

How Machine-Learning helps in the subtleties of the spectral function reconstruction

— *what we learned from solving inverse problems via Deep Learning*

施舒哲 清华大学

refs:

SS, Zhou, Zhao, Mukherjee, Zhuang, Phys. Rev. D **105**, 014017;
Wang, **SS**, Zhou, Phys. Rev. D **106**, L051502;
SS, Wang, Zhou, Comput.Phys.Commun. 282 (2023) 108547.

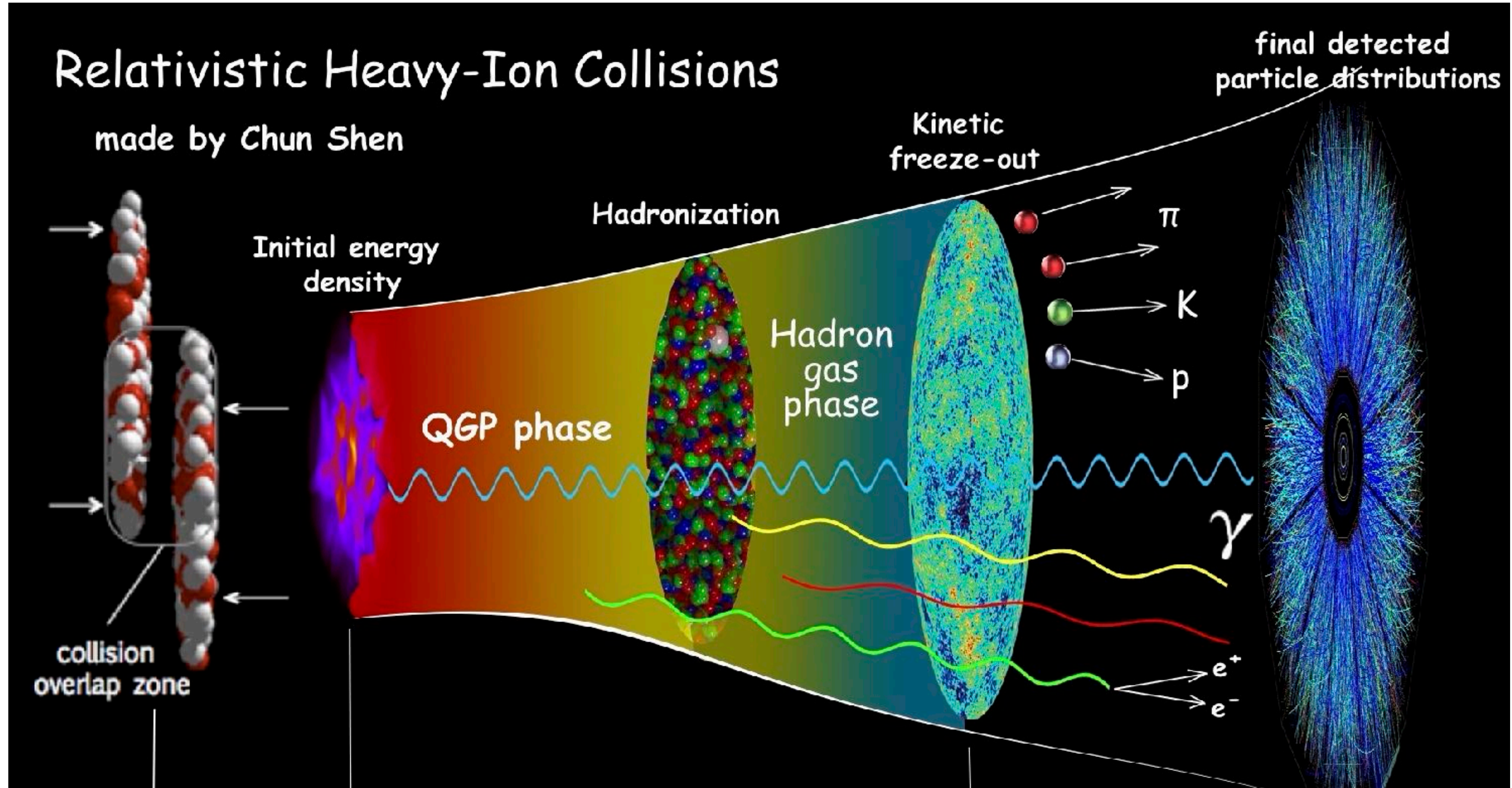
a recent review:

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

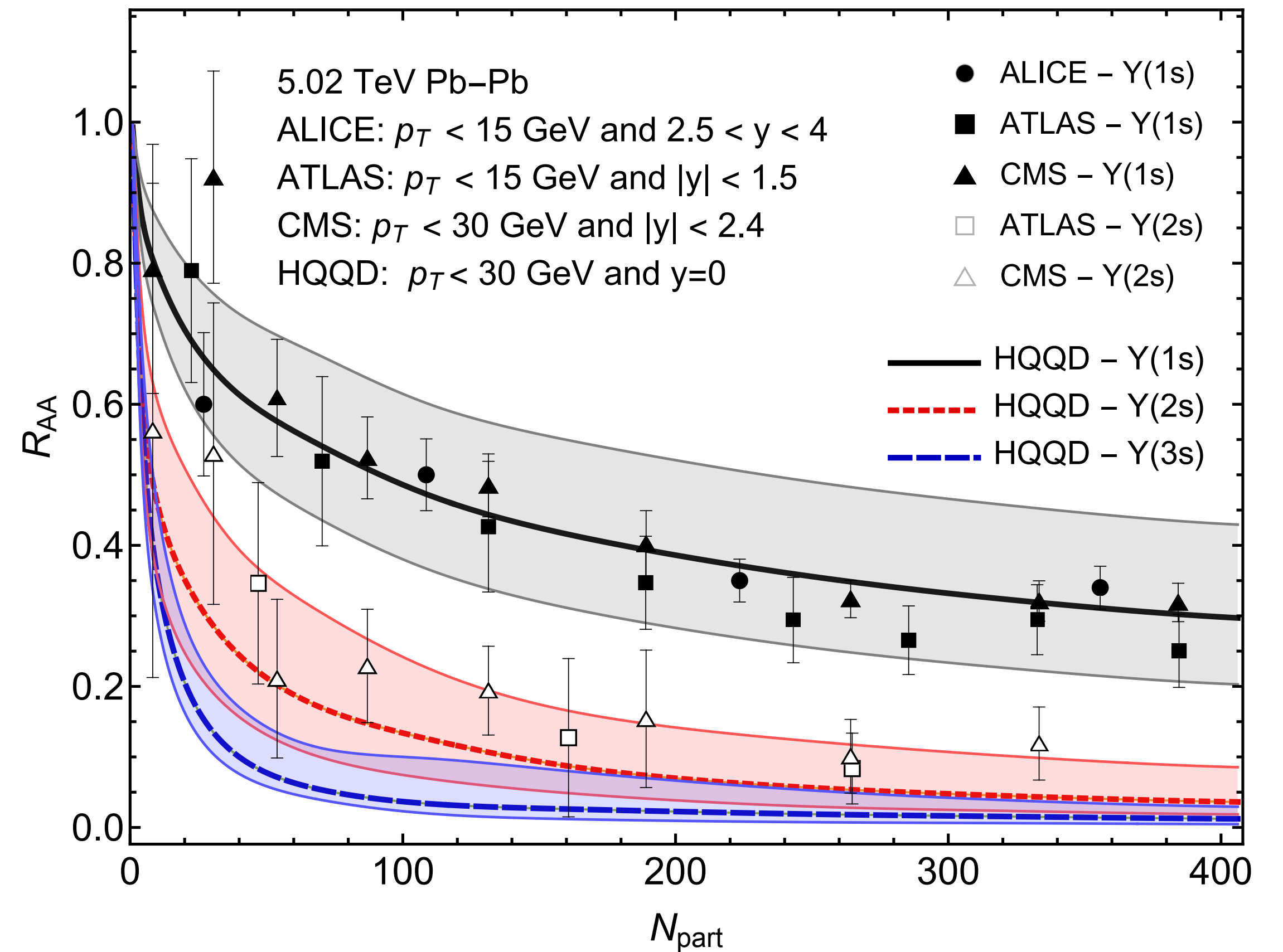
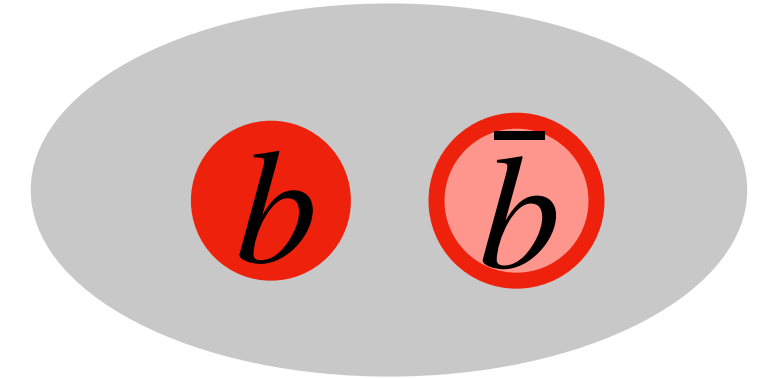
Outline

- Quarkonium potential
- Difficulties in spectral function reconstruction

Relativistic Heavy-Ion Collisions



- In heavy-ion collisions, quarkonium production serves as a probe of the QGP.



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- Accurate understanding of the in-medium heavy-quark interaction?
 - Real potential modified by color-screening
 - Imaginary potential arises due to $(Q\bar{Q})_1 \rightarrow (Q\bar{Q})_8$, Landau damping, ...

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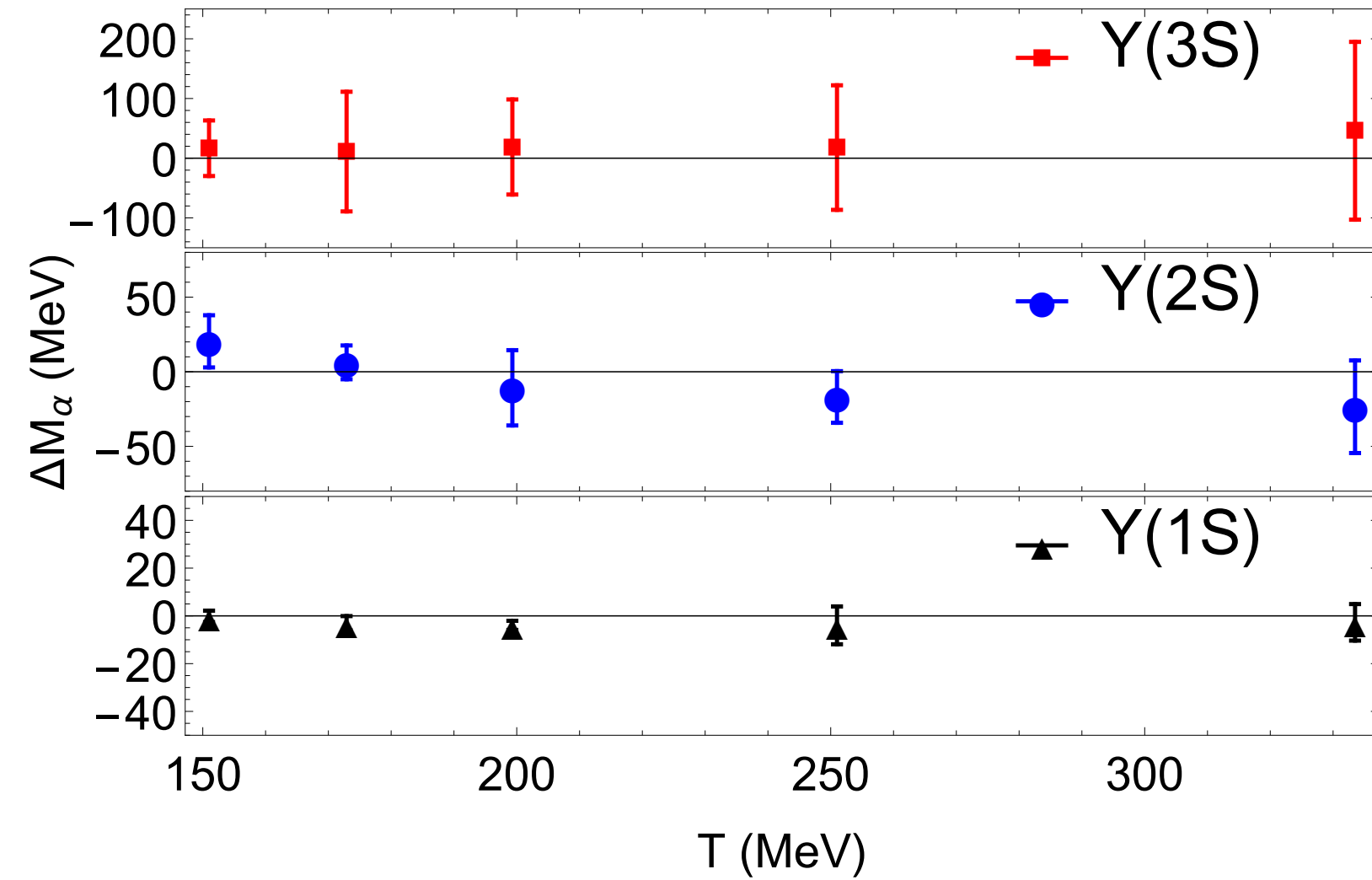
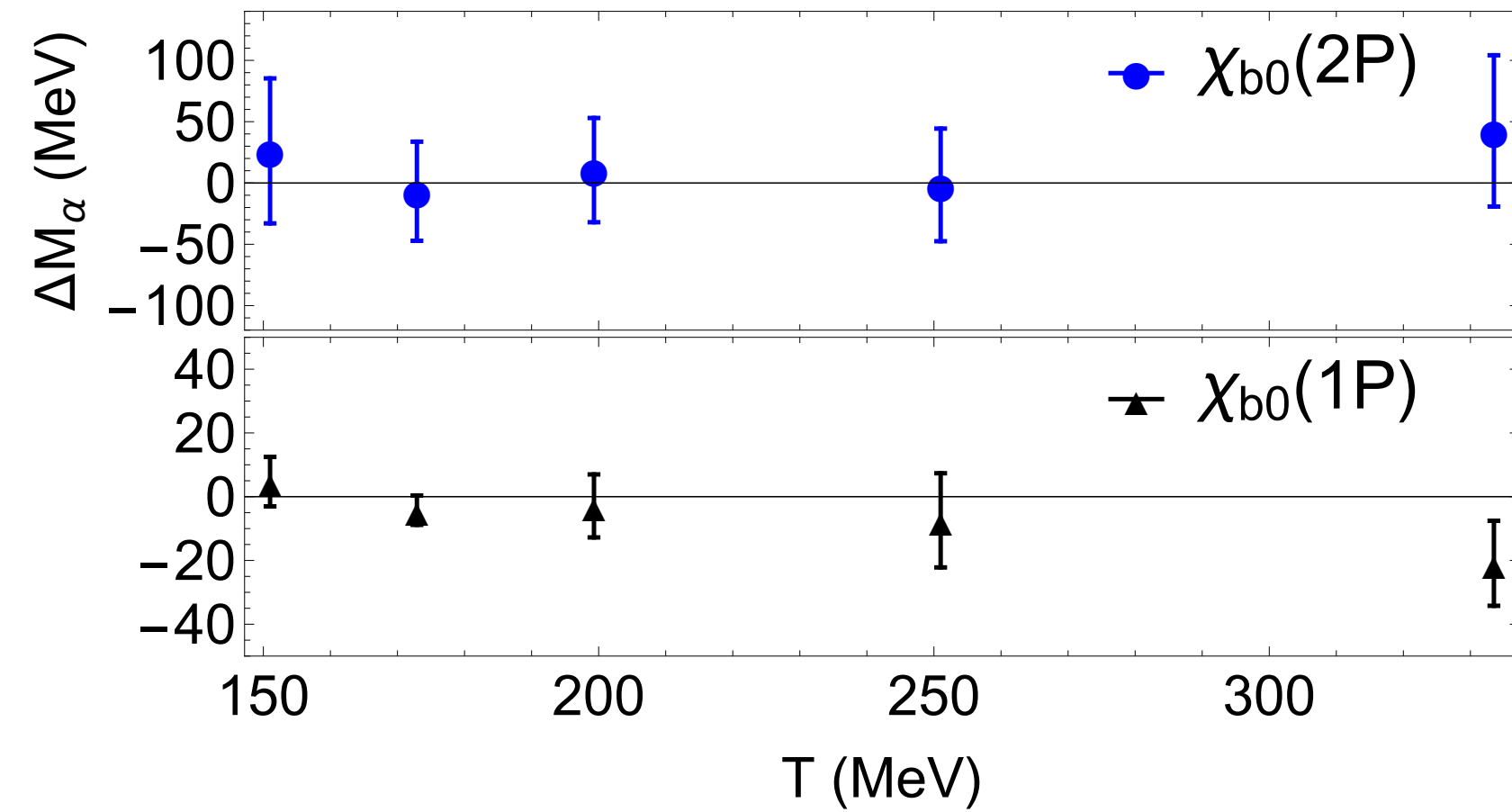
Hard Thermal Loop potentials

$$V_R(T, r) = \frac{\sigma}{\mu_D} \left(2 - (2 + \mu_D r) e^{-\mu_D r} \right) - \alpha \left(\mu_D + \frac{e^{-\mu_D r}}{r} \right) + B,$$

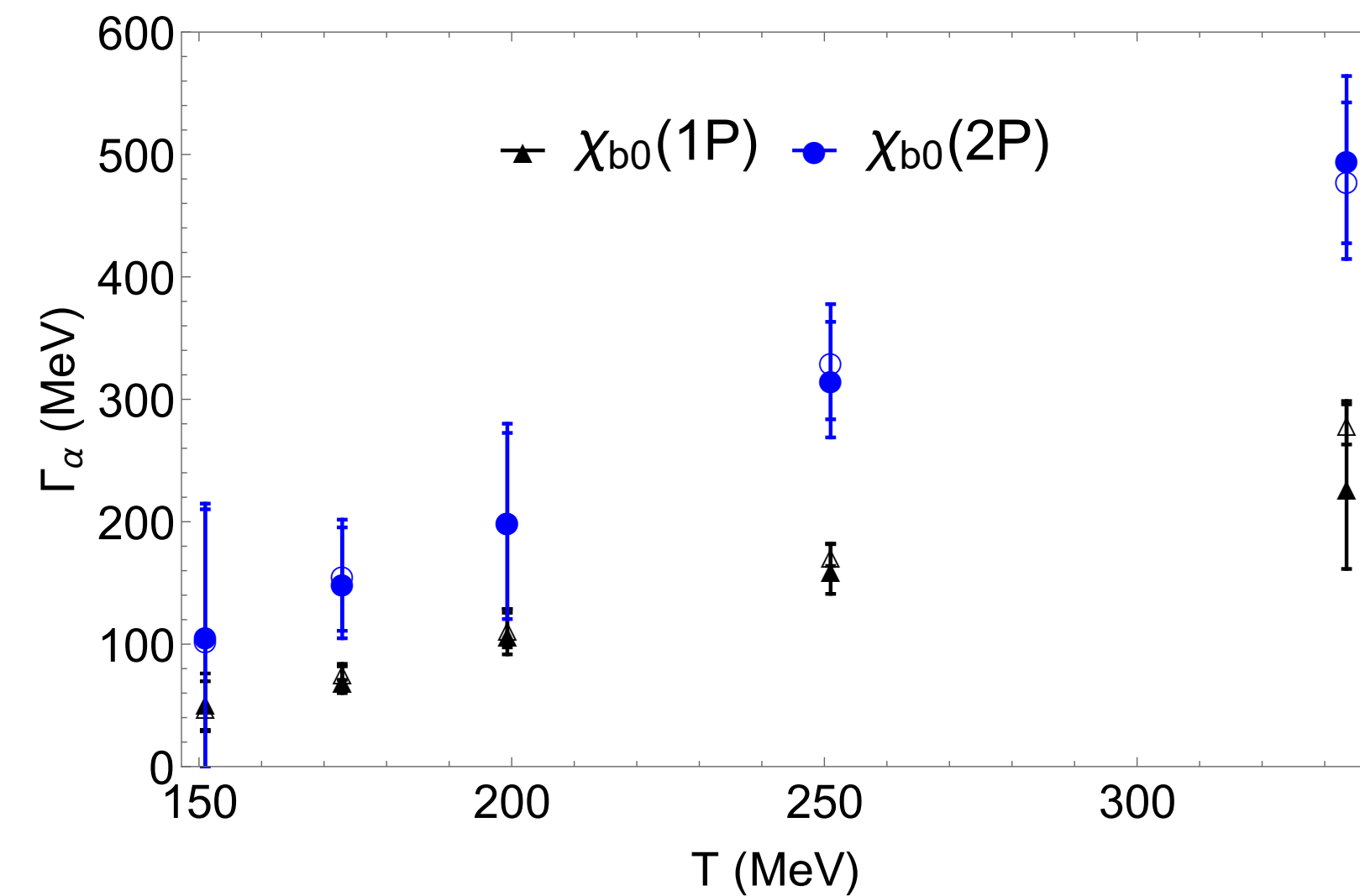
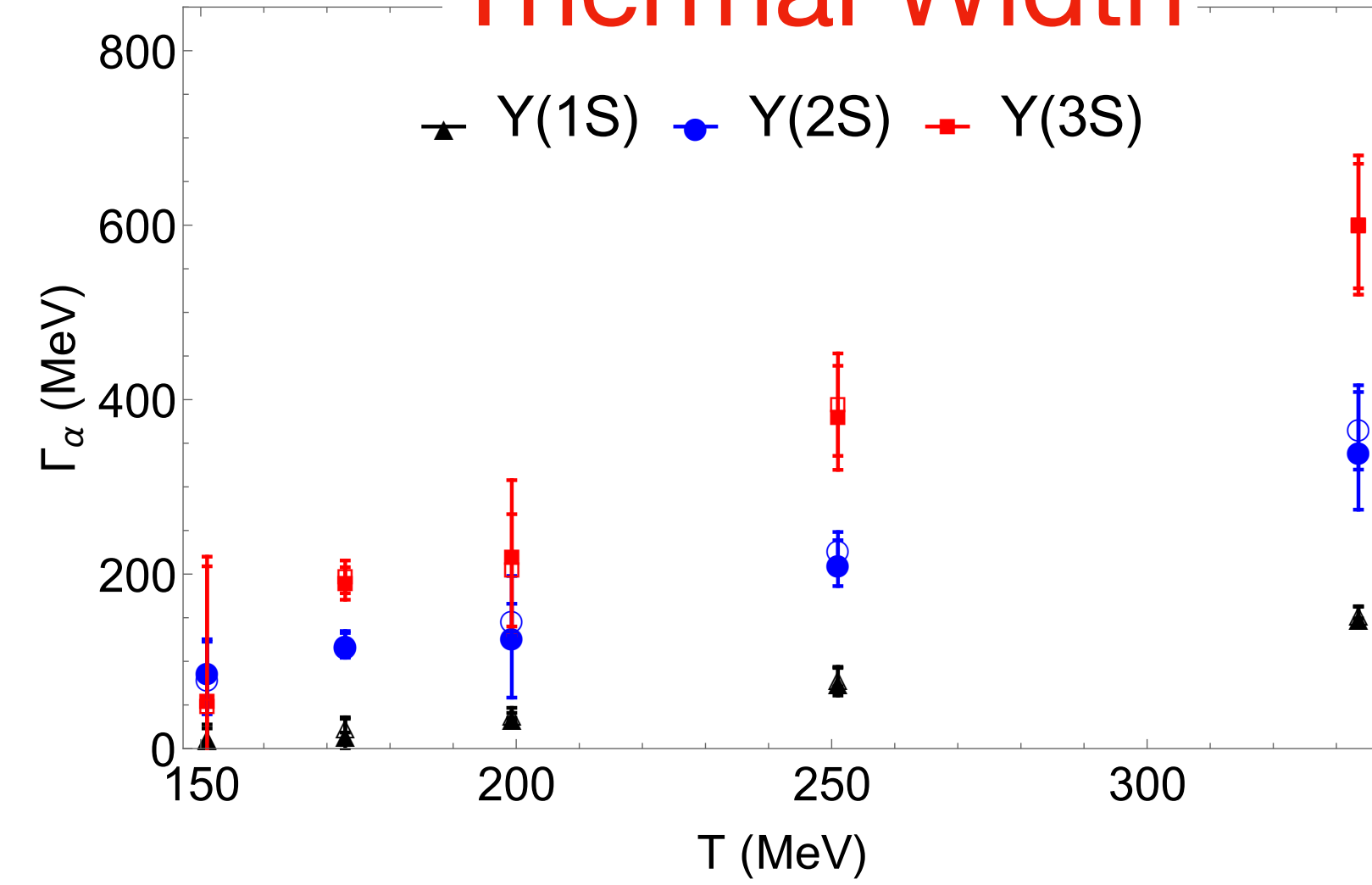
$$V_I(T, r) = -\frac{\sqrt{\pi}}{4} \mu_D T \sigma r^3 G_{2,4}^{2,2} \left(\begin{matrix} -\frac{1}{2}, -\frac{1}{2} \\ \frac{1}{2}, \frac{1}{2}, -\frac{3}{2}, -1 \end{matrix} \middle| \frac{\mu_D^2 r^2}{4} \right) - \alpha T \phi(\mu_D r).$$

see e.g., Laine, Philipsen, Romatschke, and Tassler, JHEP 03, 054 (2007)

Mass



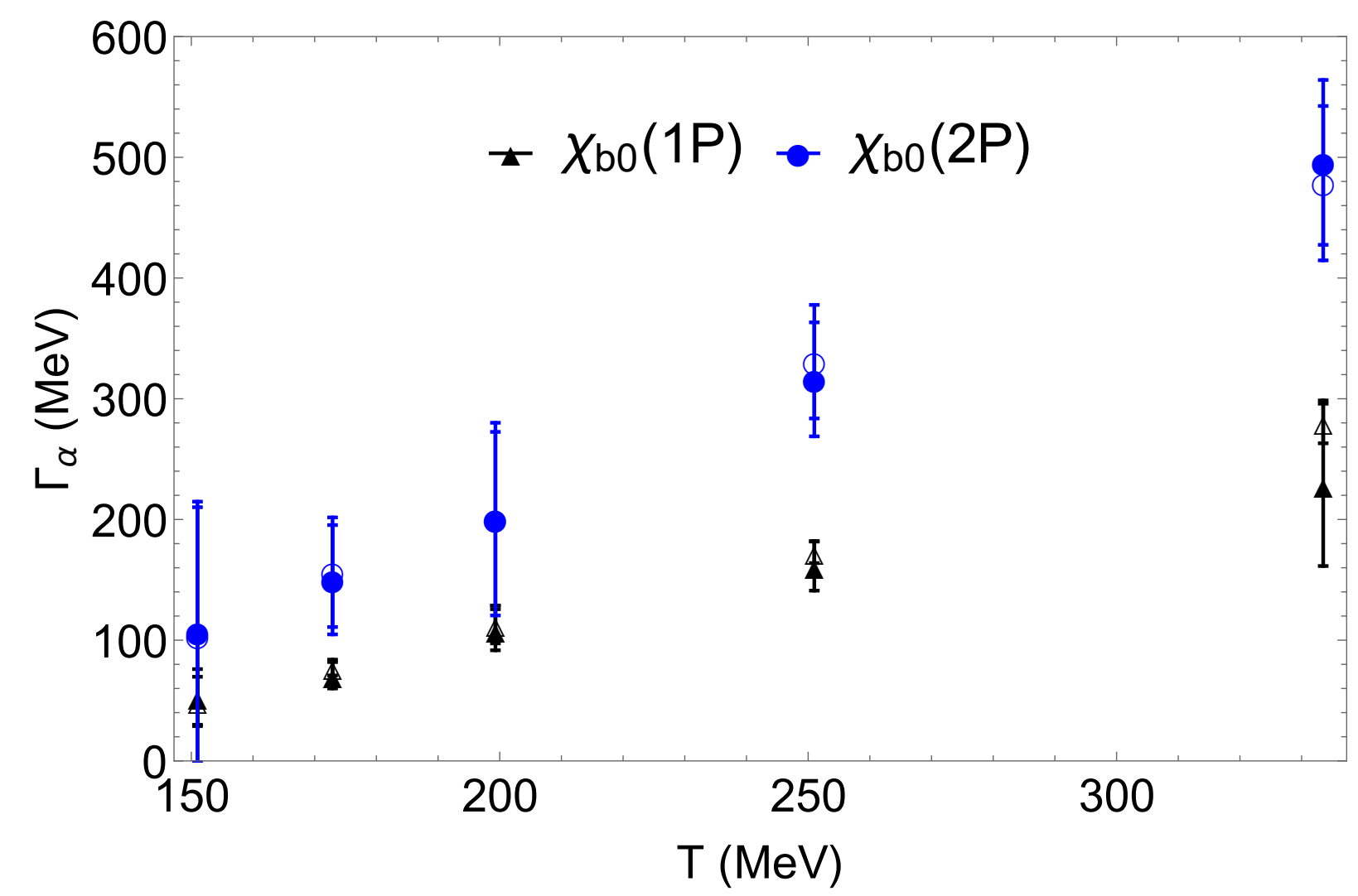
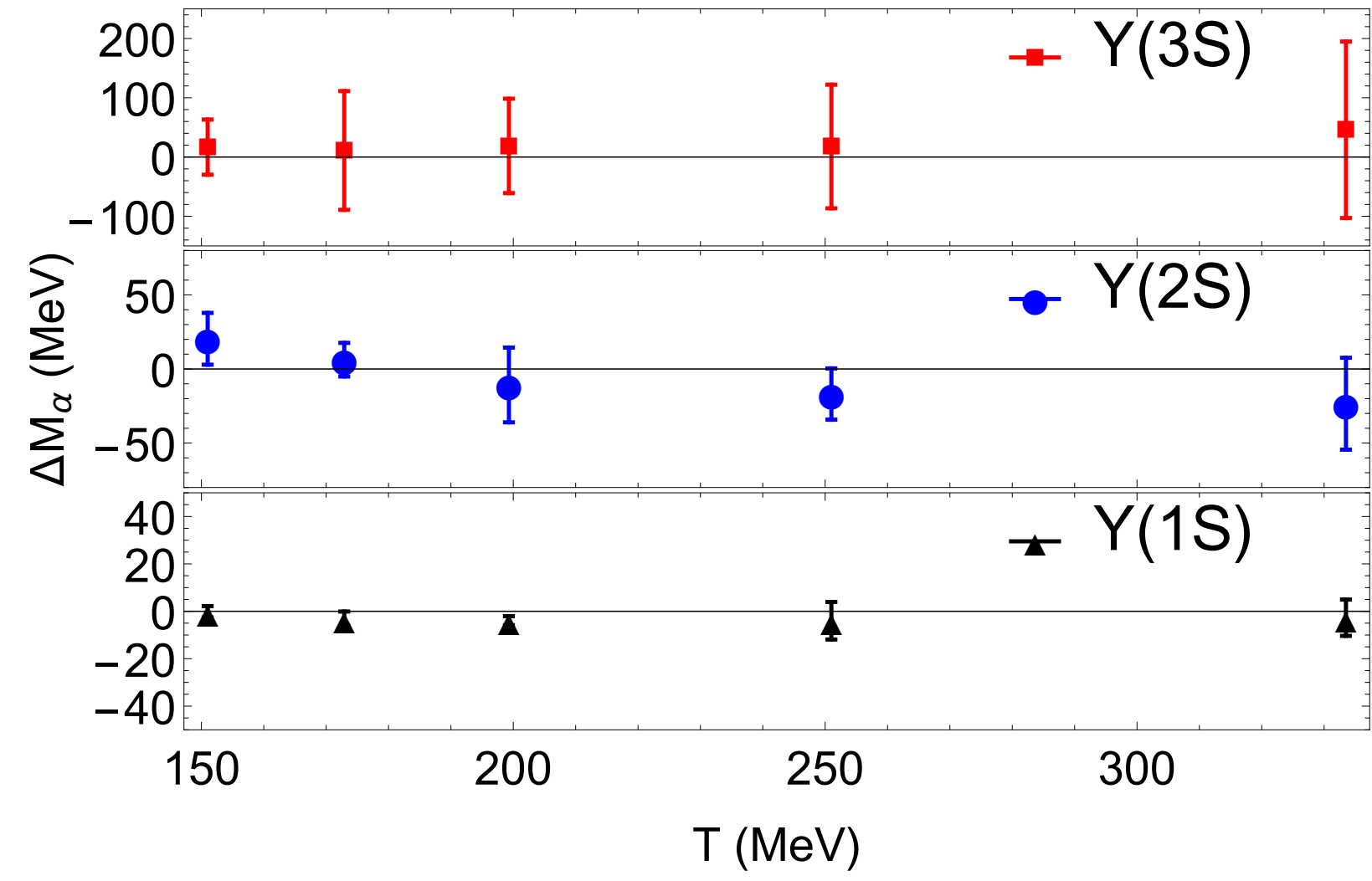
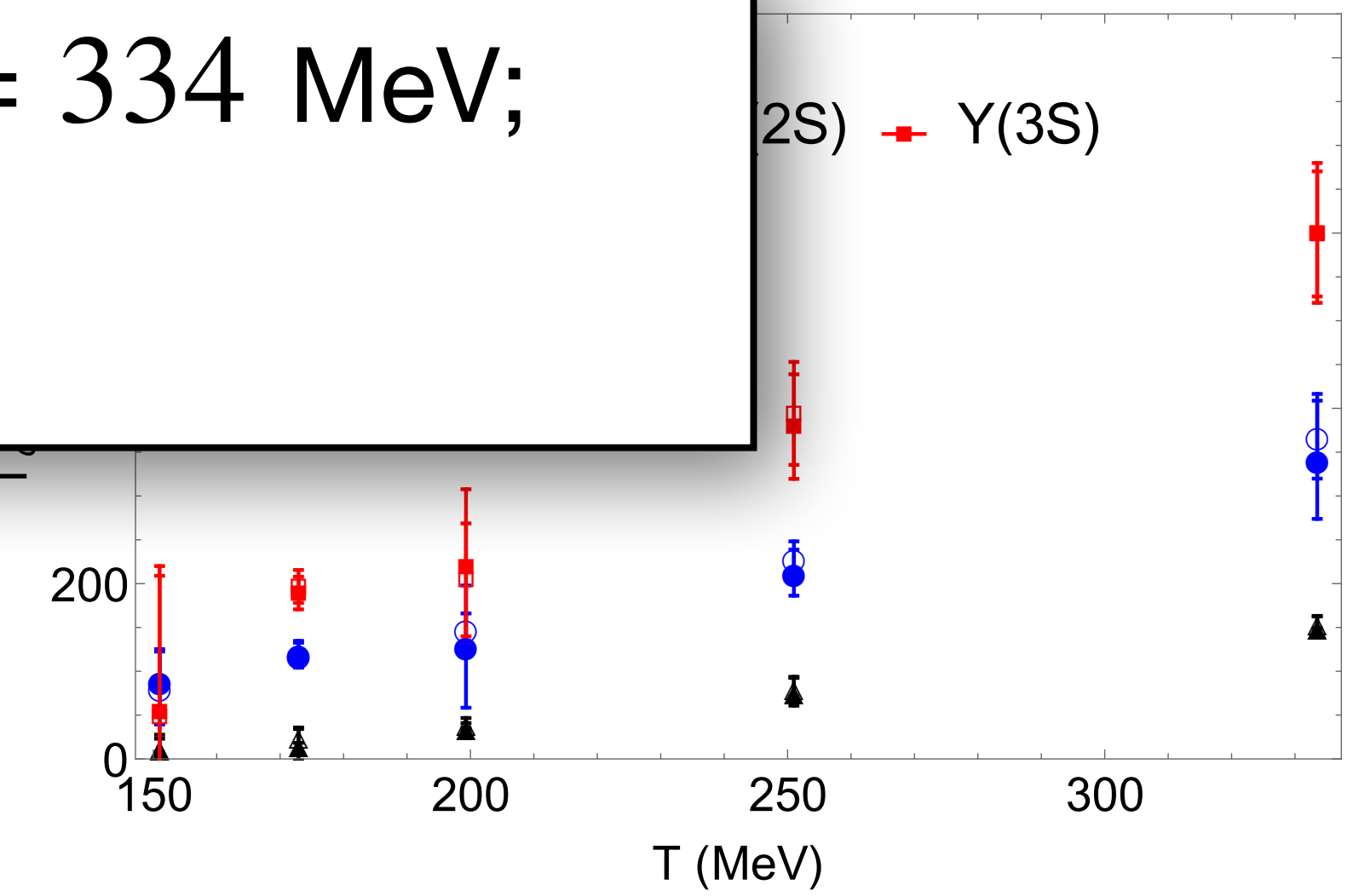
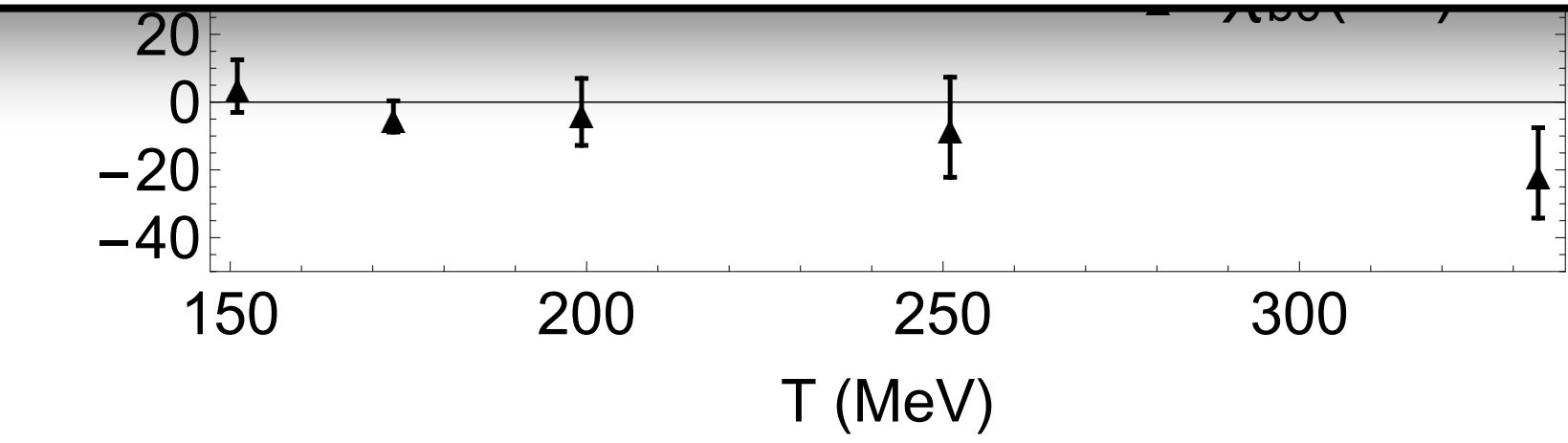
Thermal Width



