From lQCD to in-medium Heavy Quark interactions via Deep Learning

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With :

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ErUM-Data IDT

Introduction

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

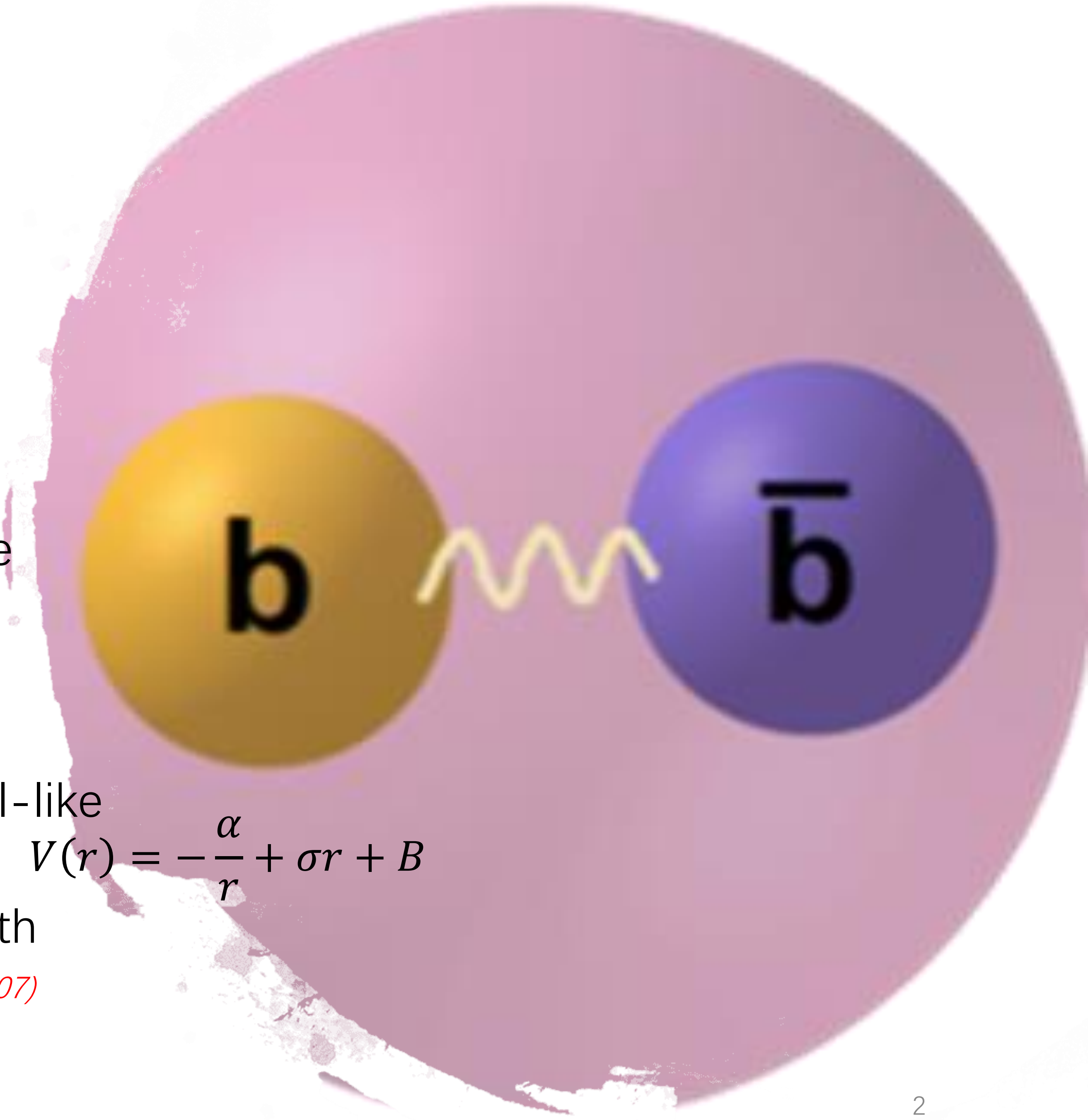
- Produced via Hard Processes from early stage
- 'Calibrated' QCD Force – HQ interaction

In Vacuum : NR potential (NRQCD) , Cornell-like

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

In Medium : Color Screening , Thermal Width

Laine, et.al, JHEP(2007)



Potential model : Shrödinger Eq.

