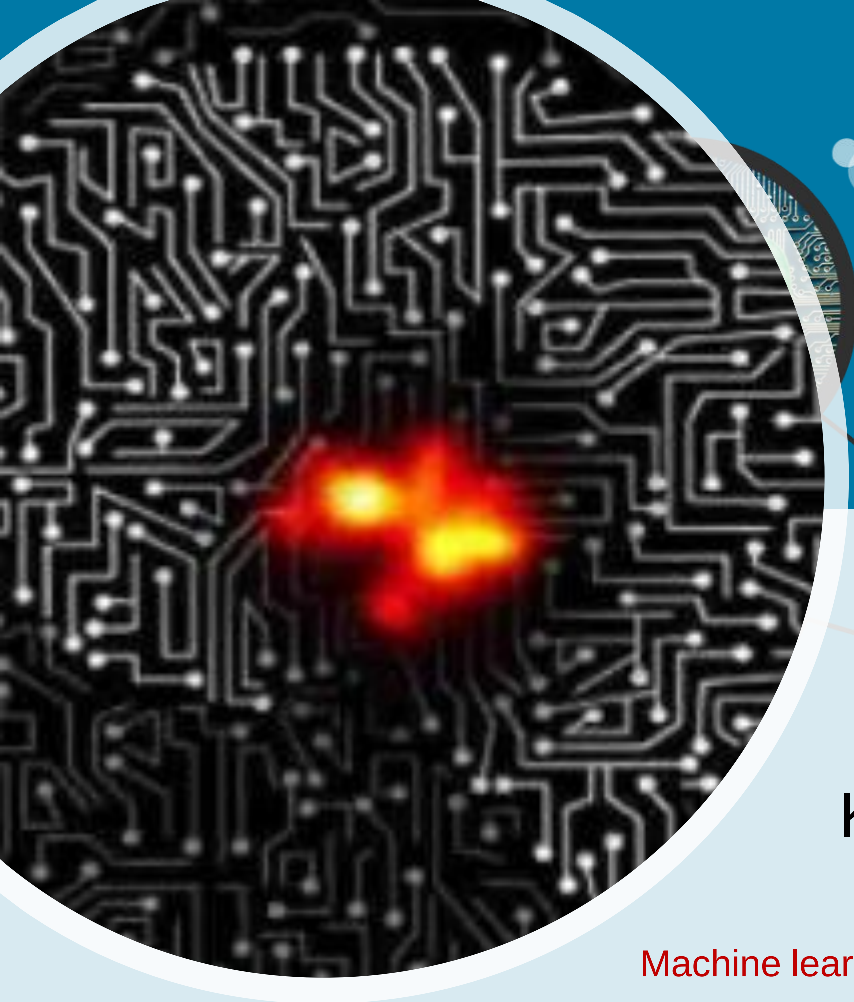


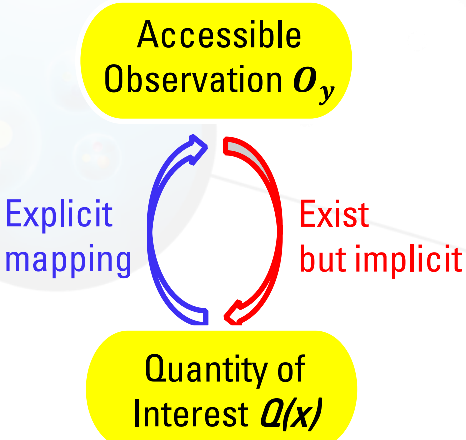
FIAS Frankfurt Institute for Advanced Studies

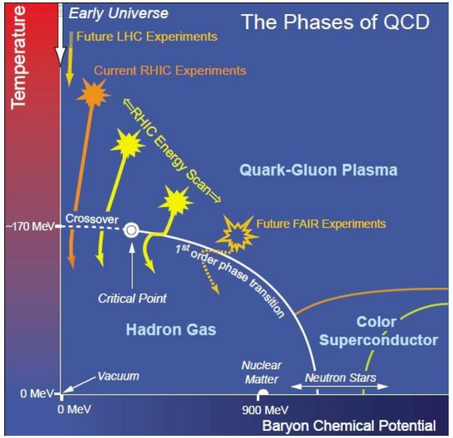
Deep Learning Inverse Problems in Extreme QCD Matter Studies

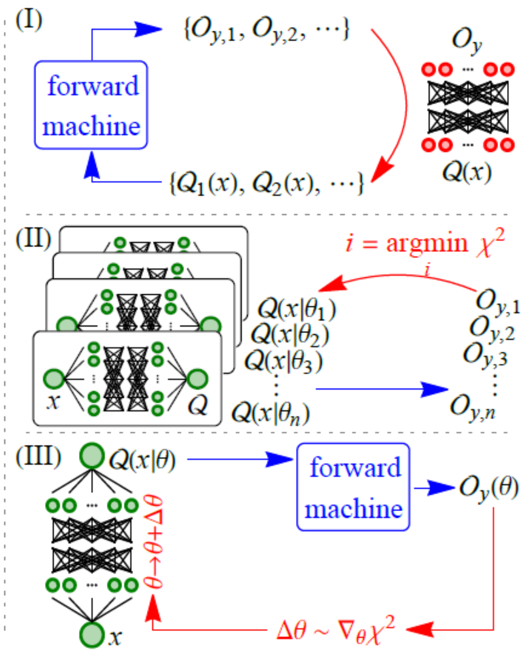
Kai Zhou (FIAS)

Machine learning for lattice field theory and beyond – ECT*

Overview : Inverse Problems Solving with ML







- Direct inverse mapping capturing : with Supervised Learning
- Statistical approach to χ^2 fitting : Bayesian Reconstruction for posterior or Heuristic (Generic) Algorithm to min.

$$\chi^2 = \sum_y \left(\frac{\mathcal{F}_y[Q_{\rm NN}(x|\boldsymbol{\theta})] - \mathcal{O}_y}{\Delta \mathcal{O}_y} \right)^2$$

- Automatic Differentiation : fuse physical prior into reconstruction via differentiable programming strategy

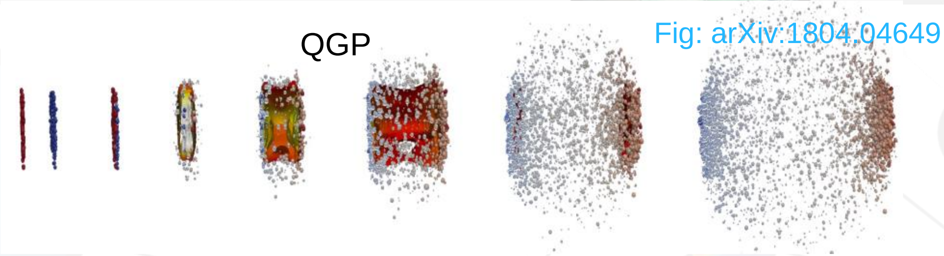
$$\frac{1}{2}\nabla_{\boldsymbol{\theta}} \chi^2 = \sum_y \frac{\mathcal{F}_y[Q_{\rm NN}(x|\boldsymbol{\theta})] - \mathcal{O}_y}{(\Delta \mathcal{O}_y)^2} \int {\rm d}x \frac{\delta \mathcal{F}_y[Q(x)]}{\delta Q(x)} \bigg|_{Q(x) = Q_{\rm NN}(x|\boldsymbol{\theta})} \nabla_{\boldsymbol{\theta}} Q_{\rm NN}(x|\boldsymbol{\theta})$$

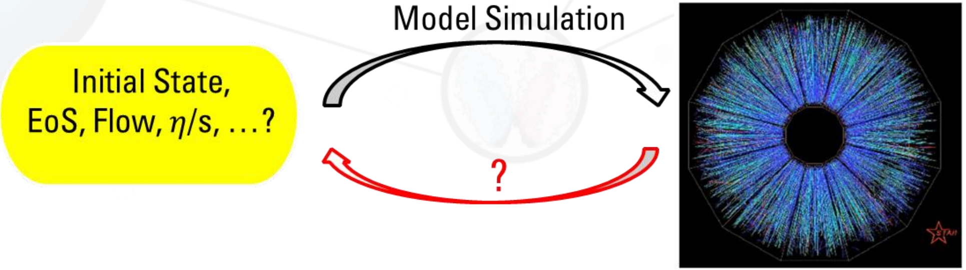
- Hot/Dense matter study from <u>Heavy Ion Collisions</u>
- Physics Inference from <u>LQCD</u> Data
- Dense matter study from <u>Neutron Star</u> observational

1, QCD matter EoS identification from Heavy Ion Collisions with Deep Learning

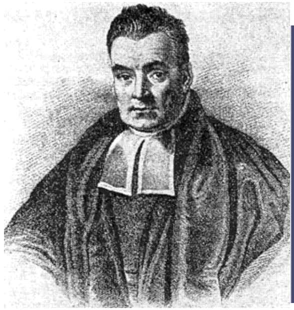
Nature Communications 9 (2018), no.1, 210
JHEP 12 (2019) 122
Eur.Phys.J.C 80 (2020) 6, 516
Phys. Lett. B 811 (2020)
JHEP 21 (2021) 184
Phys. Rev. D 103 (2021) 11, 116023
arXiv:2211.11670

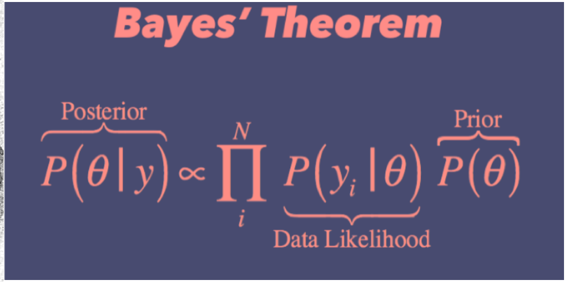
Challenge in HIC and Machine Learning

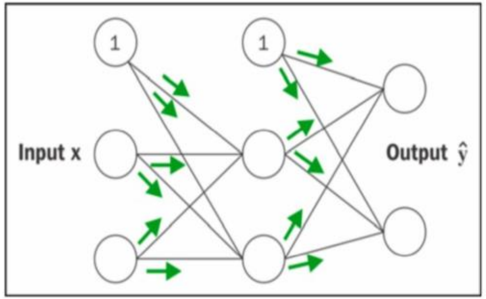




- Uncertainties in HIC modeling
- Multiple parameters entangle with multiple observables
- **How to disentangle different factors to reveal fundamental physics from the dynamical environment?**