R. Larsen, S. Meinel, S. Mukherjee, and P. Petreczky:

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

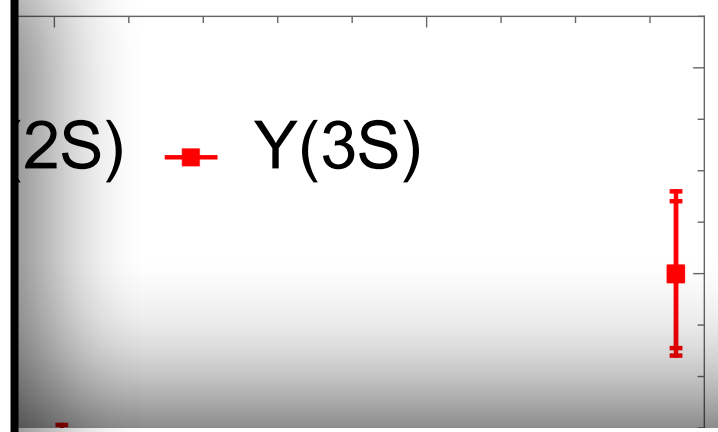
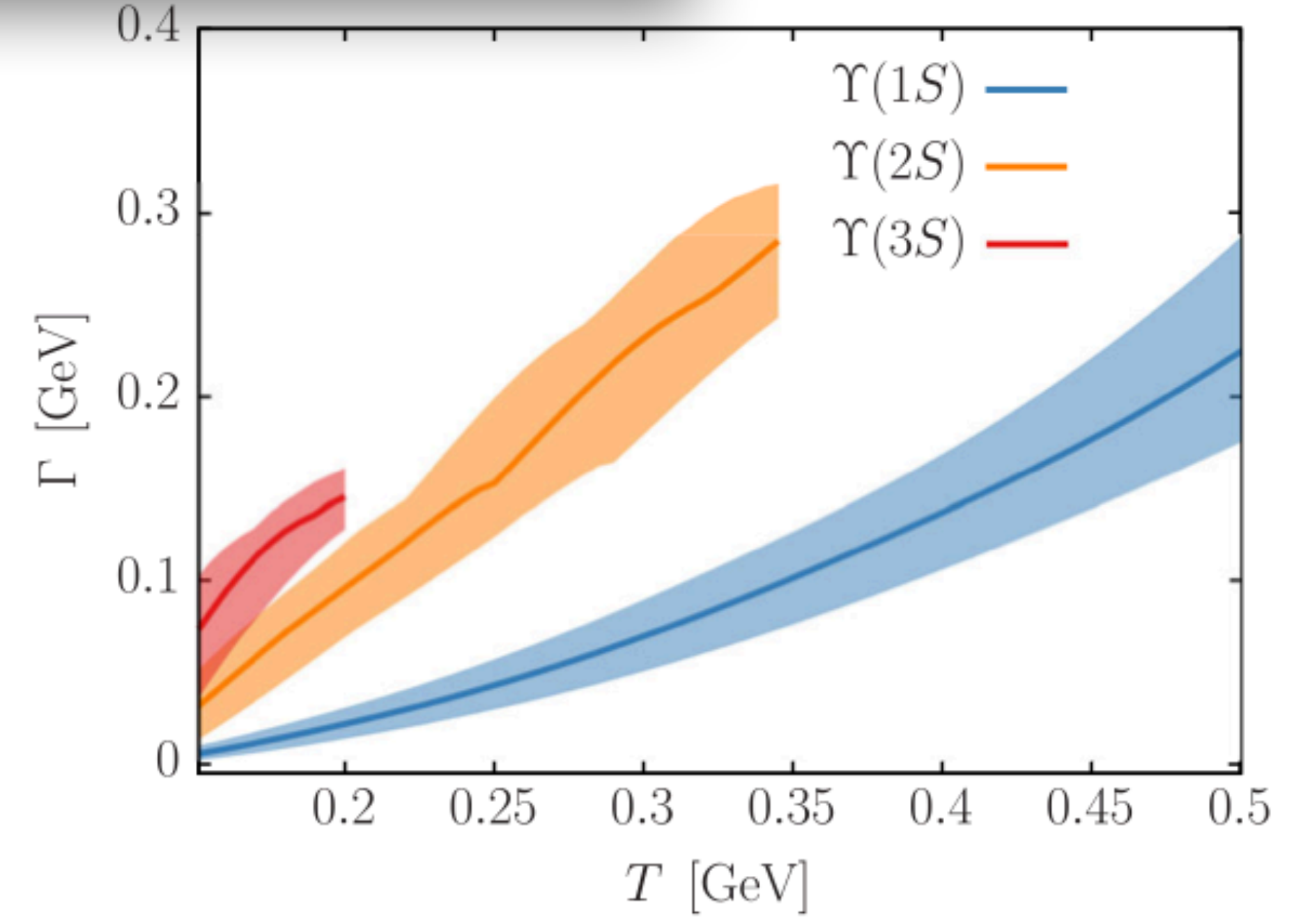
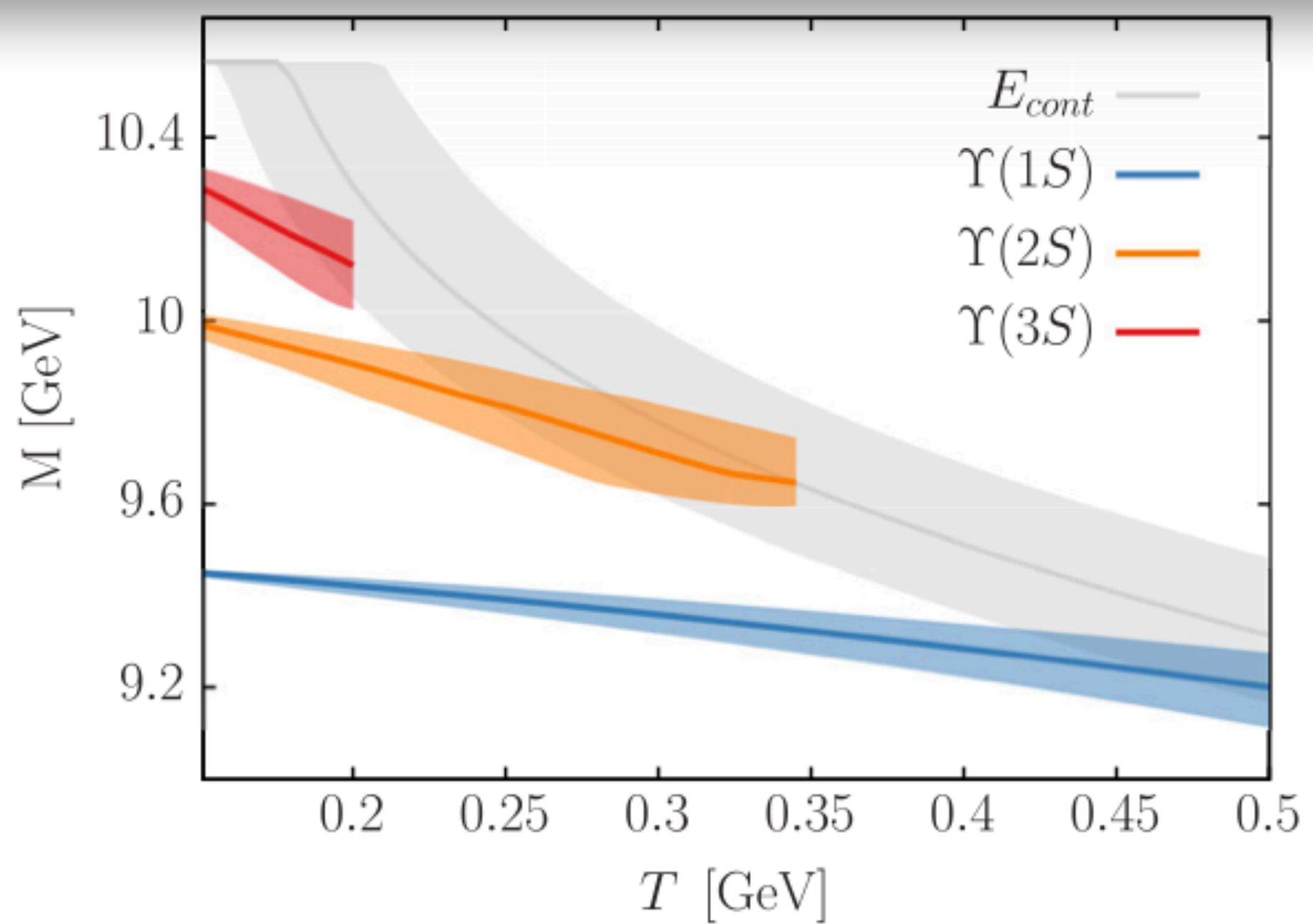
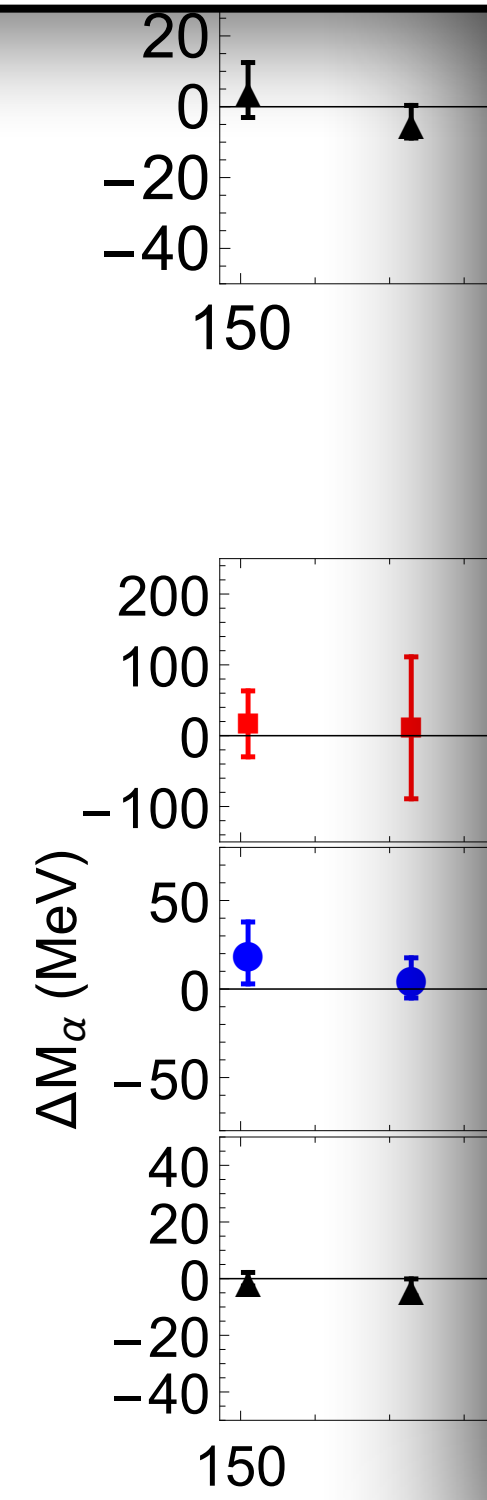
High excitations (2P, 3S) can survive at $T = 334$ MeV;
 Mass - mild temperature dependence;
 Thermal width - quantitatively larger.



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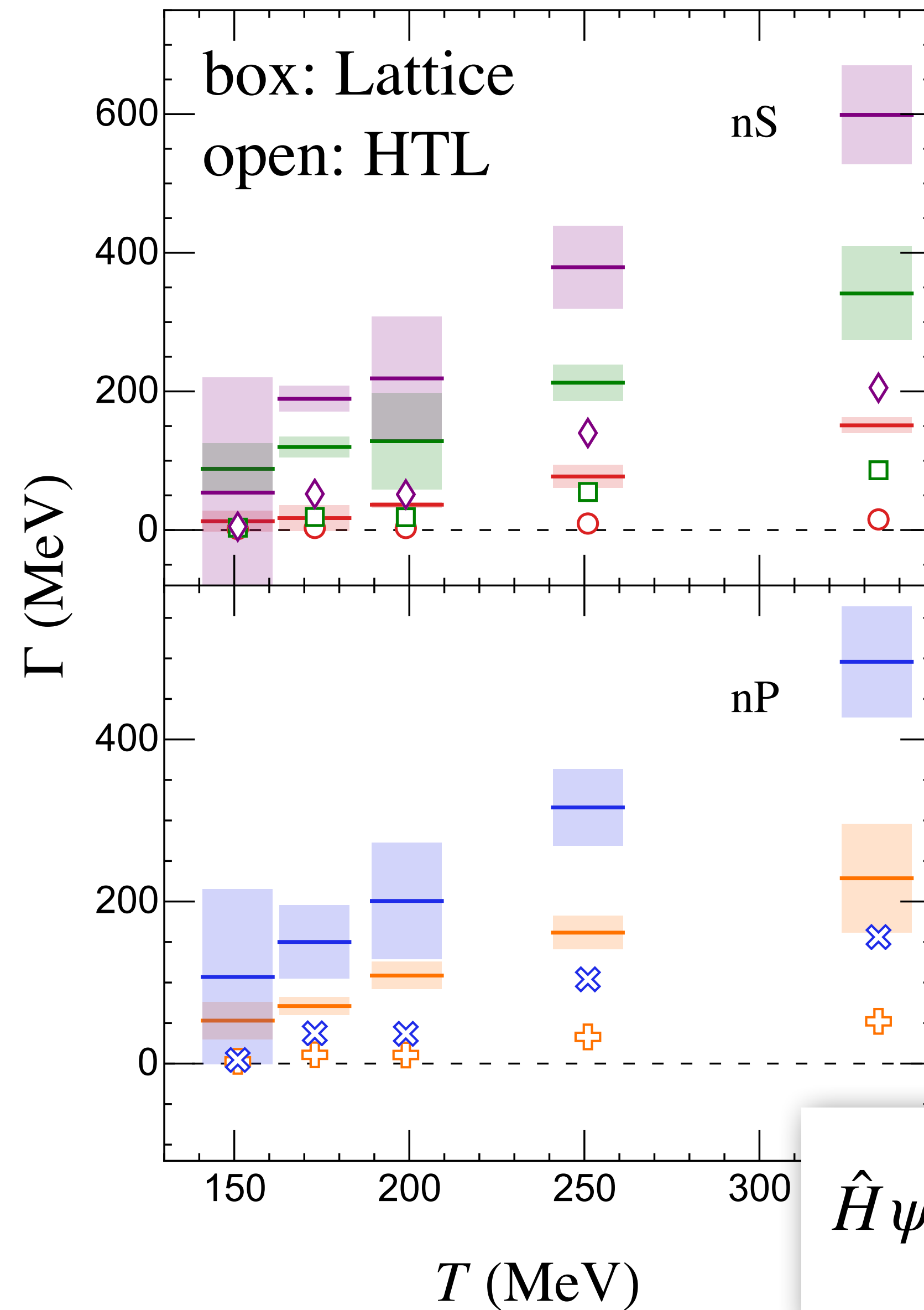
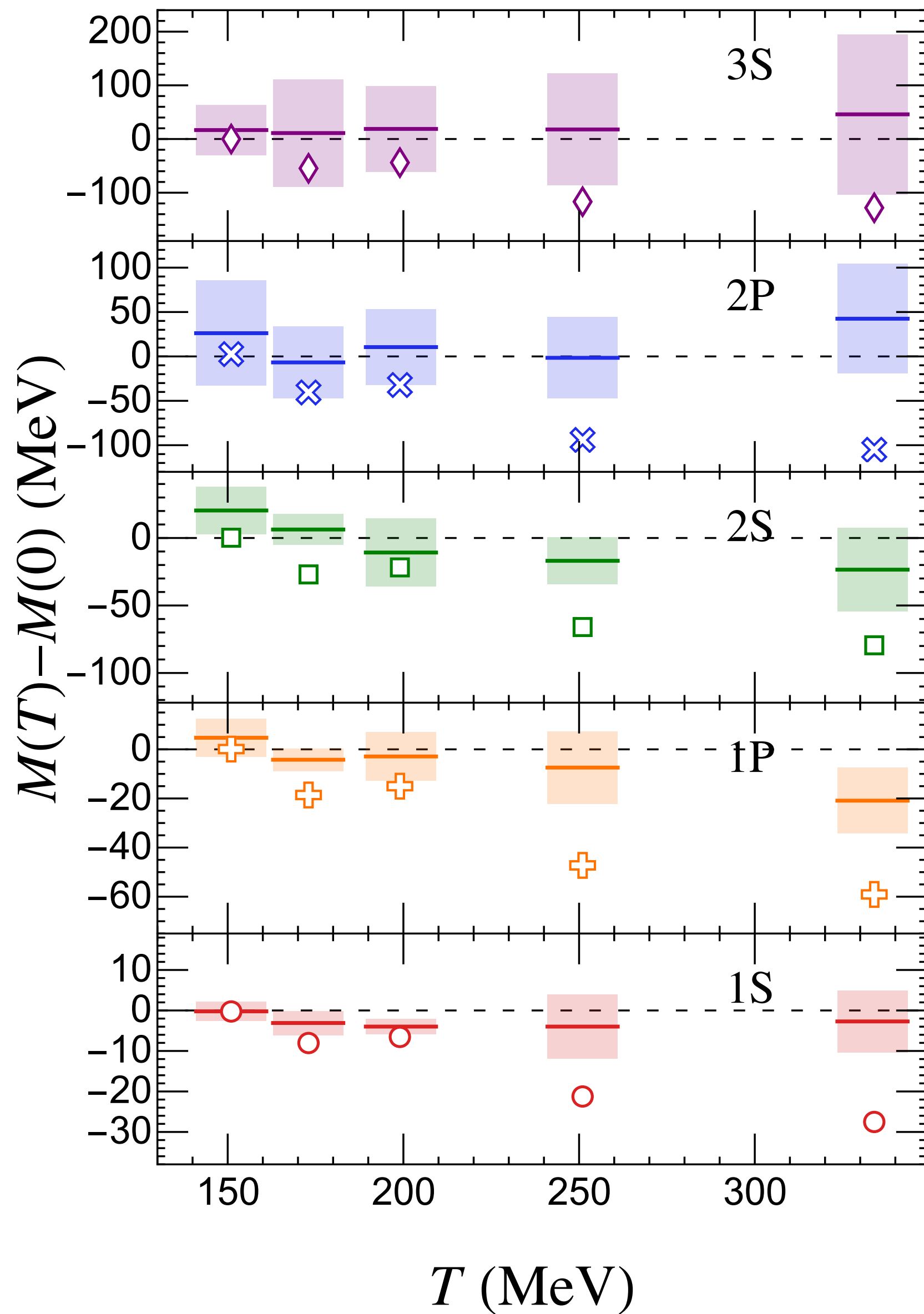
High excitations (2P, 3S) can survive at $T = 334$ MeV;
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D. Lafferty and A. Rothkopf, PhysRevD.101.056010(2020)

R. Larsen, S. Meinel, S. Mukherjee, and P. Petreczky:
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Can we understand the new lattice result using Hard Thermal Loop potential?

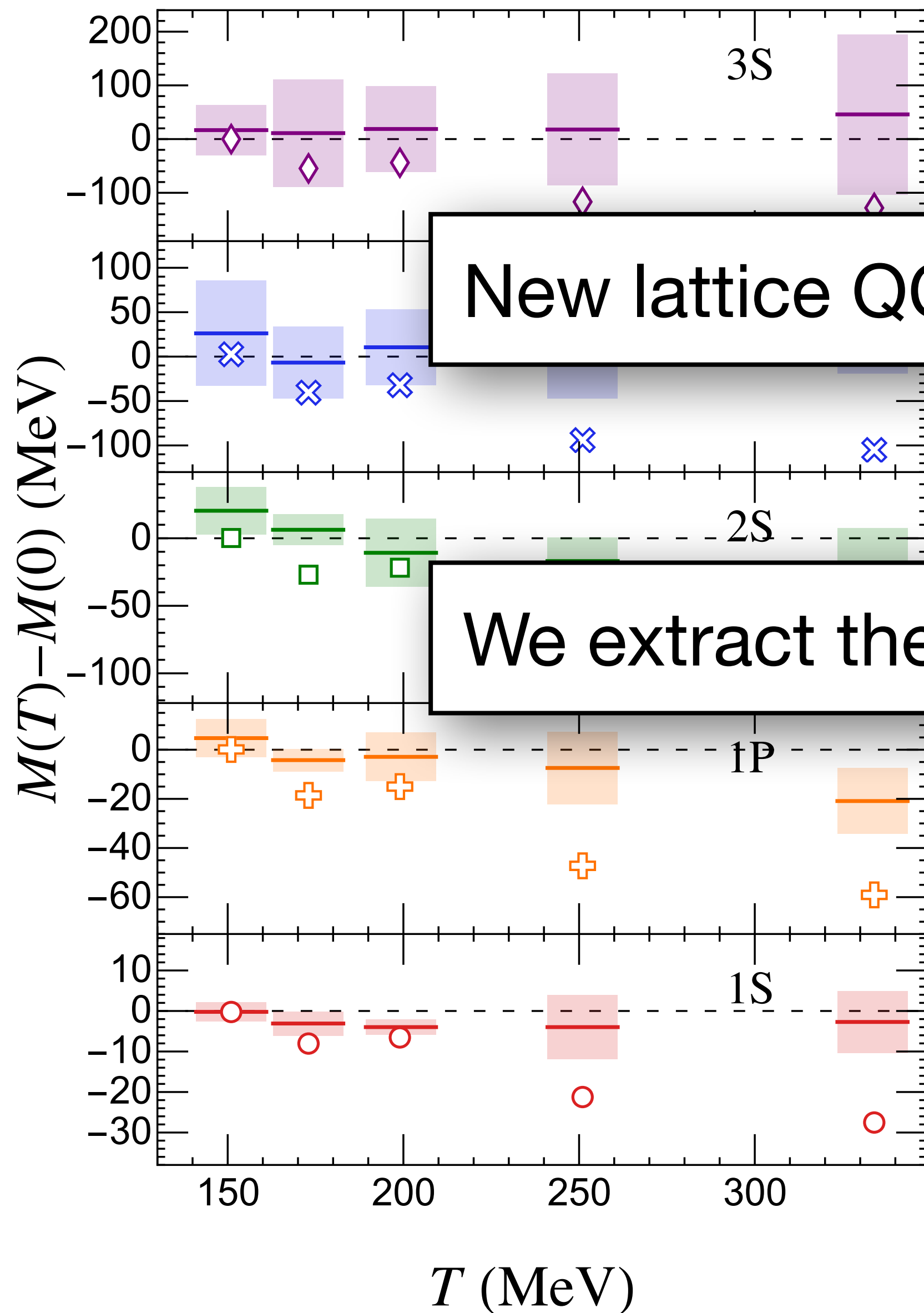


$m_D(T)$ fitted by LQCD

$$V(T, r) = V_R(T, r) + i V_I(T, r)$$

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

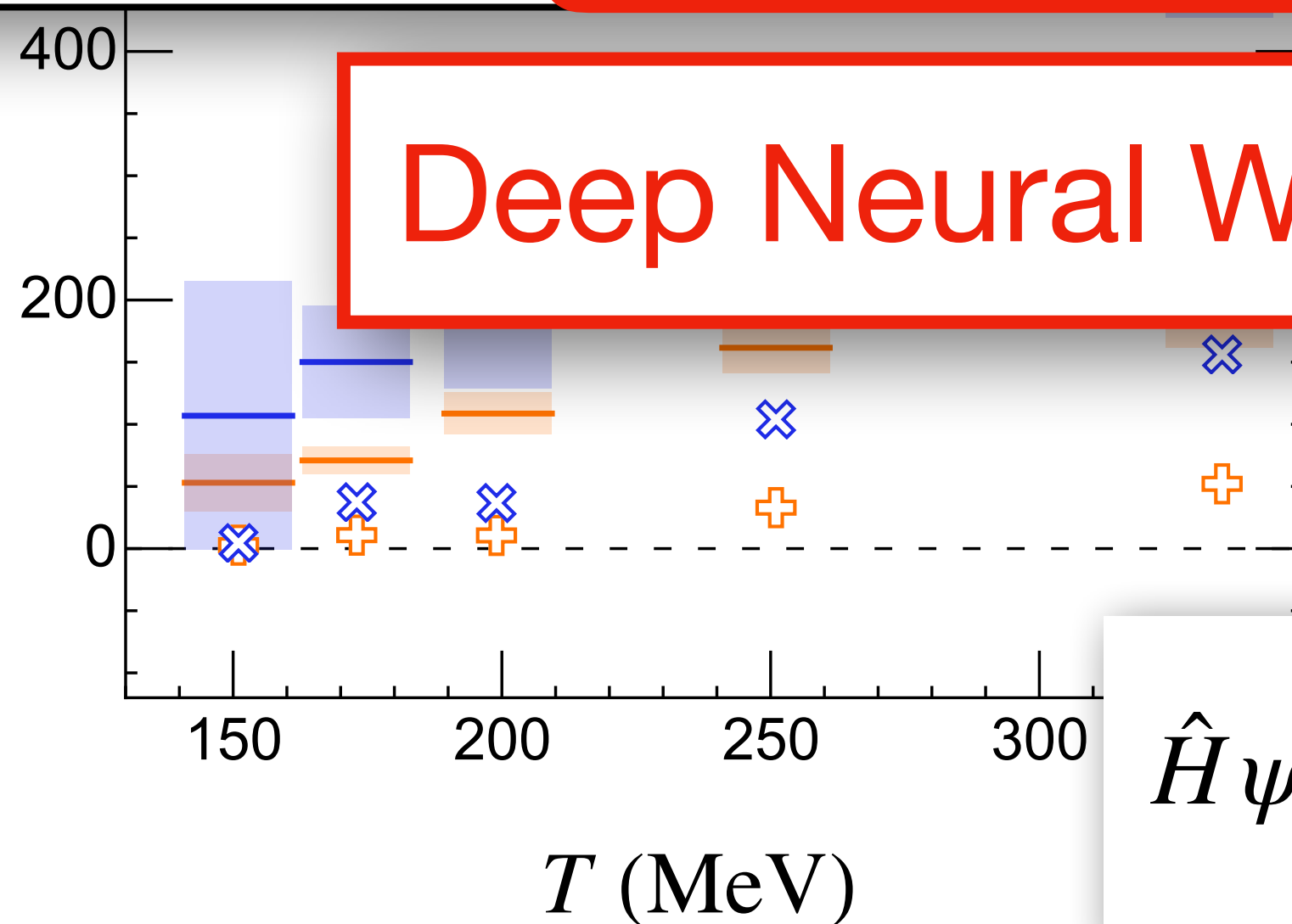
Can we understand the new lattice result using Hard Thermal Loop potential?



New lattice QCD results cannot be explained by the HTL potential

We extract the potential in a model-independent way

Deep Neural Works (DNN)

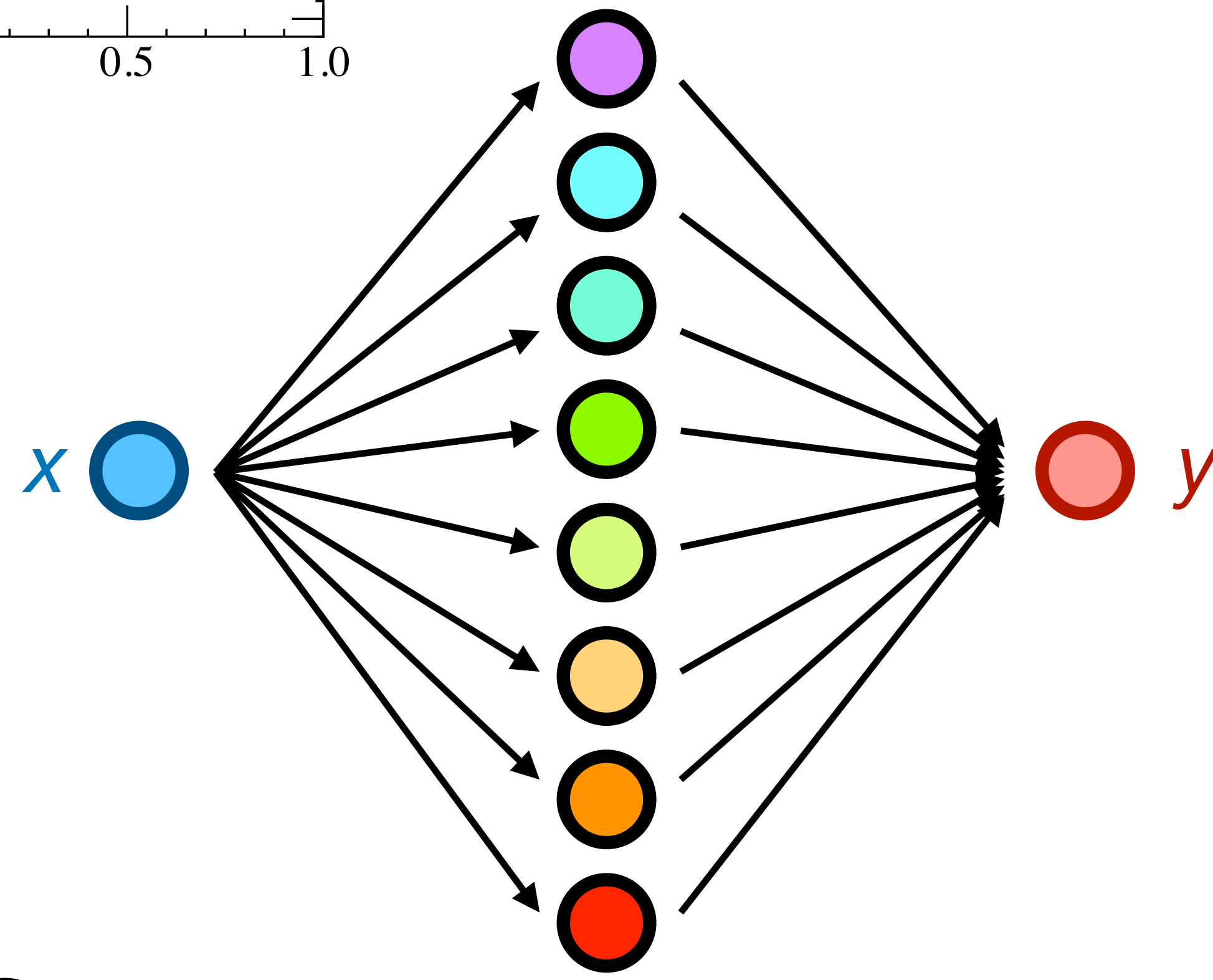
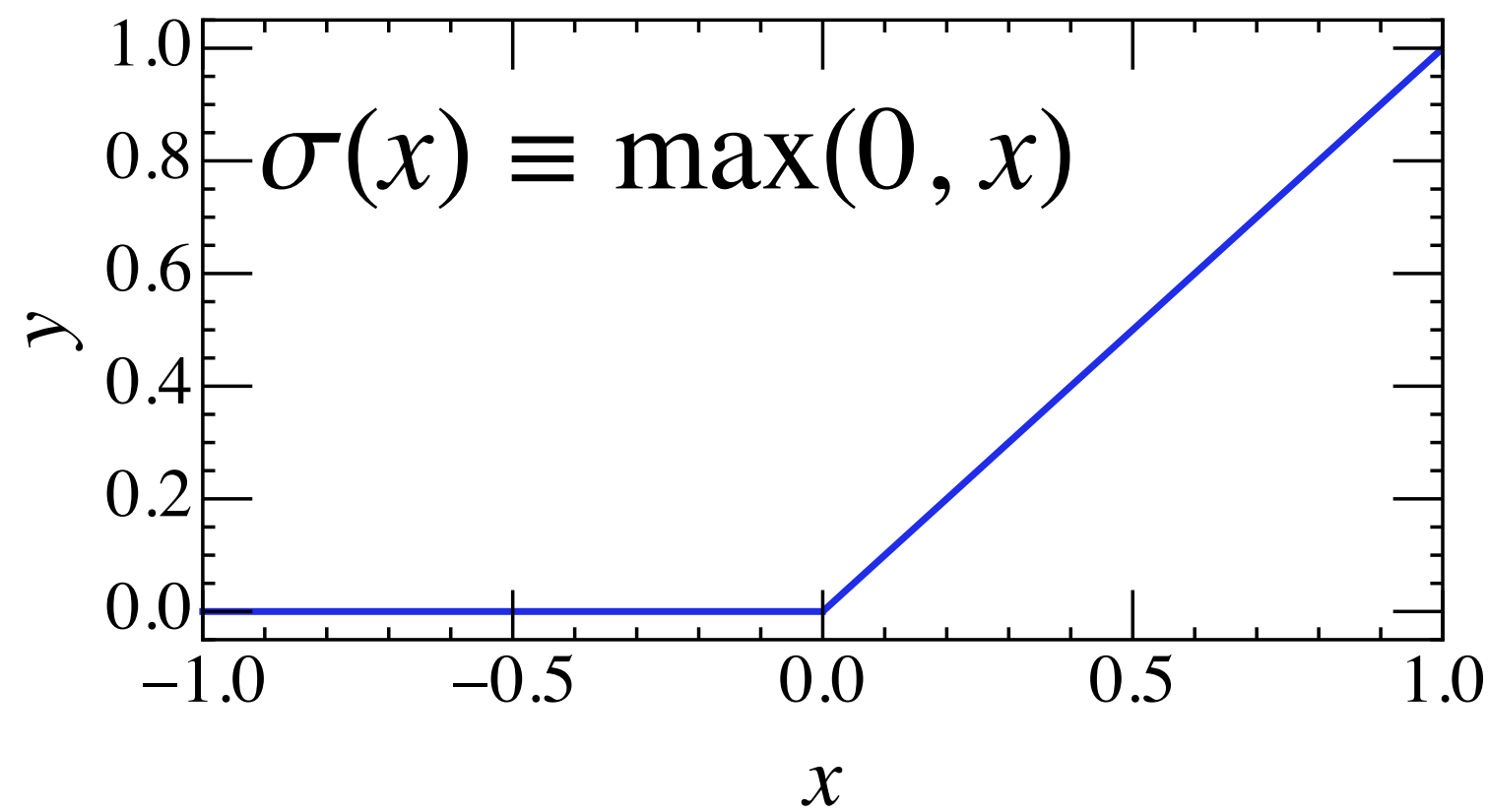
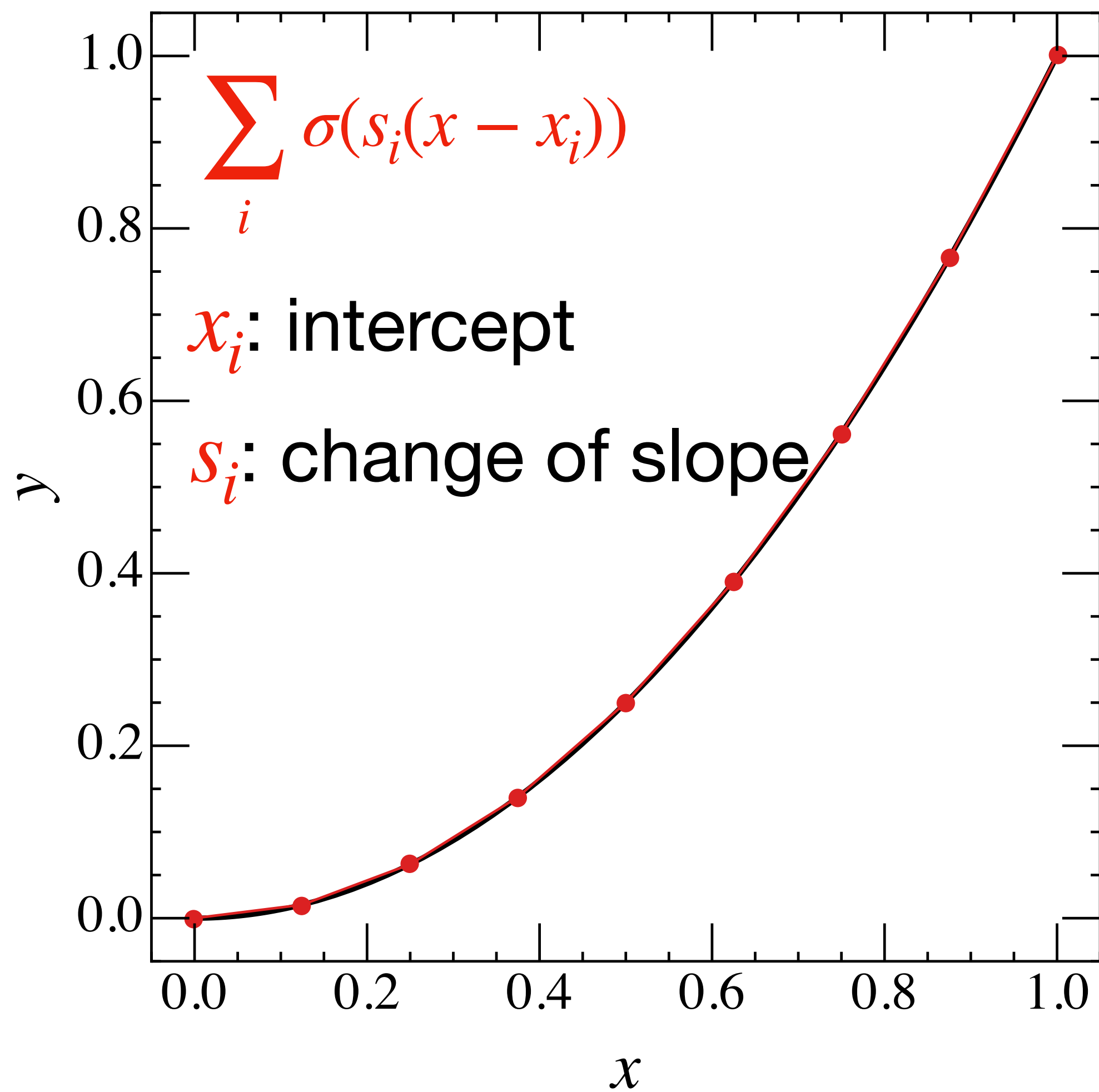


$$V(T, r) = V_R(T, r) + i V_I(T, r)$$

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What are Deep Neural Networks?