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

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

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

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

Inverse Power method

H.W.Crater, JCP(1994)

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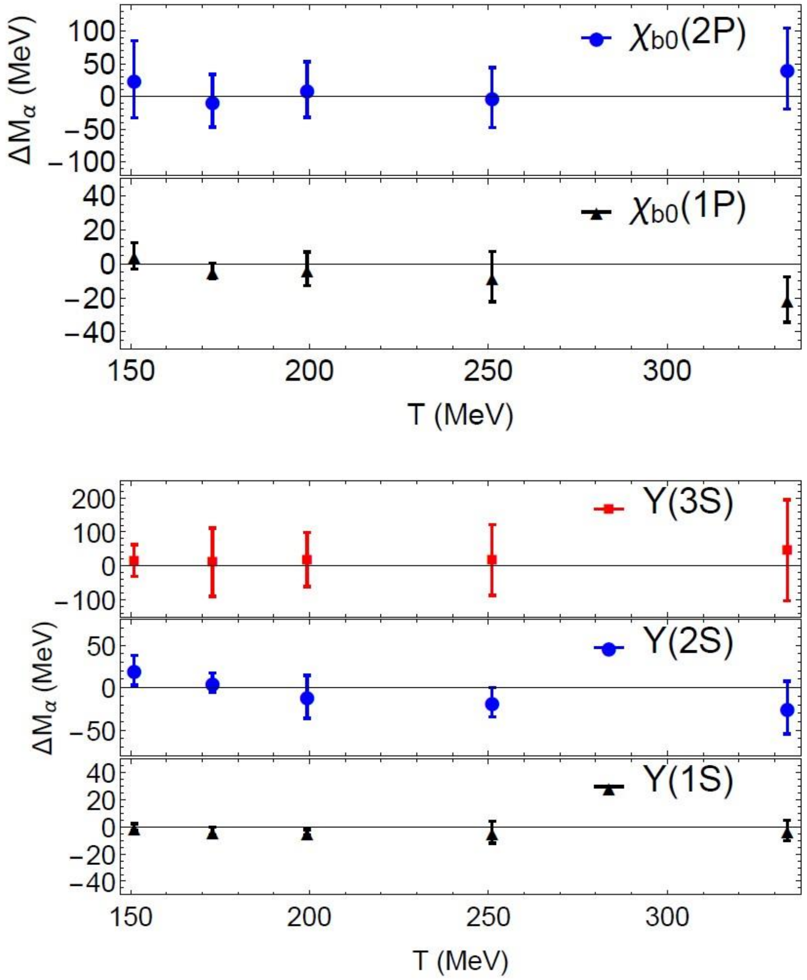
?