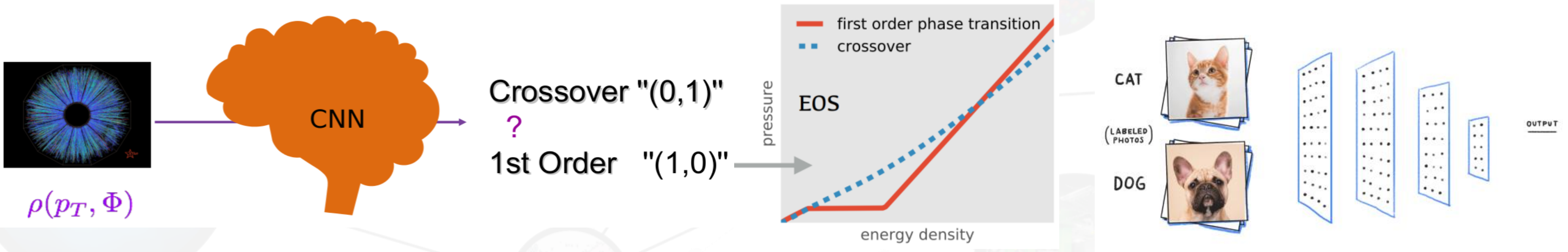


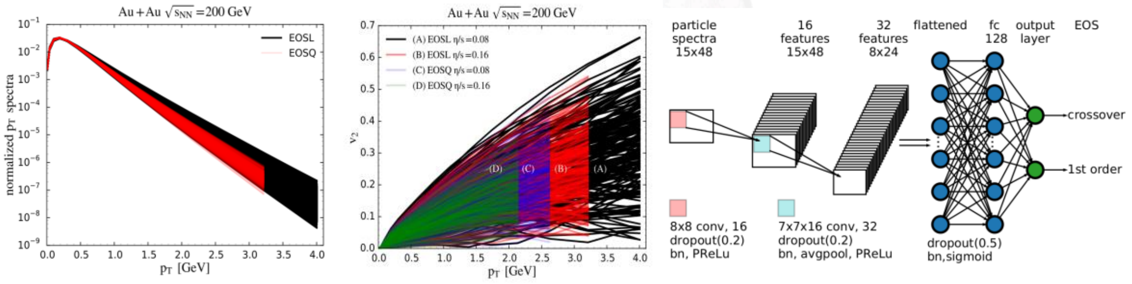
Universal approximator

Differentiable programming

Gradient based optimization

Direct inverse mapping? CNN make the road





- Conventional obs. hard to distinguish
- Strongly influence from initial fluctuations and other uncertainties
- 95% event-by-event accuracy!
- Robust to initial conditions, eta/s

Conclusion : Information of early dynamics can survive to the end of the hydrodynamics and encoded with in the final state raw spectra, immune to evolution's uncertainties, with deep CNN we can decode it back.

L.G.Pang, **K. Zhou**, N.Su et al., **Nature Commu.9 (2018), no.1, 210**

The EoS parameterization, the flow and transverse kinetic energy measurements

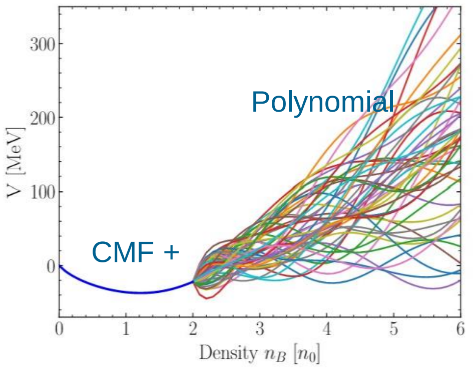
- Hadronic cascade dominant
- **UrQMD model** adapted to any density dependent EoS →

  via density dependent potential

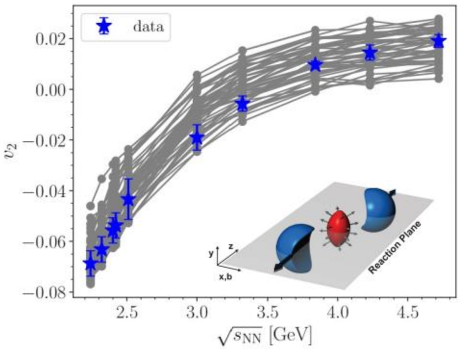
  Eur.Phys.J.C82(2022)5,417

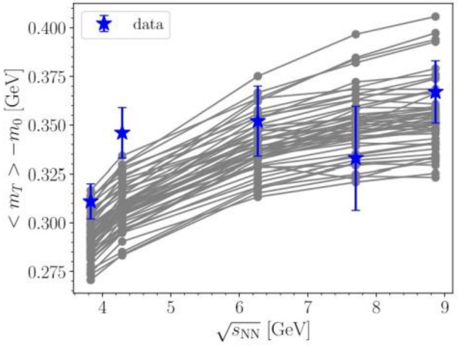
$$\dot{\mathbf{r}}_i = \frac{\partial \mathbf{H}}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i = -\frac{\partial \mathbf{H}}{\partial \mathbf{r}_i}$$

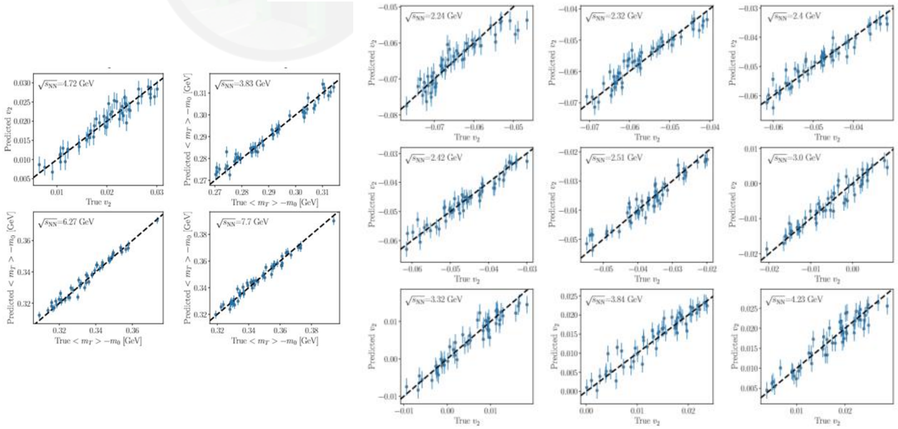
$$\dot{\mathbf{p}}_i = -\frac{\partial \mathbf{H}}{\partial \mathbf{r}_i} = -\frac{\partial \mathbf{V}}{\partial \mathbf{r}_i} = -\left(\frac{\partial V_i}{\partial n_i} \cdot \frac{\partial n_i}{\partial \mathbf{r}_i}\right) - \left(\sum_{j \neq i} \frac{\partial V_j}{\partial n_j} \cdot \frac{\partial n_j}{\partial \mathbf{r}_i}\right)$$



Evidence : proton's v2 and transverse kinetic energy





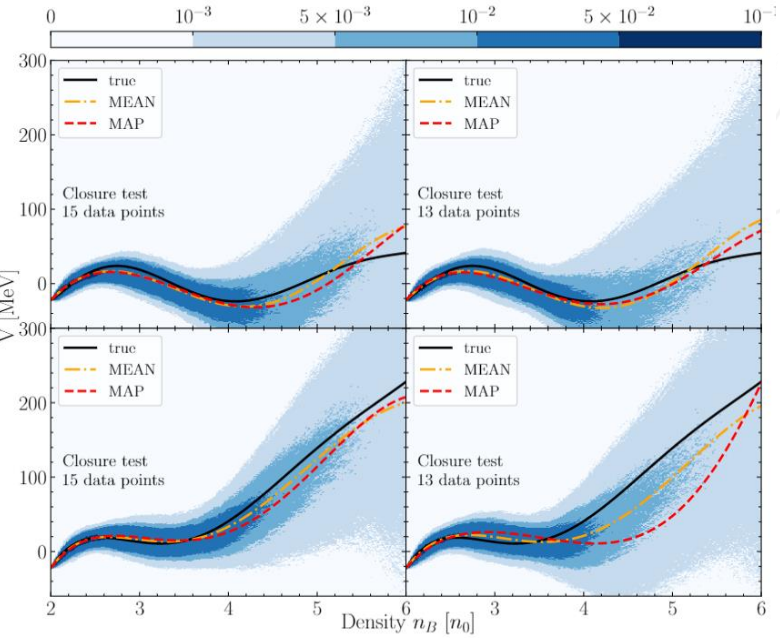


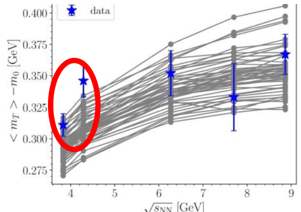
- Gaussian Process **Emulator** : $Obs_i(\boldsymbol{\theta}) \sim GP(\mu(\boldsymbol{\theta}), \kappa(\boldsymbol{\theta}, \boldsymbol{\theta}'))$
- The trained emulator <u>predict observables well: R^2</u> ~ 0.9

M.OK, J. Steinheimer, H. Stoecker, K. Zhou, arXiv:2211.11670

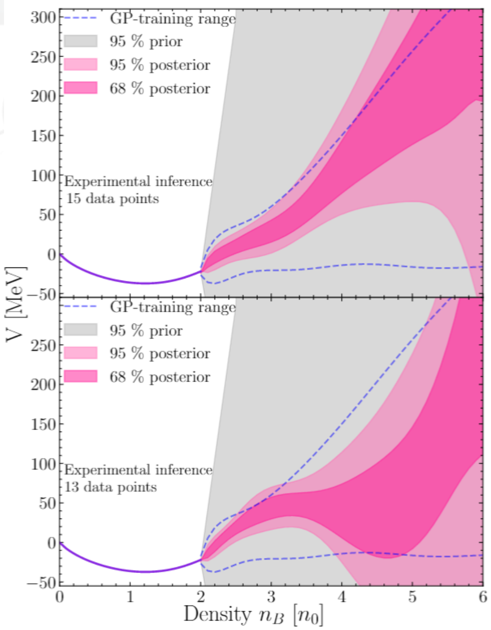
EoS reconstruction Closure tests, with Exp. Data, Predictability