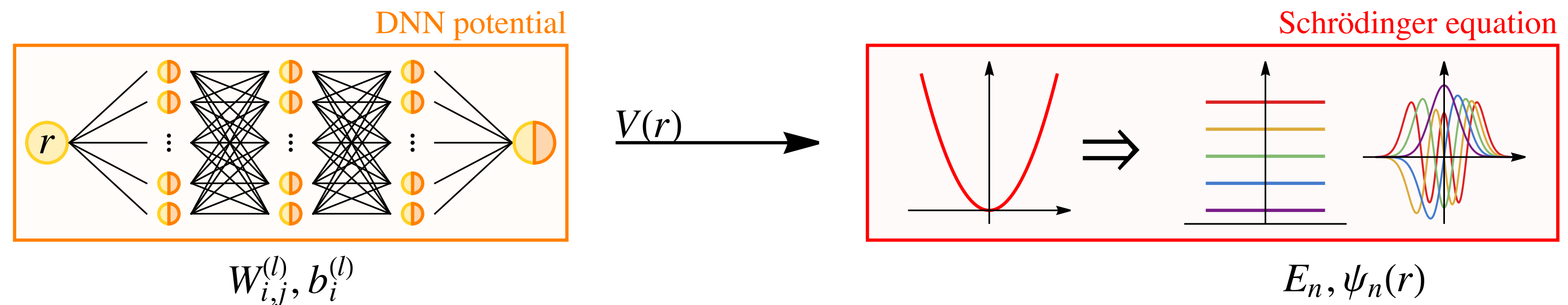
--- a general parameterization scheme to approximate continuous functions.



each  represents one of $\sigma(s_i(x - x_i))$

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

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



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

$$E_n, \psi_n(r)$$

update

$$\Delta W_{i,j}^{(l)} \sim -\frac{\partial \chi^2}{\partial W_{i,j}^{(l)}}$$

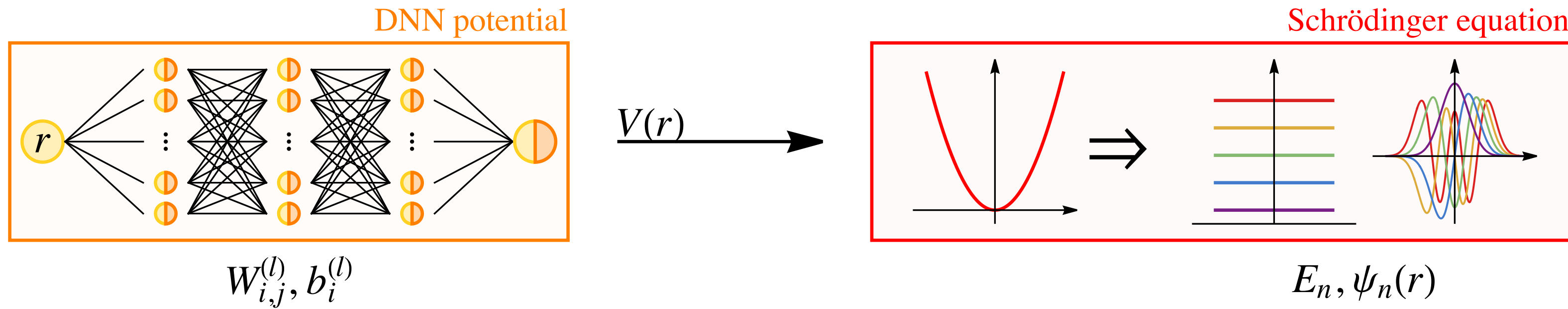
$$\Delta b_i^{(l)} \sim -\frac{\partial \chi^2}{\partial b_i^{(l)}}$$

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

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

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

- parameterize the potential $V(r | \theta)$, minimize $\chi^2 \equiv \sum_i \left(\frac{E_{\theta,i} - E_i}{\delta E_i} \right)^2$
- a **gradient-descent** based method:
 - goal -- find the θ -point that $\nabla_{\theta} \chi^2 = 0$
 - update θ iteratively according to $\Delta \theta \propto \nabla_{\theta} \chi^2$



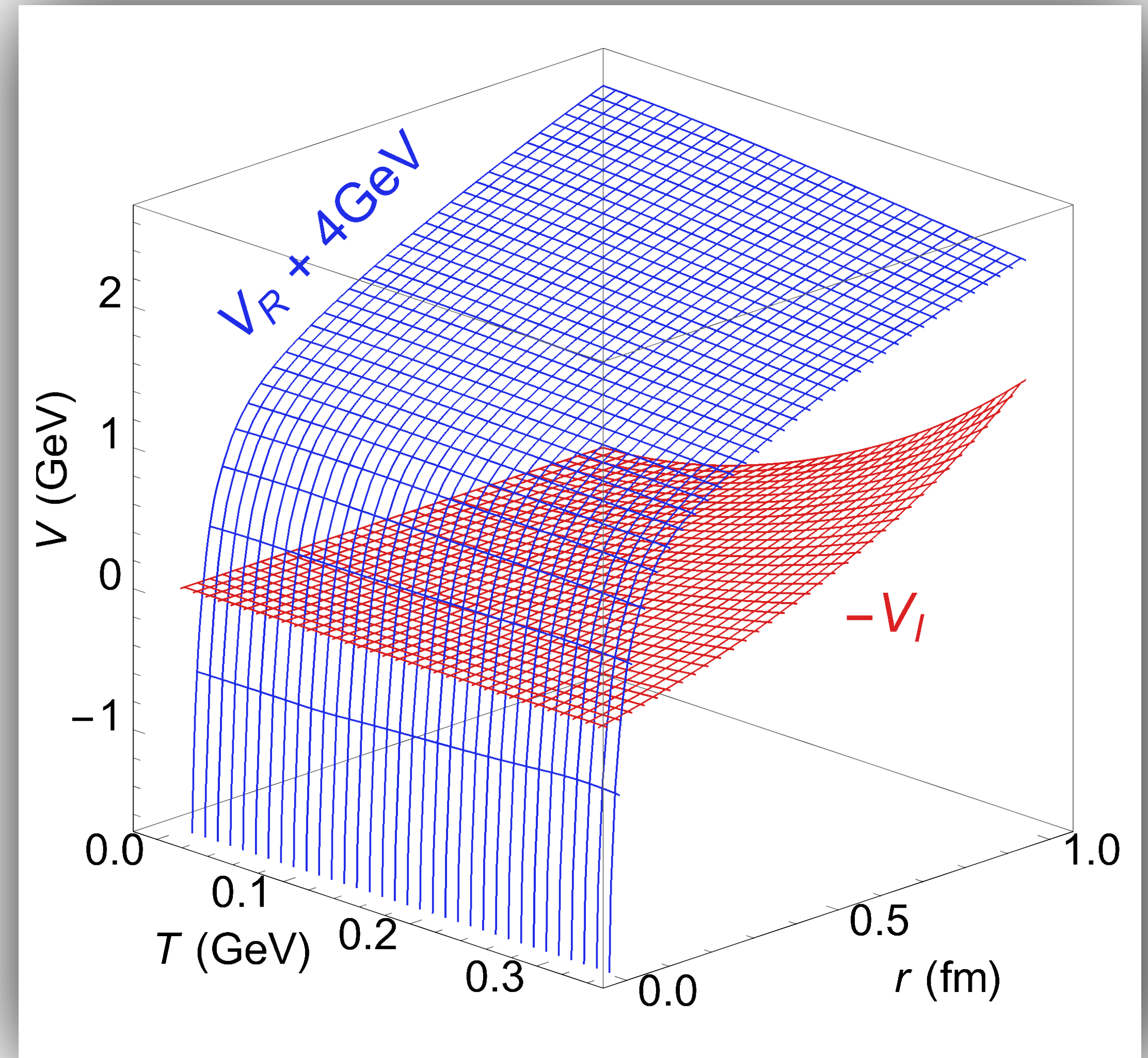
$$\chi^2 = \sum_n \left(\frac{E_n - E_n^{\text{tgt}}}{\Delta_n} \right)^2$$

$$\frac{\delta \chi^2}{\delta V(r)} \longleftarrow \Delta W_{i,j}^{(l)} \sim -\frac{\partial \chi^2}{\partial W_{i,j}^{(l)}}, \quad \Delta b_i^{(l)} \sim -\frac{\partial \chi^2}{\partial b_i^{(l)}}$$

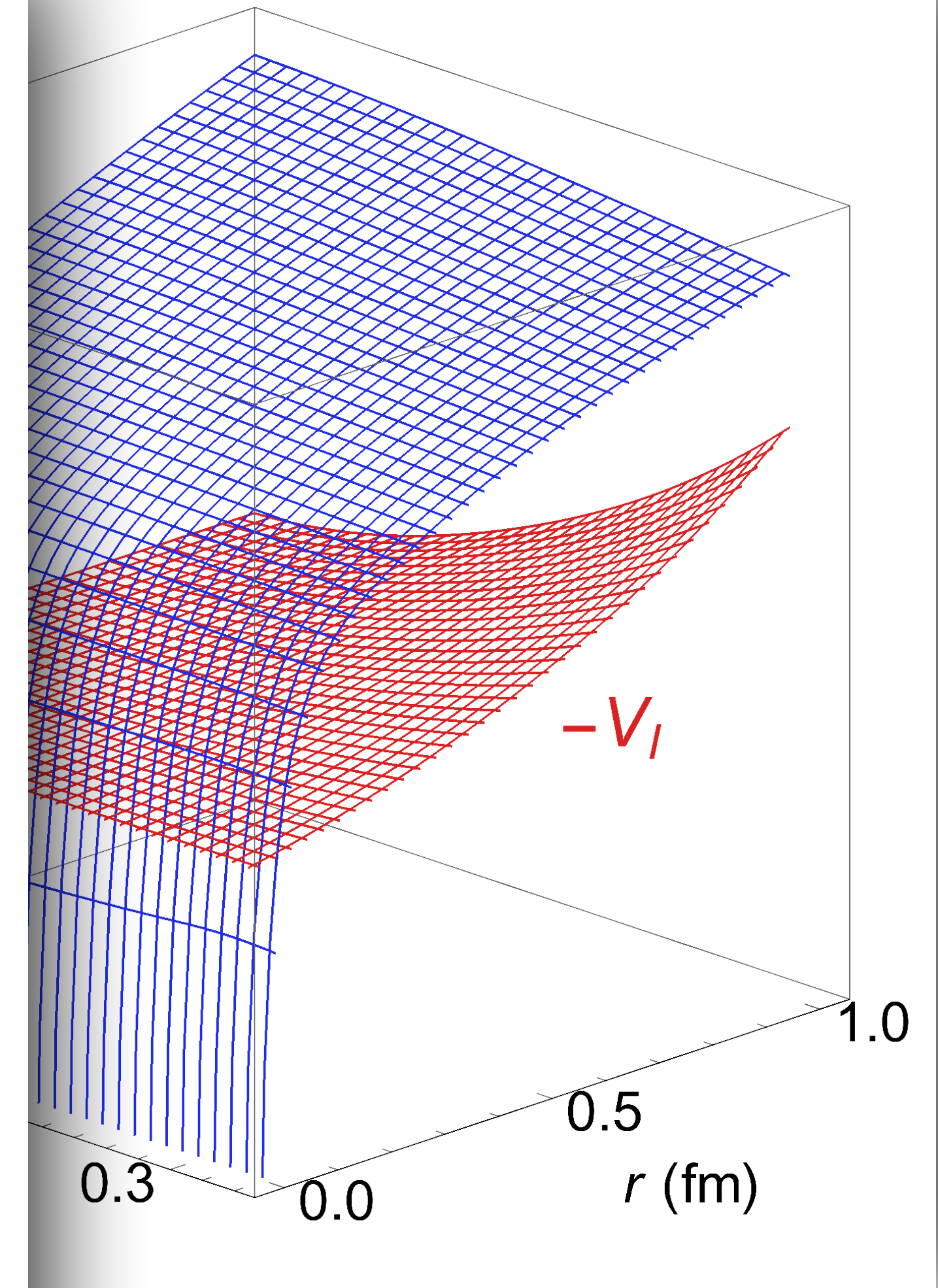
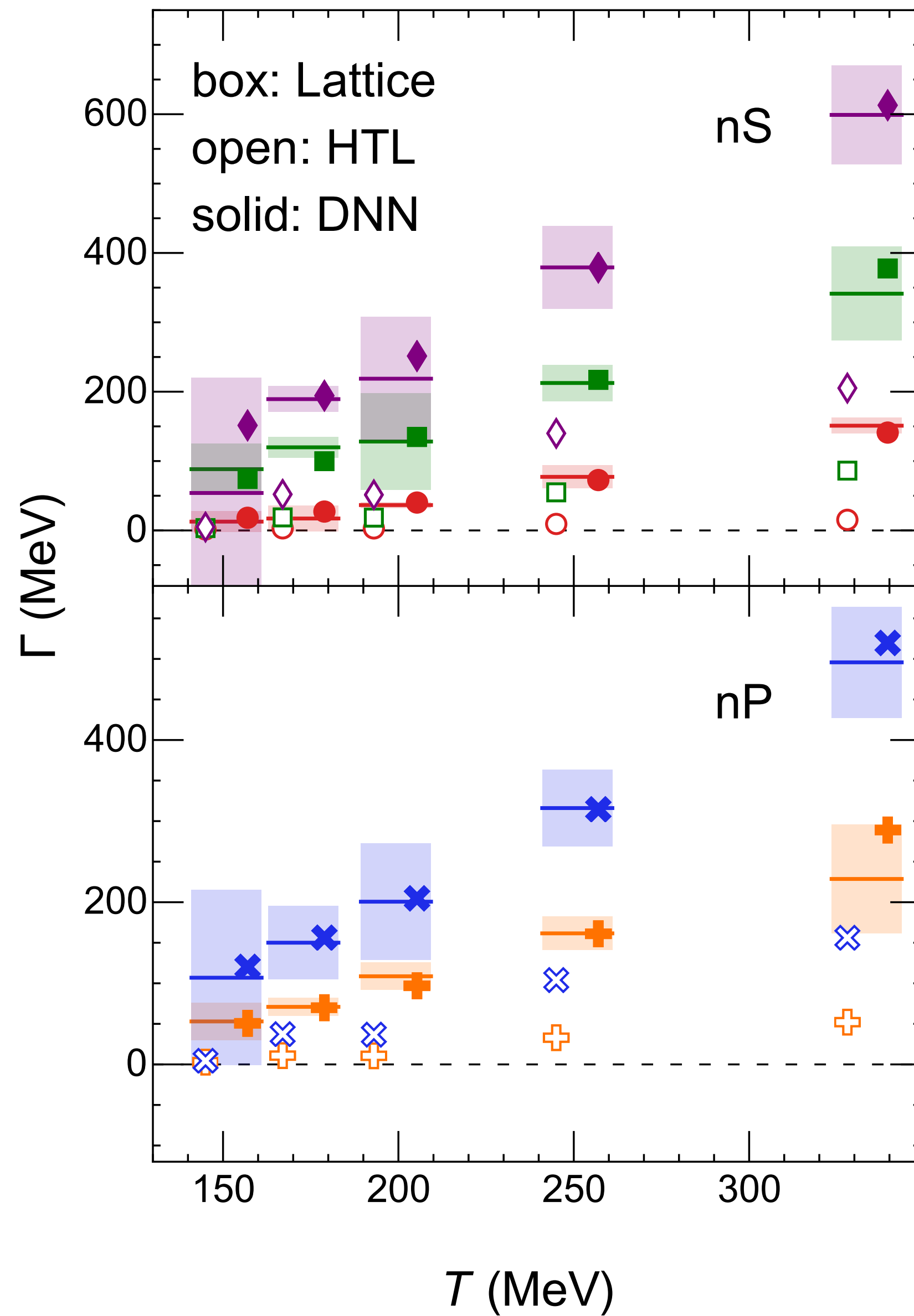
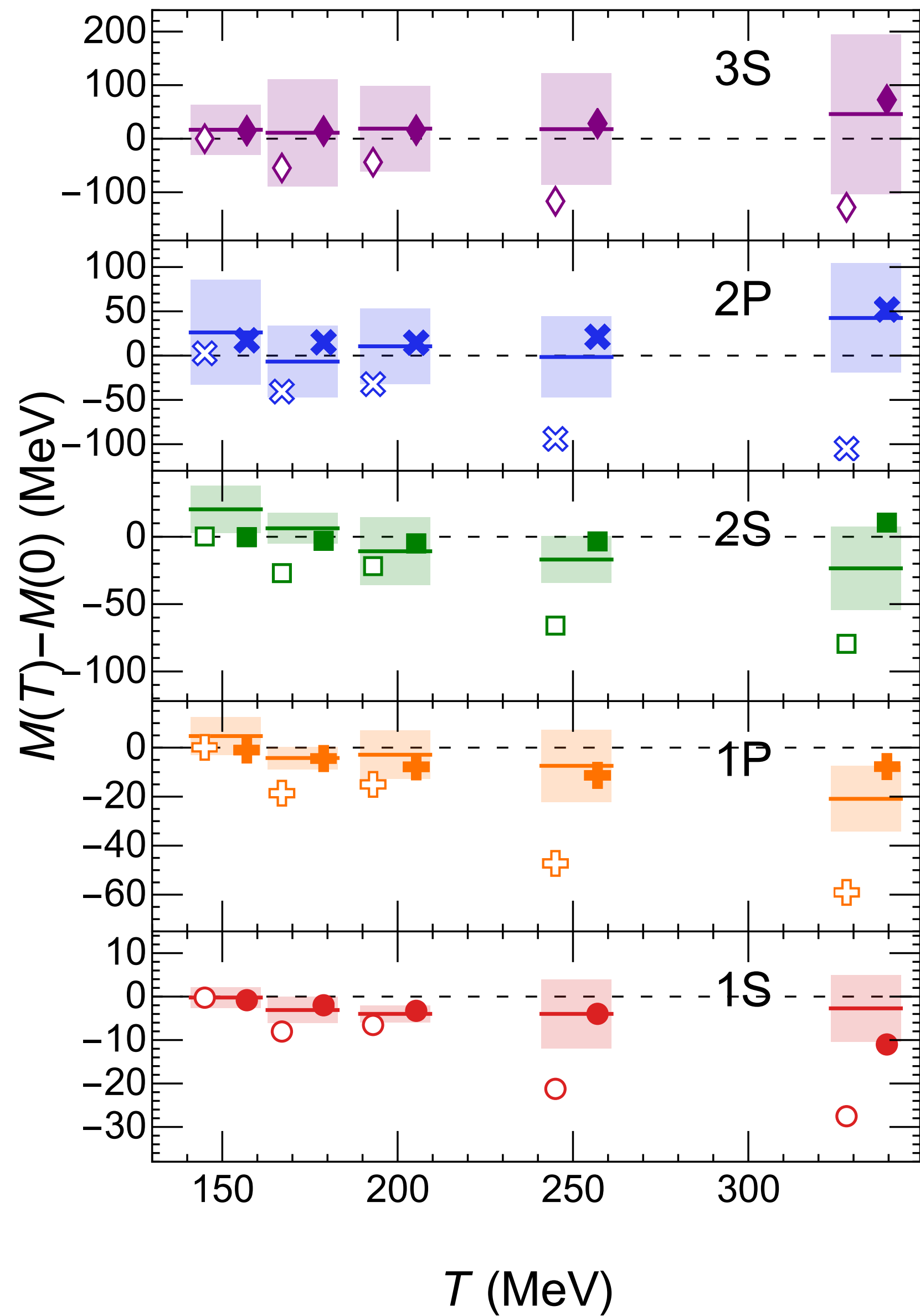
update

Finite Temperature Heavy-Quark Potential

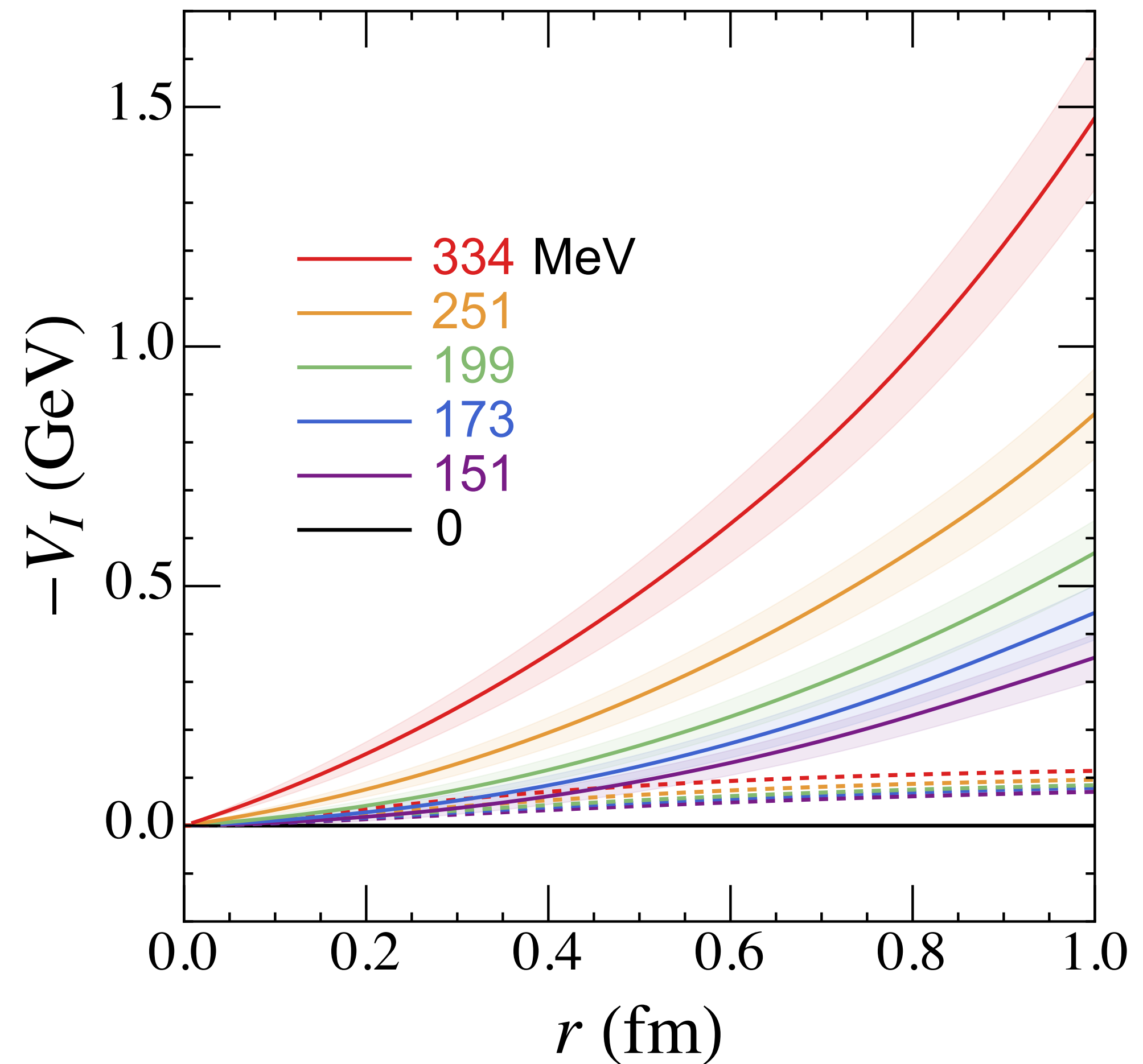
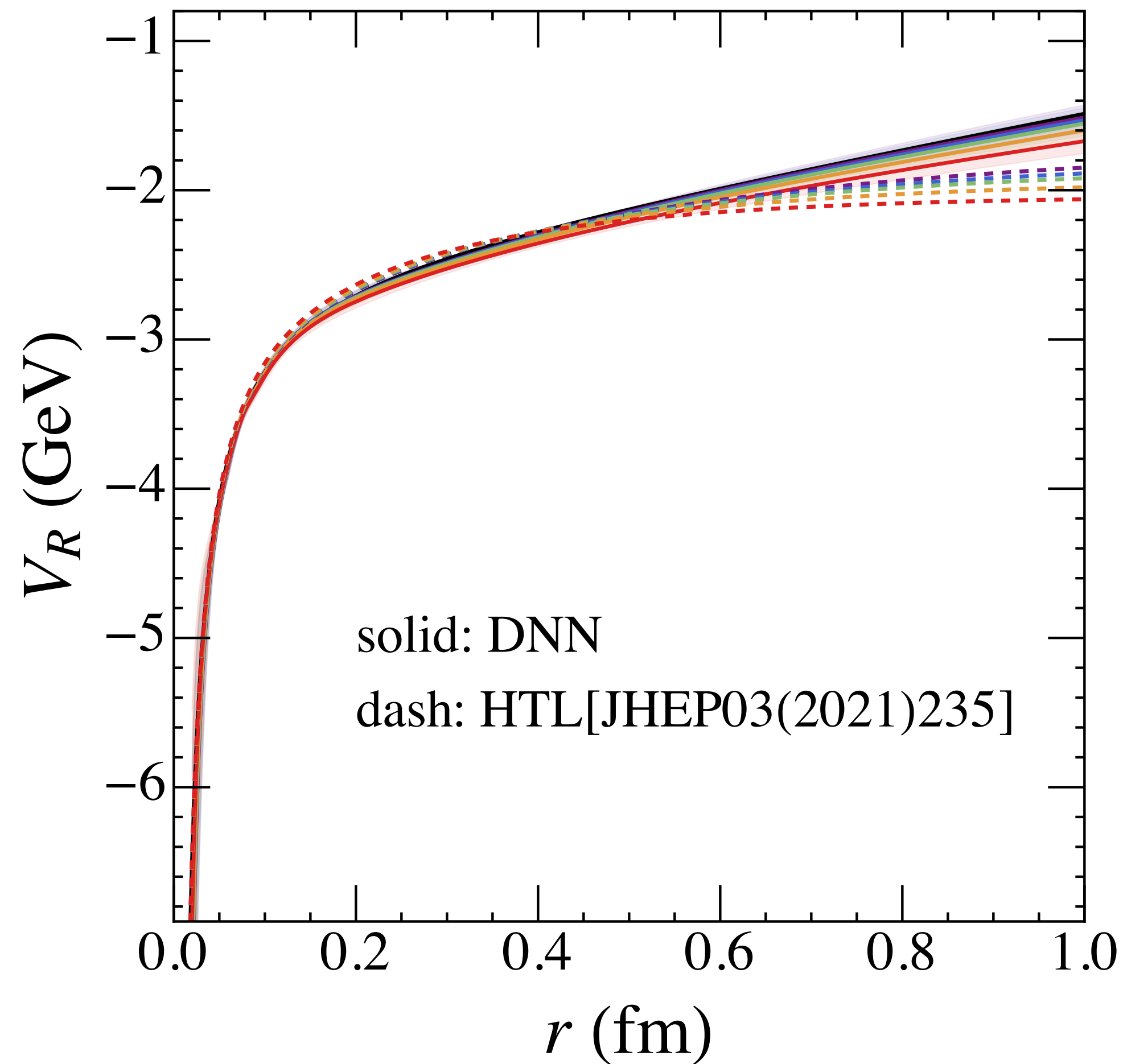
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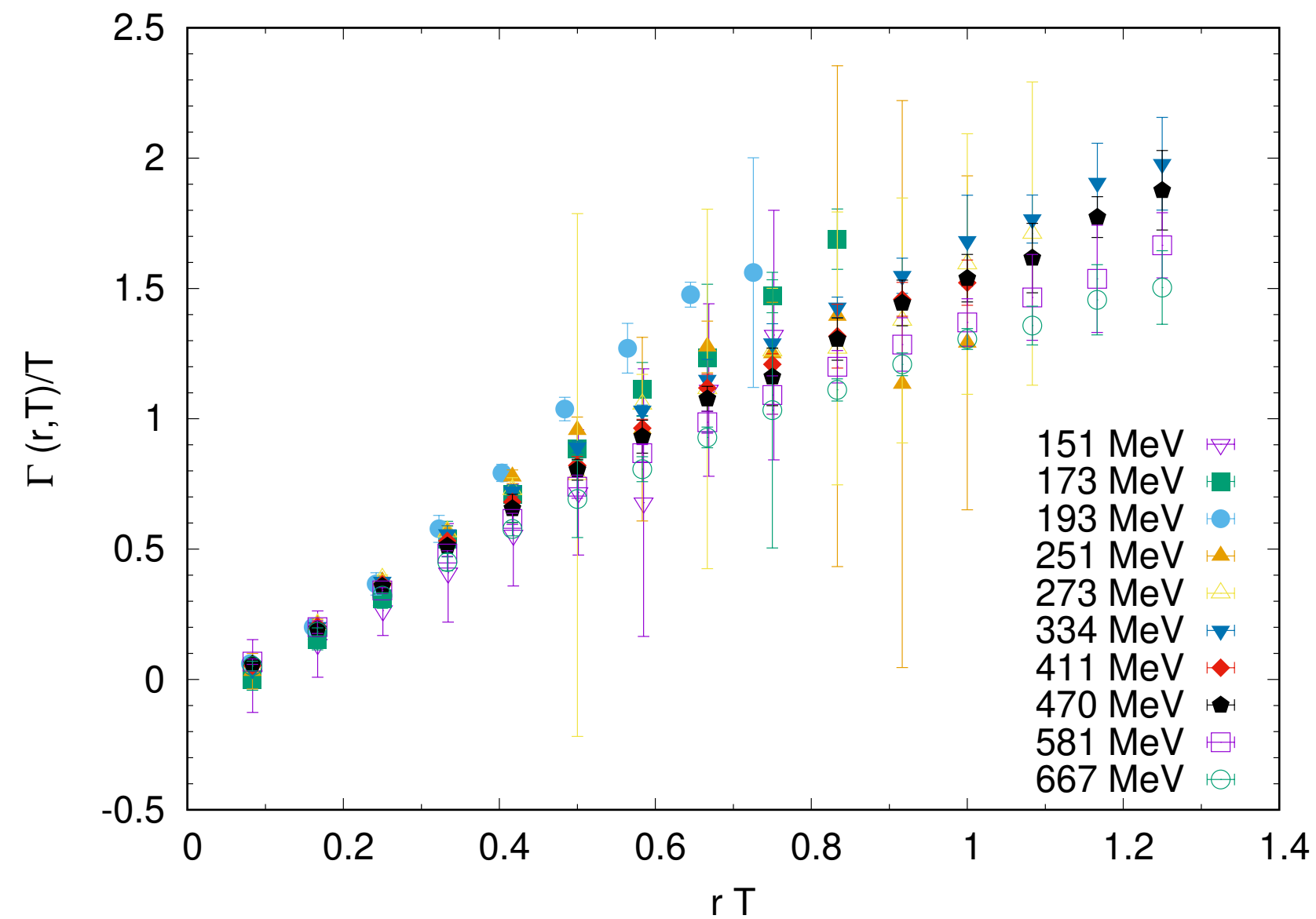
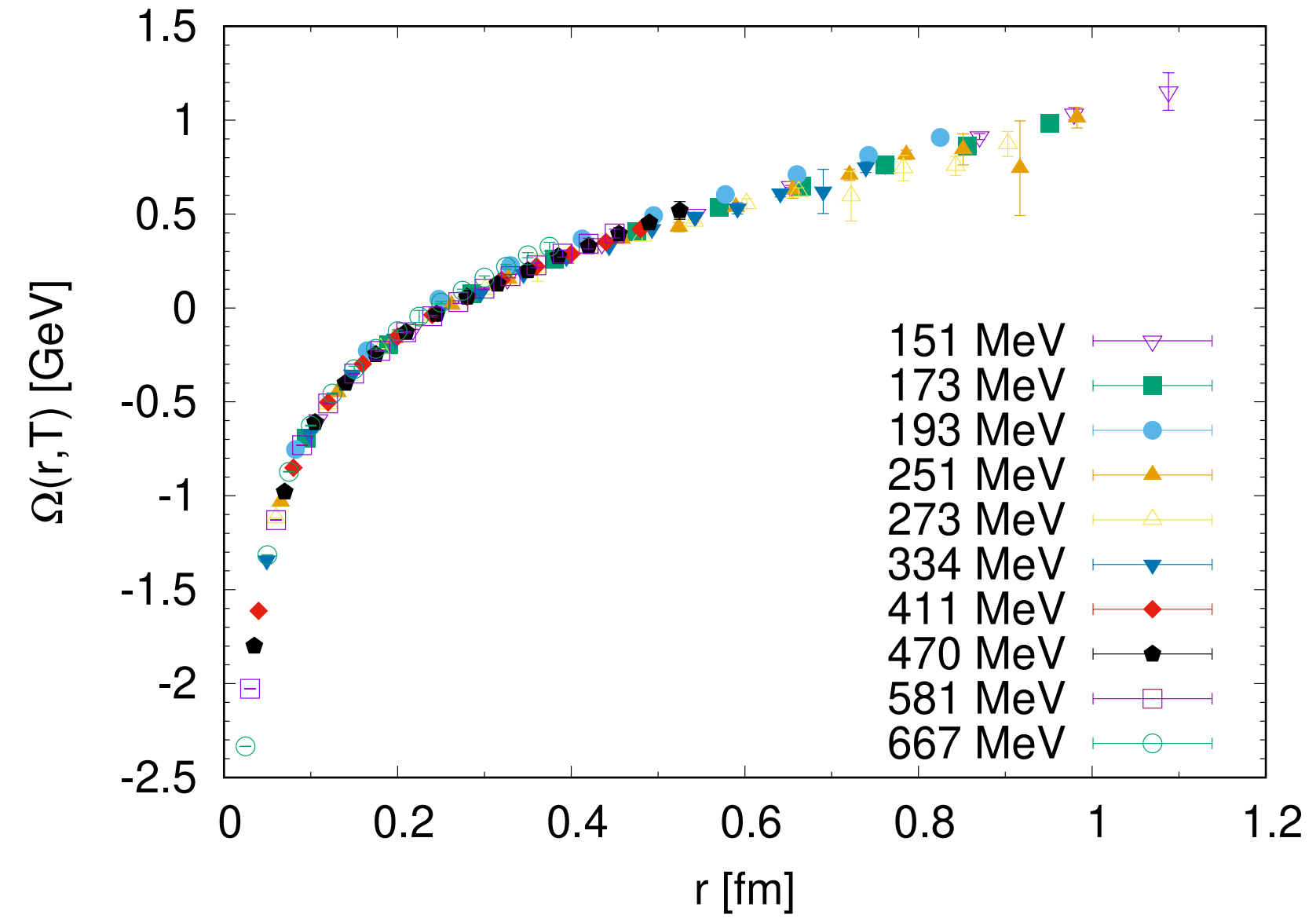
Finite Temperature Heavy-Quark Potential



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



Reason of the difference?