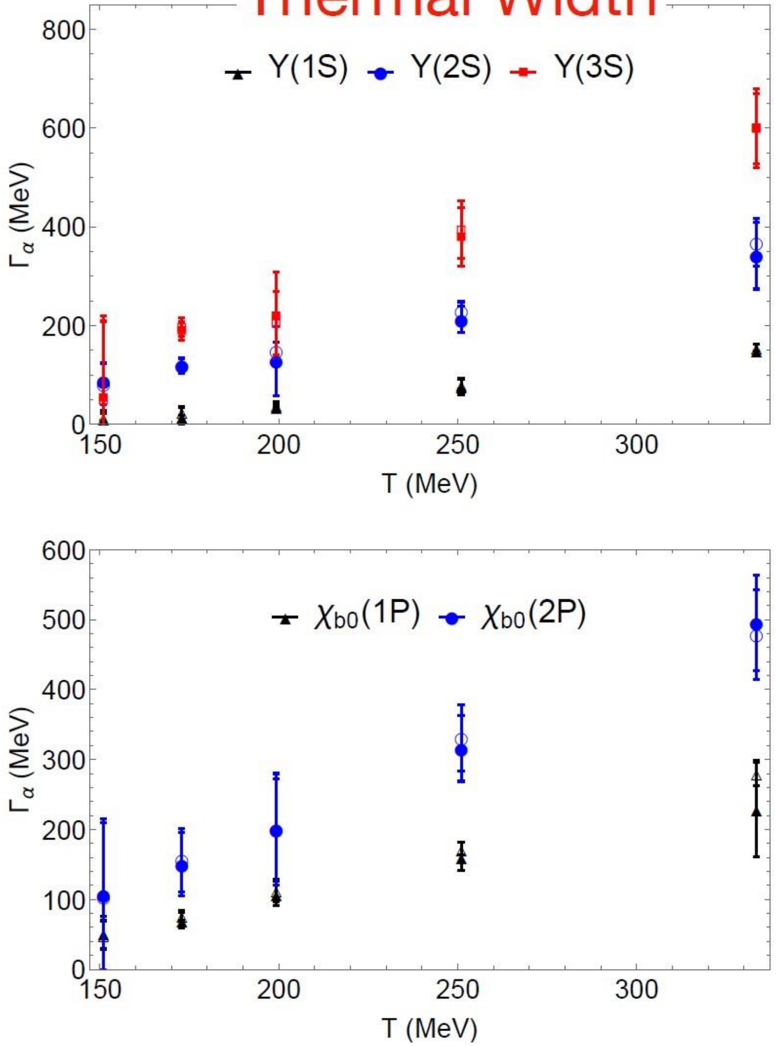
Inverse Problem

lQCD measured mass and thermal width for Bottomonium with finite HQ mass

Mass

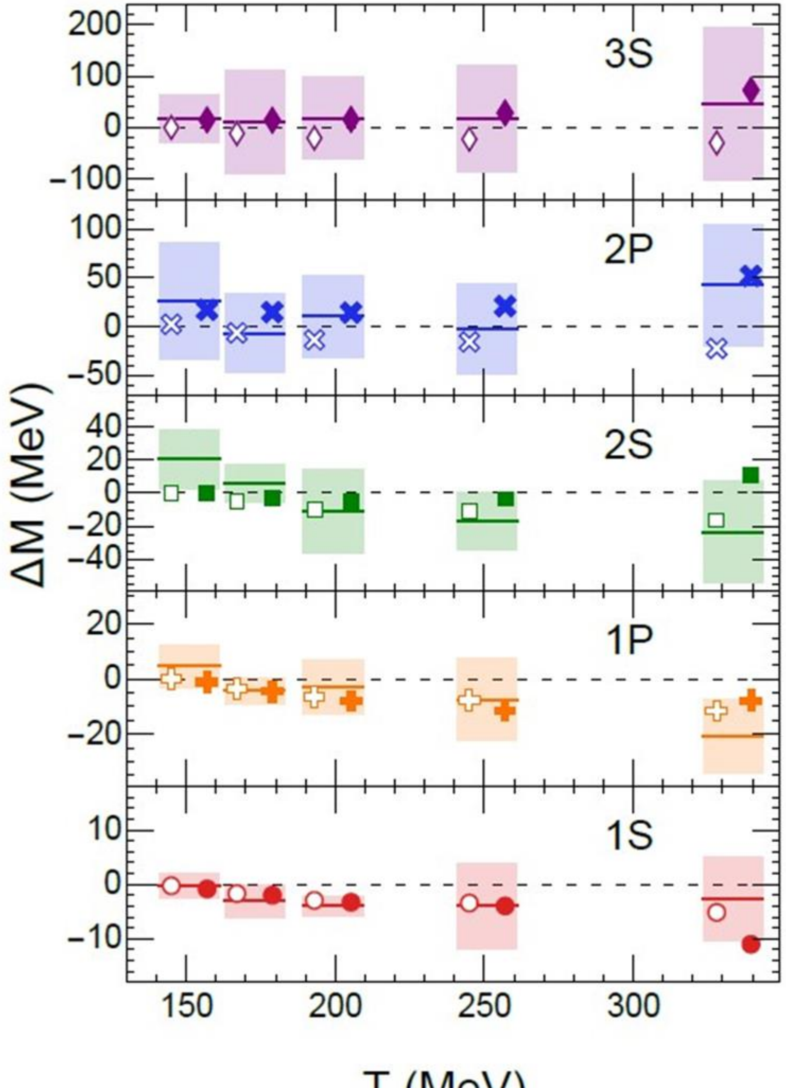