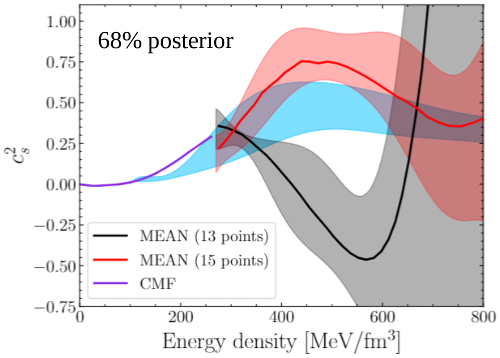
- **Posterior** ~ Likelihood * Prior

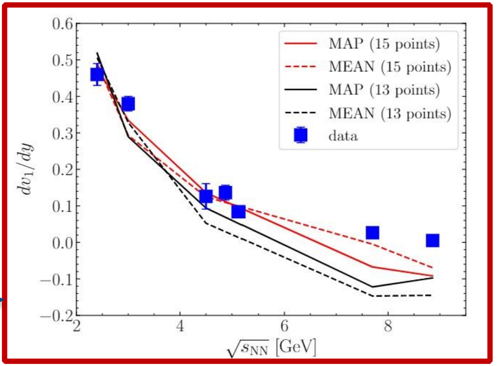




- With real experimental data







Test the extracted EoS on <u>different observables</u> (not used in Bayesian analysis)

arXiv:2211.11670

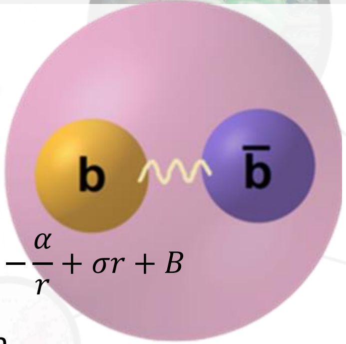
2, From LQCD to physics analysis

Shuzhe Shi, Kai Zhou, Jiaxing Zhao, Swagato Mukherjee, Pengfei Zhuang
Phys. Rev. D 105 (2022) 1, 1

Fu-Peng Li, Hong-Liang Lue, Long-Gang Pang, Guang-You Qin,
arXiv:2211.07994

Introduction, Potential Model, Inverse Shroedinger Eq.

Large mass scale : $m_Q >> \Lambda_{QCD}, T, p$

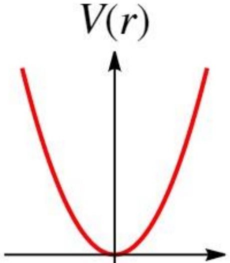


- Hard Process production in early stage
- 'Calibrated' QCD Force – HQ interaction

Vacuum: NRQCD, Cornell-like $V(r) = -\frac{\alpha}{r} + \sigma r + B$

Medium: Color Screening, Thermal width

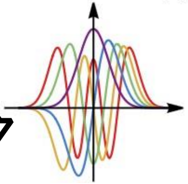
Laine, et.al, JHEP(2

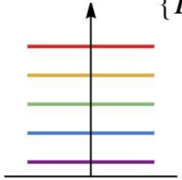


$$V(T,r) = V_R(T,r) + i \cdot V_I(T,r)$$

Inverse Power method

H.W.Crater, JCP(1994)





$$\begin{cases} \mathrm{Re}[E_n] = m - 2m_b \\ \mathrm{Im}[E_n] = -\Gamma \end{cases}$$

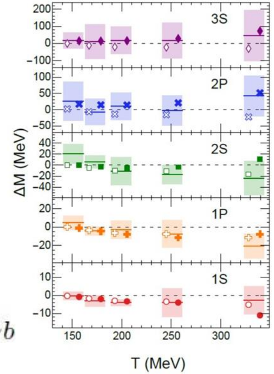
?

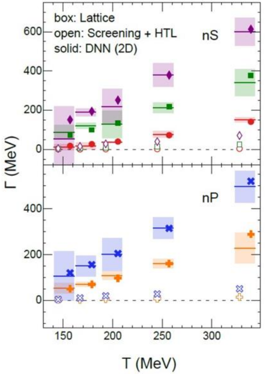
Large mass scale :

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

M. Strickland, et.at., PRC(2015) PRD(2018), PLB(2020)

New lQCD results cannot be explained by Perturbative HTL-inspired potentials !

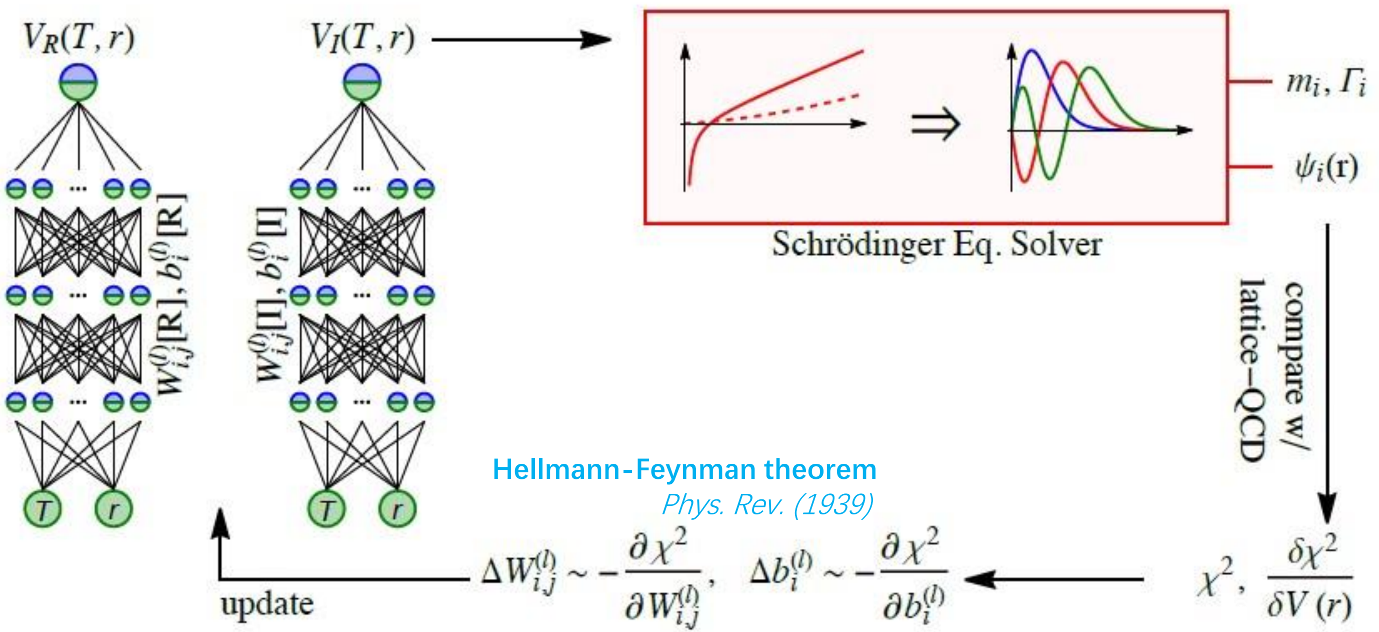




R. Larsen, et.al, PRD(2019), PLB(2020), PRD(2020)

How to extract effective potential given limited spectroscopy ?

Flow chart for "DNN + Schrödinger Eq."



Hellmann-Feynman theorem
Phys. Rev. (1939)

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

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

$$\chi^2 = \sum_{T,i} \frac{(m_{T,i} - m_{T,i}^{\mathrm{lattice}})^2}{(\delta m_{T,i}^{\mathrm{lattice}})^2} + \frac{(\Gamma_{T,i} - \Gamma_{T,i}^{\mathrm{lattice}})^2}{(\delta \Gamma_{T,i}^{\mathrm{lattice}})^2}$$

$$J(\boldsymbol{\theta}) = \frac{1}{2}\chi^2(\boldsymbol{\theta}) + \frac{\lambda}{2}\boldsymbol{\theta}\cdot\boldsymbol{\theta},$$

$$T \in \{0, 151, 173, 199, 251, 334\} \ \mathrm{MeV}$$
$$i \in \{1\mathrm{S}, 2\mathrm{S}, 3\mathrm{S}, 1\mathrm{P}, 2\mathrm{P}\}$$

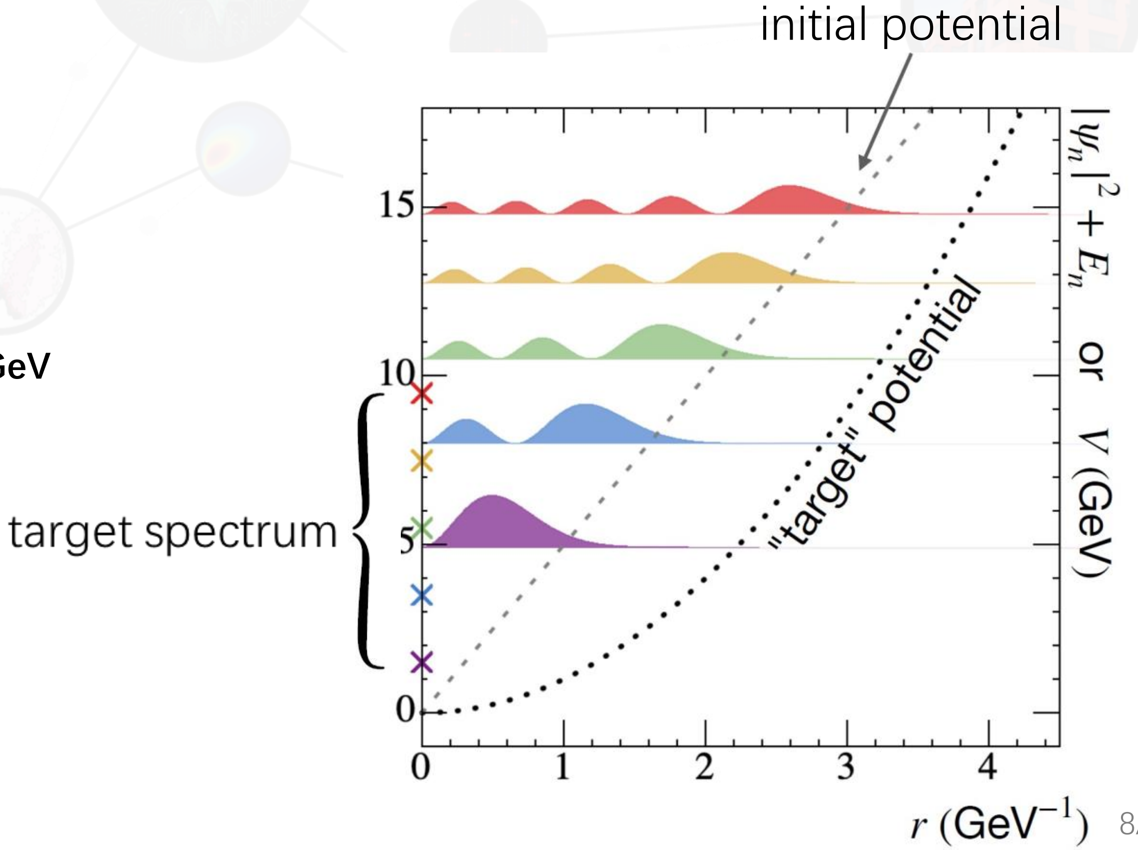
Phys. Rev. D 105 (2022) 1, 1

Proof of Concept

limited spectrum { En } to continuous interaction V(r) ?