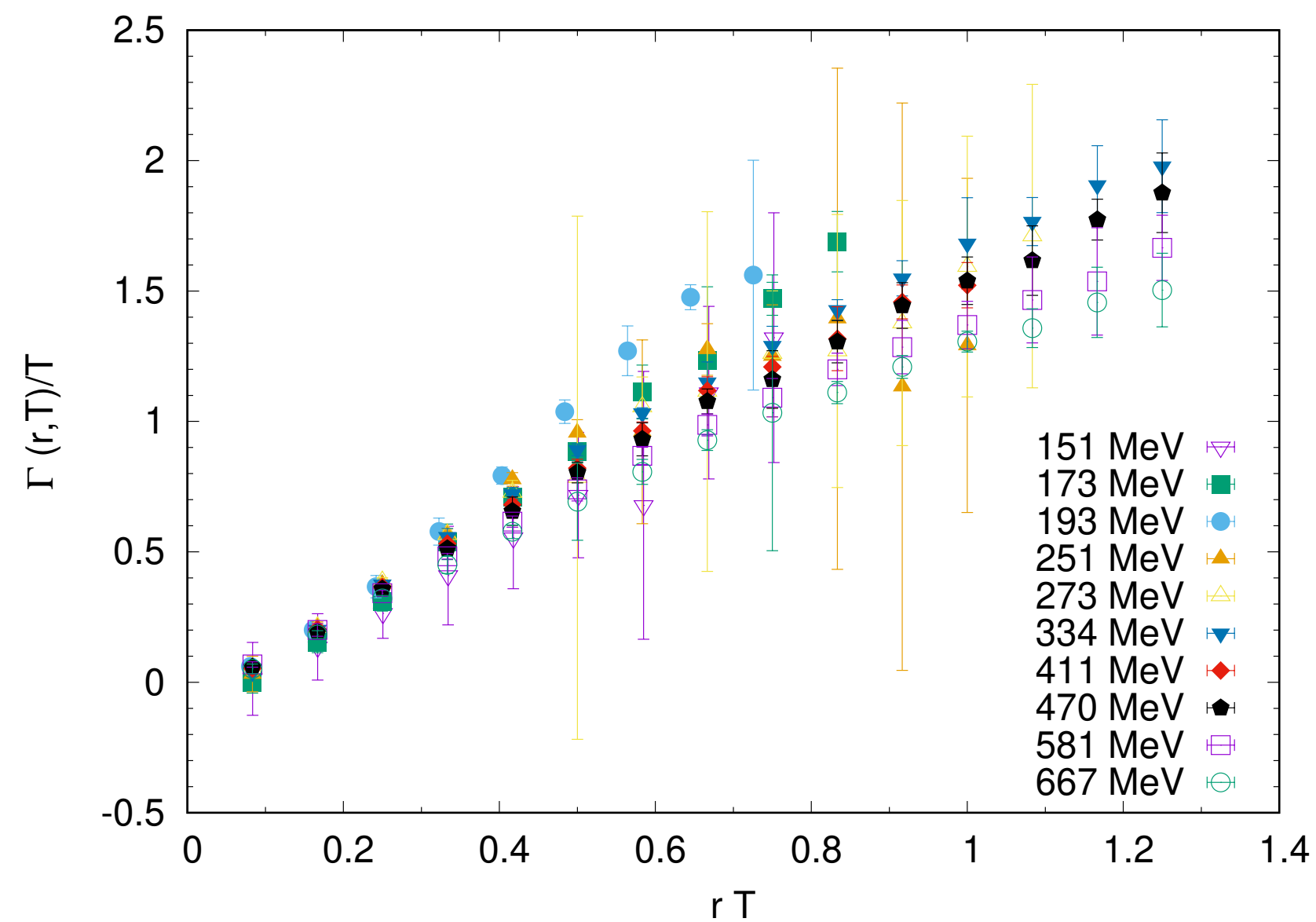
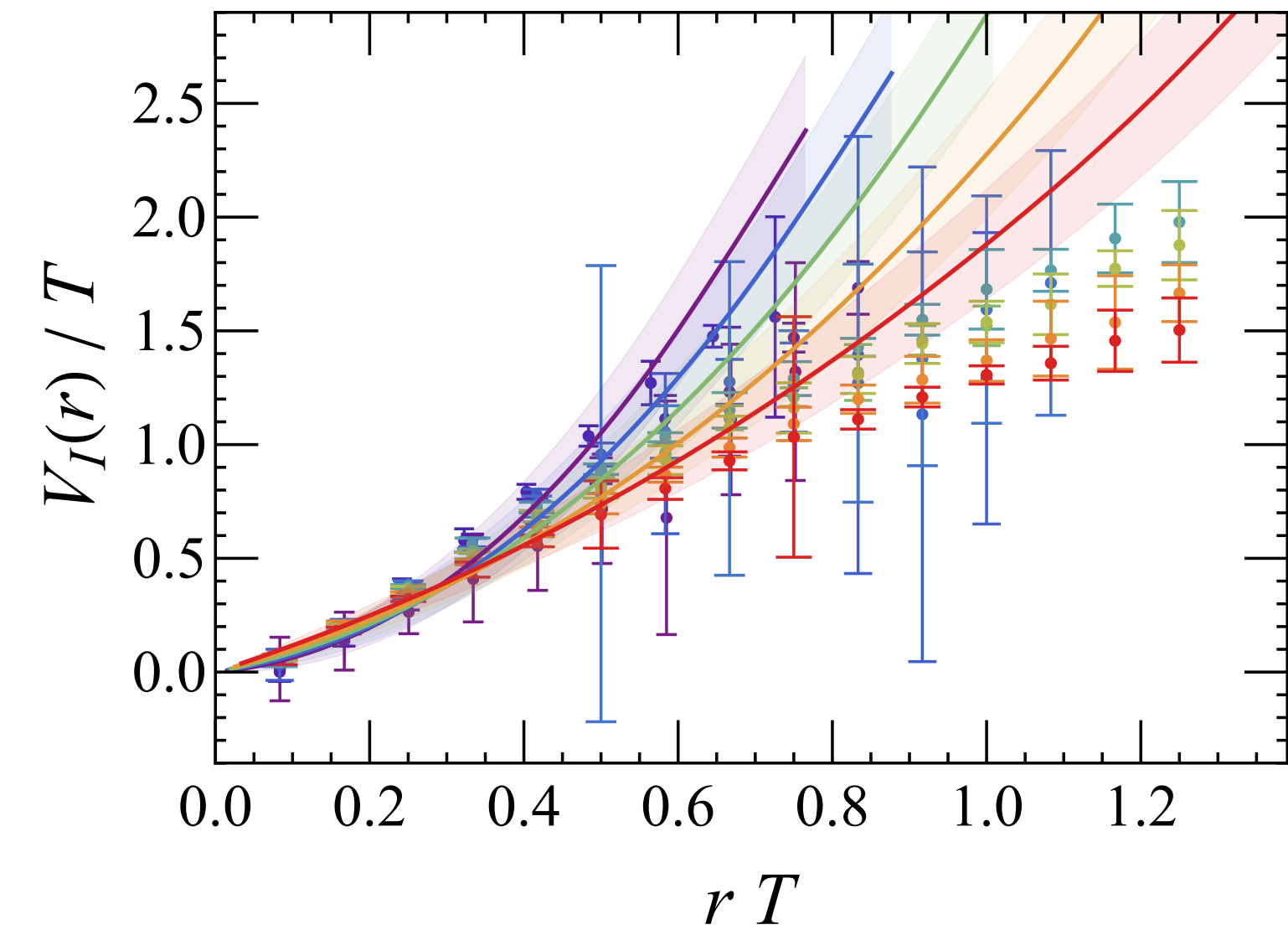
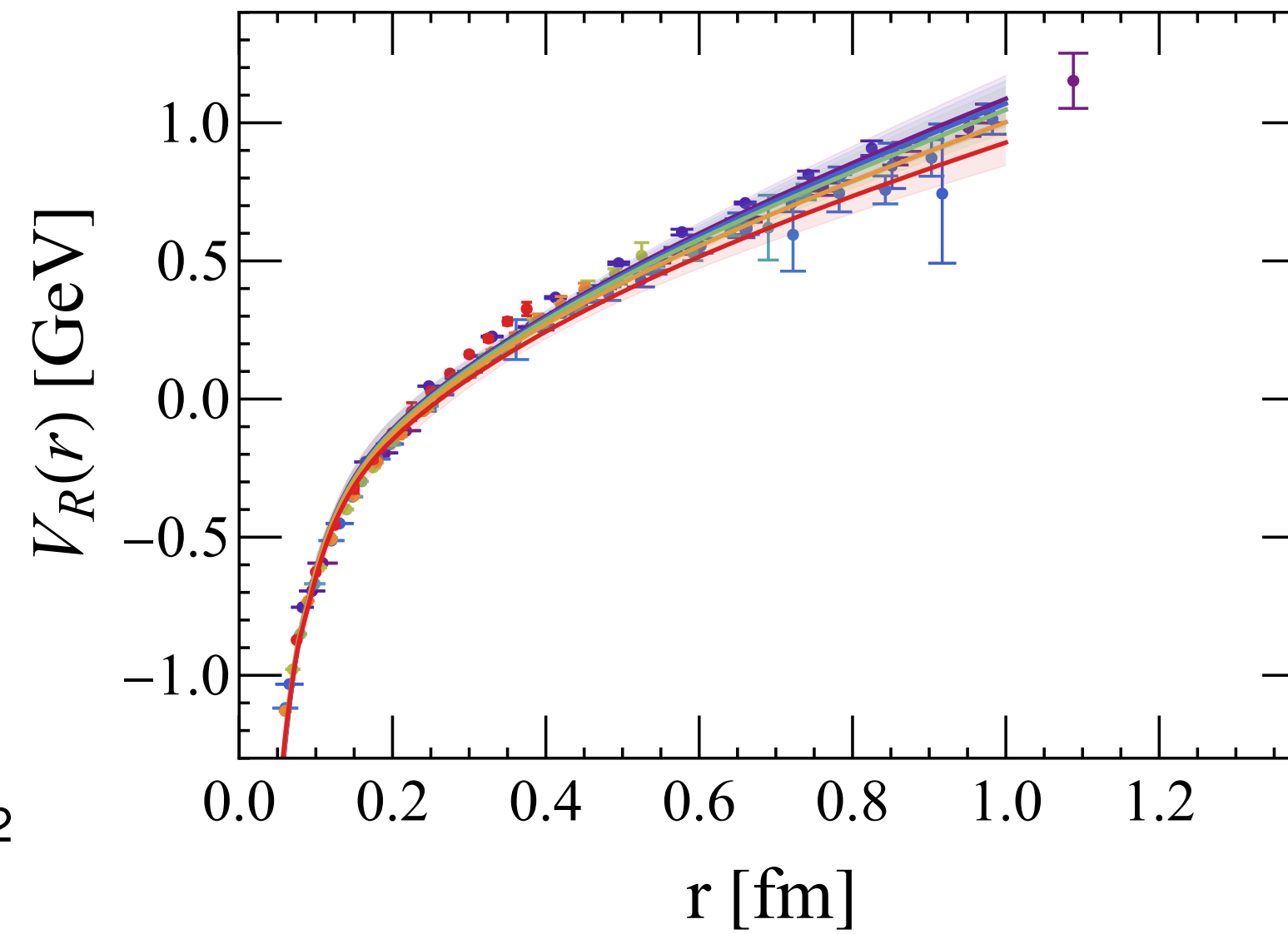
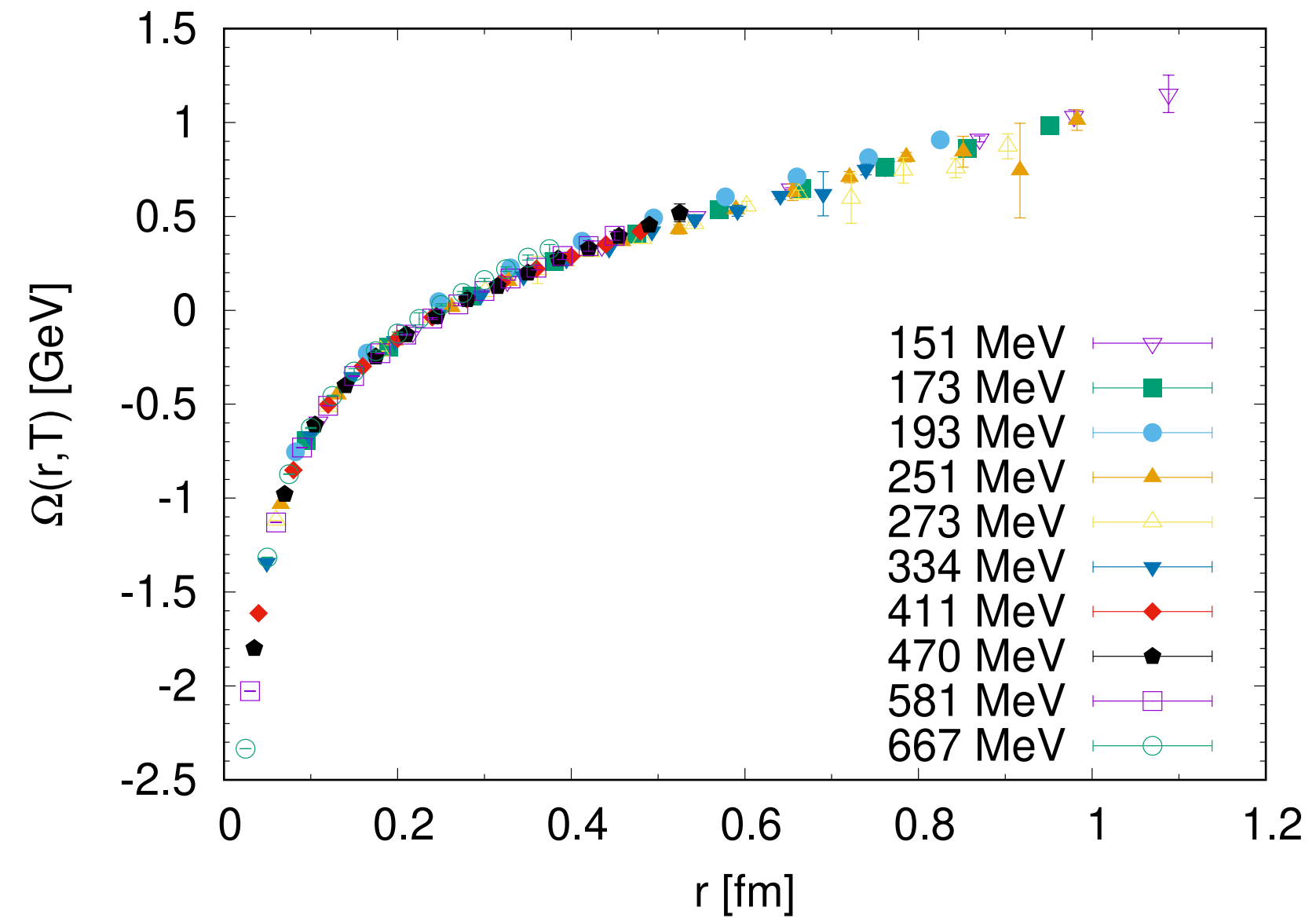
PHYSICAL REVIEW D **105**, 054513 (2022)

Static quark-antiquark interactions at nonzero temperature from lattice QCD

Dibyendu Bala,¹ Olaf Kaczmarek,¹ Rasmus Larsen,² Swagato Mukherjee,³ Gaurang Parkar,² Peter Petreczky,³ Alexander Rothkopf,² and Johannes Heinrich Weber⁴

(HotQCD Collaboration)

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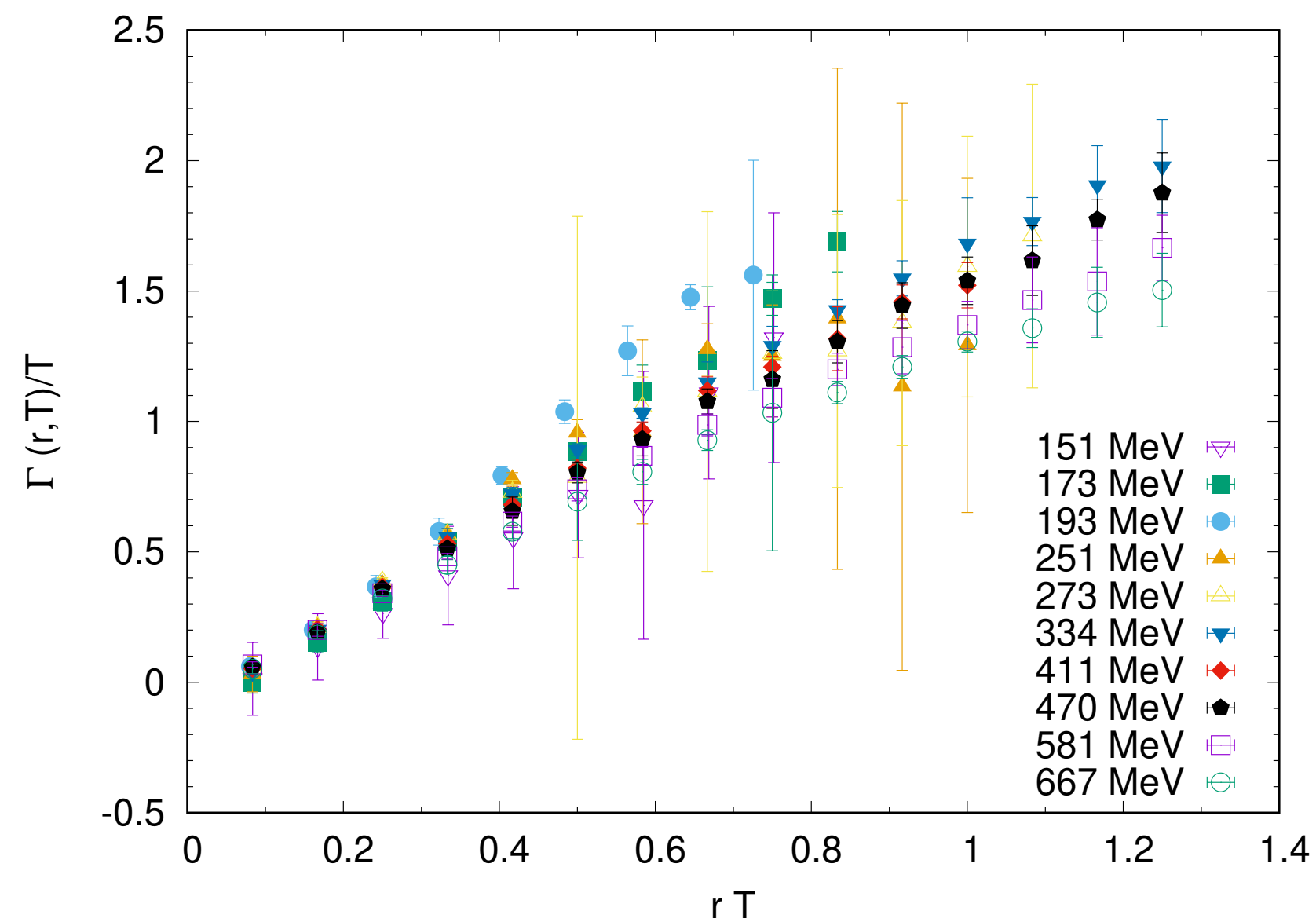
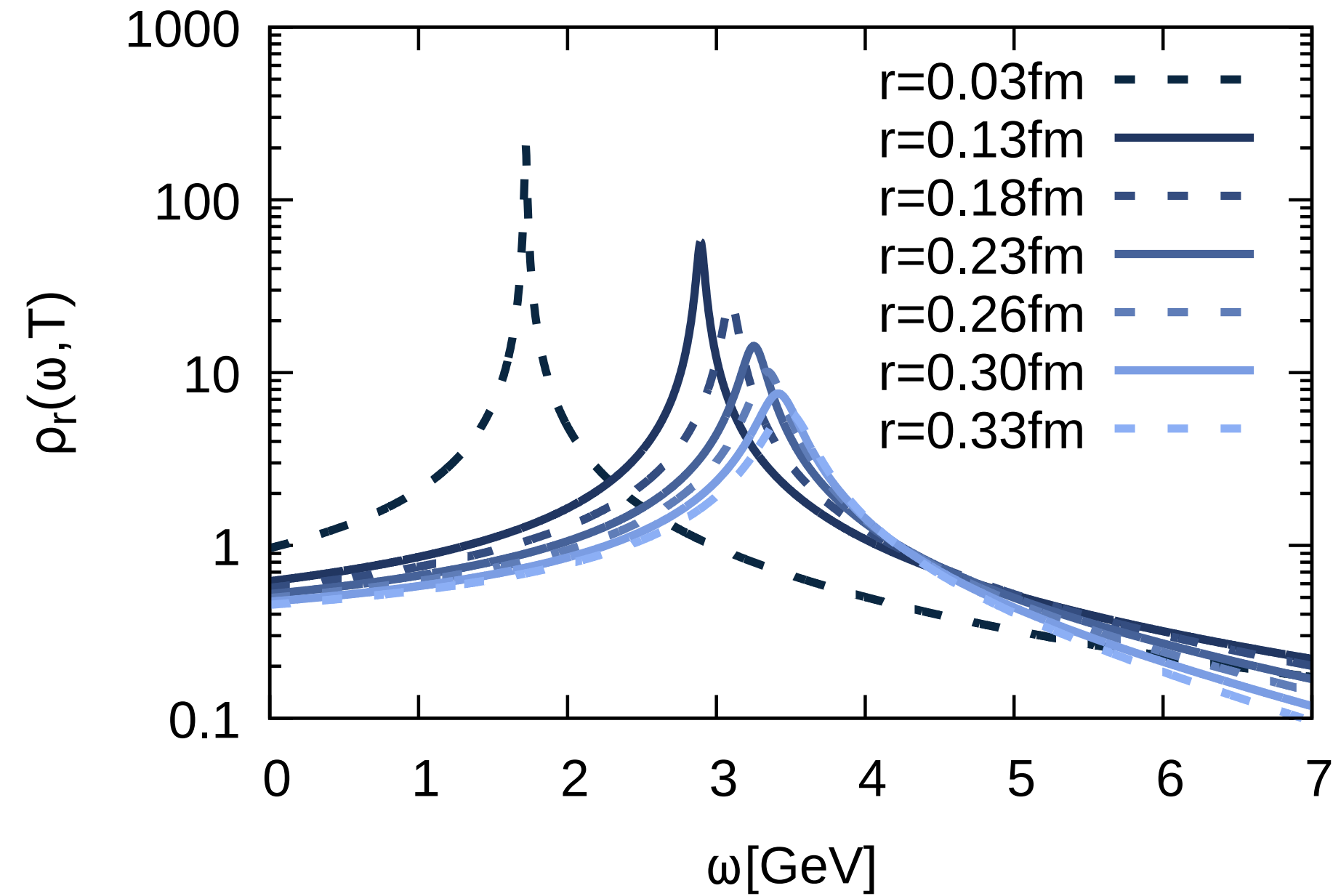
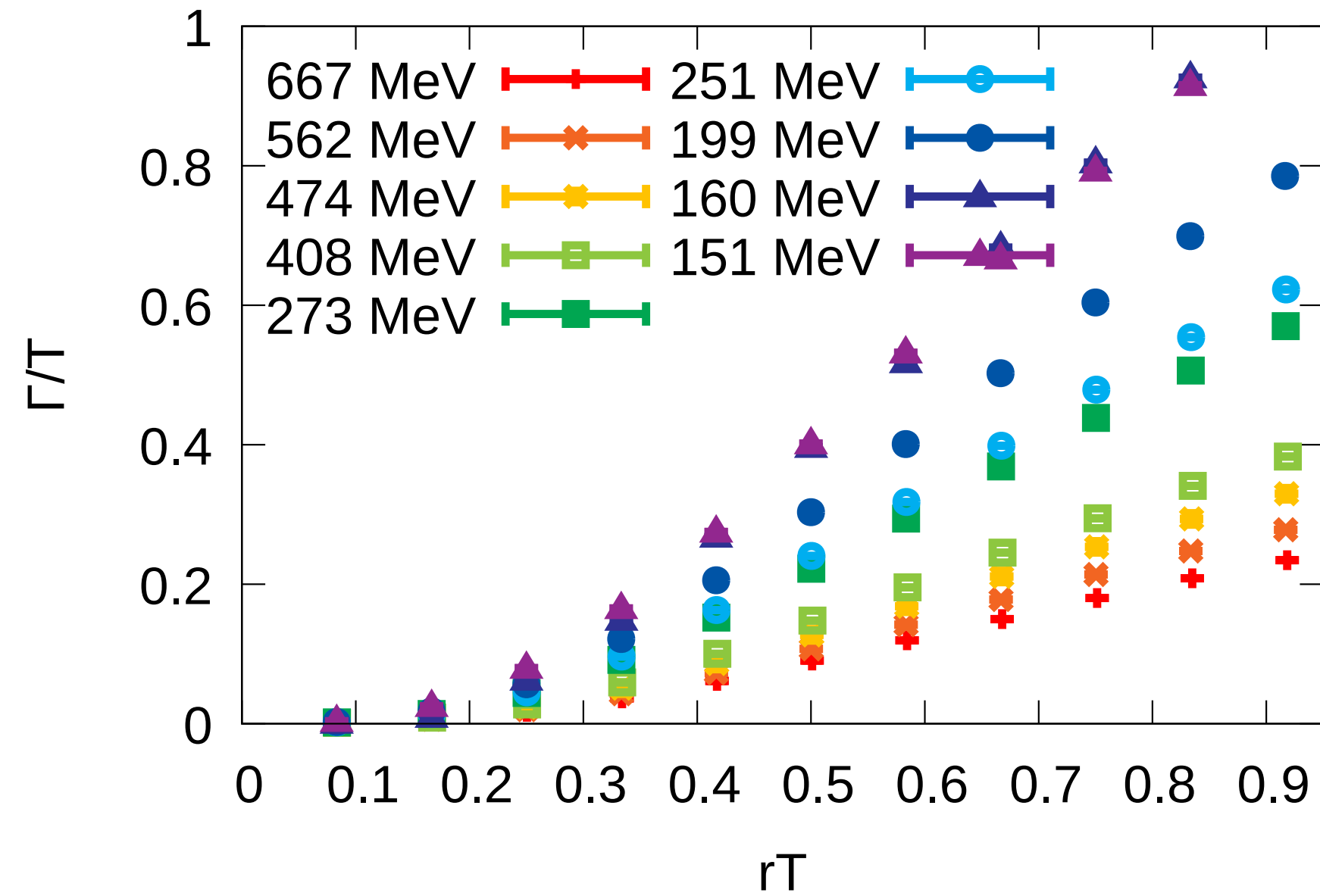
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Problem # II:

spectral function reconstruction

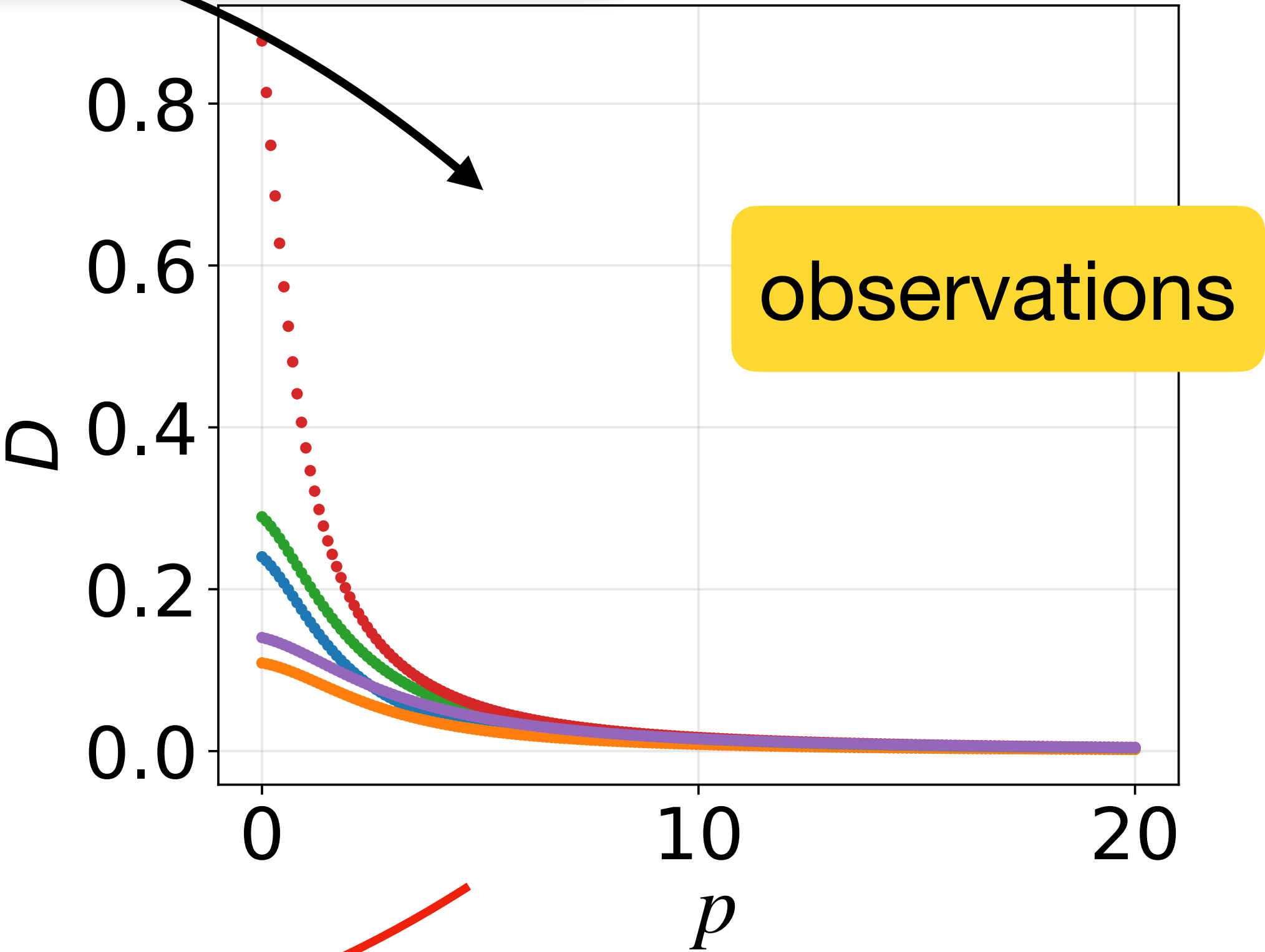
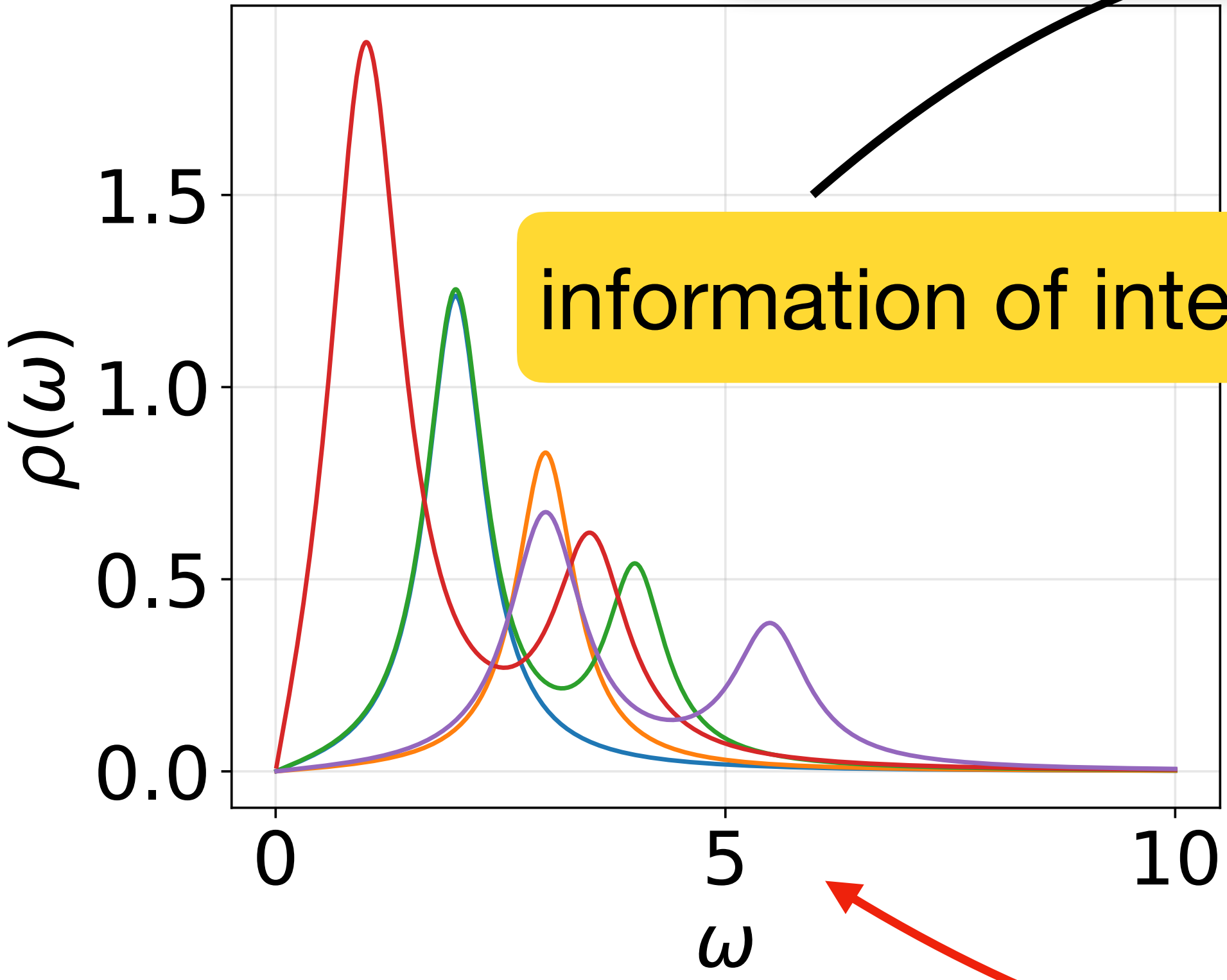
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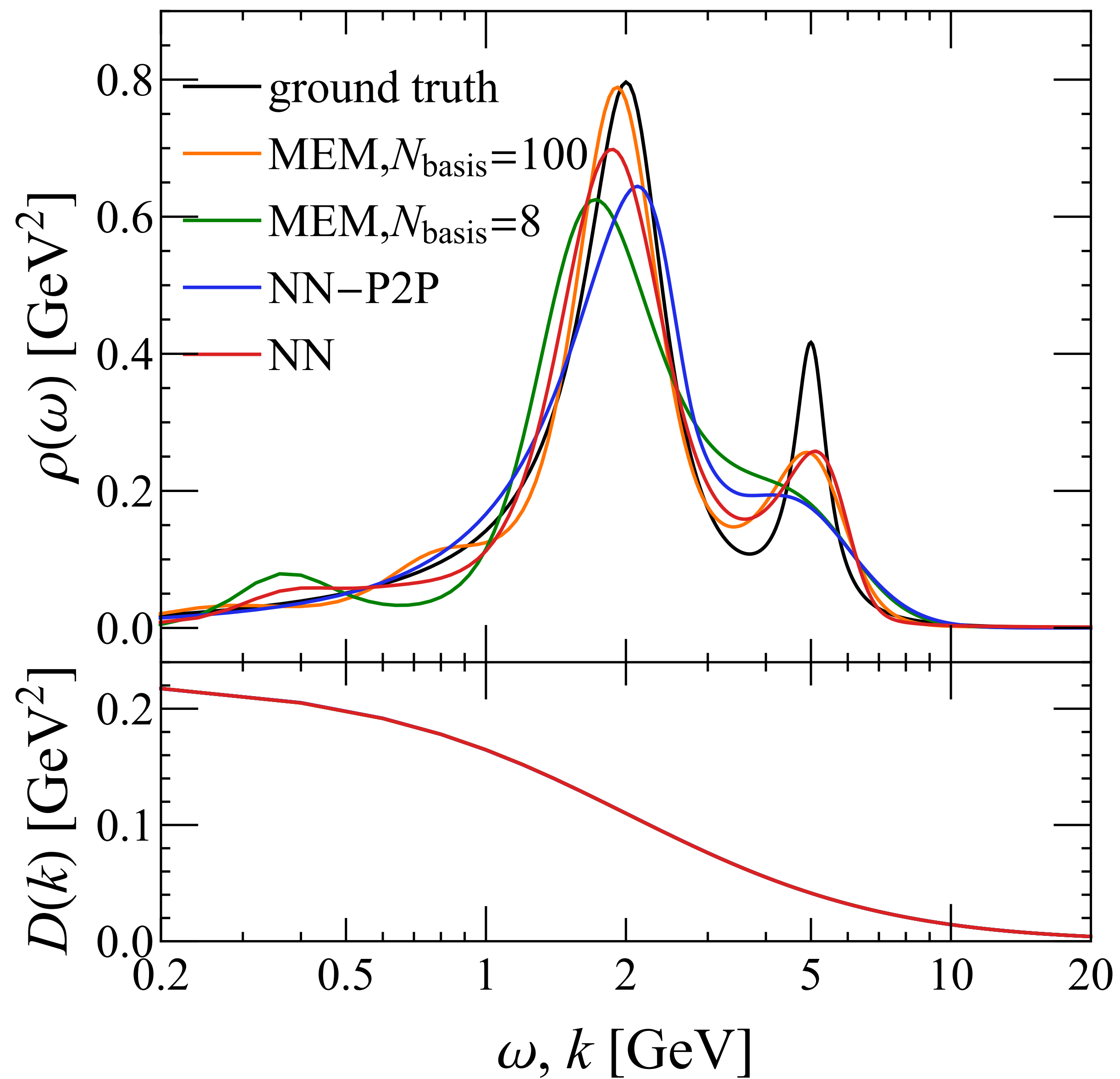
3. spectral function \Leftrightarrow correlation

$$D(p) = \int_0^\infty K(p, \omega) \rho(\omega) d\omega$$

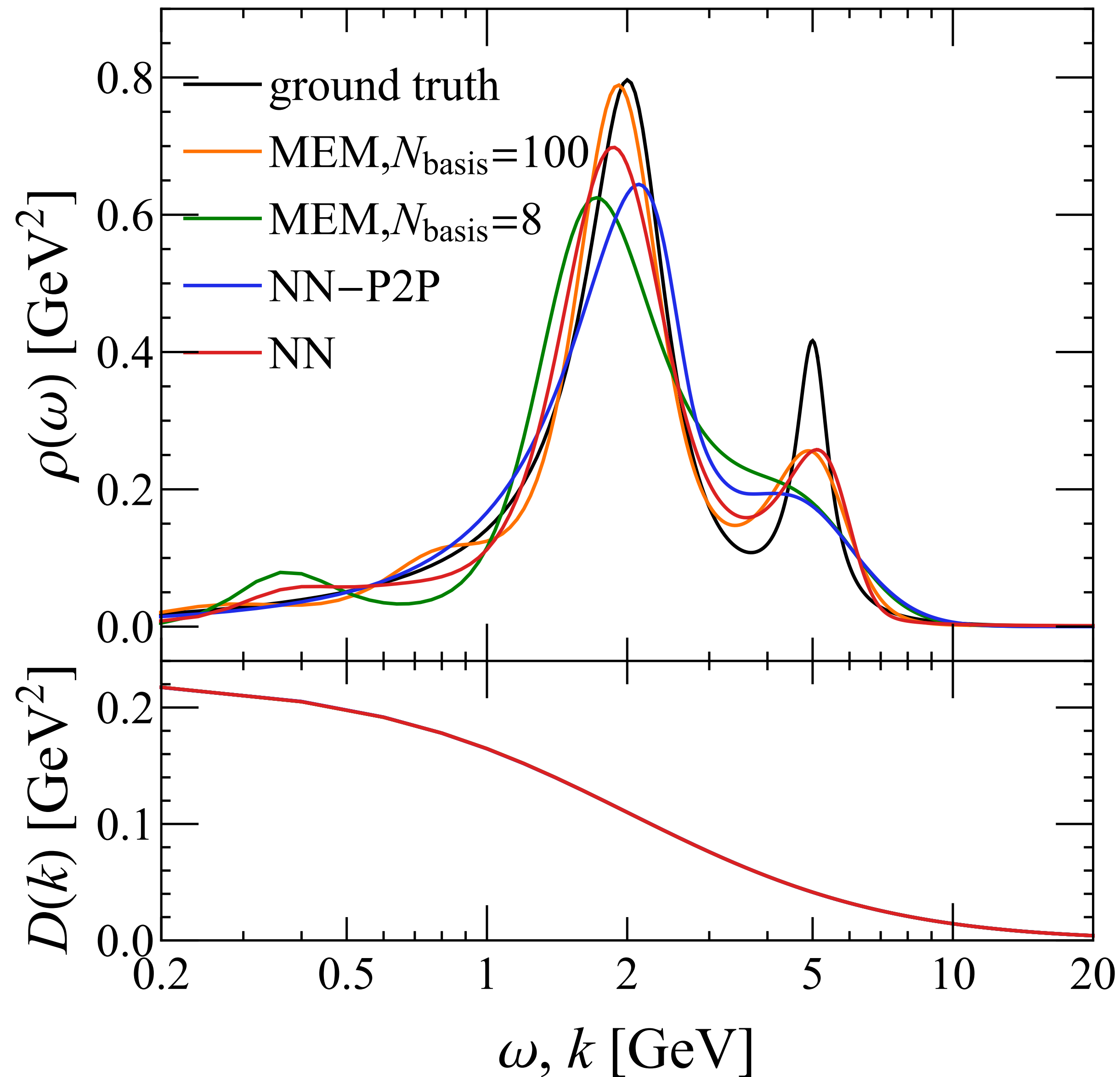
$$K(p, \omega) \equiv \frac{\pi^{-1} \omega}{\omega^2 + p^2}$$



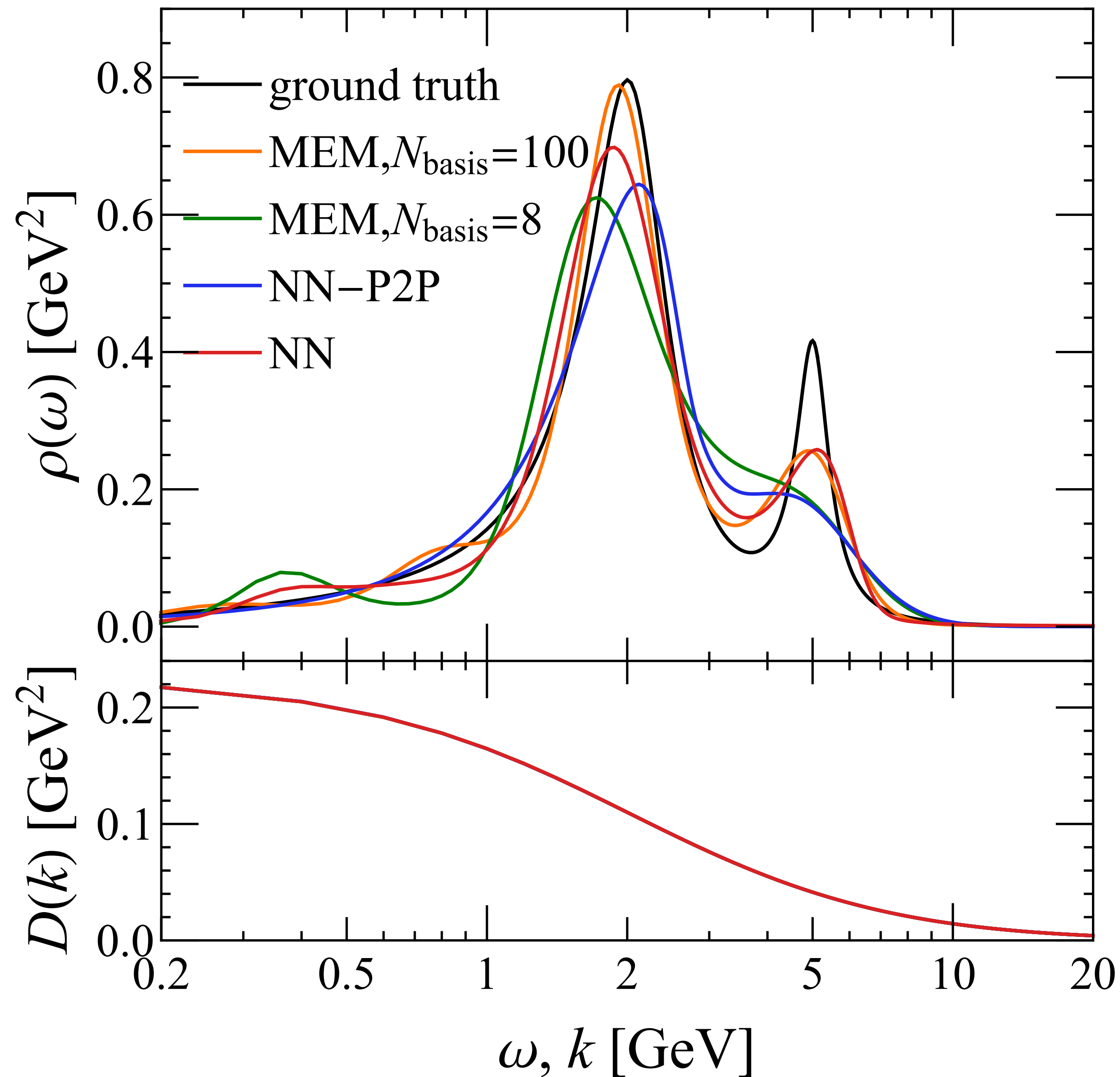
Can one learn the spectral function from correlation?