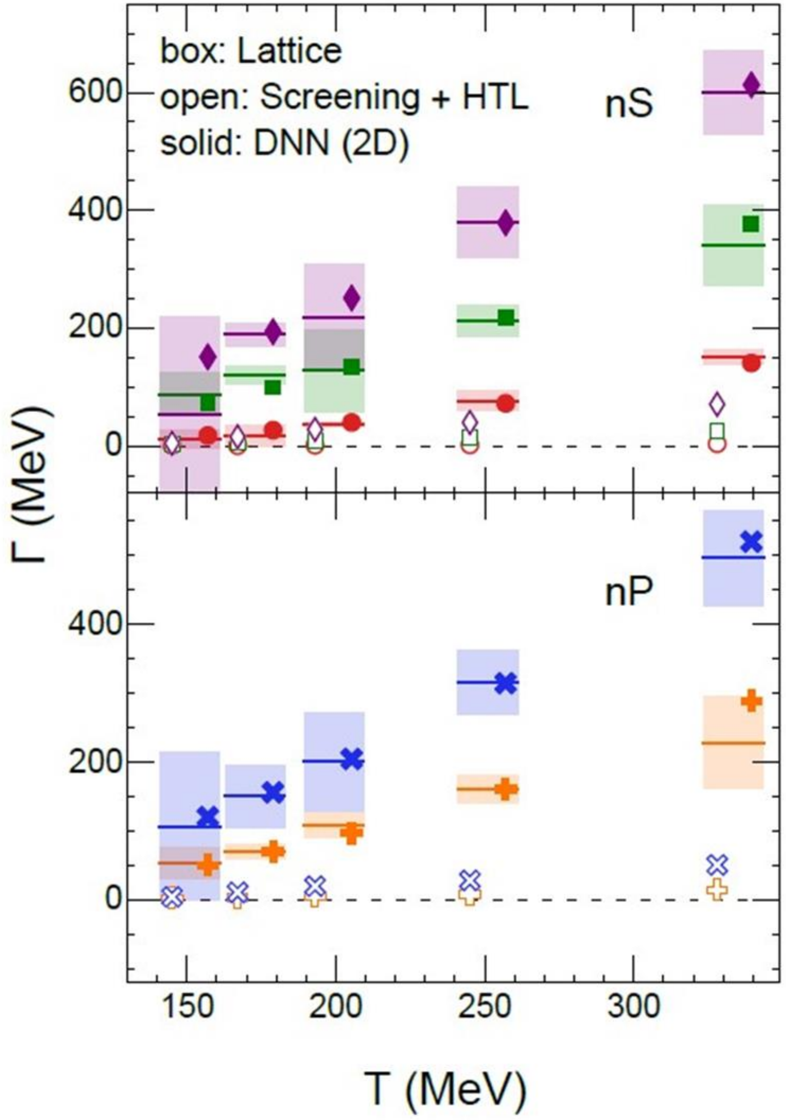
Thermal Width



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

lQCD measured (color box) m and width and best fit of **HTL**(open symbol) and **DNNs** (solid symbol)



