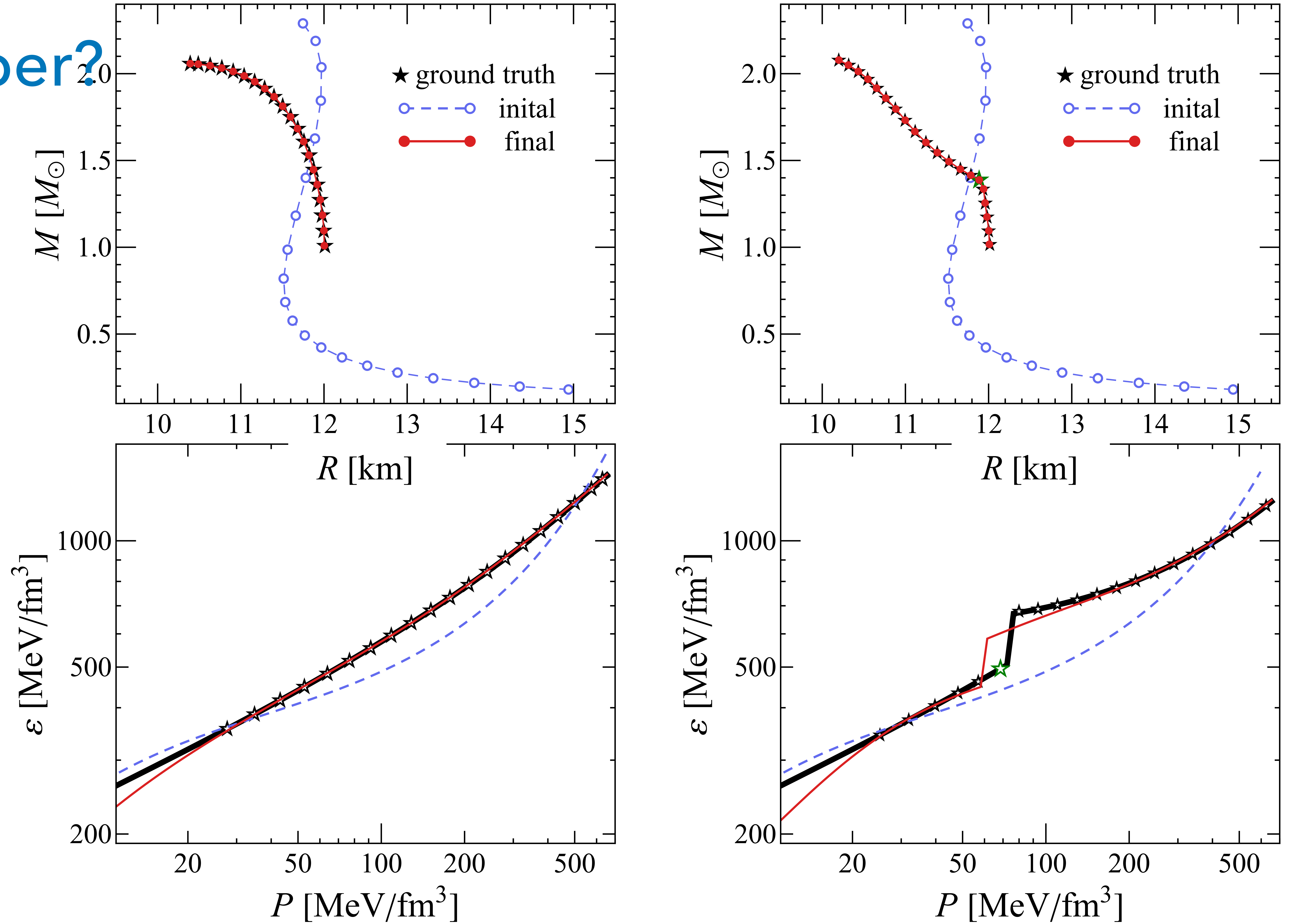
able to capture first-order phase transition

[unknown at training]