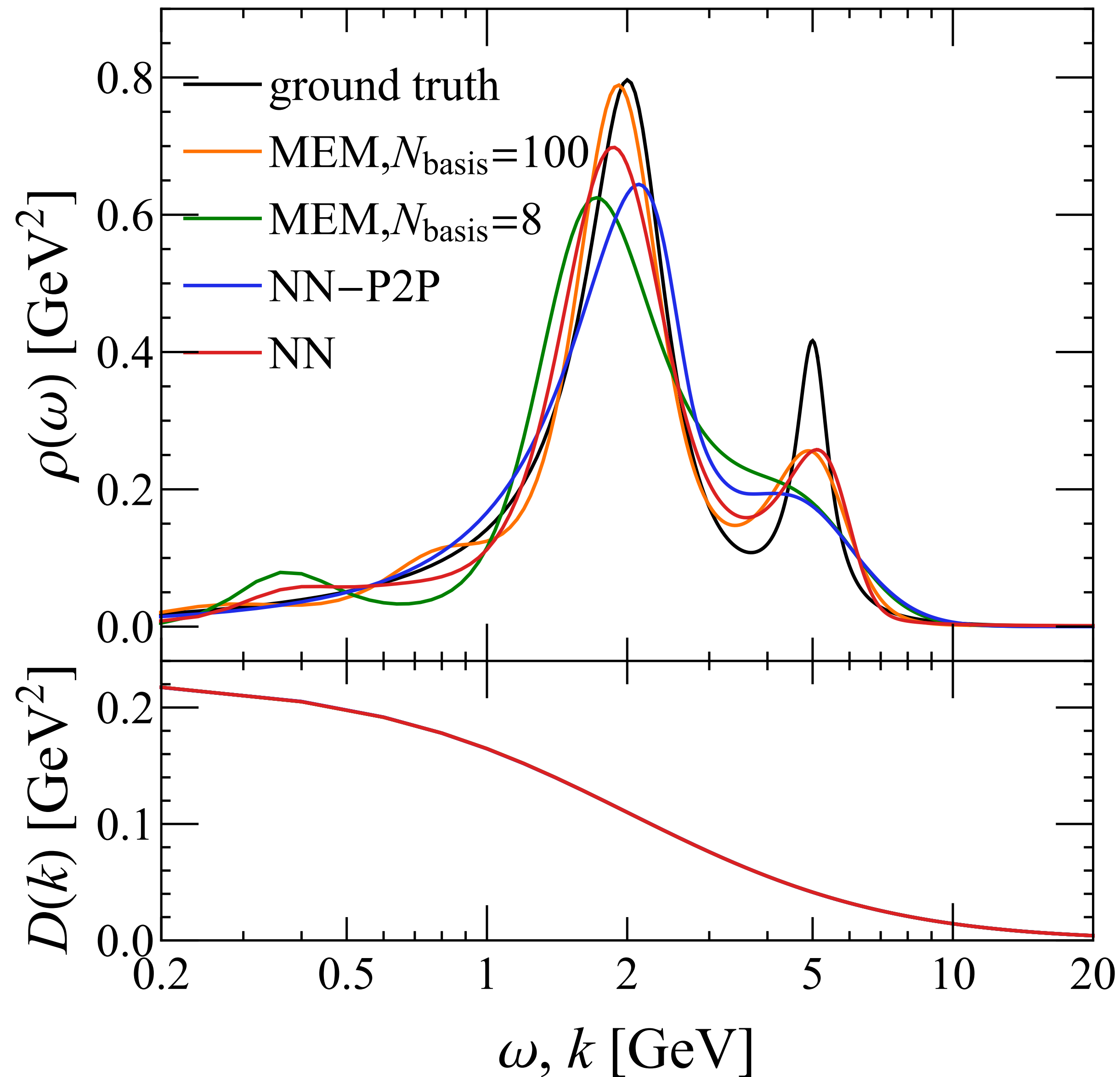
Can one learn the spectral function from correlation?



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



- ill-conditioned?
 - one needs more points in ω than that were given in k
- resolved by increasing # of k -points?



- 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!!!

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

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 $[0, +\infty)$.

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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:

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

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

eigenfunctions and eigenvalues of KL convolution:

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

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

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

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

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

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

$$\tilde{\rho}_{\pm}(s) = \tilde{D}_{\pm}(s) / \lambda_s$$

$$\frac{1}{\pi} \int_0^{\infty} \frac{\omega \, d\omega}{\omega^2 + k^2} \psi_{\pm,s}(\omega) = \lambda_s \psi_{\pm,s}(k),$$

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

$$\widetilde{D}_{\pm}(s) = \int_0^{+\infty} \frac{k dk}{a^2} D(k) \psi_{\pm,s}(k)$$

$$\widetilde{\rho}_{\pm}(s) = \widetilde{D}_{\pm}(s) / \lambda_s$$

$$\frac{1}{\pi} \int_0^{\infty} \frac{\omega d\omega}{\omega^2 + k^2} \psi_{\pm,s}(\omega) = \lambda_s \psi_{\pm,s}(k),$$

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

$$\tilde{D}_{\pm}(s) = \int_0^{+\infty} \frac{k dk}{a^2} D(k) \psi_{\pm,s}(k)$$

$$\rho(\omega) = \sum_{i=\pm} \int_{-\infty}^{+\infty} \frac{ds}{2} \tilde{\rho}_{\pm}(s) \psi_{i,s}(\omega)$$

$$\tilde{\rho}_{\pm}(s) = \tilde{D}_{\pm}(s) / \lambda_s$$

$$\frac{1}{\pi} \int_0^{\infty} \frac{\omega d\omega}{\omega^2 + k^2} \psi_{\pm,s}(\omega) = \lambda_s \psi_{\pm,s}(k),$$

eigenfunctions and eigenvalues of KL convolution:

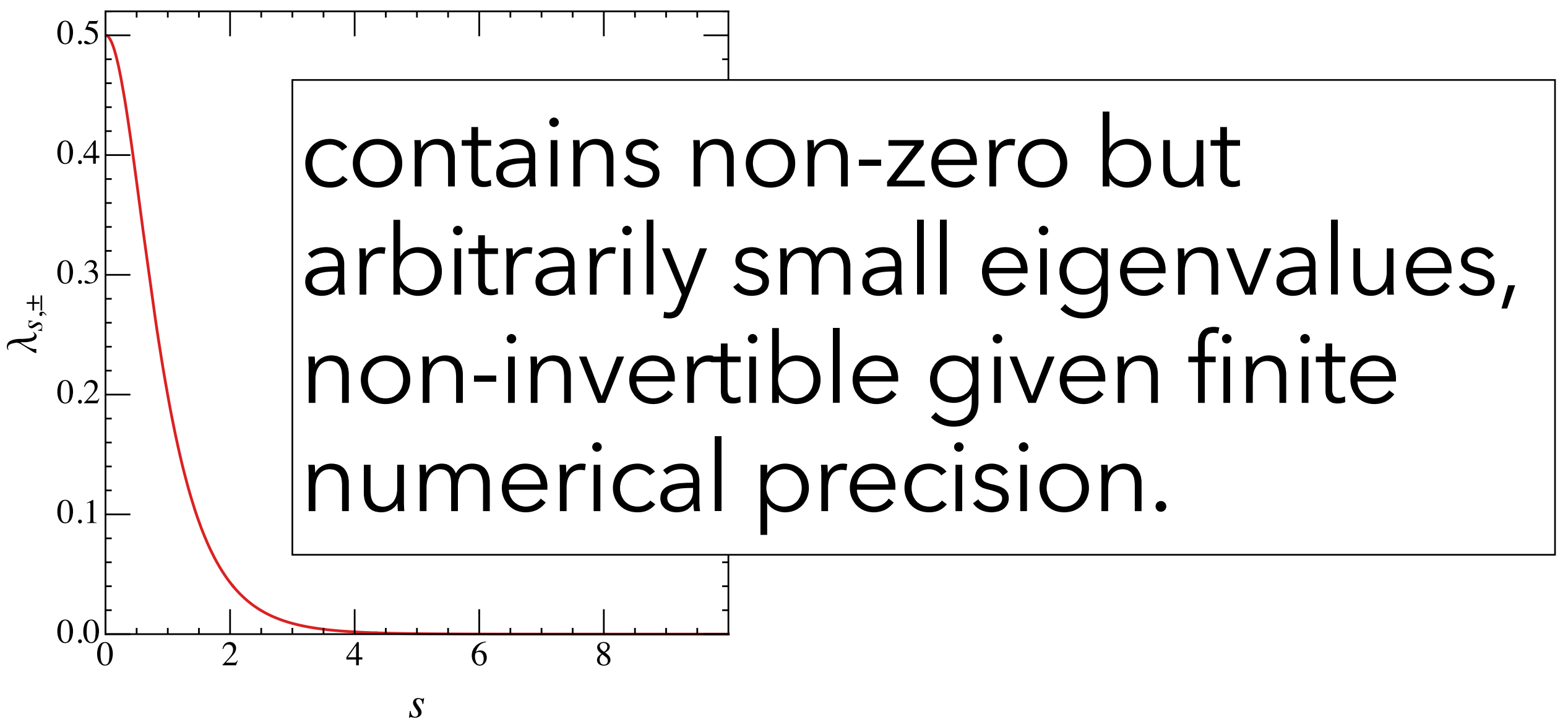
$$D(k) = \frac{1}{\pi} \int_0^\infty \frac{\omega d\omega}{\omega^2 + k^2} \rho(\omega)$$

$$\tilde{D}_\pm(s) = \int_0^{+\infty} \frac{k dk}{a^2} D(k) \psi_{\pm,s}(k)$$

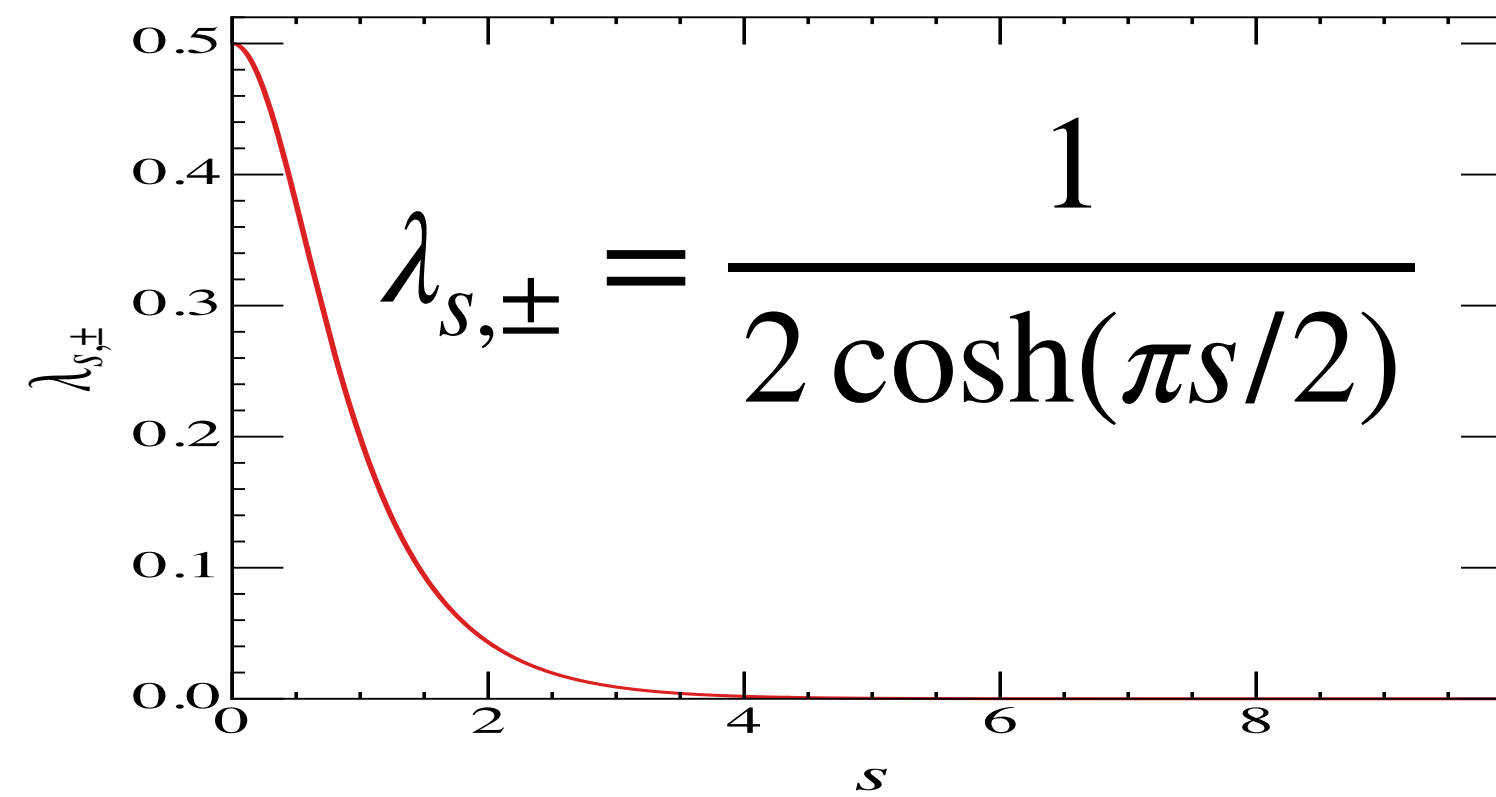
$$\rho(\omega) = \sum_{i=\pm} \int_{-\infty}^{+\infty} \frac{ds}{2} \tilde{\rho}_\pm(s) \psi_{i,s}(\omega)$$

$$\tilde{\rho}_\pm(s) = \tilde{D}_\pm(s) / \lambda_s$$

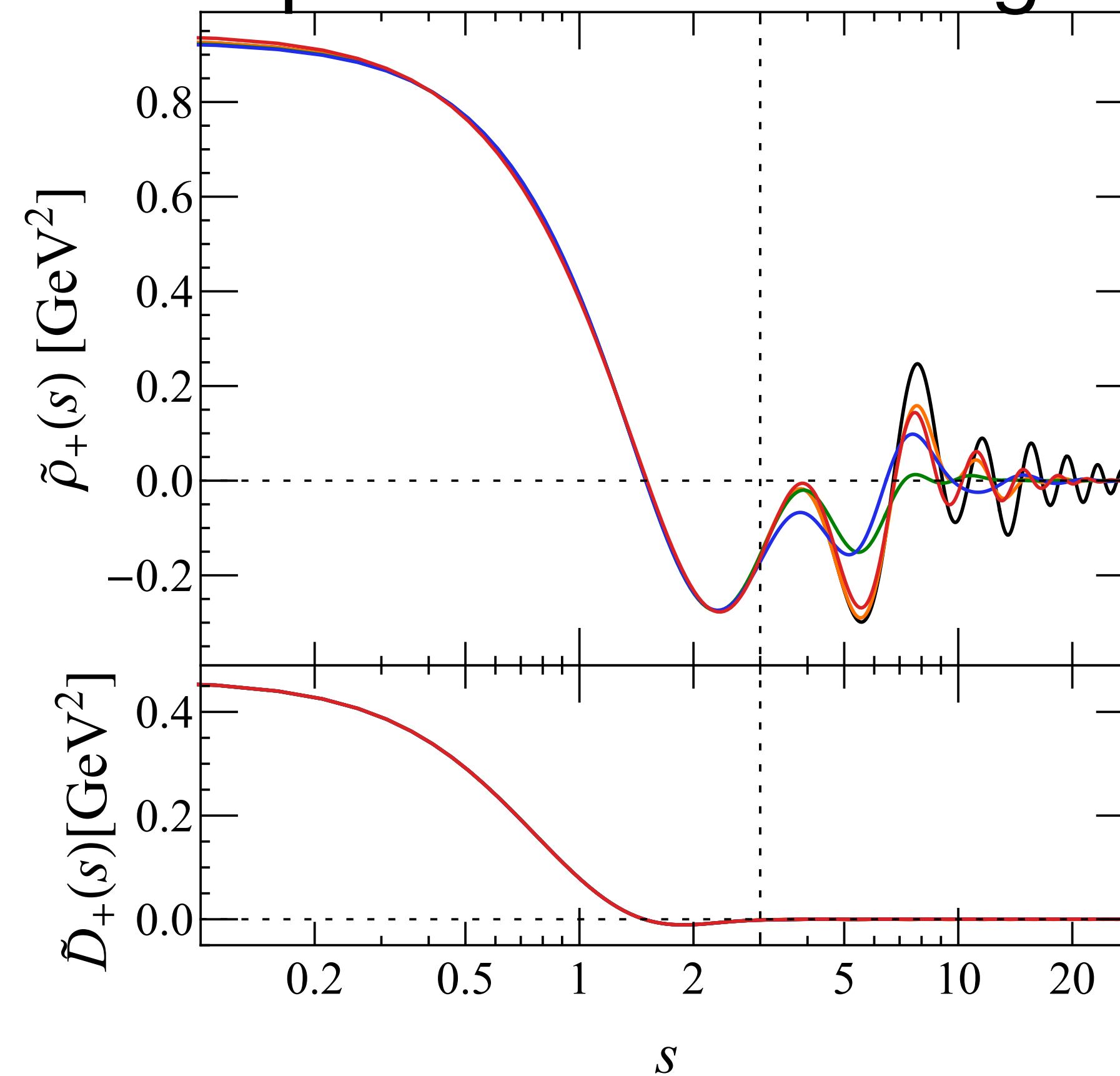
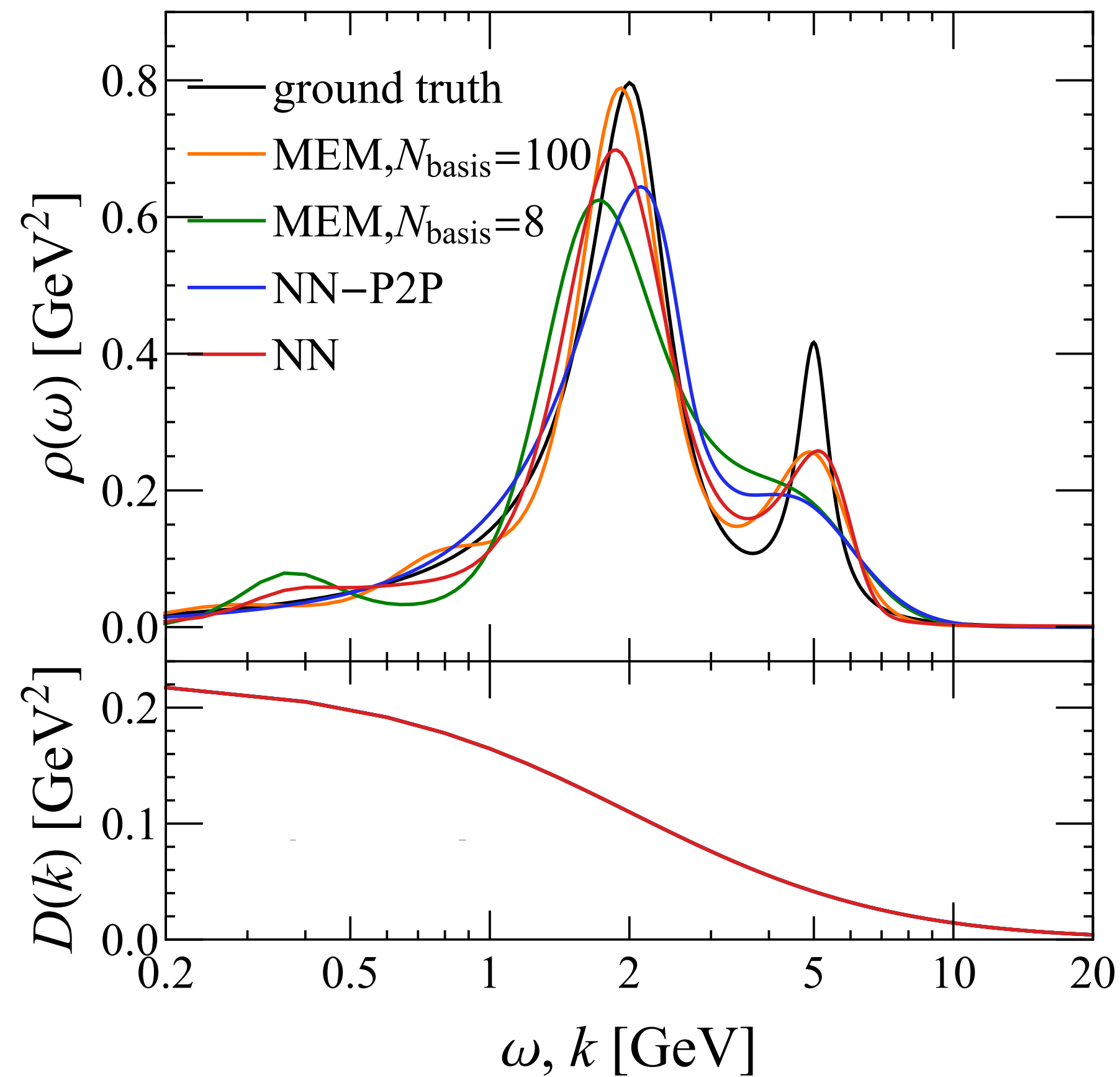
$$\lambda_{s,\pm} = \frac{1}{2 \cosh(\pi s/2)}$$



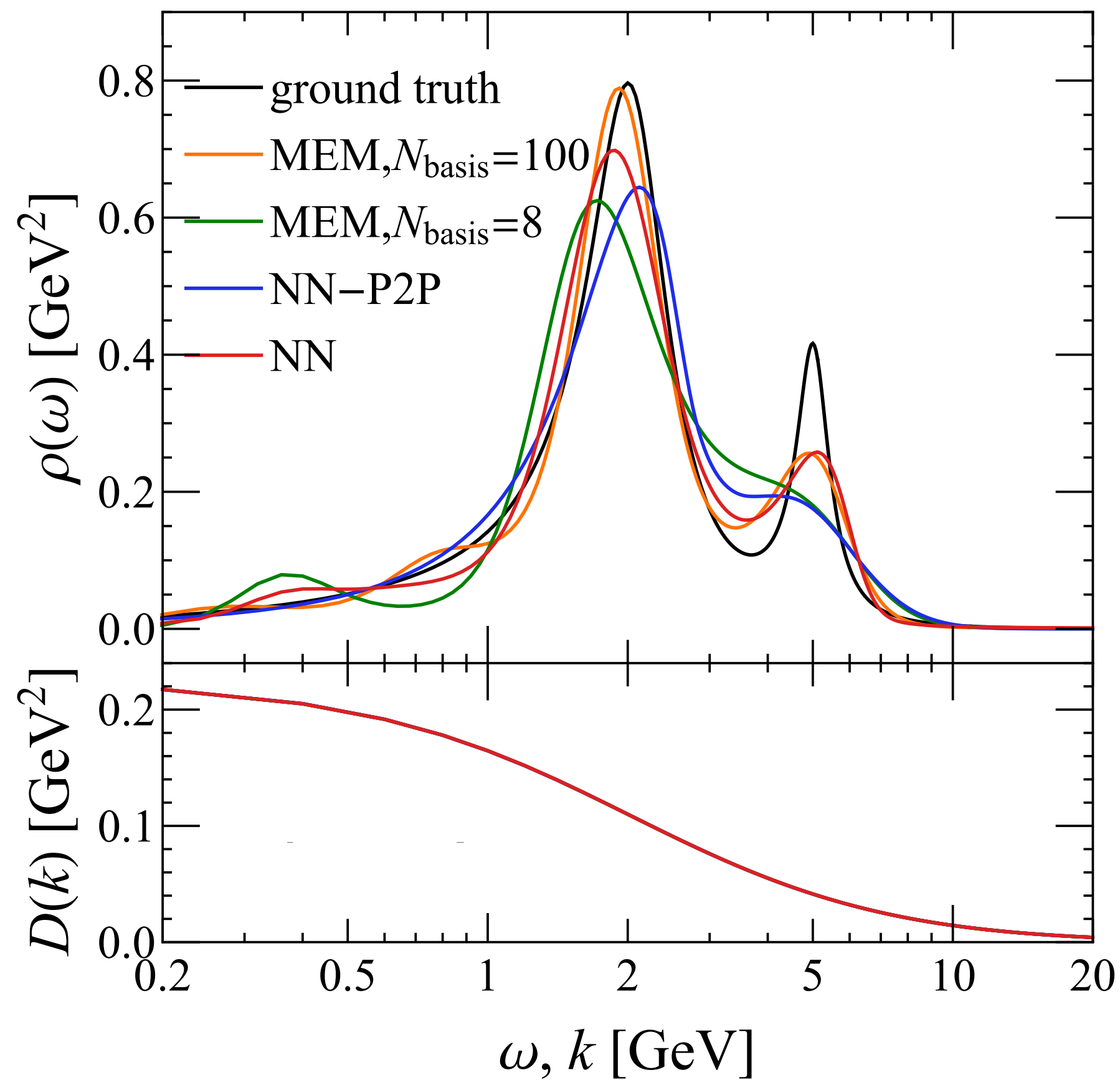
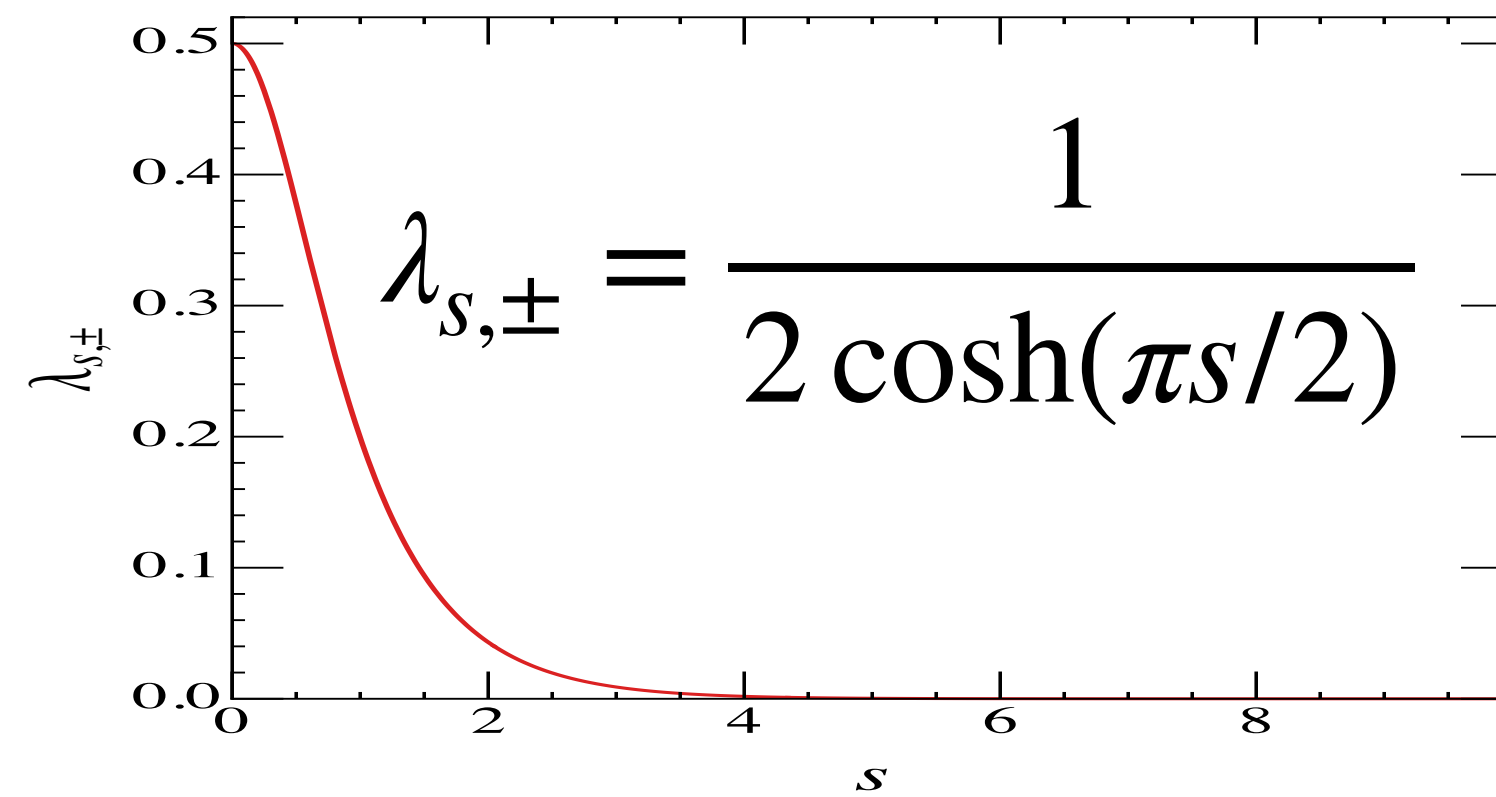
$$\psi_{s,+}(x) = \frac{\cos(s \ln(x/a))}{\sqrt{\pi x/a}}$$



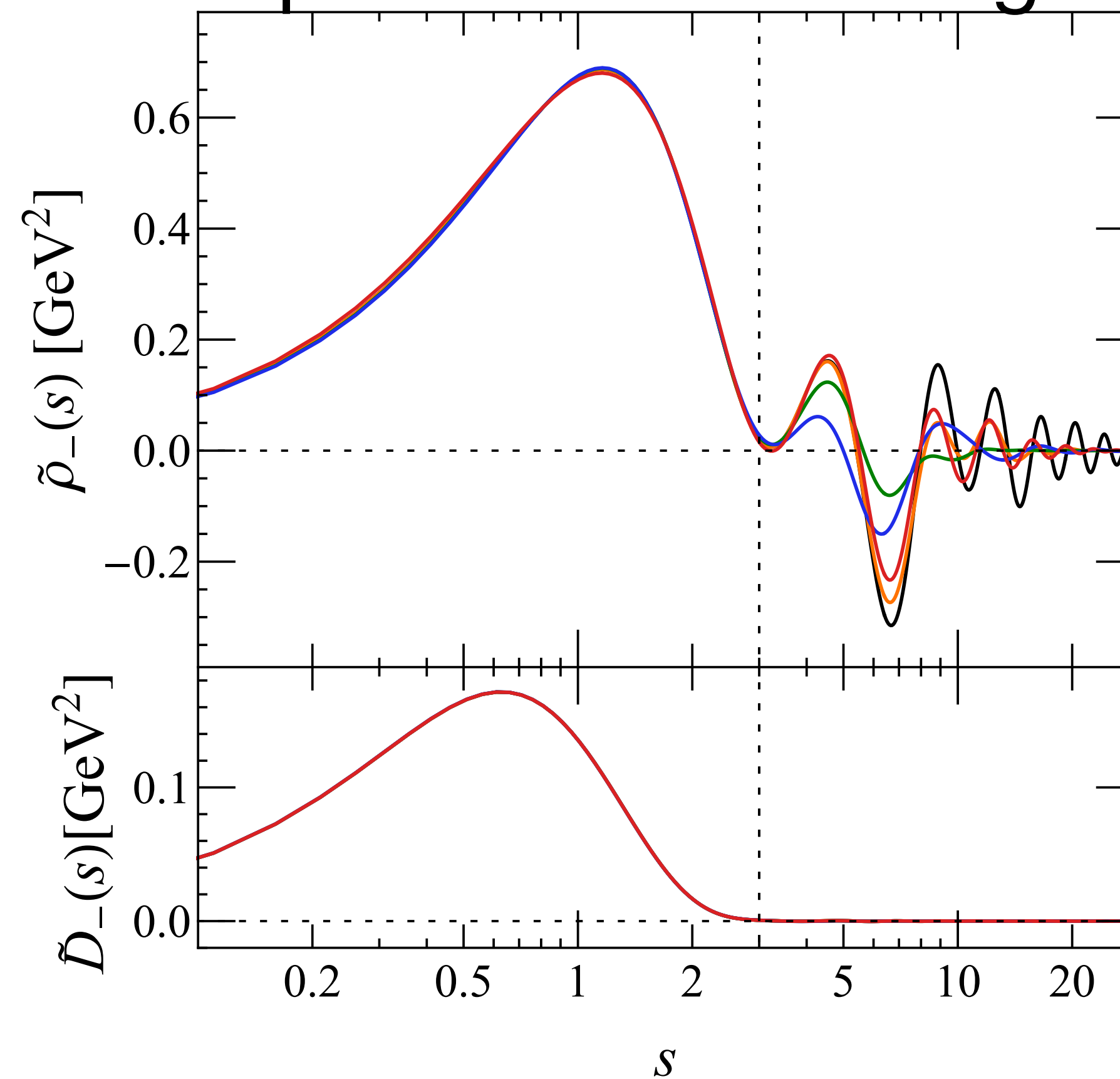
decomposition into the eigen-space



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



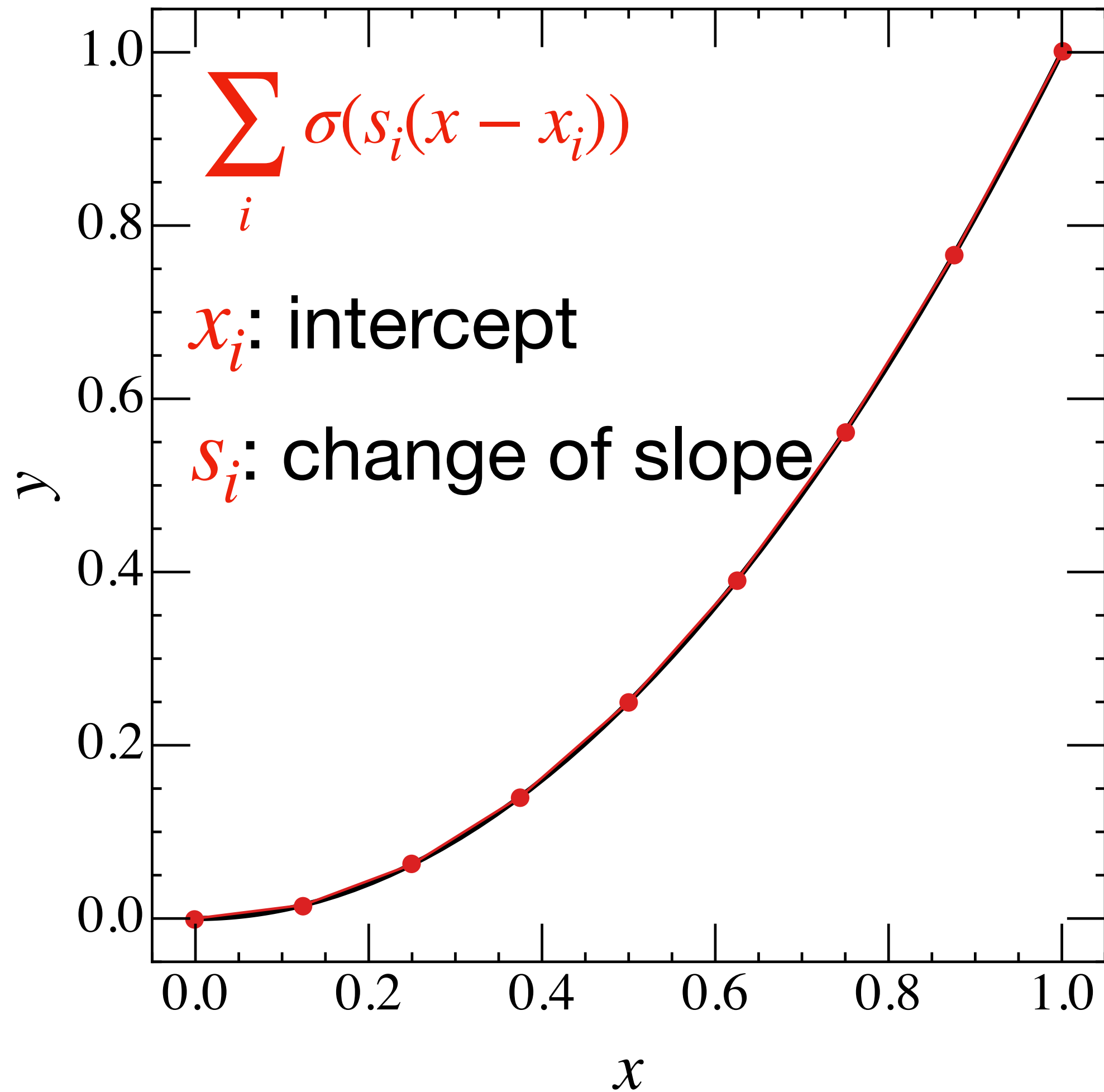
decomposition into the eigen-space



Then, why Deep Learning?