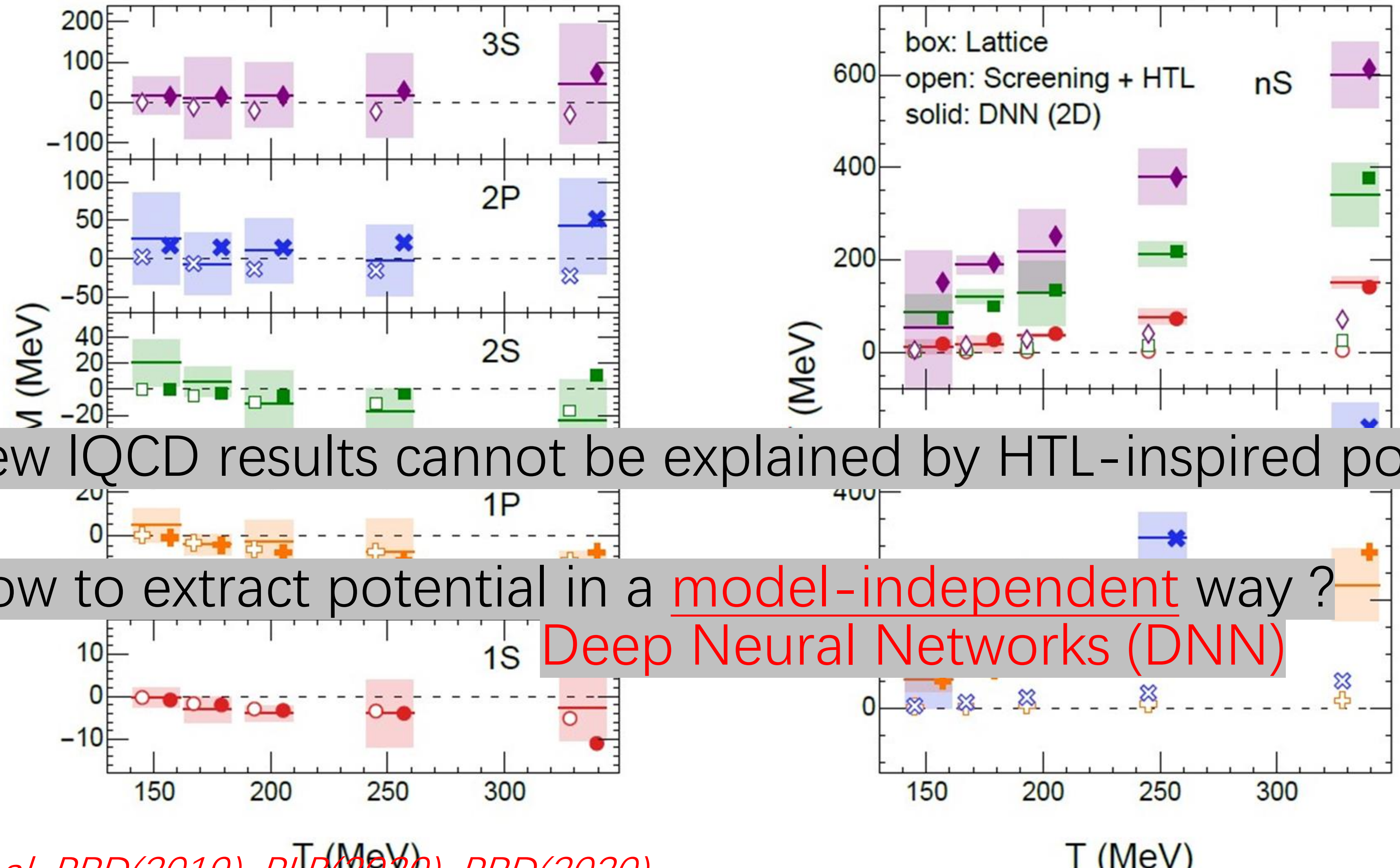


$$V_R(T,r) = \frac{\sigma}{\mu_D}\Big(2-(2+\mu_D r)e^{-\mu_D r}\Big) - \alpha\Big(\mu_D + \frac{e^{-\mu_D r}}{r}\Big) + B\,,$$

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

HTL from “A. Rothkopf, et.al, PRD(2020)”

lQCD measured (color box) m and width and best fit of **HTL**(open symbol) and **DNNs** (solid symbol)