~~Black: ground truth~~

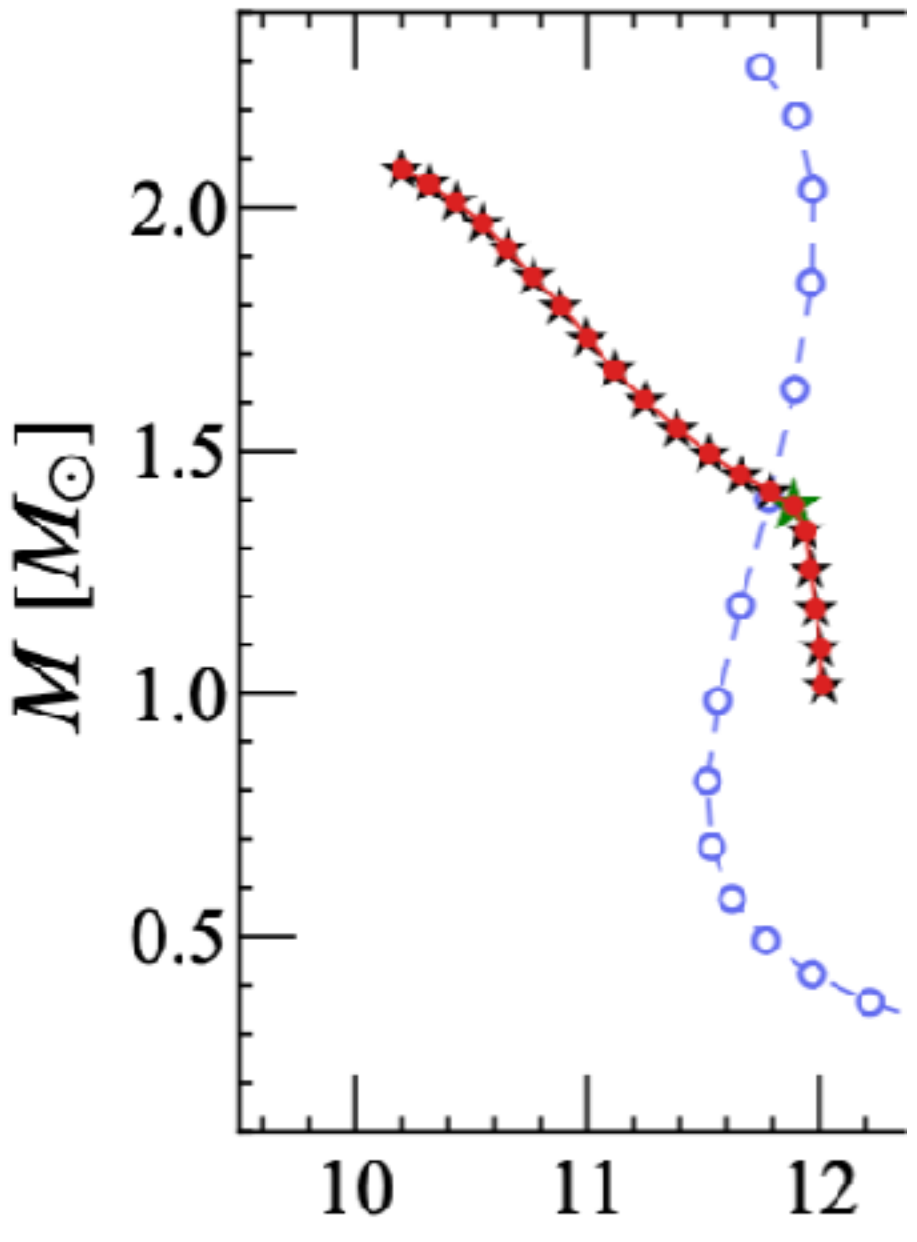
Red: DNN recons.