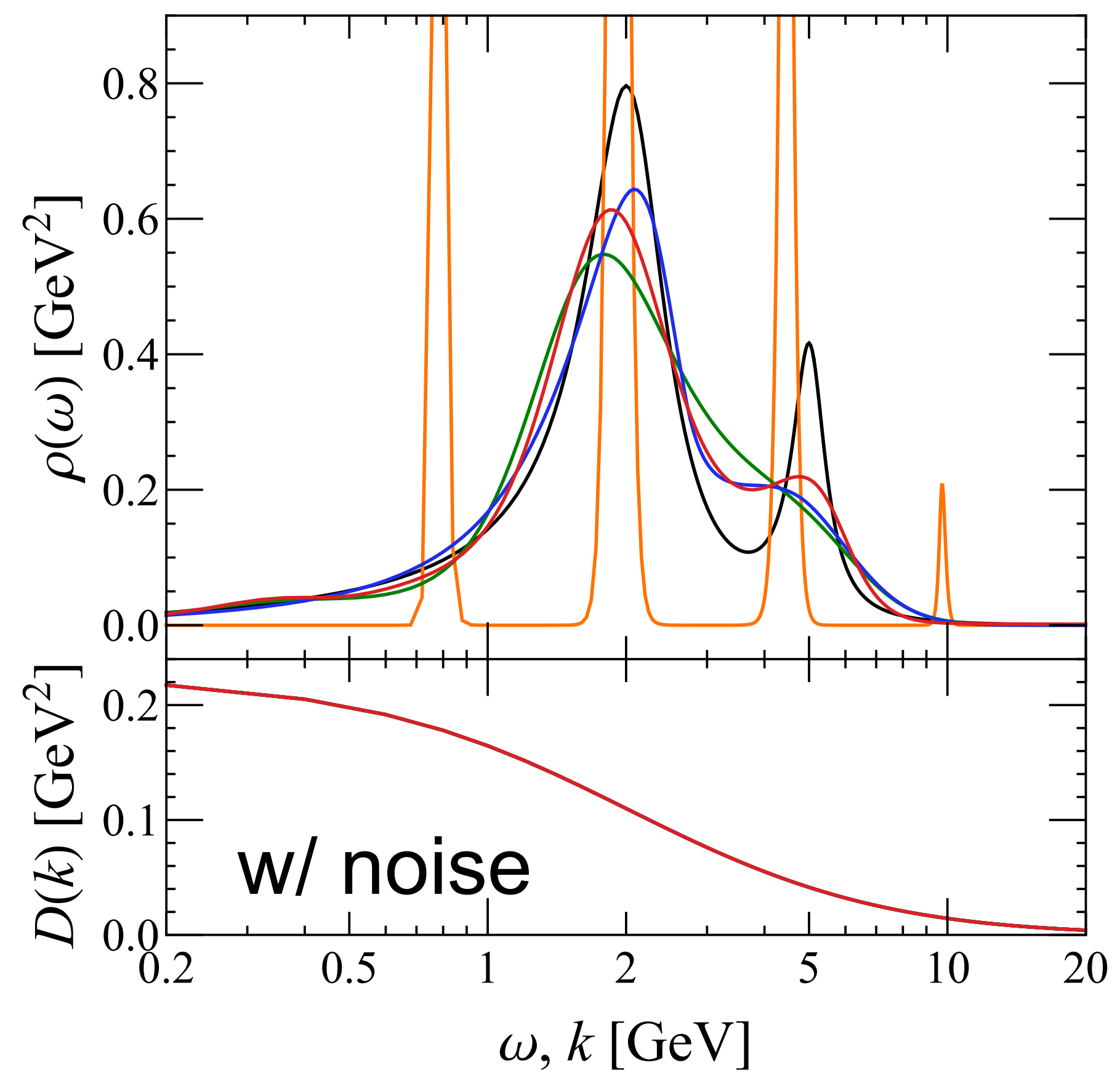
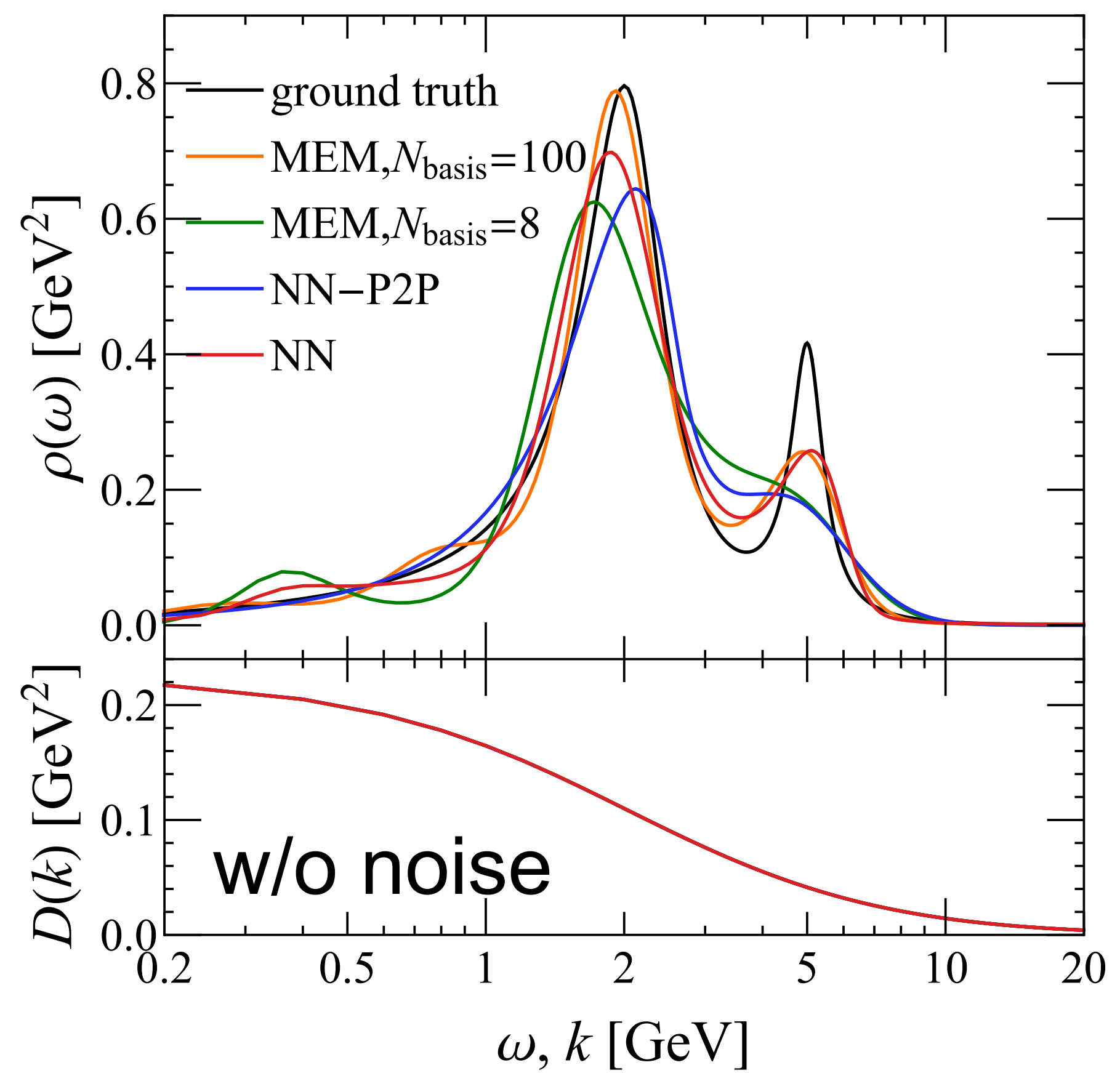
DNN is a natural implementation of smoothness regularization!

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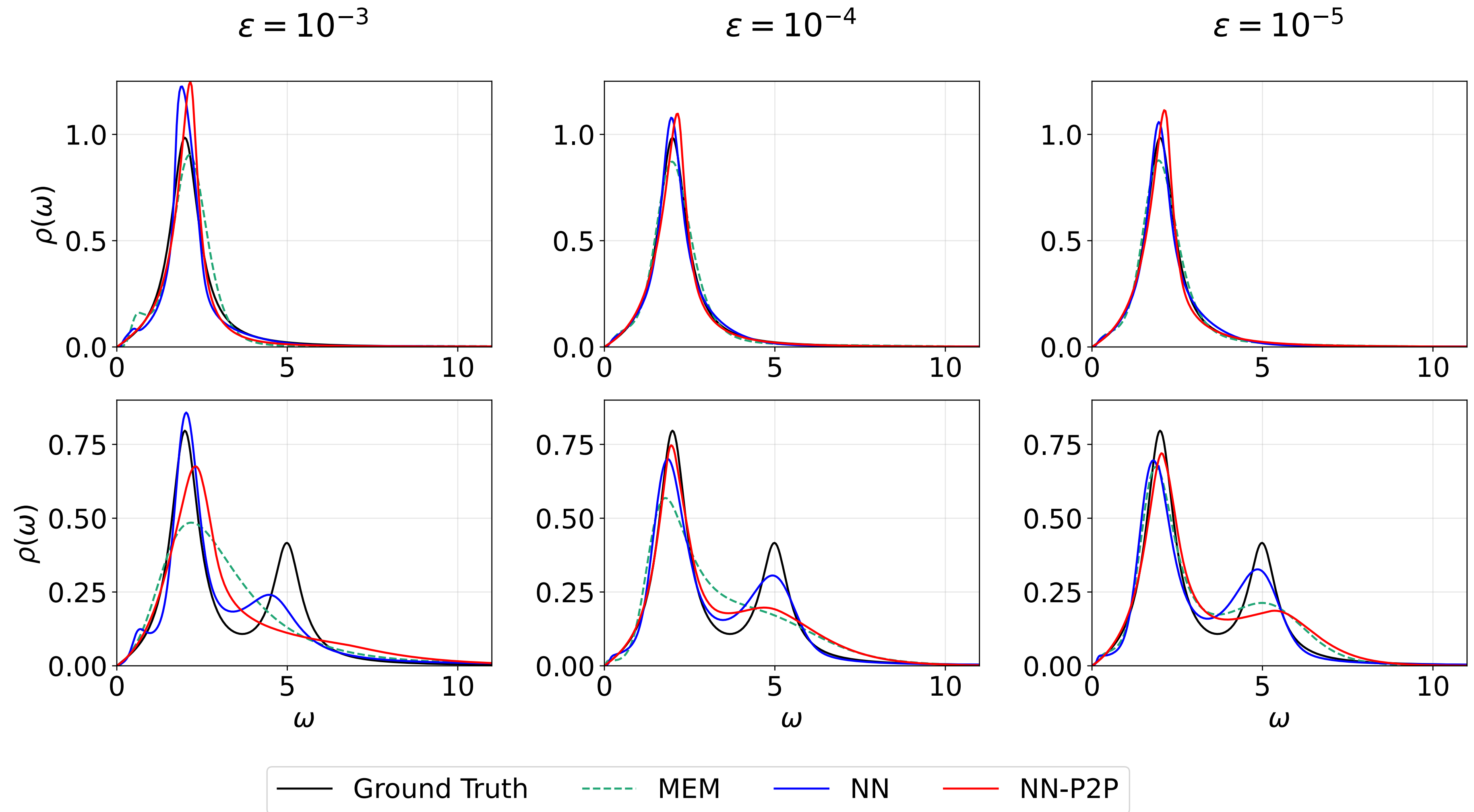


minimizing $\sum_i s_i^2 \leftrightarrow$ imposing smoothness

Robustness against larger noise



Robustness against larger noise



Summary

- New algorithm employing DNN to solve inverse problems;
- Extracted HF complex $V(T, r)$;
- Reconstructing spectral function ...

Summary

- New algorithm employing DNN to solve inverse problems;
- Extracted HF complex $V(T, r)$;
- Reconstructing spectral function ... **is ill-posed!!!**
 - **physics-based parameterization**
 - **real time evolution?**
 - **supervised learning?**

Machine learning spectral functions in lattice QCD

S.-Y. Chen (Hua-Zhong Normal U., LQLP and CCNU, Wuhan, Inst. Part. Phys.), H.-T. Ding (Hua-Zhong Normal U., LQLP and CCNU, Wuhan, Inst. Part. Phys.), F.-Y. Liu (Hua-Zhong Normal U., LQLP and CCNU, Wuhan, Inst. Part. Phys. and Eotvos U.), G. Papp (Eotvos U.), C.-B. Yang (Hua-Zhong Normal U., LQLP and CCNU, Wuhan, Inst. Part. Phys.)

Oct 26, 2021

25 pages

e-Print: [2110.13521](https://arxiv.org/abs/2110.13521) [hep-lat]

View in: [ADS Abstract Service](#)

eigenfunctions and eigenvalues of KL convolution:

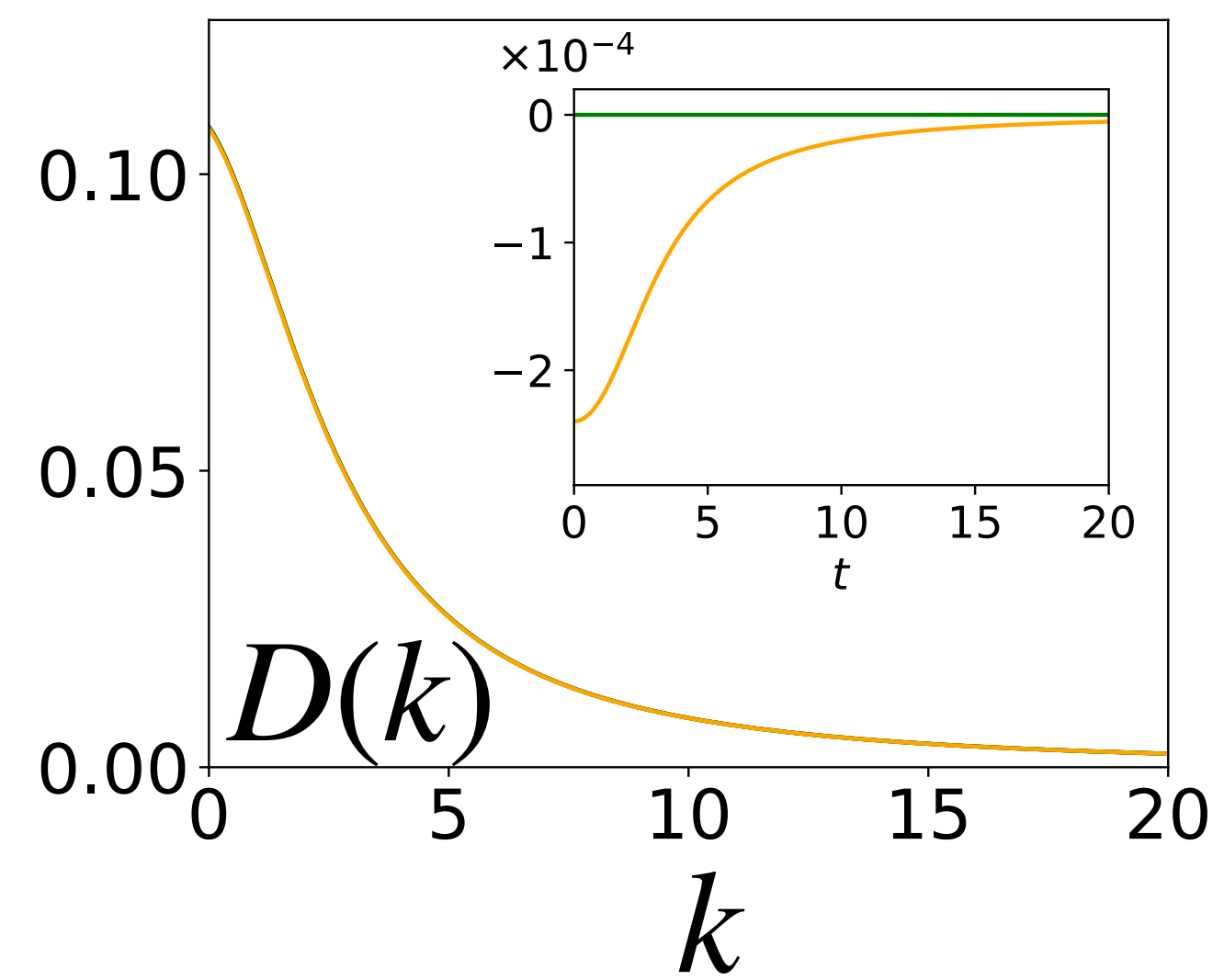
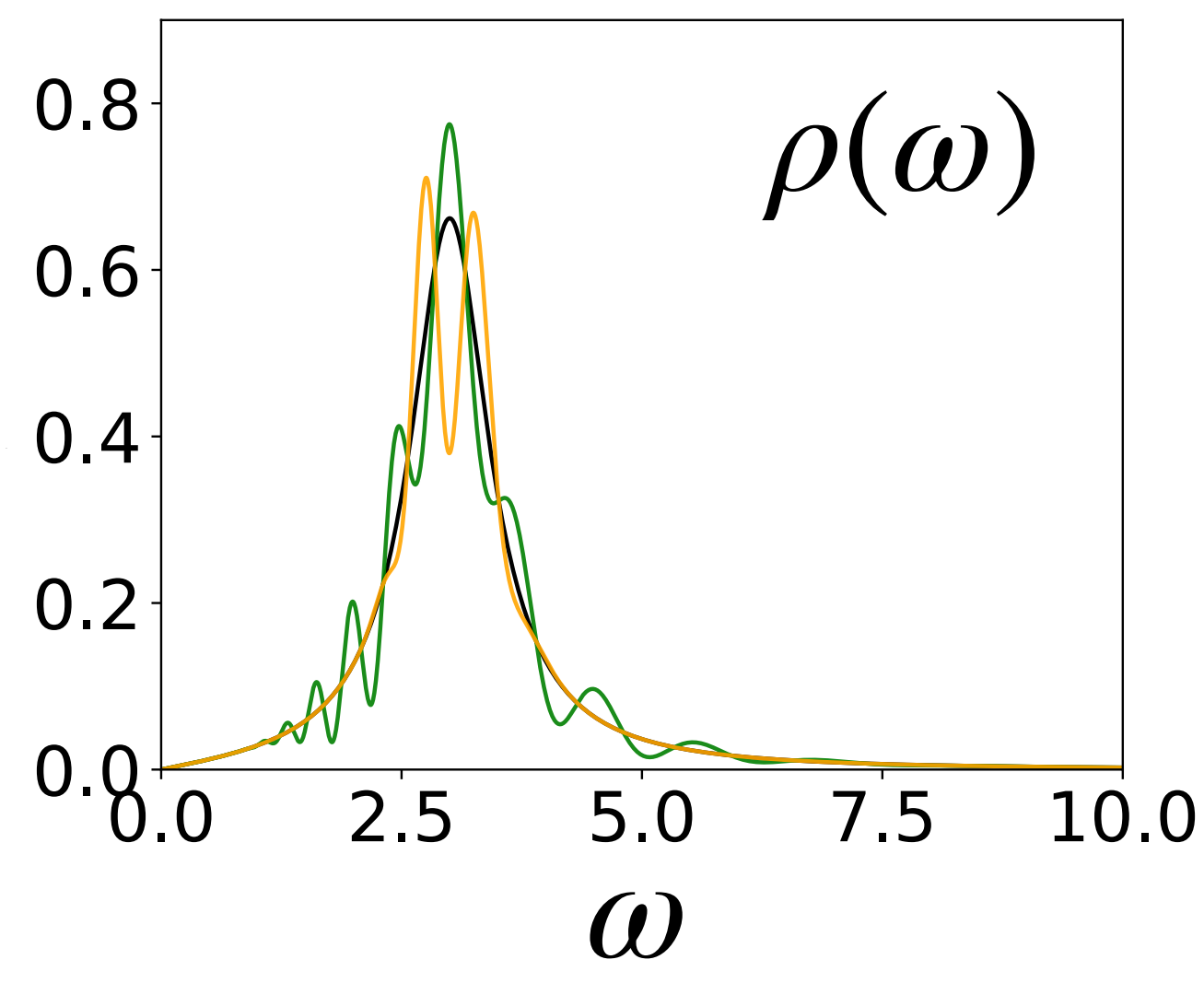
$$\frac{1}{\pi} \int_0^\infty \frac{\omega d\omega}{\omega^2 + k^2} \psi(\omega) = \lambda \psi(k),$$

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

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

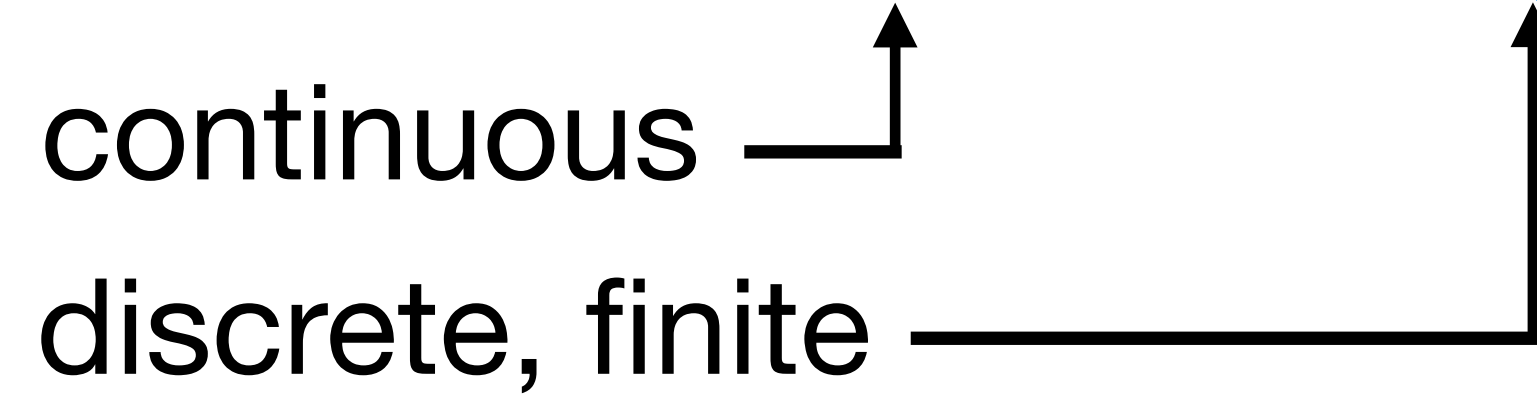
$$\psi_{s,-}(x) = \frac{\sin(s \ln(x/a))}{\sqrt{\pi x/a}},$$

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



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

continuous \rightarrow
discrete, finite \rightarrow

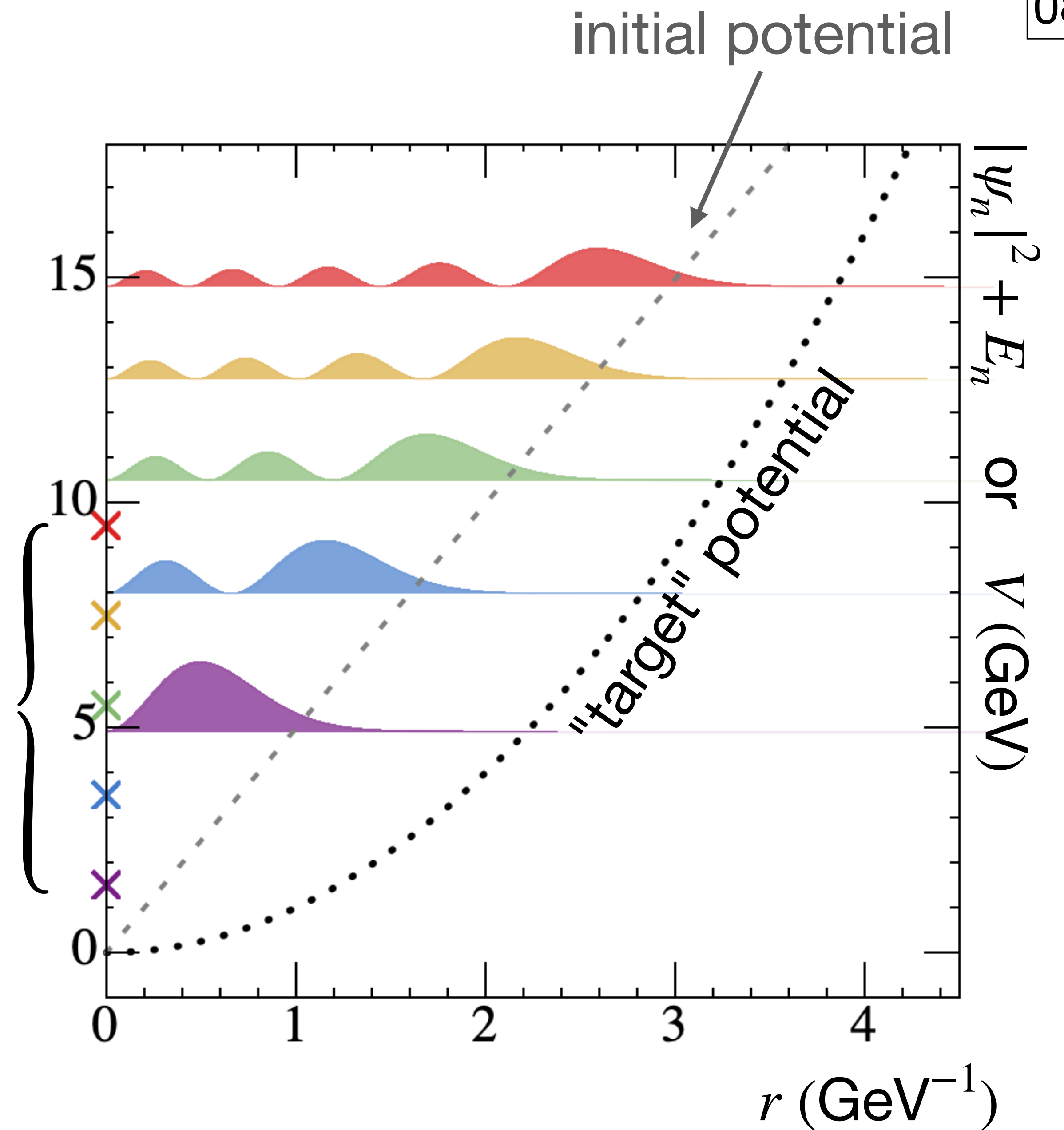


Can we really learn $V(r)$ from $\{E_n\}$?

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

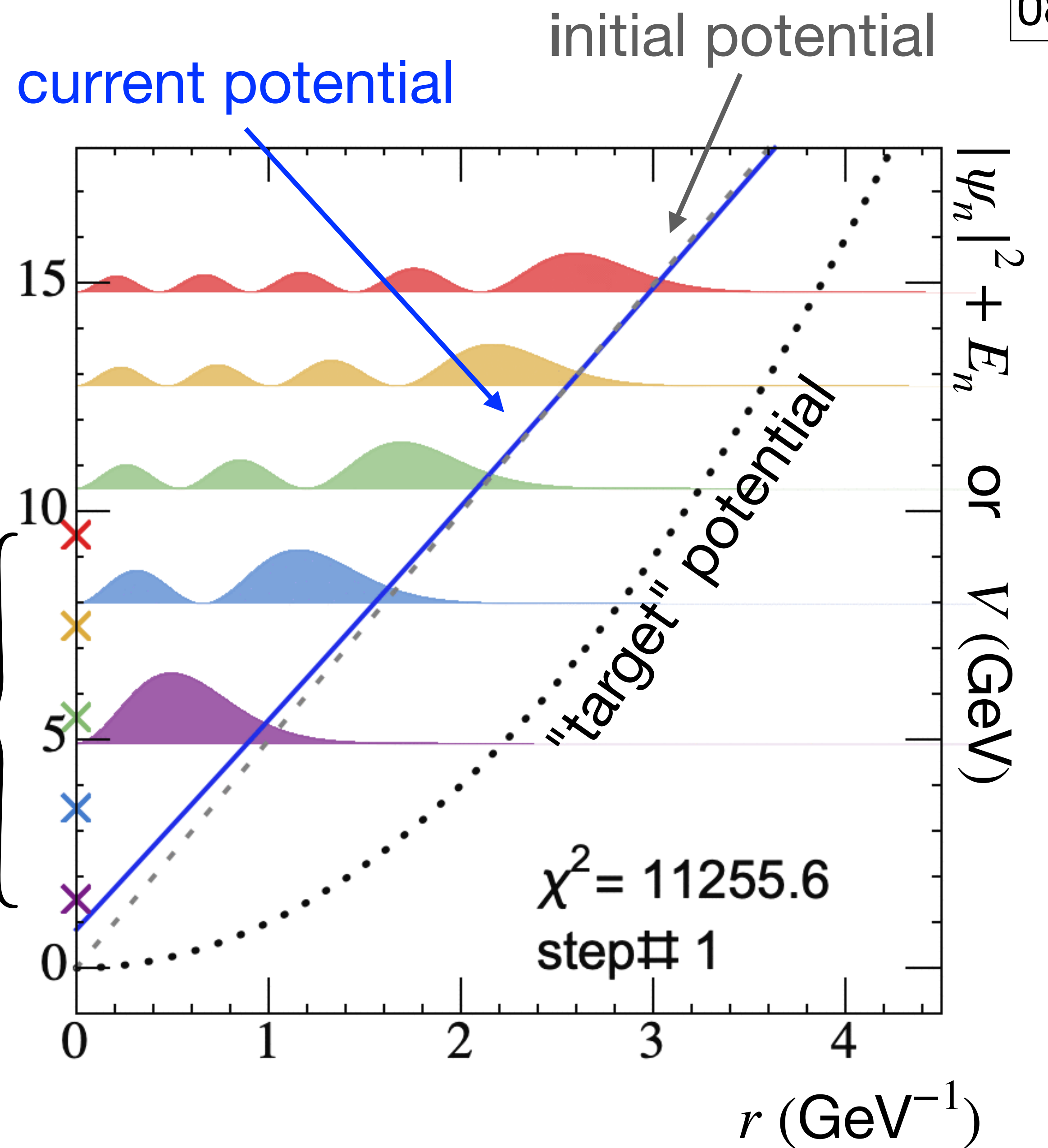


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Test - Can we recover a known complex $V(T, r)$?

- Start with a known potential

$$V_R(T, r) = \frac{\sigma}{\mu_D} \left(2 - (2 + \mu_D r) e^{-\mu_D r} \right) - \alpha \left(\mu_D + \frac{e^{-\mu_D r}}{r} \right) + B,$$

$$V_I(T, r) = -\frac{\sqrt{\pi}}{4} \mu_D T \sigma r^3 G_{2,4}^{2,2} \left(\begin{matrix} -\frac{1}{2}, -\frac{1}{2} \\ \frac{1}{2}, \frac{1}{2}, -\frac{3}{2}, -1 \end{matrix} \middle| \frac{\mu_D^2 r^2}{4} \right) - \alpha T \phi(\mu_D r).$$

- Compute $\{m_n, \Gamma_n\}$ at

$$T = \{0, 151, 173, 199, 251, 334\} \text{ MeV}$$

- Learn the potential using DNN

Test - Can we recover a known complex $V(T, r)$?

-- Yes!

- Start with a known potential (solid line)

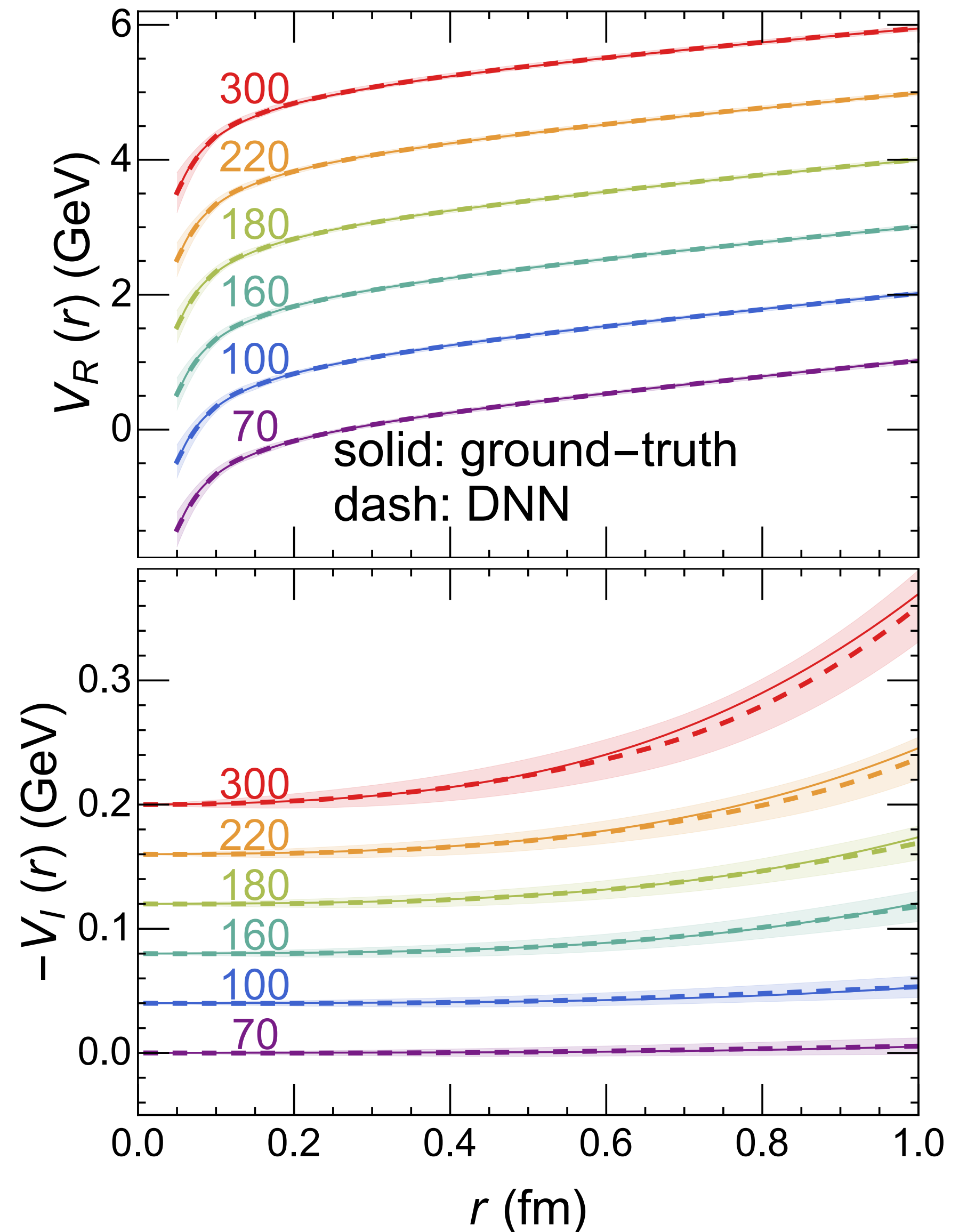
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- Learn the potential using DNN (dash + band)



Test - Can we recover a known complex $V(T, r)$?

extrapolation is risky!