Learn V(r) from 5 eigenvalues :

{ En } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV



Proof of Concept

limited spectrum { En } to continuous interaction V(r) ?

Learn V(r) from 5 eigenvalues :

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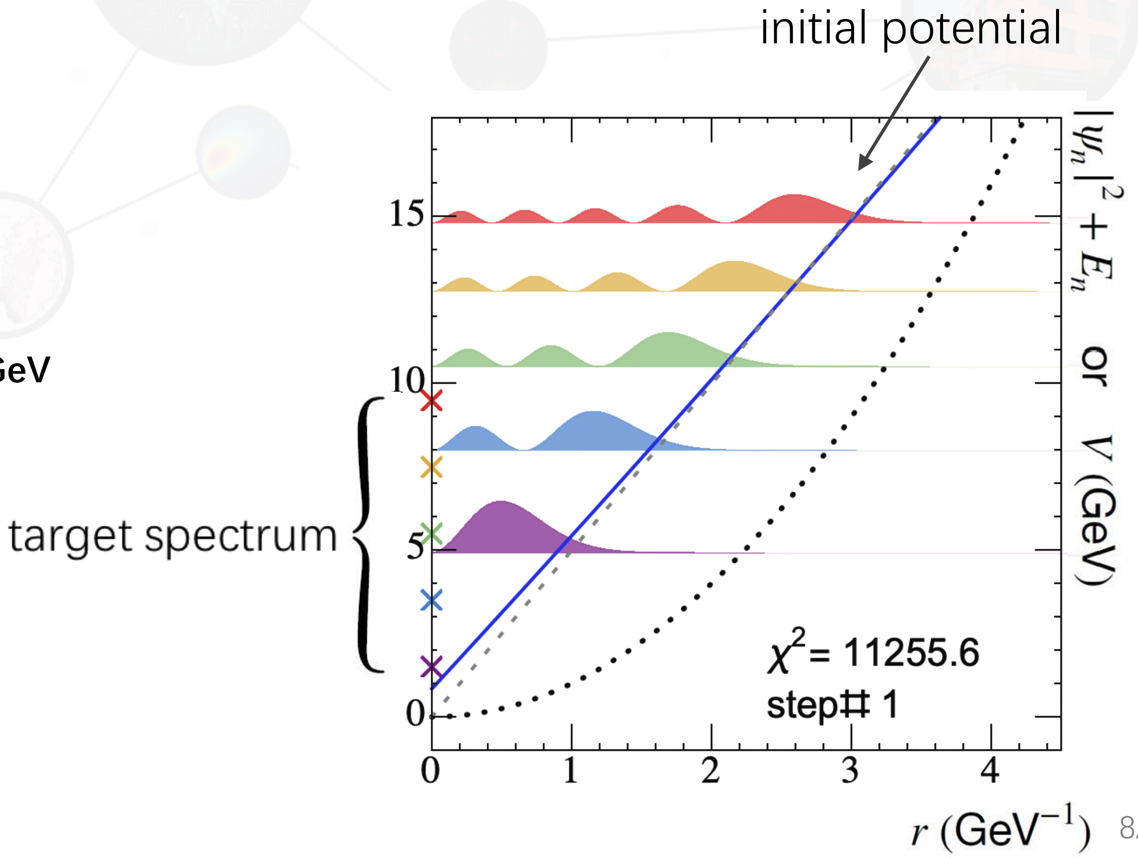


Proof of Concept

limited spectrum { En } to continuous interaction V(r) ?

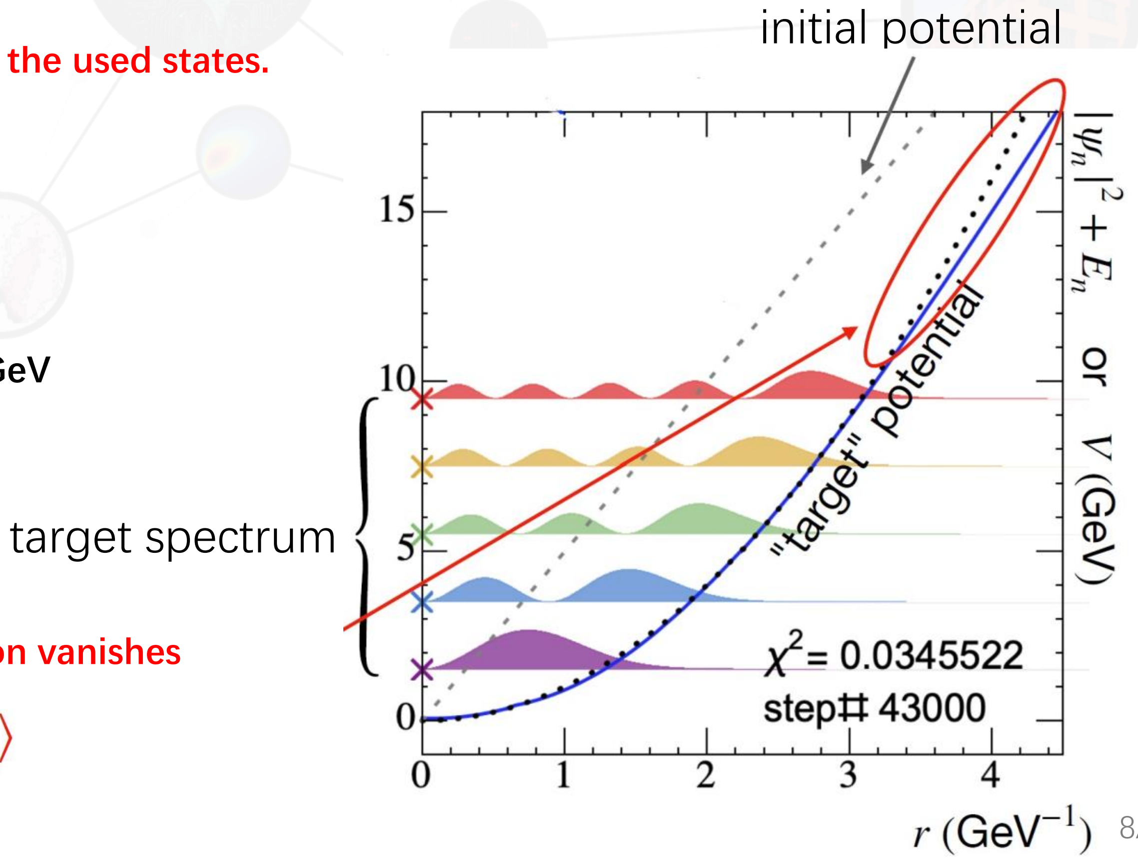
-- Yes! But to some range decided by the used states.

Learn V(r) from 5 eigenvalues :

{ En } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV

Deviation @ given states' wavefunction vanishes

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



Closure Test – suppose HTL is true

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

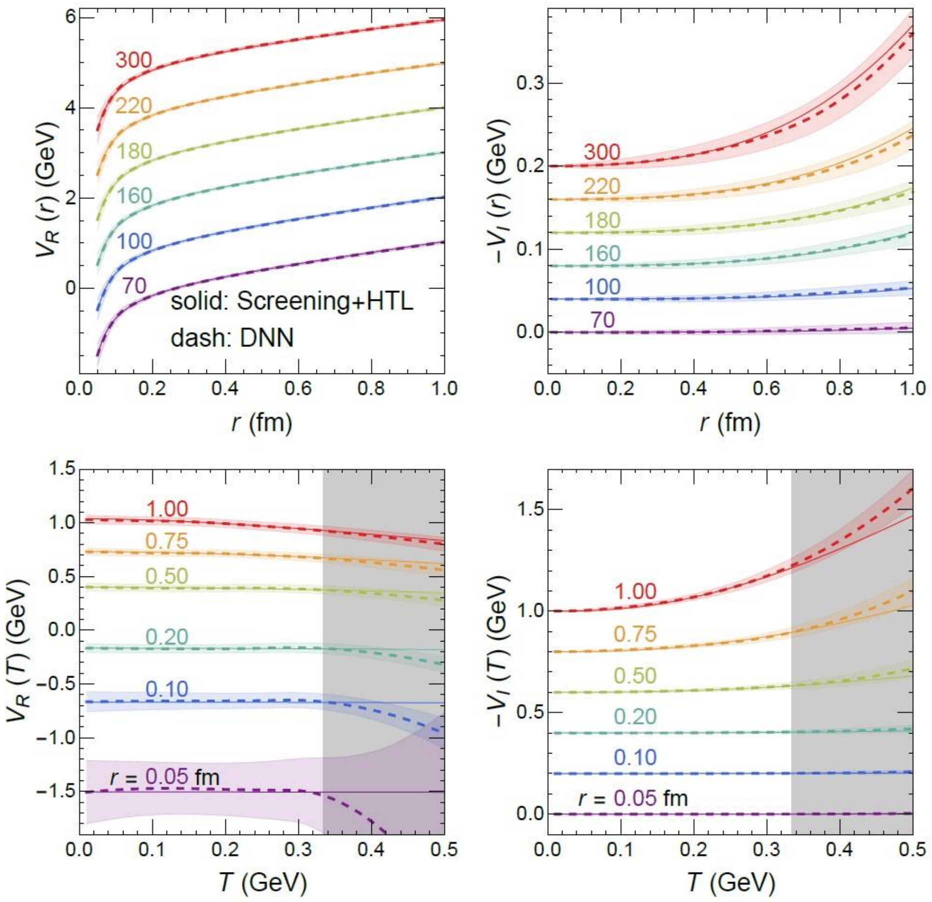
$$V_I(T,r) = -\frac{\sqrt{\pi}}{4}\mu_D T \sigma r^3 G^{2,2}_{2,4}\left(\begin{matrix}-\frac{1}{2},-\frac{1}{2} \\ \frac{1}{2},\frac{1}{2},-\frac{3}{2},-1\end{matrix}\middle|\frac{\mu_D^2 r^2}{4}\right) - \alpha T\,\phi(\mu_D r)\,,$$

$m_b = 4.676$ GeV, $\alpha = 0.39$,
$\sigma = 0.223\ \mathrm{GeV}^2$, $B = 0$ GeV,
assume that $\mu_D(T) = T/2$.