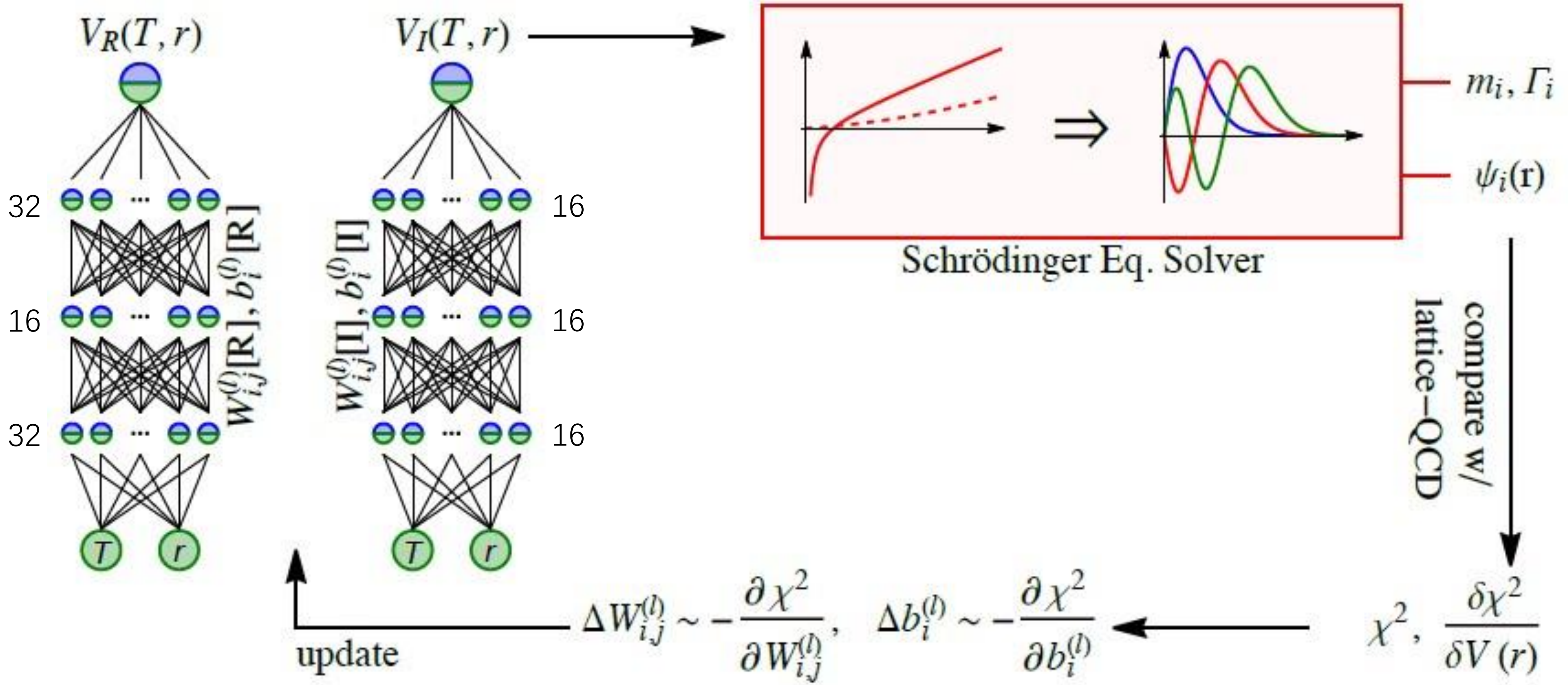
New lQCD results cannot be explained by HTL-inspired potential

How to extract potential in a <u>model-independent</u> way ?