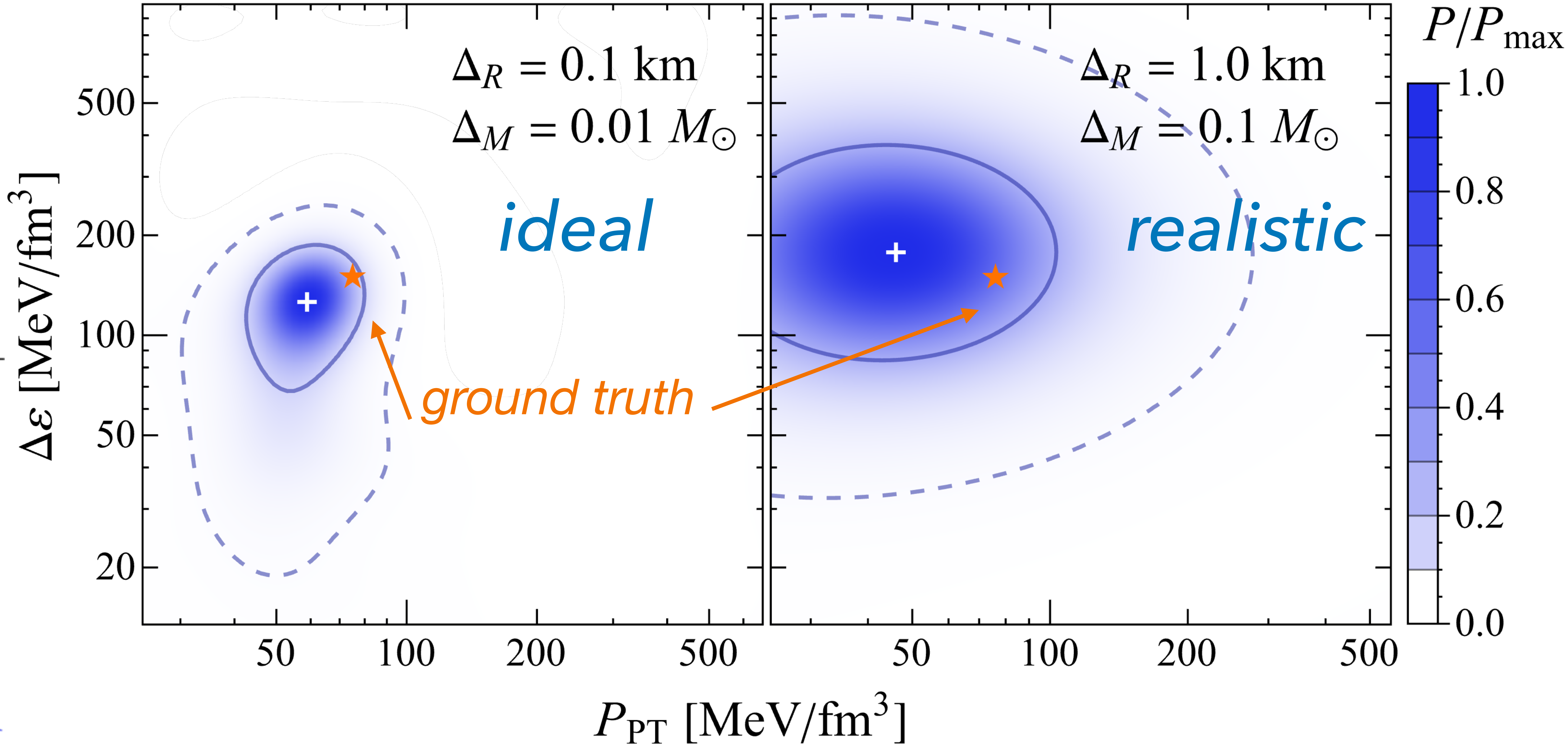
reconstruction w/ finite number?



reconstruction power for different uncertainties

marginal posterior distribution of phase transition pressure and latent heat





assign different level of uncertainties and perform BA.

Summary

- Develop new algorithm employing DNN to solve inverse problems.

- Extracted HF complex $V(T, r)$ from LQCD results of bottomonium m and Γ.

- Can be applied to learn Neutron Star EOS from Mass-Radius observations.

- Discussed application and limitations in reconstructing spectral function.