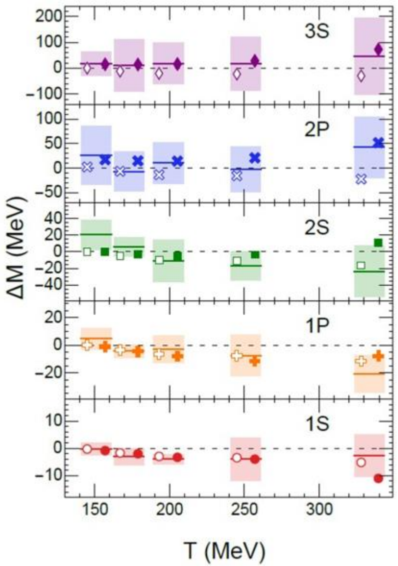
Provide mass and width of

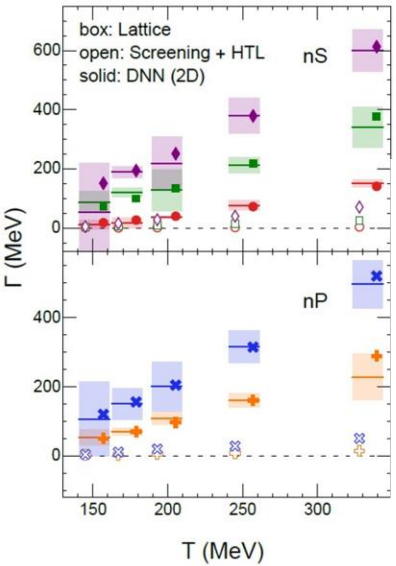
1S, 2S, 3S, 1P, and 2P states.

@$(0, 151, 173, 199, 251, 334)$ MeV



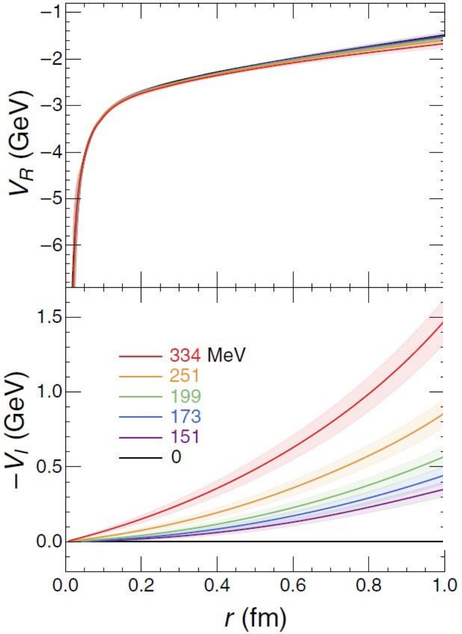
Best Fit of lQCD mass and width from HTL (open symbols) and DNNs (solid symbols)

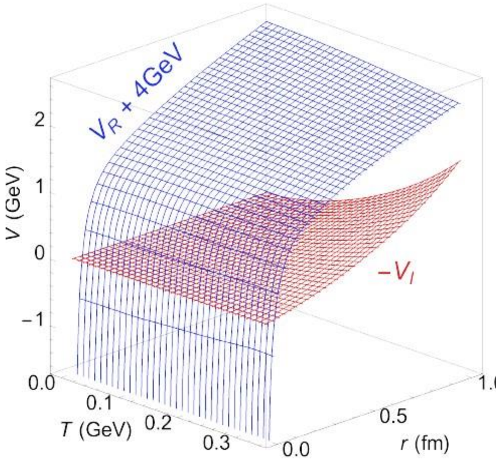




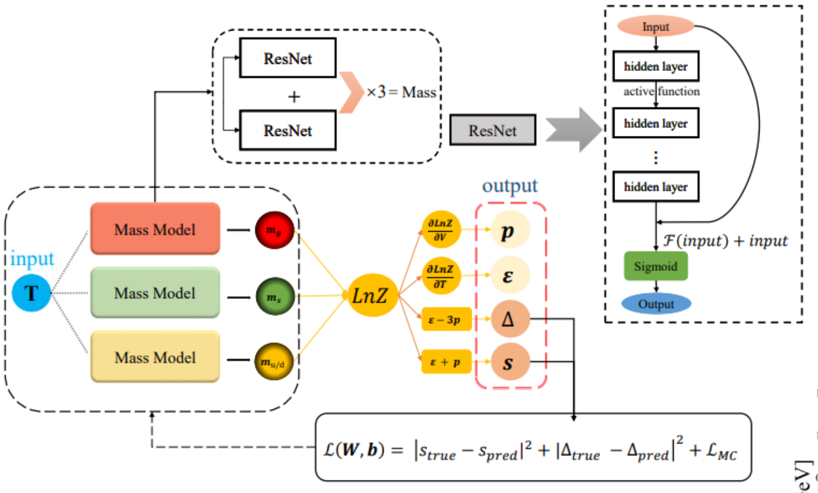
Chi2-per-data=16.5/30

The reconstructed T, r dependent potential





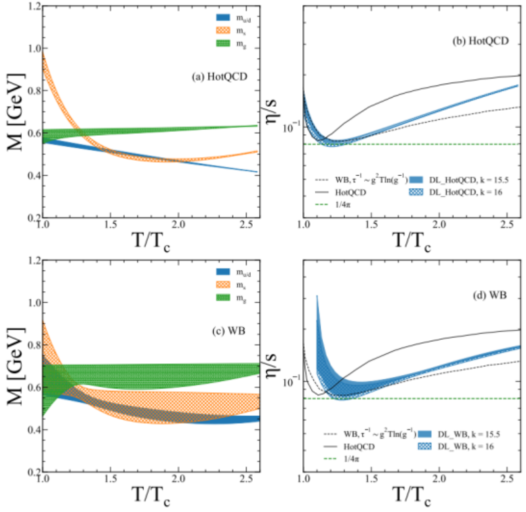
Quasi-particle analysis of lQCD thermodynamics

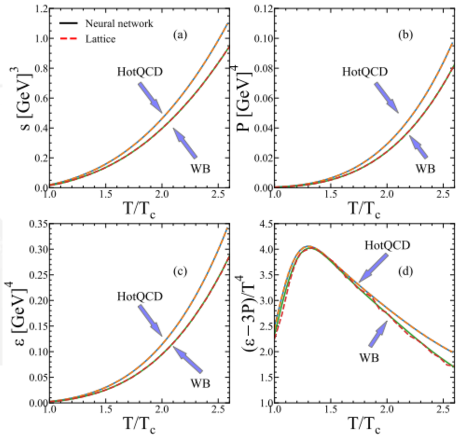


$$\ln Z_g(T) = -\frac{16V}{2\pi^2}\int_0^\infty p^2 dp \ln\left[1-\exp\left(-\frac{1}{T}\sqrt{p^2+m_g^2(T)}\right)\right], \quad (2)$$

$$\ln Z_{q_i}(T) = +\frac{12V}{2\pi^2}\int_0^\infty p^2 dp \ln\left[1+\exp\left(-\frac{1}{T}\sqrt{p^2+m_{q_i}^2(T)}\right)\right], \quad (3)$$

F.Li, H. Lue, L. Pang and G. Qin, arXiv:2211.07994



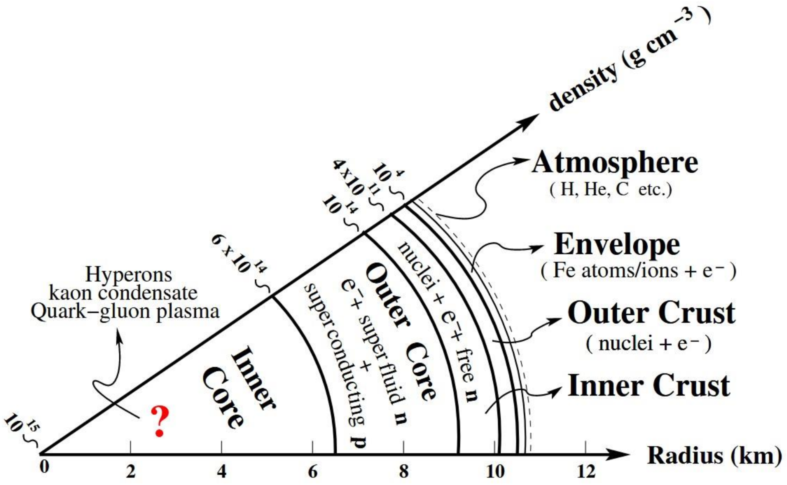


3, Dense matter EoS reconstruction for Neutron Star from M-R observation

JCAP08(2022)071   (arXiv:2201.01756)
arXiv:2209.0xxxx (soon)

From EoS to Stellar Structure (MR)

- Mass ~ 2 solar masses
- Radii ~ 10 km
- Densities ~ 8 ρ_0



- Gravity ← → Pressure

$$\frac{dP}{dr} = -\frac{G}{r^2}\left(\rho + \frac{P}{c^2}\right)\left(m + 4\pi r^3\frac{P}{c^2}\right)\left(1 - \frac{2Gm}{c^2 r}\right)^{-1}$$

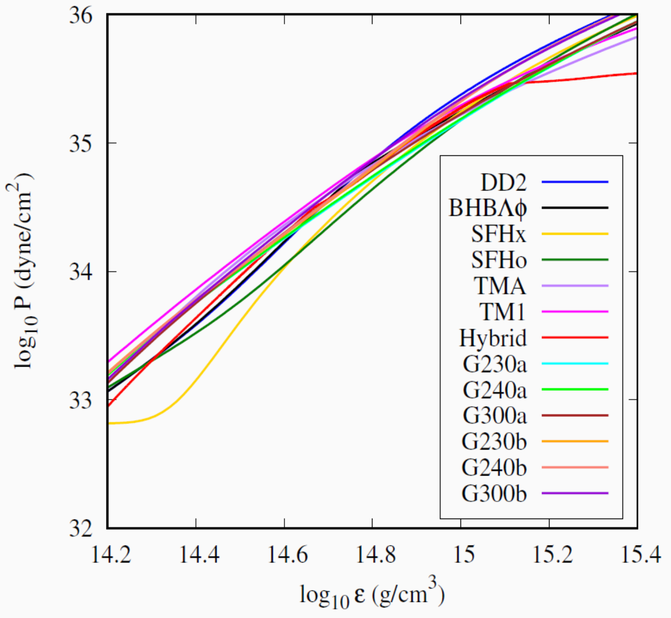
$$M = m(R) = \int_0^R 4\pi r^2 \rho \, dr$$