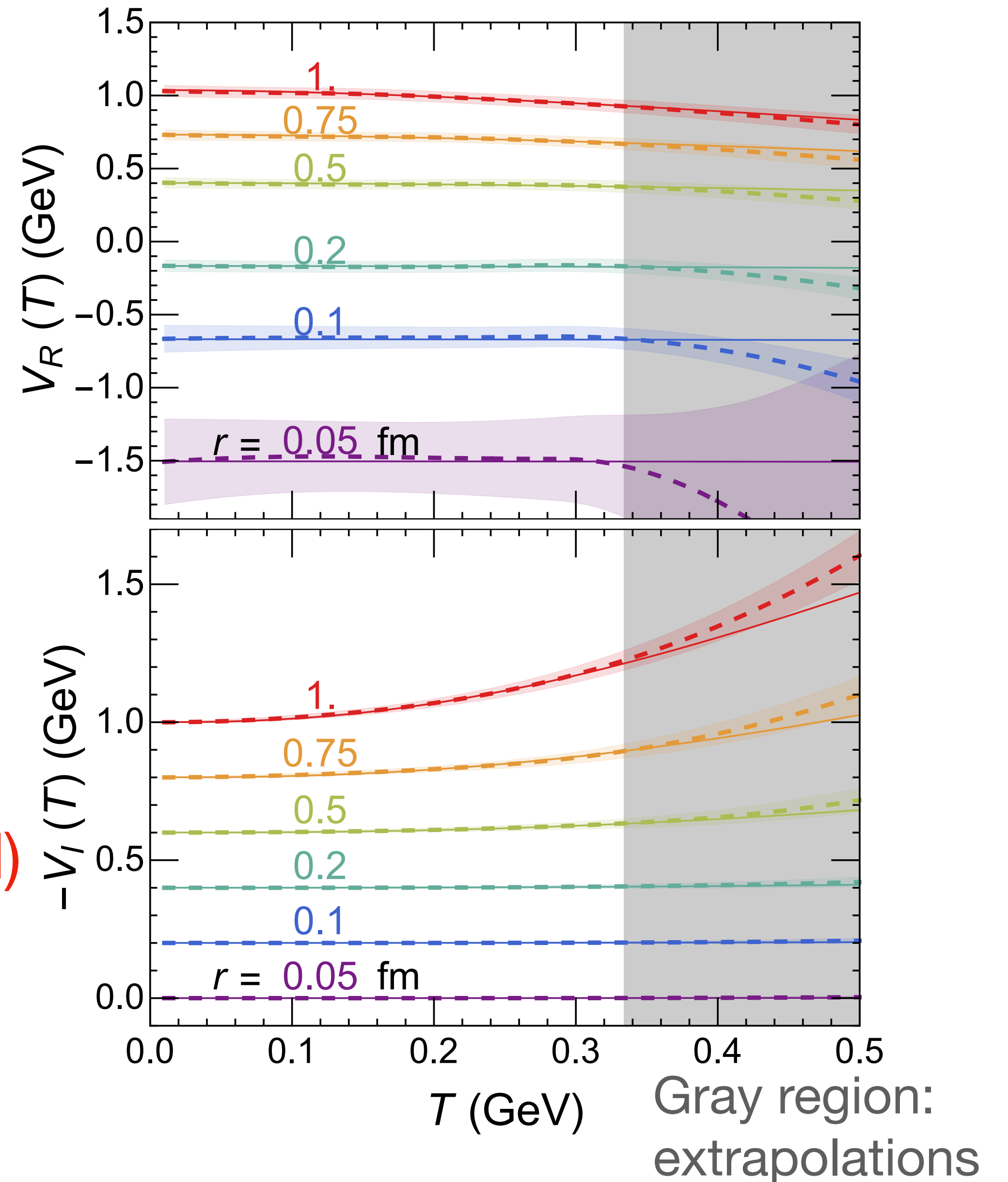
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- Compute $\{m_n, \Gamma_n\}$ at $T = \{0, 151, 173, 199, 251, 334\}$ MeV

- Learn the potential using DNN (dash + band)



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

- parameterize the potential $V(r | \boldsymbol{\theta})$, **scan** the whole $\boldsymbol{\theta}$ -space,

$$\text{minimize } \chi^2 \equiv \sum_i \left(\frac{E_{\boldsymbol{\theta},i} - E_i}{\delta E_i} \right)^2$$

- a **gradient-descent** based method:

- goal -- find the $\boldsymbol{\theta}$ -point that $\nabla_{\boldsymbol{\theta}} \chi^2 = 0$
- update $\boldsymbol{\theta}$ iteratively according to $\Delta \boldsymbol{\theta} \propto \nabla_{\boldsymbol{\theta}} \chi^2$

$$\nabla_{\boldsymbol{\theta}} \chi^2 = 2 \sum_i \frac{E_{\boldsymbol{\theta},i} - E_i}{(\delta E_i)^2} \nabla_{\boldsymbol{\theta}} E_{\boldsymbol{\theta},i}$$

$$\nabla_{\boldsymbol{\theta}} E_{\boldsymbol{\theta},i} = \langle \psi_i | \nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}) | \psi_i \rangle$$

- general unbiased parameterization scheme? Deep Neural Network!

How to compute the likelihood (density) distribution of V_{θ}

$$P(V_{\theta})dV = \text{Posterior}(\boldsymbol{\theta} \mid \text{data})d^N\boldsymbol{\theta}$$

- Sample $\{\boldsymbol{\theta}_i\}$ according to a reference distribution: $P(\boldsymbol{\theta}) = \tilde{P}(\boldsymbol{\theta})$;
- Each data point corresponds to the element volume $d^N\boldsymbol{\theta}_i = 1/\tilde{P}(\boldsymbol{\theta}_i)$;
- Compute $V_{\boldsymbol{\theta}_i}(r)$, $\chi_{\boldsymbol{\theta}_i}^2$, and $\text{Posterior}(\boldsymbol{\theta}_i \mid \text{data})$;
- For given r , histogram $V_{\boldsymbol{\theta}_i}(r)$ with weights

$$w_i = P(V_{\boldsymbol{\theta}_i})dV_i = \text{Posterior}(\boldsymbol{\theta}_i)/\tilde{P}(\boldsymbol{\theta}_i)$$

- In practice:

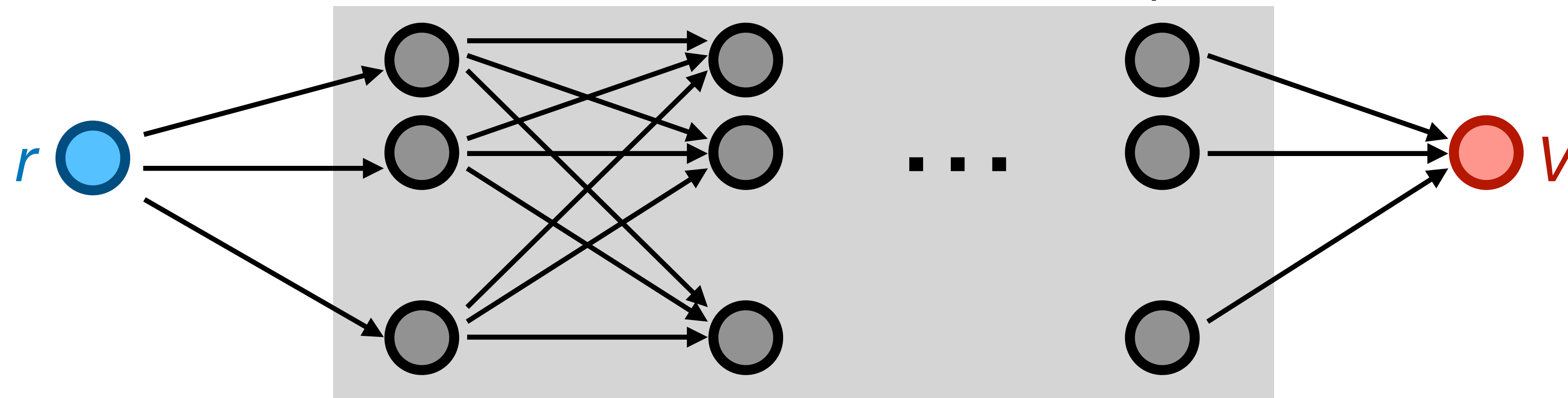
$$\tilde{P}(\boldsymbol{\theta}) = (2\pi)^{-N_{\theta}/2} \sqrt{\det[\Sigma^{-1}]} \times \exp\left[-\frac{\Sigma_{ab}^{-1}}{2}(\theta_a - \theta_a^{\text{opt}})(\theta_b - \theta_b^{\text{opt}})\right] \quad \Sigma_{ab}^{-1} = \lambda\delta_{ab} + \frac{1}{2} \frac{\partial^2 \chi^2(\boldsymbol{\theta})}{\partial\theta_a \partial\theta_b}$$

What are Deep Neural Networks?

--- a general parameterization scheme to approximate continuous functions.

$$V(r) \approx V_{\text{DNN}}(r \mid \text{parameters})$$

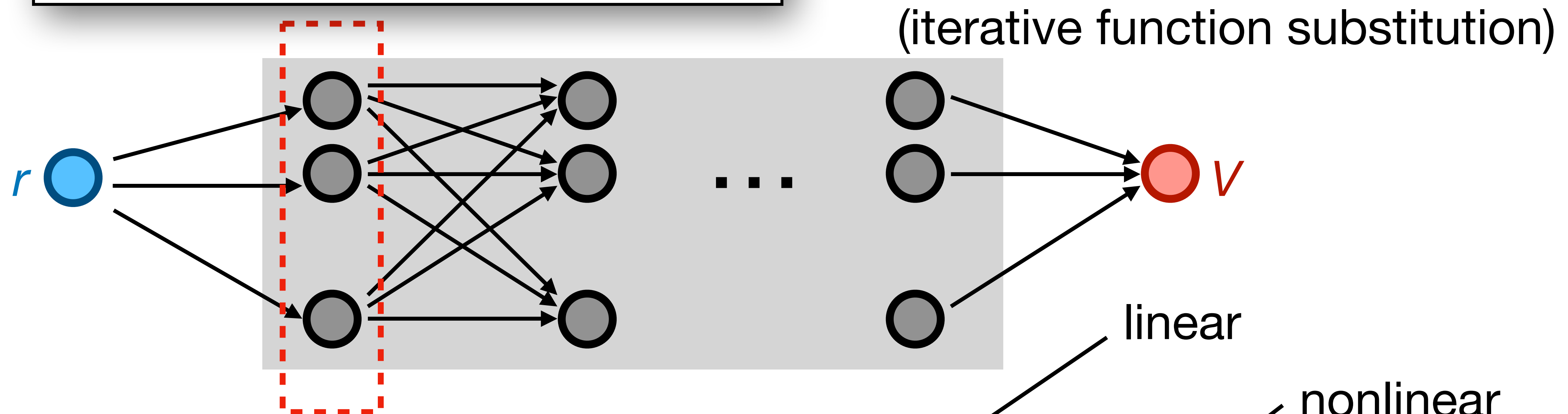
(iterative function substitution)



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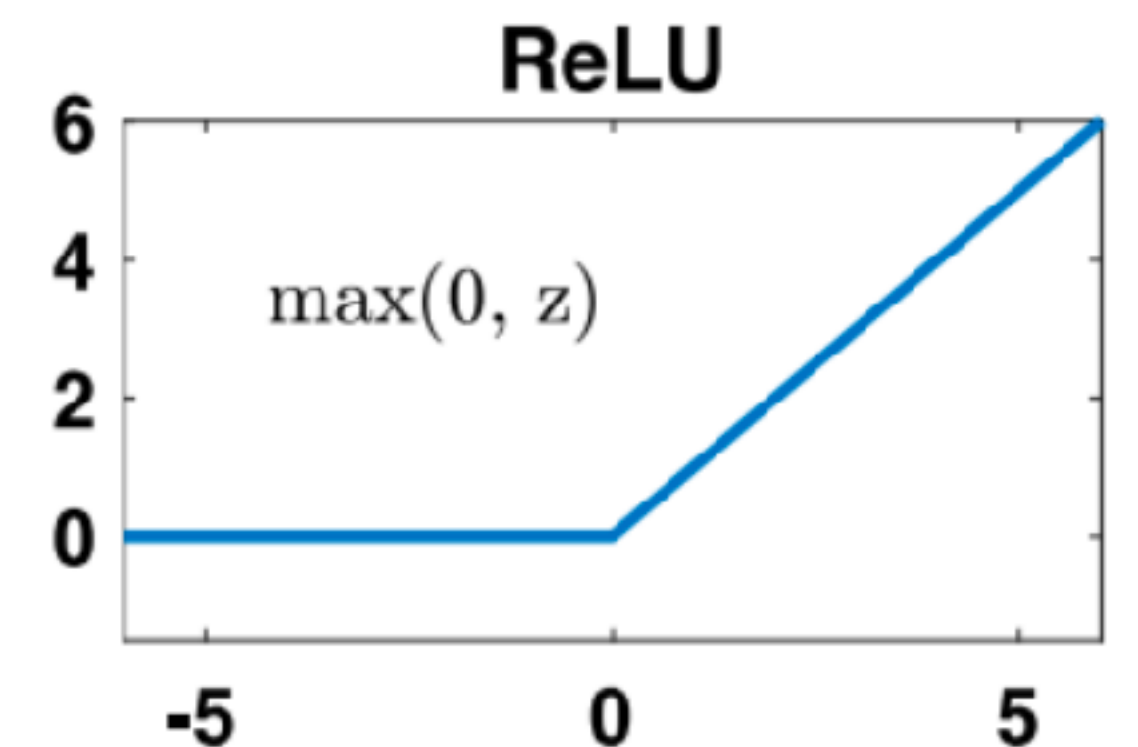
Each \bullet is an intermediate function ($a_i^{(l)}$):

- At the first layer:

$$z_i^{(1)} = b_i^{(1)} + W_{i,1}^{(1)} r,$$

$$a_i^{(1)} = \sigma(z_i^{(1)})$$

nonlinear

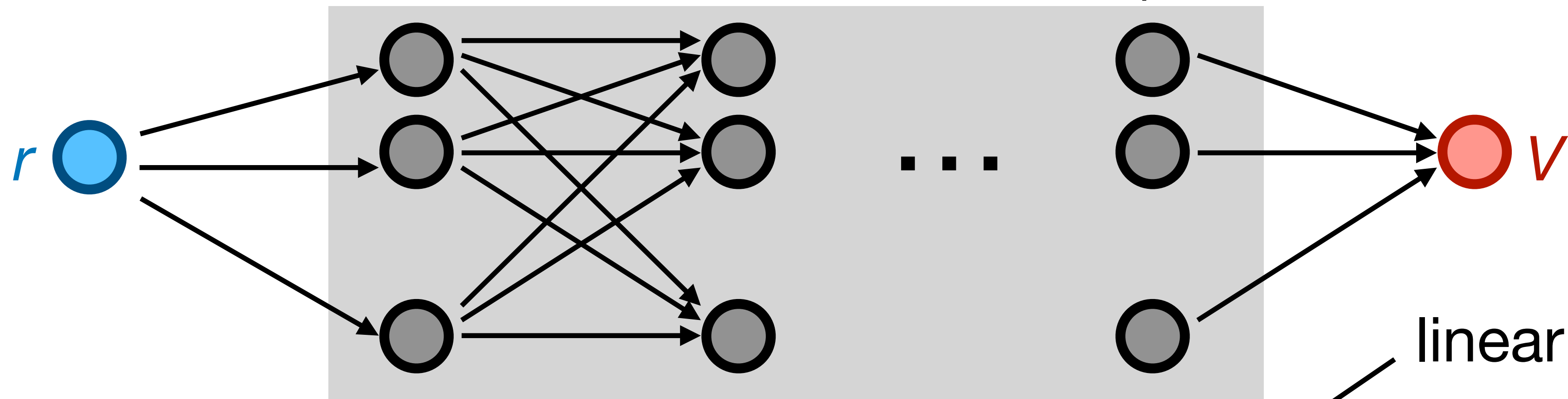


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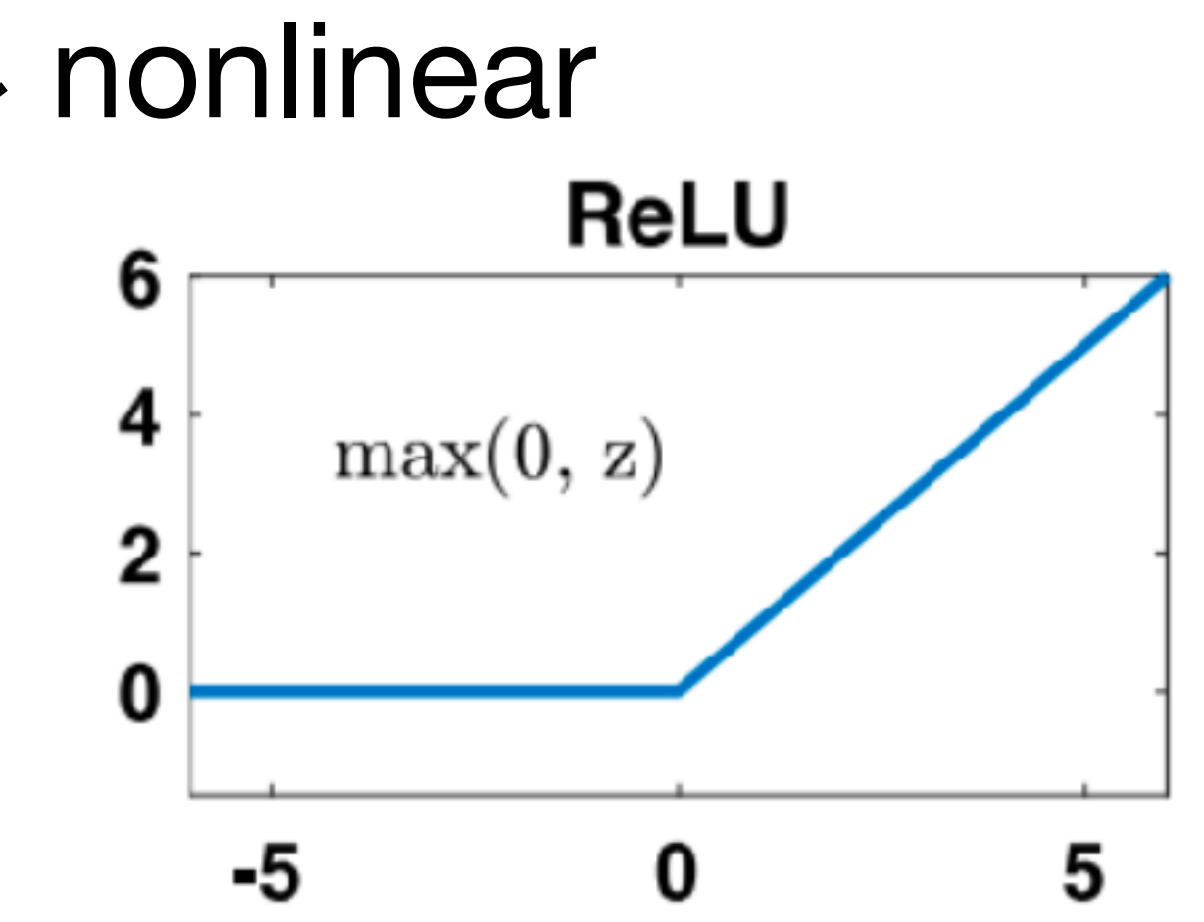
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Each \bullet is an intermediate function ($a_i^{(l)}$):

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- At later layers:

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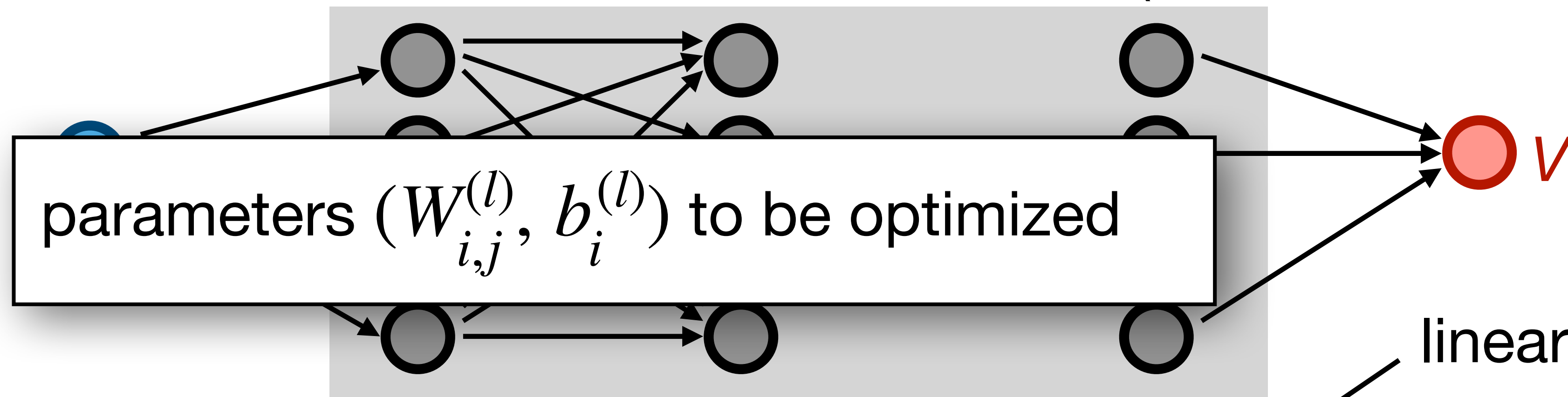


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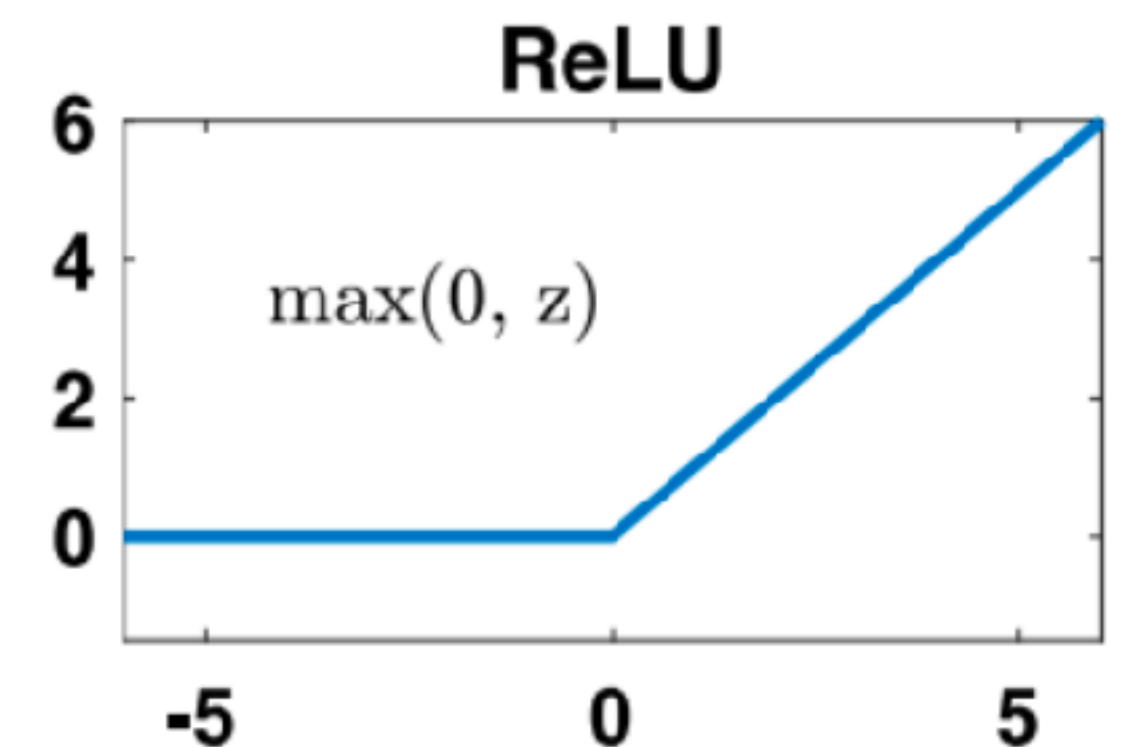
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nonlinear



Backup

information of interest

observations

potential $V(x)$

energy level $\{E_n\}$

E. o. S. $\varepsilon(P)$

mass-radius $M(R)$

information of interest

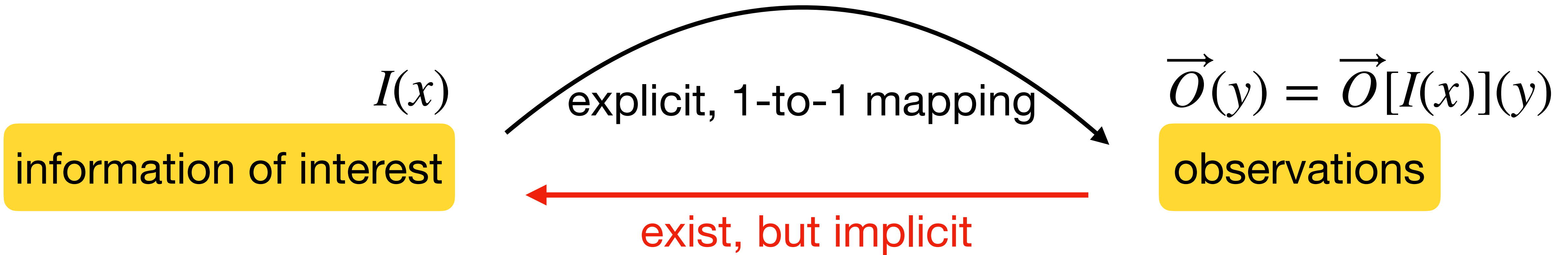
observations

potential $V(x)$

energy level $\{E_n\} = \{E_n\}[V(r)]$

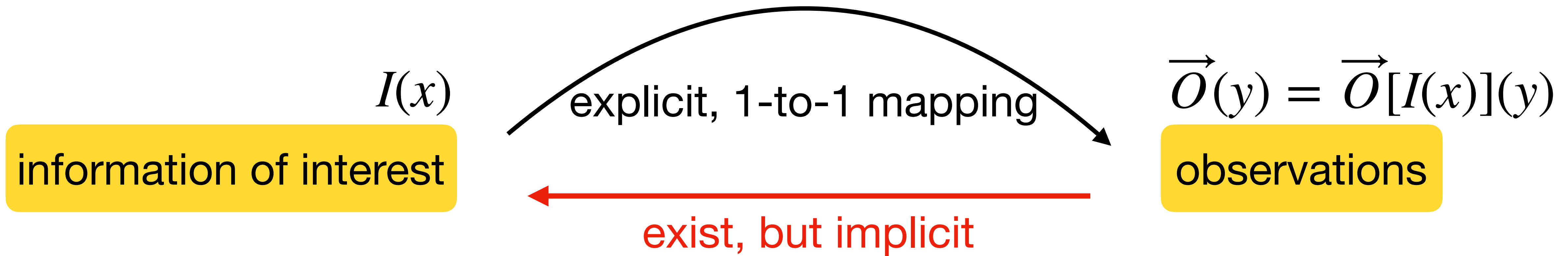
E. o. S. $\varepsilon(P)$

mass-radius $M(R) = M[\varepsilon(P)](R)$



potential $V(x)$ energy level $\{E_n\} = \{E_n\}[V(r)]$

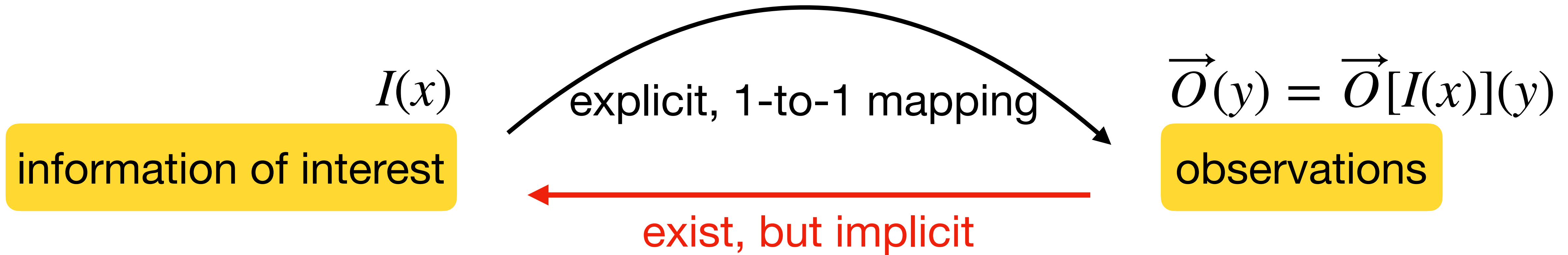
E. o. S. $\varepsilon(P)$ mass-radius $M(R) = M[\varepsilon(P)](R)$



prepare data set $\{I_i \rightarrow \vec{O}_i\}$, use NN to learn the inverse function(al) $\{\vec{O} \rightarrow I\}$

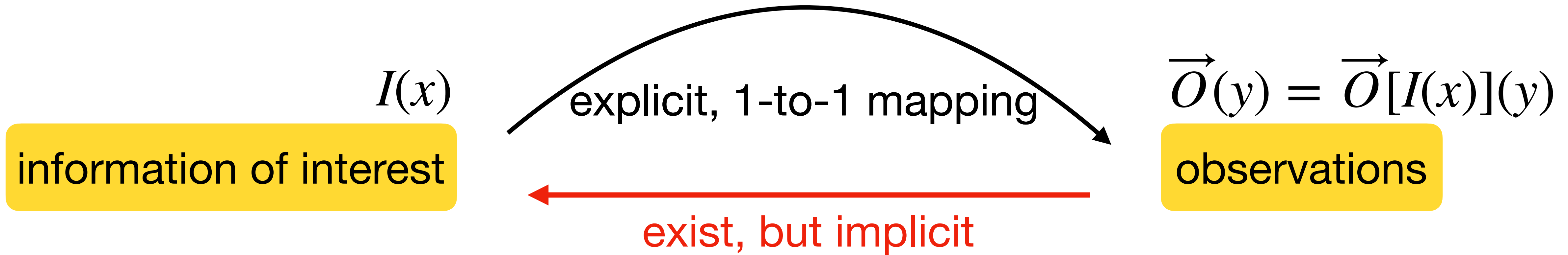
- dimension of input?
- completeness?
- bias/prior?
- uncertainty?

ref: Yuki's seminar this Monday



$$I(x) \equiv I_{\text{DNN}}(x | \theta)$$

$$\vec{O}_{\theta}(y) \equiv \vec{O}[I_{\text{DNN}}(x | \theta)](y)$$

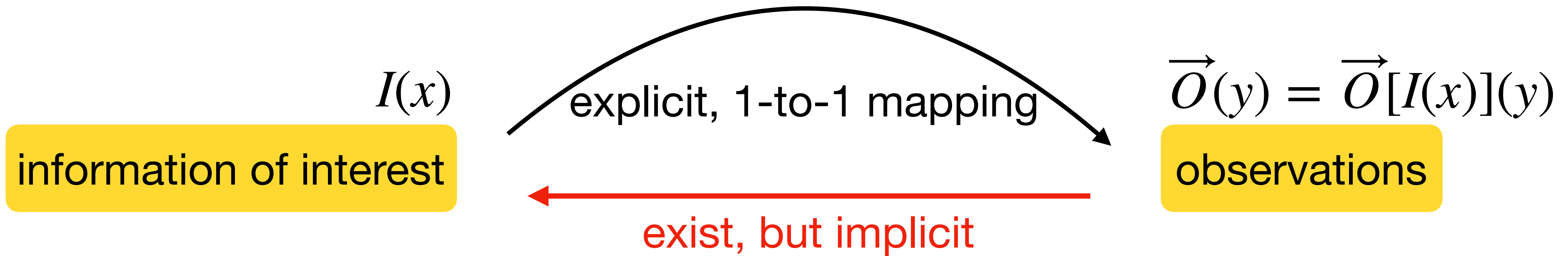


$$I(x) \equiv I_{\text{DNN}}(x | \theta)$$

$$\vec{O}_{\theta}(y_i) \equiv \vec{O}[I_{\text{DNN}}(x | \theta)](y_i)$$

loss: dist. bt/ *reconstructed* and *true* obsv.

$$J_{\theta} \equiv \sum_i \left| \vec{O}_{\theta}(y_i) - \vec{O}(y_i) \right|^2$$



$$I(x) \equiv I_{\text{DNN}}(x | \theta)$$

$$\vec{O}_\theta(y_i) \equiv \vec{O}[I_{\text{DNN}}(x | \theta)](y_i)$$

$$J_\theta \equiv \sum_i \left| \vec{O}_\theta(y_i) - \vec{O}(y_i) \right|^2$$

Tune θ to minimize J_θ . Prerequisite: $\frac{\delta O(y)}{\delta I(x)}$ can be computed

$$\nabla_\theta J = 2 \sum_i [O_\theta(y_i) - O(y_i)] \int dx \frac{\delta O(y)}{\delta I(x)} \Big|_{O(y)=O_\theta(y_i)} \nabla_\theta I_{\text{DNN}}(x | \theta)$$

Problem # III:

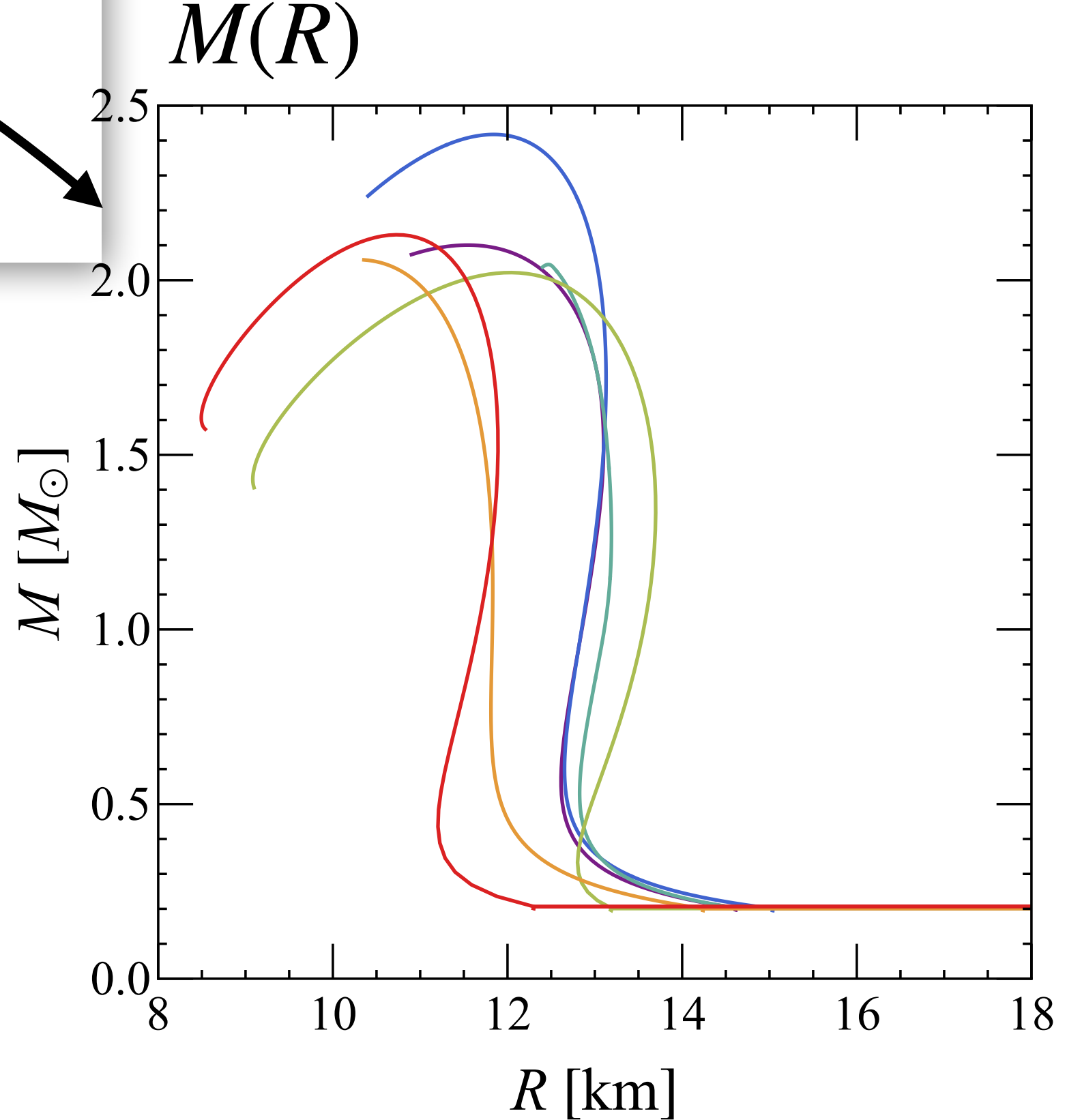
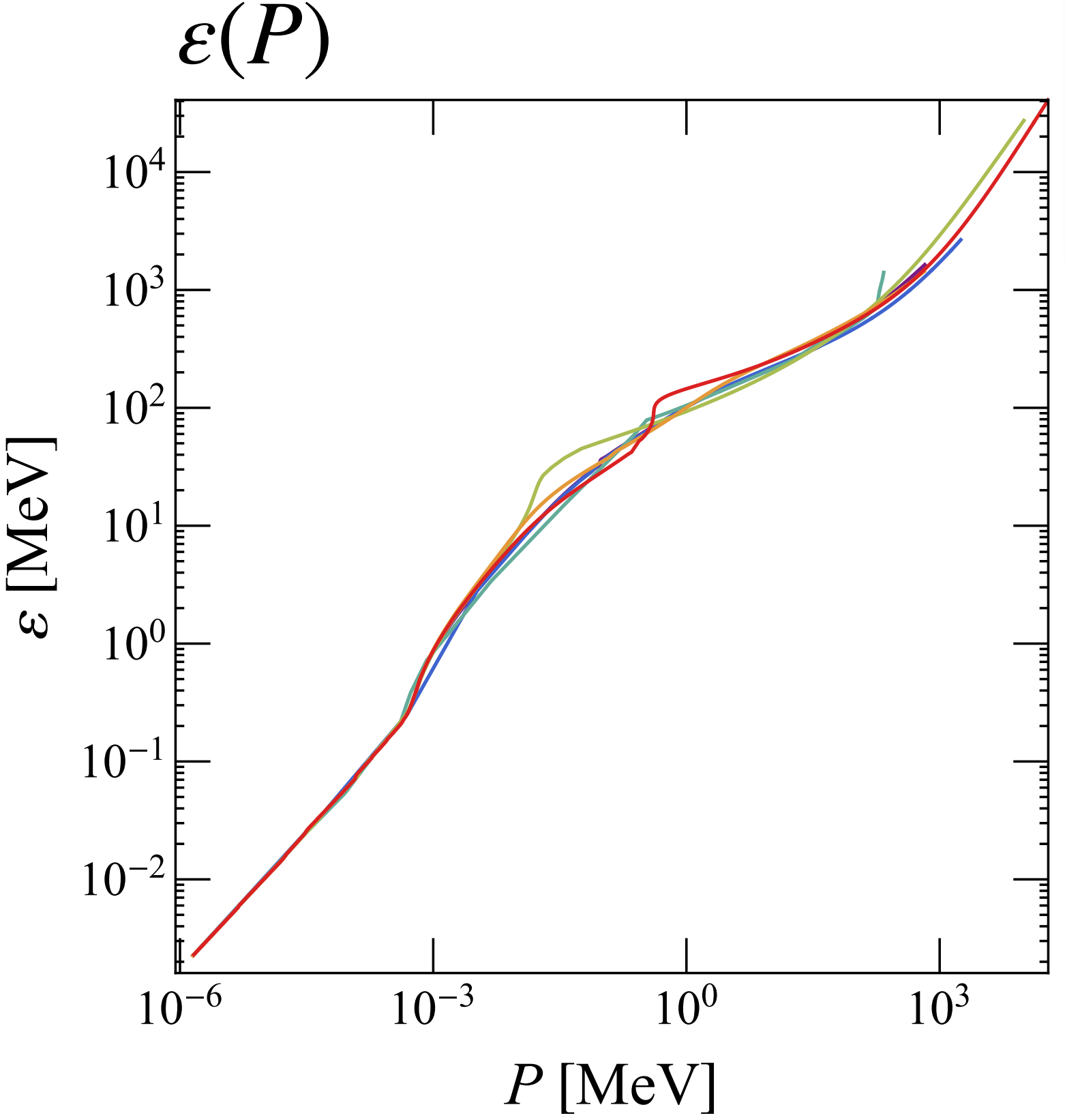
Neutron Star: EoS \Leftrightarrow {M,R}

reference: Soma, Wang, **SS**, Stoecker, Zhou,
JCAP08 (2022) 071; 2209.08883; in progress.