- Dense matter Equation of State

$$P(\rho)$$

1-to-1 mapping from EoS to M(R)

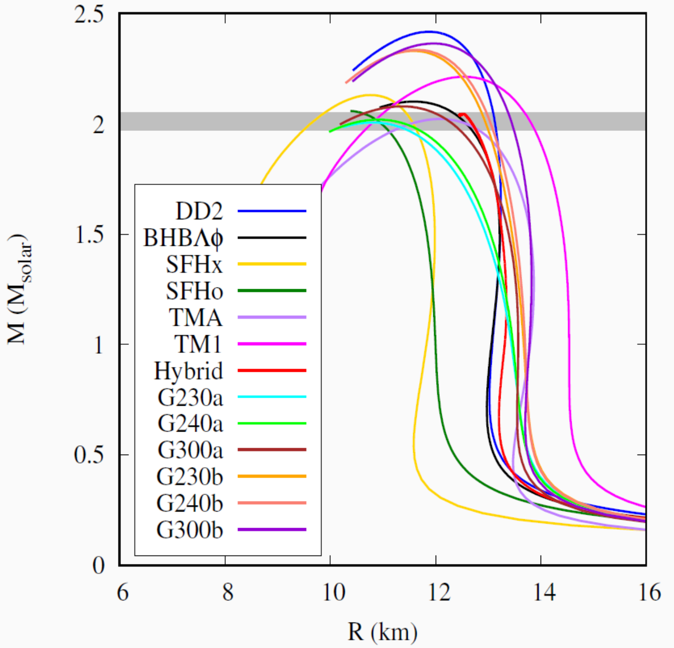
Micro to Macro



TOV solver

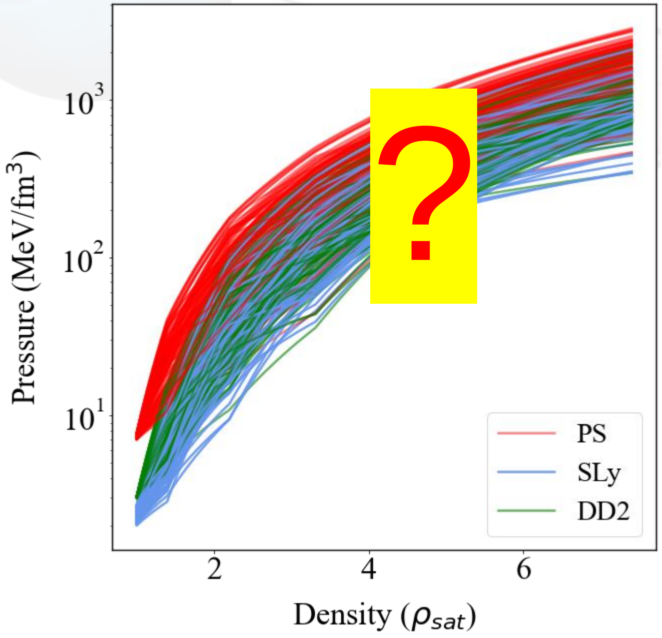
$$-\frac{dP}{dr} = \frac{[\epsilon(r) + P(r)]\,[M(r) + 4\pi r^3 P(r)]}{r[r - 2M(r)]}$$

$$\frac{dM(r)}{dr} = 4\pi r^2 \epsilon(r),$$



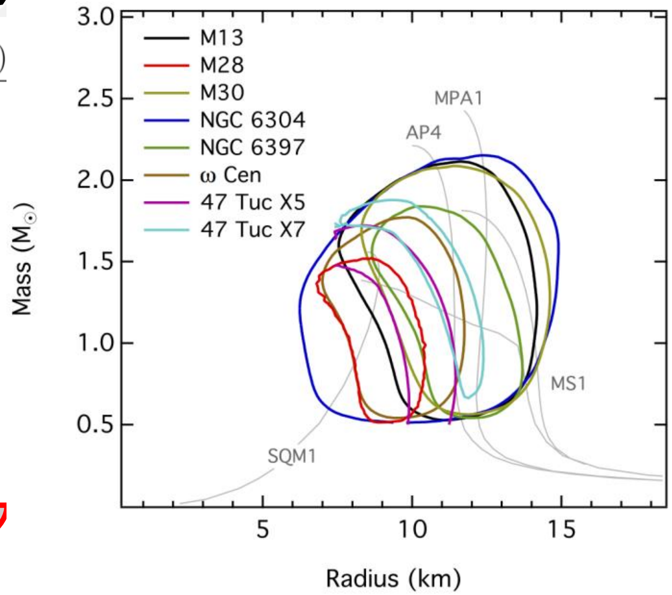
Noisy NS Observables to Equation of State ?

TOV solver



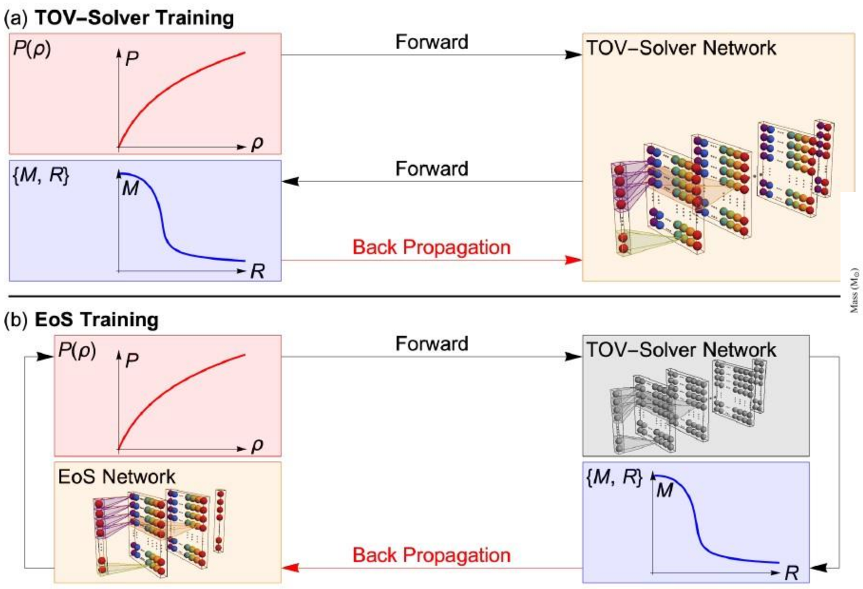
$$-\frac{dP}{dr} = \frac{[\epsilon(r) + P(r)]\,[M(r) + 4\pi r^3 P(r)]}{r[r - 2M(r)]}$$

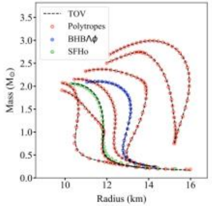
$$\frac{dM(r)}{dr} = 4\pi r^2 \epsilon(r),$$



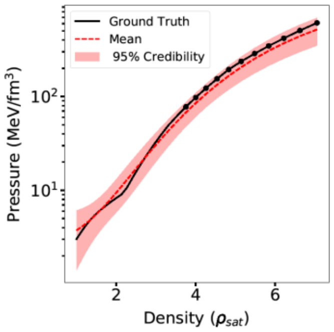
Infer matter's EoS inside NS from M(R)

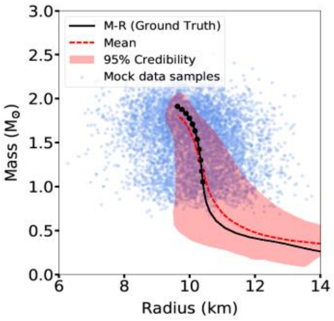
Generalized Bayesian Inference with DNN+AD:



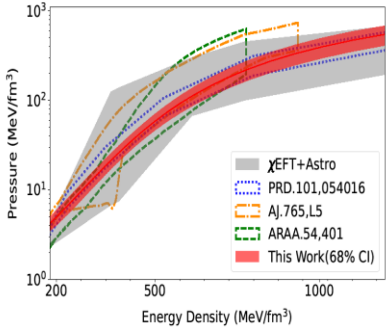


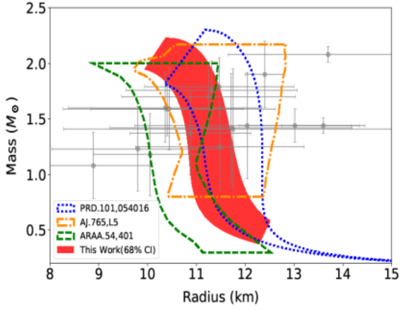
- Well validated through **Mock Tests**





- With **real observable** we reconstruct the NS EoS also

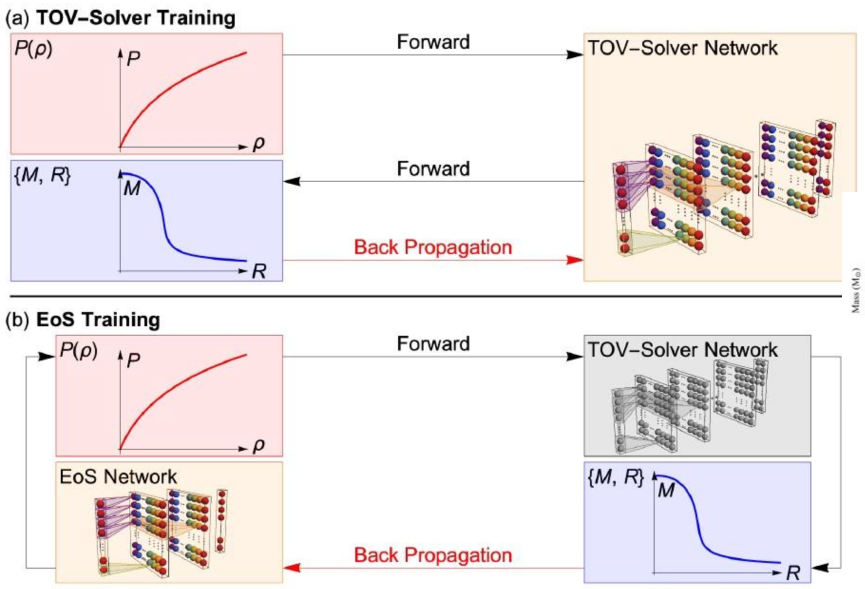


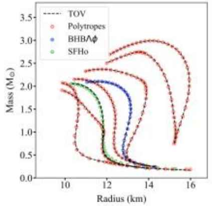


*S.Soma, **K. Zhou***, et.al., JCAP98(2022)071, Phys.Rev.D107(2023)083028*

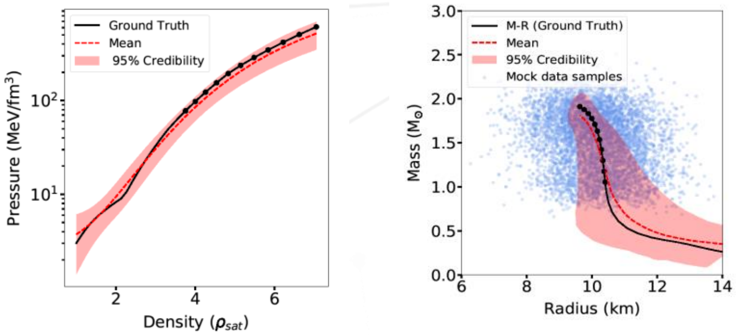
Infer matter's EoS inside NS from M(R)

Generalized Bayesian Inference with DNN+AD:

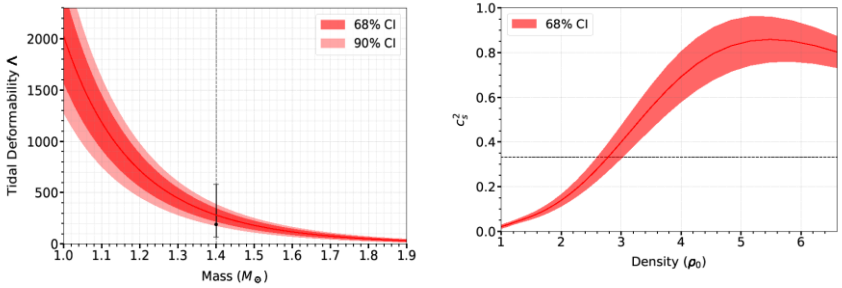




- Well validated through Mock Tests

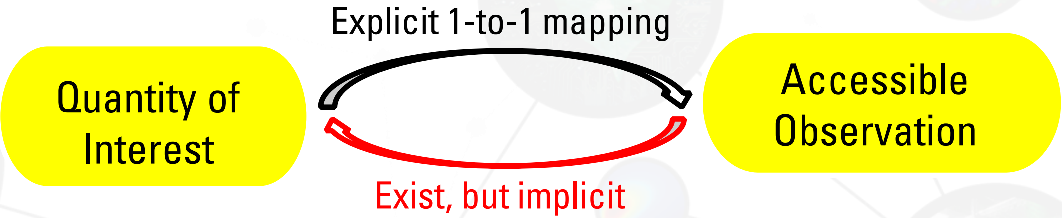


- With real observable we reconstruct the NS EoS also



*S.Soma, **K. Zhou***, et.al., JCAP98(2022)071, Phys.Rev.D107(2023)083028*

Summary : Inverse Problems



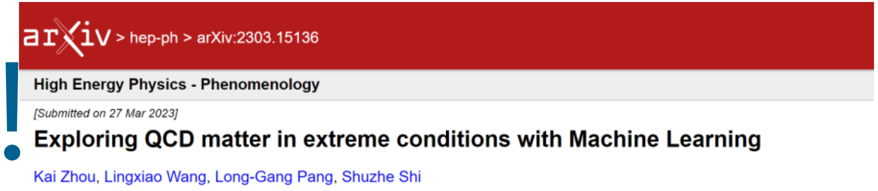
- Physics Priors are needed, coult be put into :

1, **training data** **(Implicit) :** **DL (network)** learn the inverse mapping directly :
general mapping, avoid case-specific retraining

2, **inference process** **(Explicit) :** Chi2 fit+**Bayesian** inference+Gradient Descent :
Automatic differentiation and Network representation

If interested, for more discussion for QCD matter exploration with ML see Review: arXiv:2303.15136

Thanks !


arXiv > hep-ph > arXiv:2303.15136

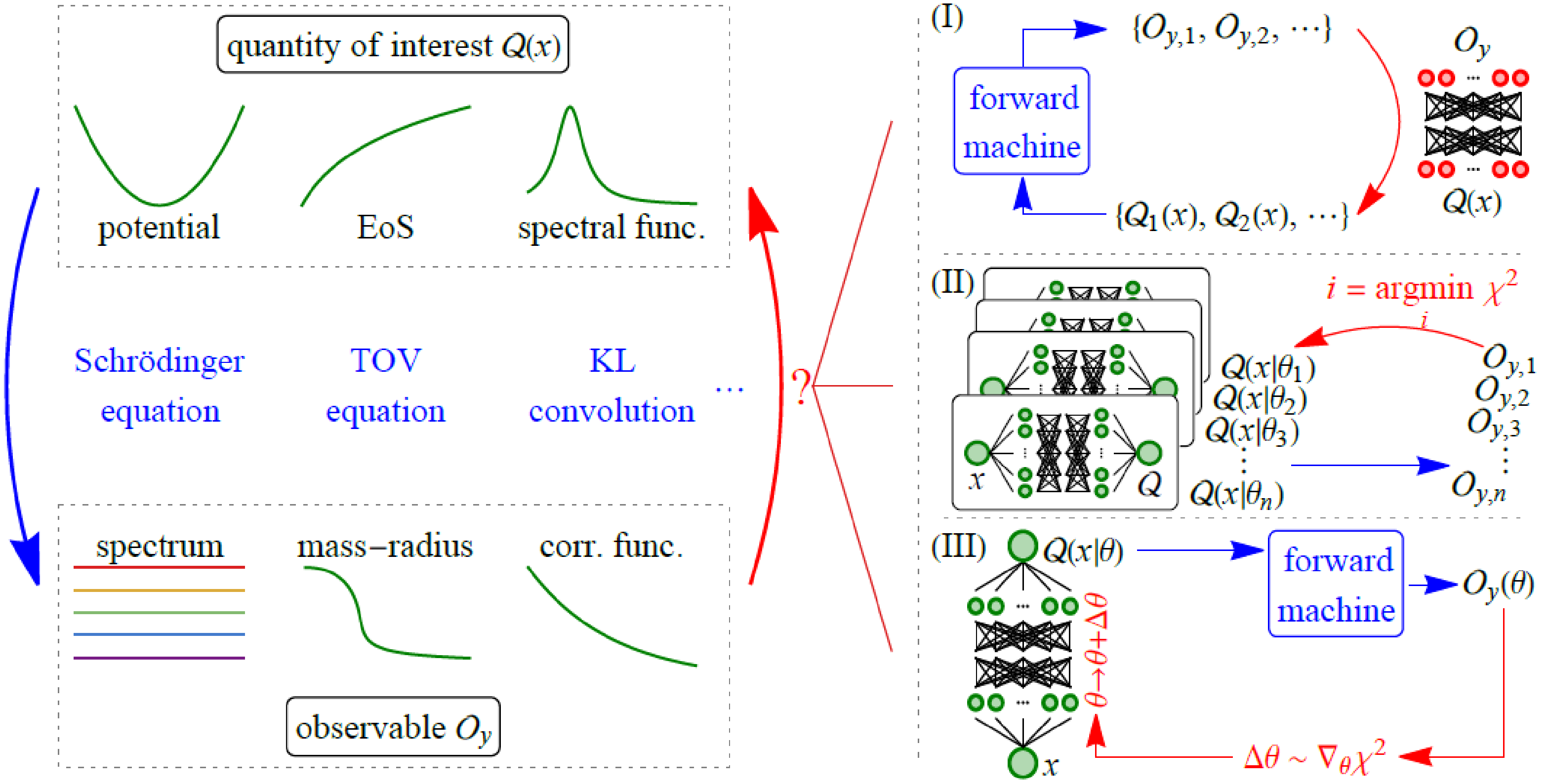
High Energy Physics - Phenomenology

[Submitted on 27 Mar 2023]

Exploring QCD matter in extreme conditions with Machine Learning

Kai Zhou, Lingxiao Wang, Long-Gang Pang, Shuzhe Shi

Overview : Inverse Problems Solving



Backup

Perturbation on Schroedinger Eq.

$$\left(\frac{\hat{p}^2}{2m} + V(r)\right)|\psi_i\rangle = E_i|\psi_i\rangle,$$
$$\left(\frac{\hat{p}^2}{2m} + V(r) + \delta V(r)\right)|\psi_i'\rangle = (E_i + \delta E_i)|\psi_i'\rangle.$$

$$\Rightarrow \quad \delta m_i = \langle\psi_i|\delta V_R(r)|\psi_i\rangle,$$
$$\delta\Gamma_i = -\langle\psi_i|\delta V_I(r)|\psi_i\rangle.$$

$$|\psi_i'\rangle = |\psi_i\rangle + \sum_{j\neq i}\frac{\langle\psi_j|\delta V(r)|\psi_i\rangle}{E_i - E_j}|\psi_j\rangle.$$

Hellmann-Feynman theorem

Phys. Rev. (1939)

$$\delta V(r) = v\,\delta(r - r_k), \quad \Rightarrow$$

$$\frac{\delta m_i}{\delta V_R(r)} = -\frac{\delta\Gamma_i}{\delta V_I(r)} = |\psi_i(r)|^2,$$
$$\frac{\delta m_i}{\delta V_I(r)} = \frac{\delta\Gamma_i}{\delta V_R(r)} = 0.$$

$$\text{Posterior}(\boldsymbol{\theta}|\text{data}) \propto L(\boldsymbol{\theta}|\text{data}) \cdot \text{Prior}(\boldsymbol{\theta}).$$

$$L(\boldsymbol{\theta}|\text{data}) = P(\text{data}|\boldsymbol{\theta}) \propto \exp[-\chi^2(\boldsymbol{\theta})/2].$$

$$\text{Prior}(\boldsymbol{\theta}) \propto \exp[-\frac{\lambda}{2}\boldsymbol{\theta}\cdot\boldsymbol{\theta}].$$

$$\text{Posterior}(\boldsymbol{\theta}|\text{data}) = N_0 \exp\left[-\frac{\chi^2(\boldsymbol{\theta})}{2} - \frac{\lambda}{2}\boldsymbol{\theta}\cdot\boldsymbol{\theta}\right]$$

Sample potentials ~ $P(V_{\boldsymbol{\theta}}(T,r)) = \text{Posterior}(\boldsymbol{\theta}|\text{data})\,.$

Reference Sampler ~ $\widetilde{P}(\boldsymbol{\theta}) = (2\pi)^{-N_\theta/2}\sqrt{\det[\Sigma^{-1}]} \times \exp\left[-\frac{\Sigma^{-1}_{ab}}{2}(\theta_a - \theta^{\text{opt}}_a)(\theta_b - \theta^{\text{opt}}_b)\right]$ $\left(\Sigma^{-1}_{ab} \equiv \frac{\partial^2 J(\boldsymbol{\theta})}{\partial\theta_a\partial\theta_b}\right)$

Re-weighting with :

$\omega(\theta) = p\left(V_\theta(T,r)\right)/\tilde{p}\,(\theta)$ to grantee the sampling following posterior

Eigenvalues of the Hamiltonian (with t-independent potential) : mass and width ?