2. Neutron Star: EoS \Leftrightarrow mass-radius relation

TOV equations:

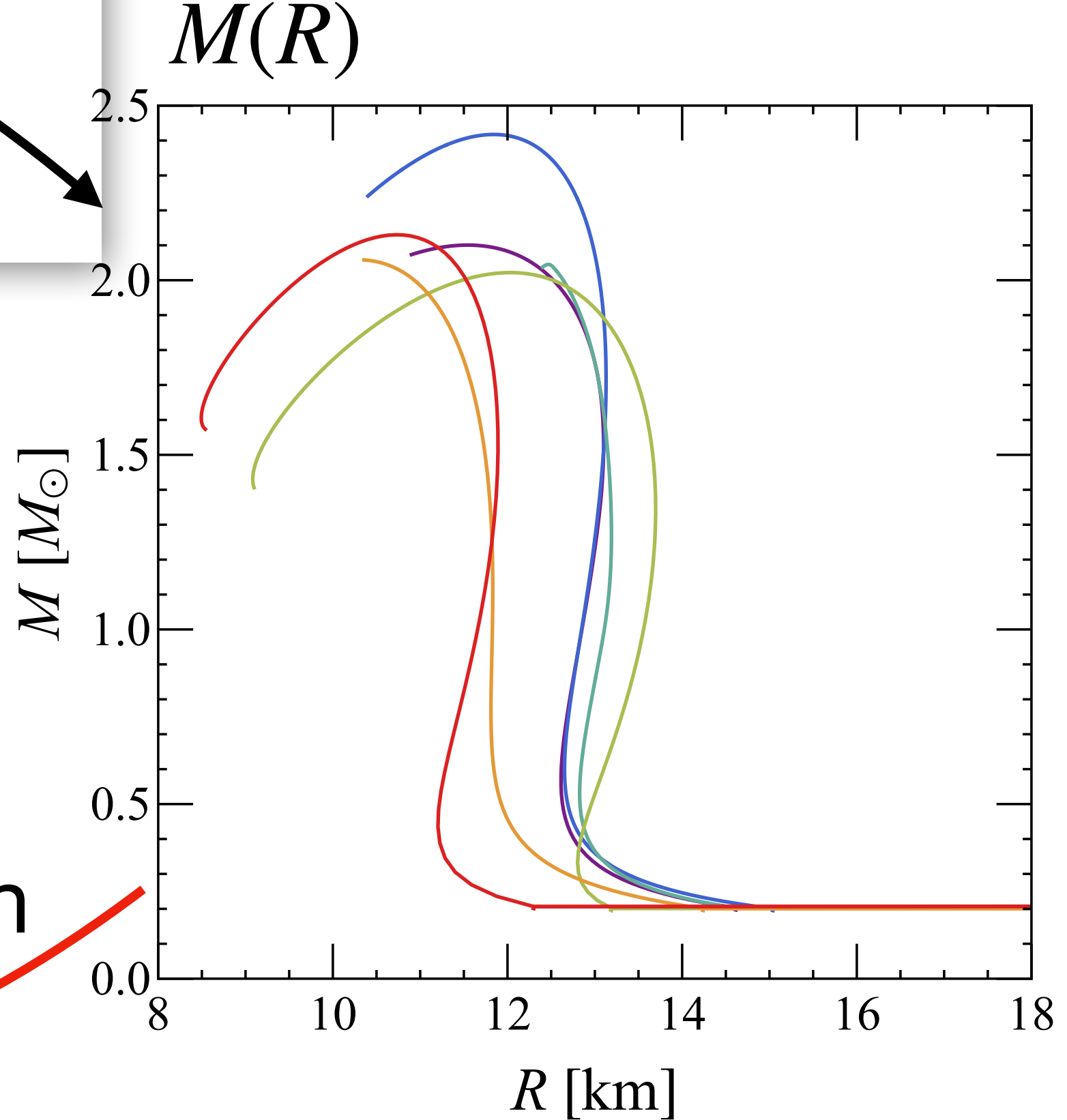
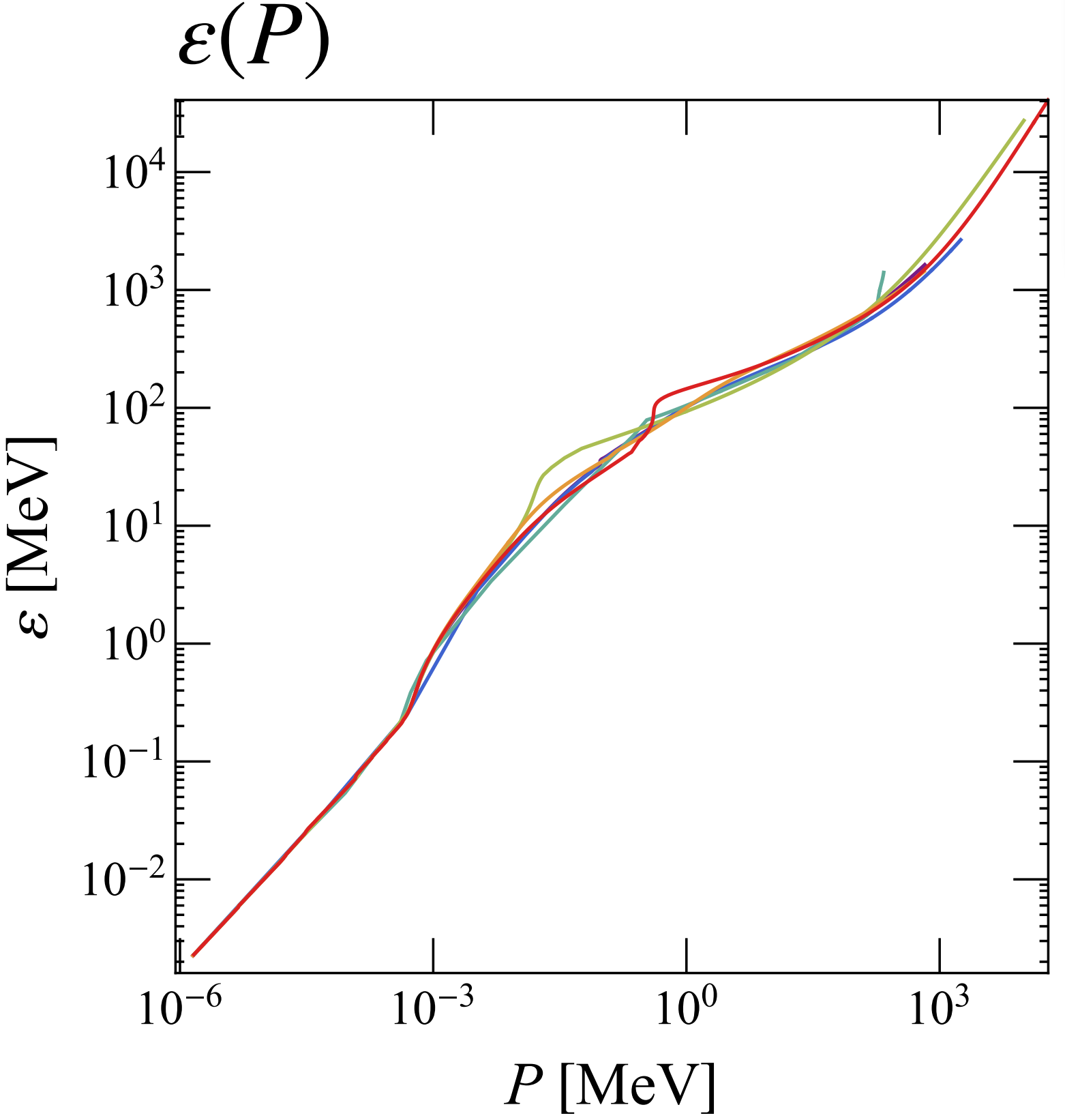
$$\frac{dP}{dr} = -\frac{(m + 4\pi r^3 P)(P + \varepsilon)}{r^2 - 2mr},$$
$$\frac{dm}{dr} = 4\pi r^2 \varepsilon,$$
$$\varepsilon = \varepsilon(P),$$



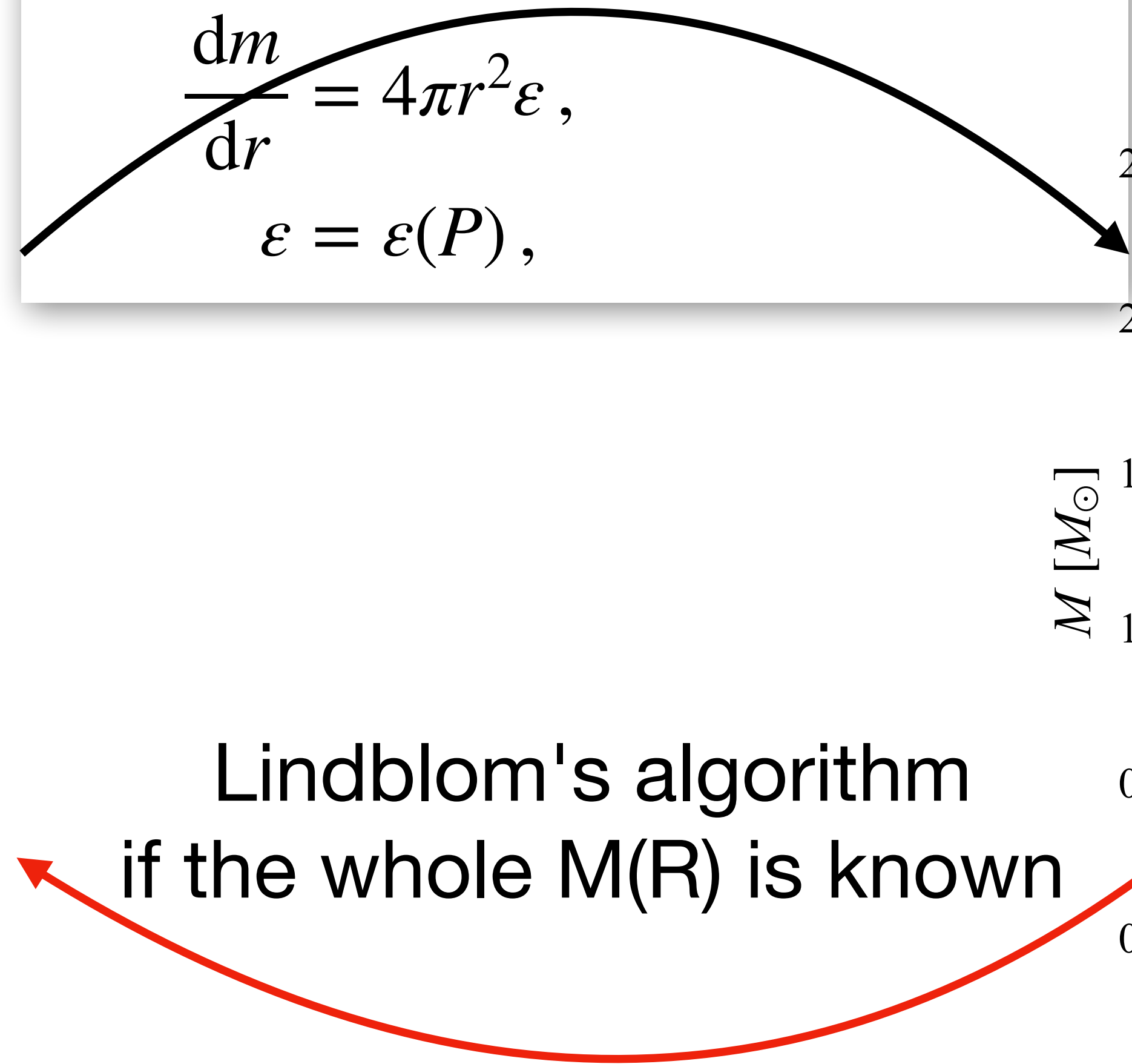
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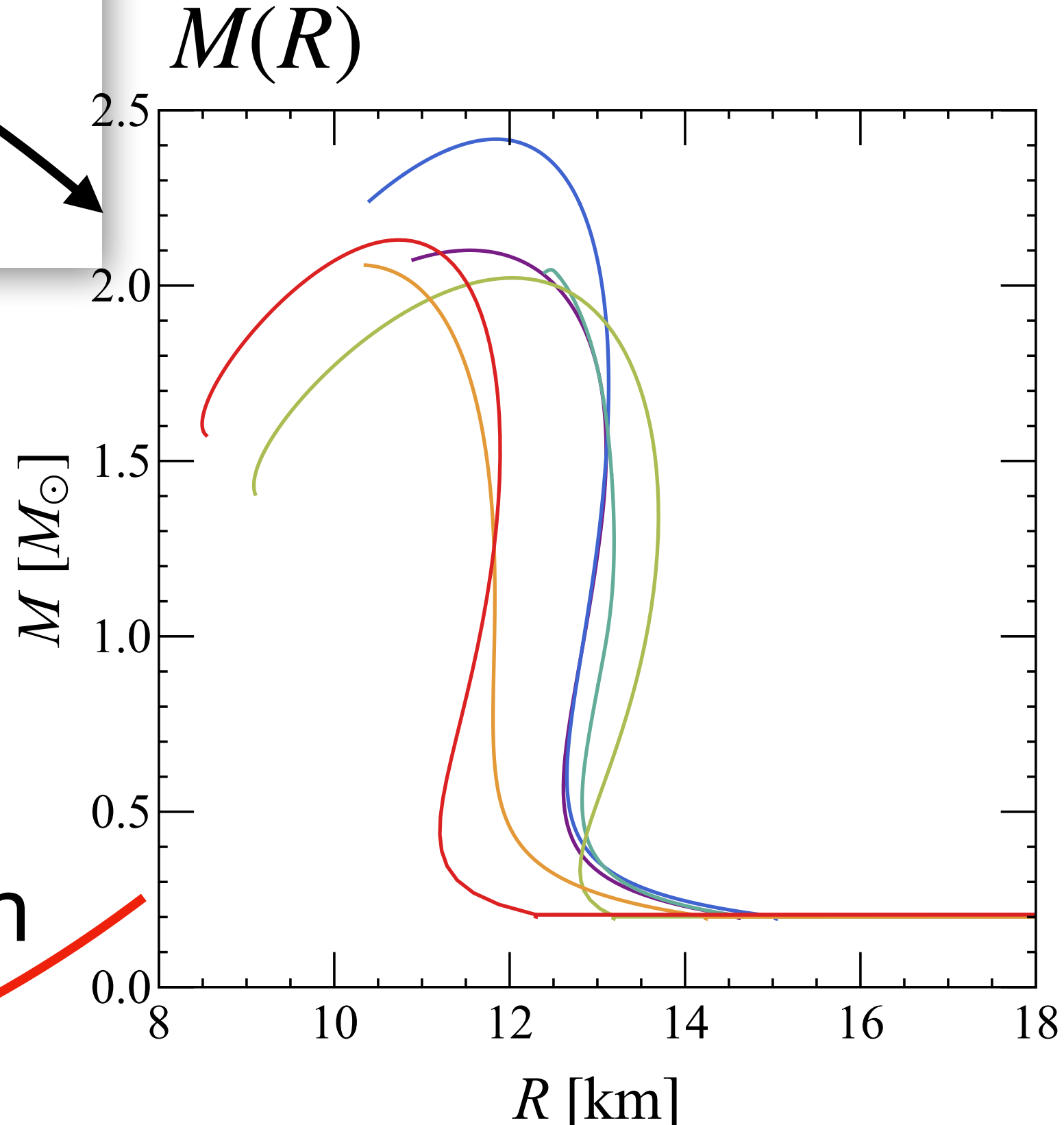
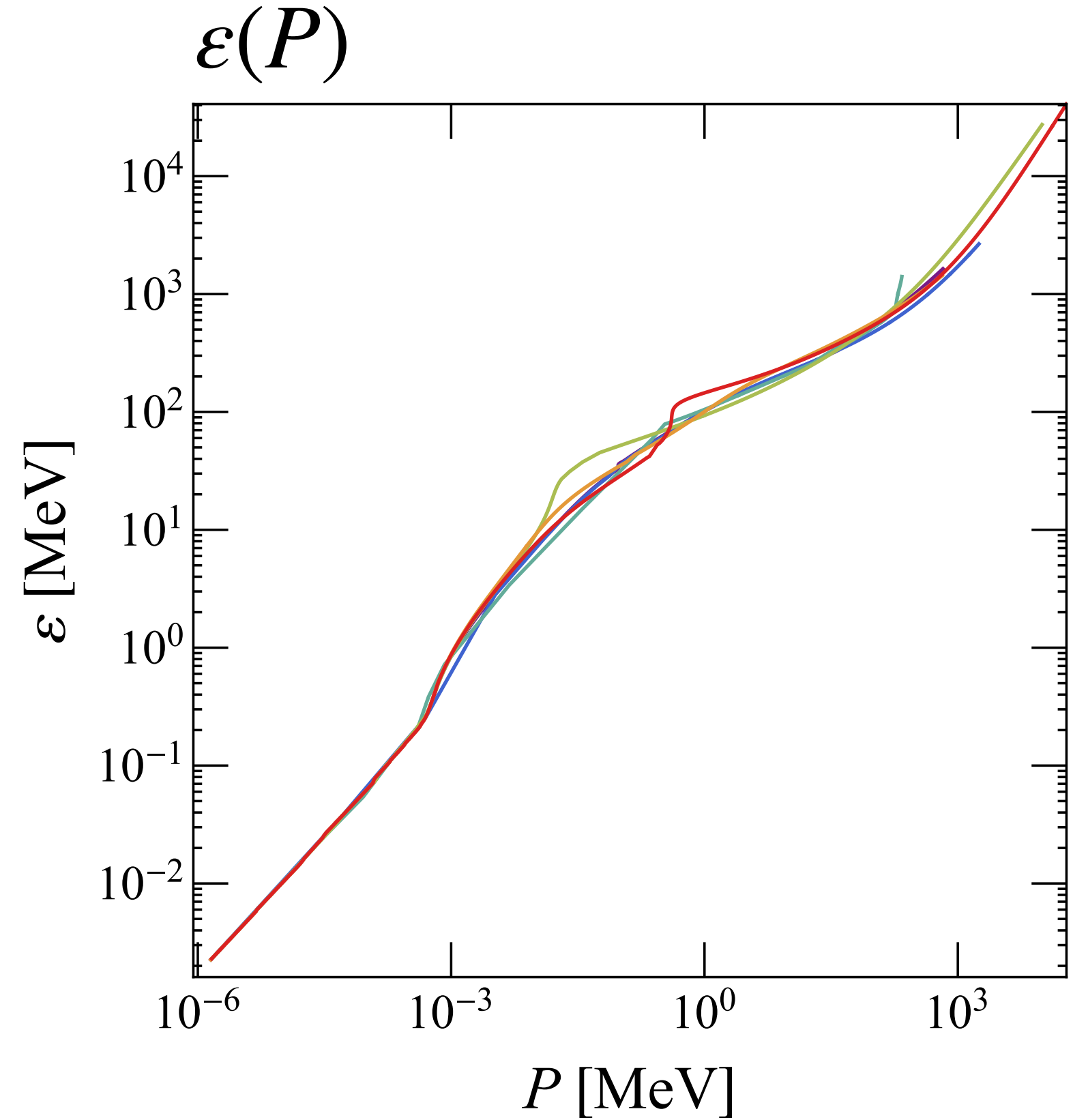
Lindblom's algorithm
if the whole $M(R)$ is known



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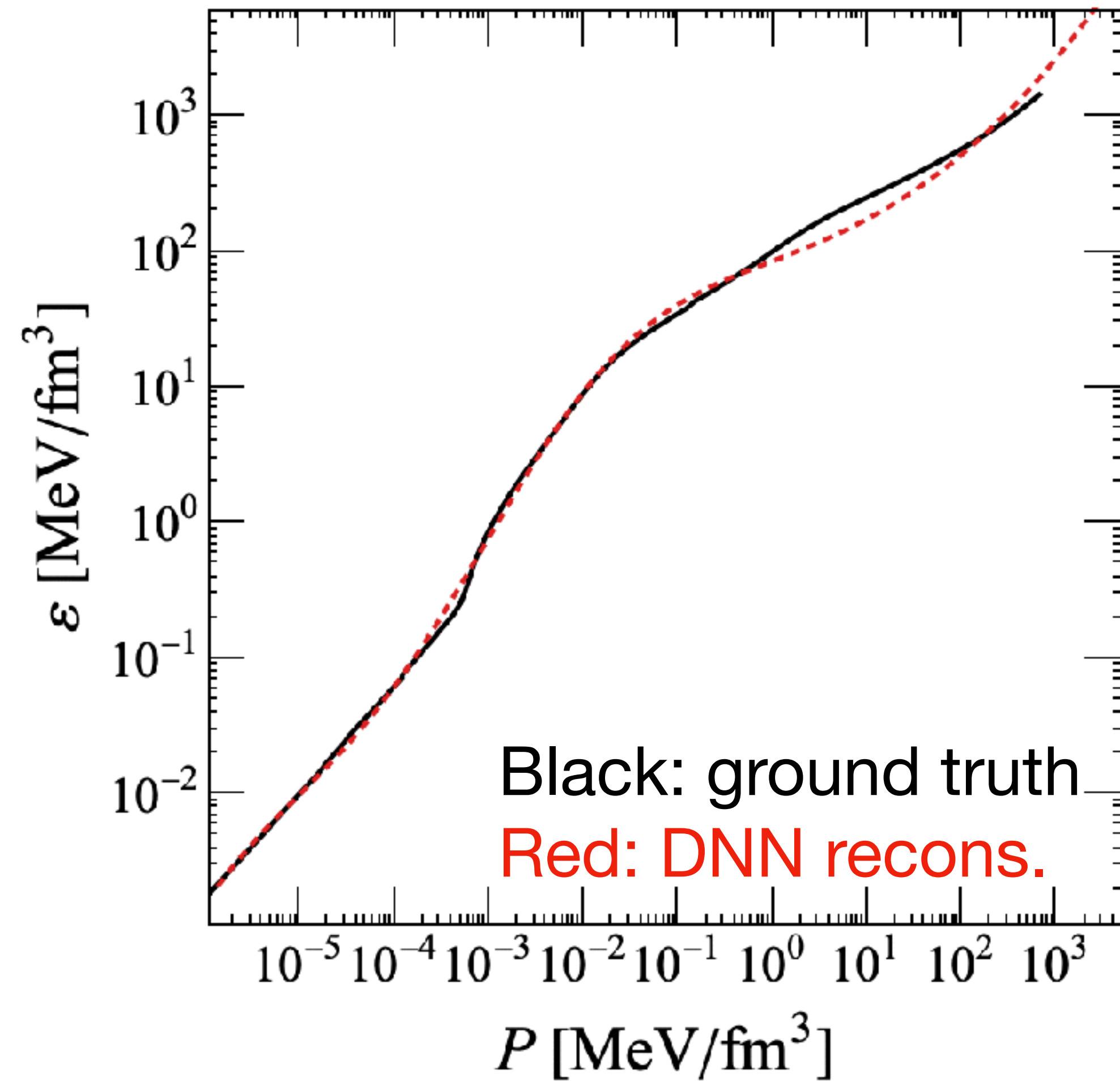
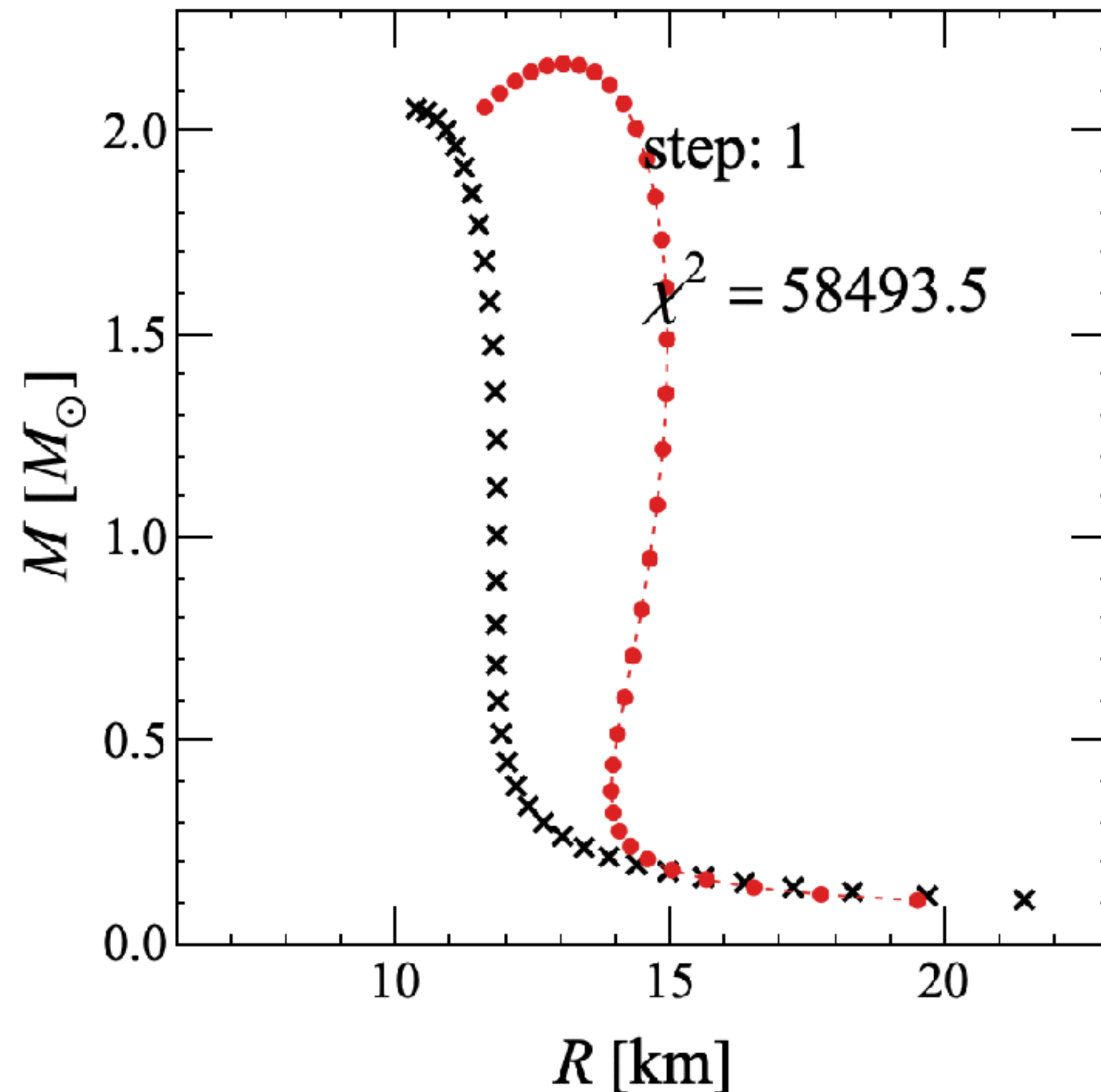
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Discrete $\{M, R\}$ observations?
Lindblom's algorithm if the whole $M(R)$ is known

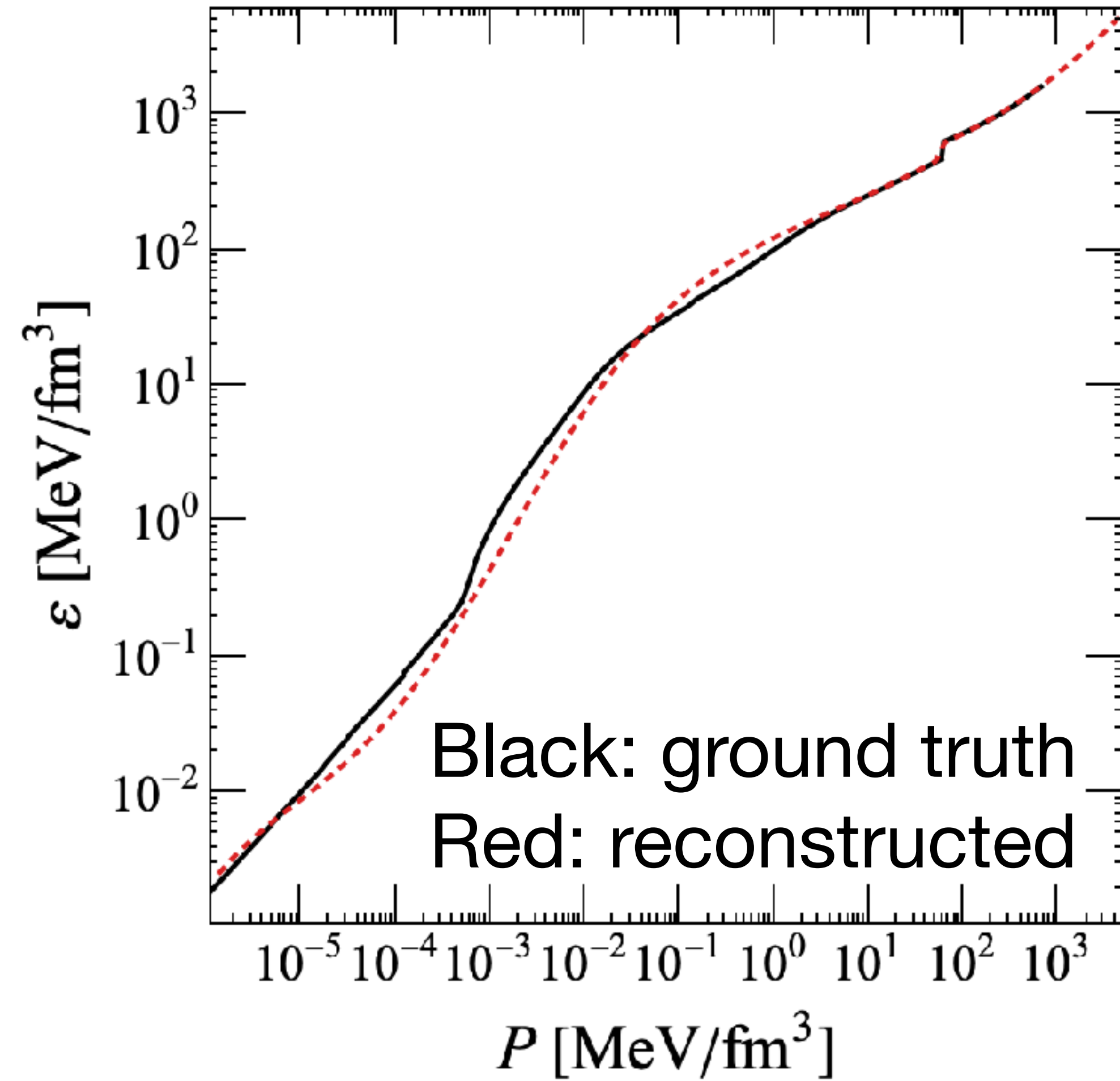
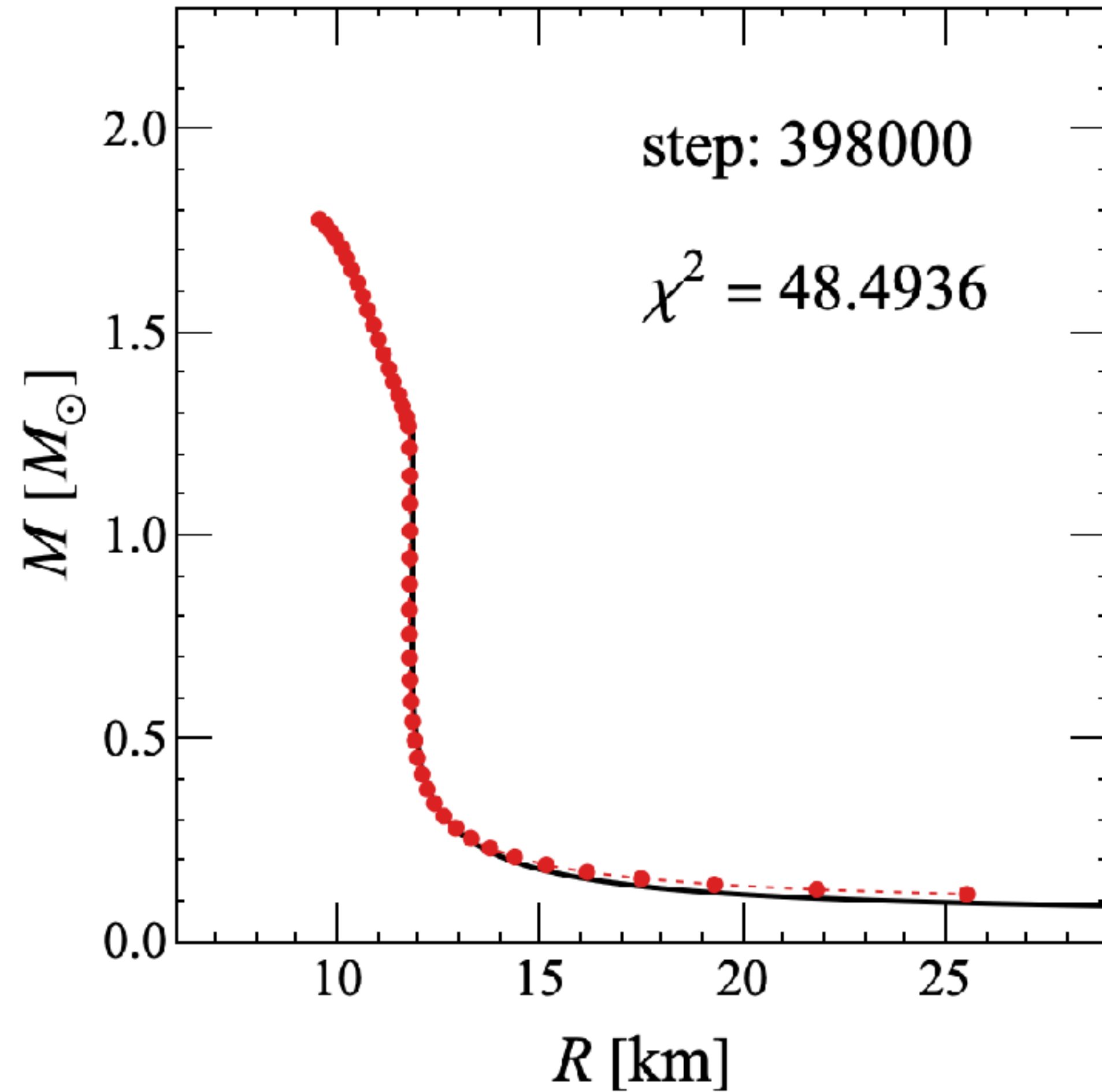


Closure test: can we learn EoS from $\{m_i, R_i\}$?



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

can we learn EoS w/ phase transition?



EoS reconstruction from real observations