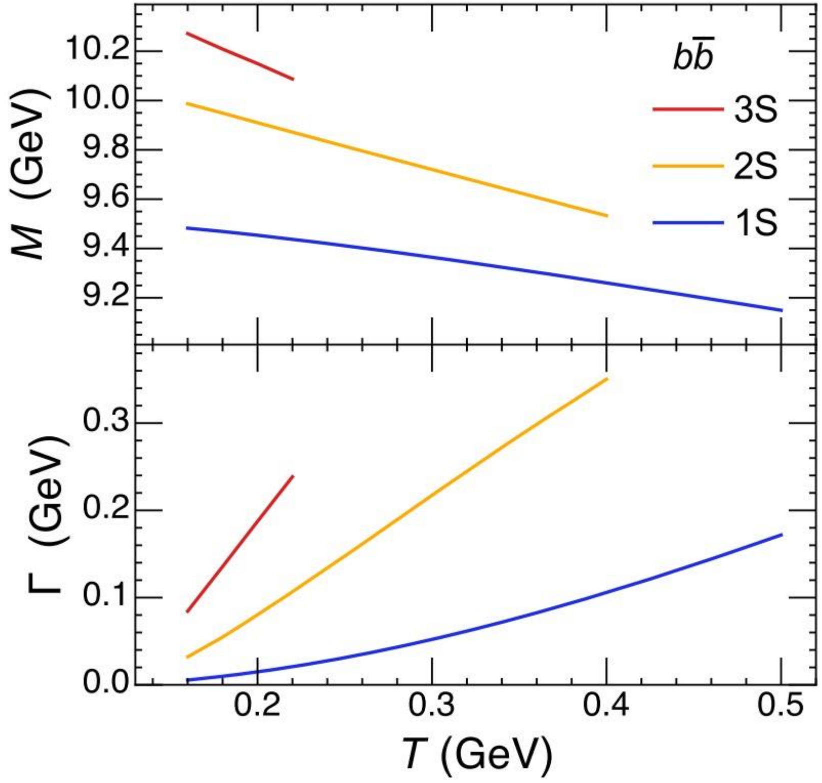
$$C^{>}(0,\mathbf{r}) = \delta^{(3)}(\mathbf{r}), \qquad \begin{cases} \hat{H}C^{>}(t,\mathbf{r}) = i\partial_t C^{>}(t,\mathbf{r}), & t>0, \\ \hat{H}^{\dagger}C^{>}(t,\mathbf{r}) = i\partial_t C^{>}(t,\mathbf{r}), & t<0. \end{cases}$$

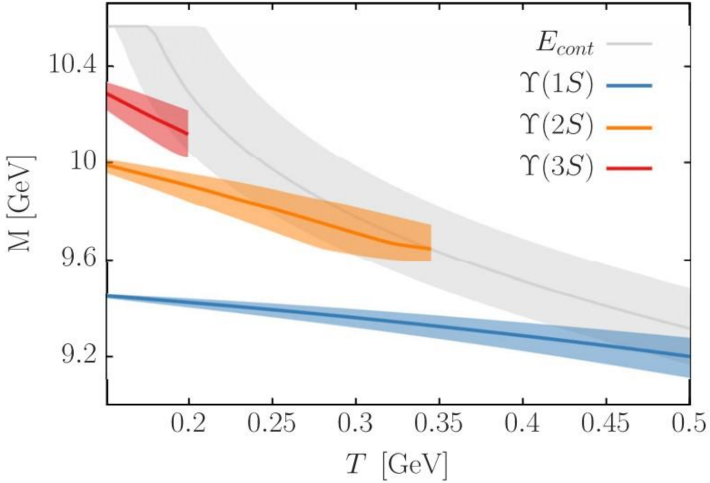
$$c_n \equiv \int \mathrm{d}^3\mathbf{r}\, C^{>}(0,\mathbf{r})\psi_n^*(\mathbf{r}) = \psi_n^*(0), \qquad C^{>}(t,\mathbf{r}) = \begin{cases} \sum_n c_n e^{-iE_n t} \times \psi_n(\mathbf{r}), & t>0, \\ \sum_n c_n^* e^{-iE_n^* t} \times \psi_n^*(\mathbf{r}), & t<0, \end{cases}$$

$$\rho(\omega) \equiv \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{i\omega t} C^{>}(t,0) = \sum_n \frac{-2|\psi_n(0)|^2\, \mathrm{Im}[E_n]}{(\omega - \mathrm{Re}[E_n])^2 + (\mathrm{Im}[E_n])^2} \Rightarrow \Gamma_n^{\mathrm{Lor}} = -\mathrm{Im}[E_n]$$

$$\rho(\omega) \propto \sum_n \exp\left[-\frac{(\omega - M_n)^2}{2\Gamma_n^2}\right]. \qquad \Gamma_n^{\mathrm{Lor}} = \sqrt{2\,\ln 2}\,\Gamma_n^{\mathrm{Gau}}$$

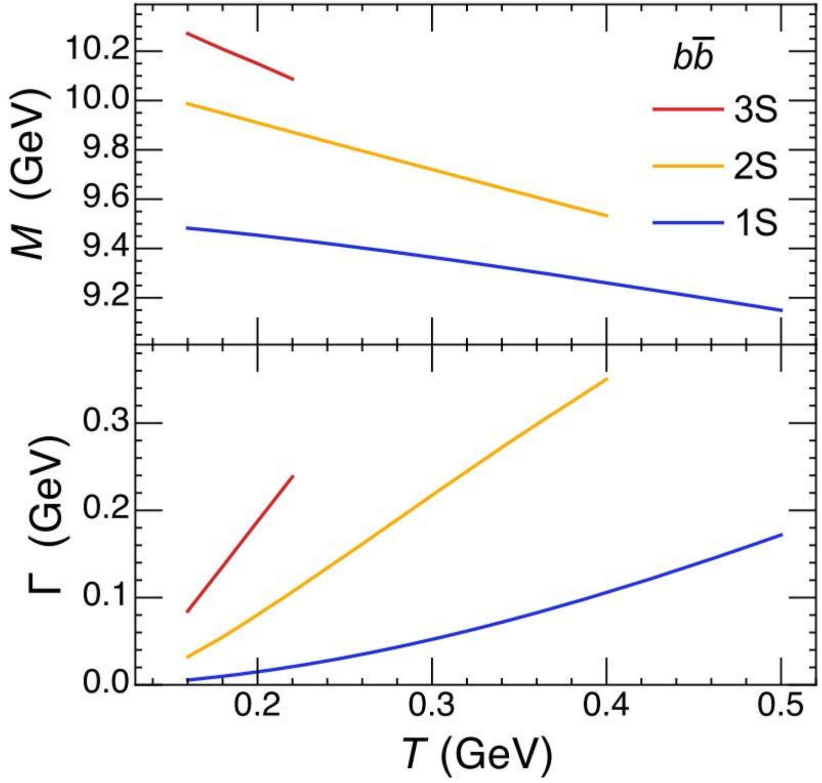
Potential model reproduce in-medium spectroscopy of others

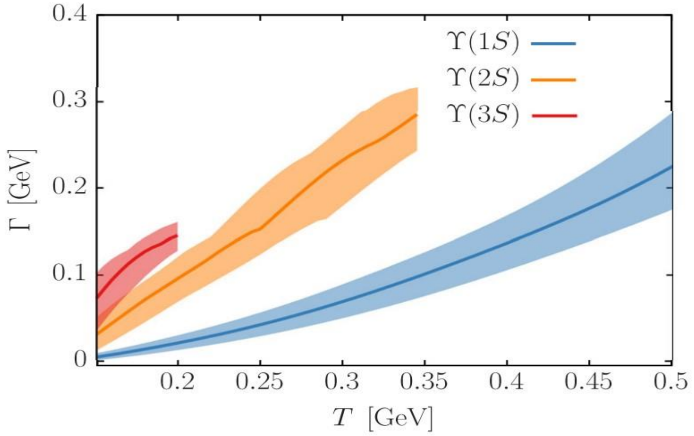




D. Lafferty and A. Rothkopf, **Phys. Rev. D 101, 056010 (2020)**

Potential model reproduce in-medium spectroscopy of others





D. Lafferty and A. Rothkopf, **Phys. Rev. D 101, 056010 (2020)**

Uncertainty estimation for NS EoS reconstruction-- reweighting

1, draw ensemble of M-R samples from measured likelihood (Gaussian approximated)

2, convert each set of M-R points into EoS via the reconstruction model

3, apply TOV-solver to convert the ensemble of EoSs to corresponding M-Rs

4, evaluate the weight for each EoS sample

$$w^{(j)} = \frac{\text{Posterior}(\boldsymbol{\theta}^{(j)}_{\text{EoS}}|\text{data})}{\text{Proposal}(\boldsymbol{\theta}^{(j)}_{\text{EoS}})} \propto \frac{P(\text{data}|\boldsymbol{\theta}^{(j)}_{\text{EoS}})\ \text{Prior}(\boldsymbol{\theta}^{(j)}_{\text{EoS}})}{P(\boldsymbol{\theta}^{(j)}_{\text{EoS}}|\text{samples}^{(j)})\ P(\text{samples}^{(j)}|\text{data})\ \text{Prior}(\text{data})},$$

$$P(\text{data}|\boldsymbol{\theta}^{(j)}_{\text{EoS}}) \propto \exp\left(-\chi^2(M_{\boldsymbol{\theta}^{(j)}_{\text{EoS}}}, R_{\boldsymbol{\theta}^{(j)}_{\text{EoS}}})/2\right)$$