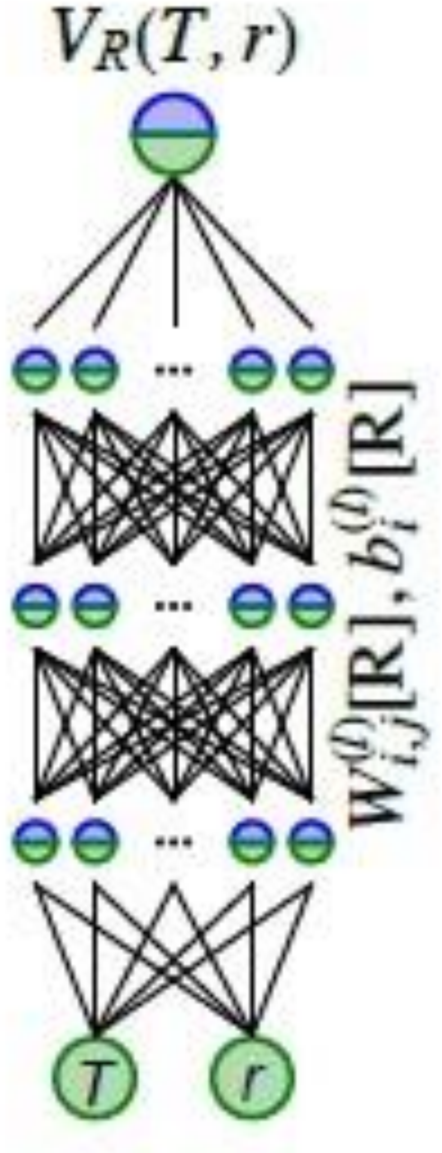
Deep Neural Networks (DNN)

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

Flow chart of HQ potential reconstruction



DNN basic :



Universal Function Approximator

$$(f: \mathbb{R}^n \to \mathbb{R}^m) \quad \vec{x} \to \vec{y}$$

$$z_i^{(l)} = b_i^{(1)} + \sum_j W_{ij}^{(l)} a_j^{(l-1)}, \qquad a_i^{(l)} = \sigma^{(l)}\left(z_i^{(l)}\right)$$

ELU

$$\longrightarrow \quad a^{(N)} = \tilde{y}(x;\theta) \qquad \theta \equiv \left\{W_{ij}^{(l)}, b_i^{(l)}\right\}$$

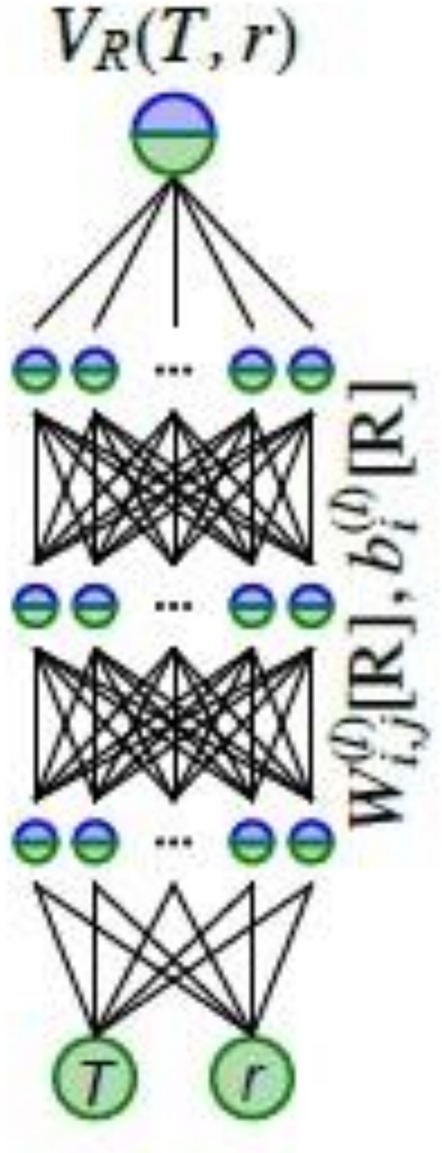
Gradient Descent for parameter tuning :

$$\Delta\theta \equiv \theta^{[k+1]} - \theta^{[k]} \sim -\nabla_\theta J(\theta)$$

Cost, e.g. : $J(\theta) = \frac{1}{2} \sum_{x \in \text{data set}} \left|\tilde{y}(\theta, x) - y(x)\right|^2 + \frac{\lambda}{2}\theta \cdot \theta$

DNN basic :

Back Propagation for Gradients



$$\frac{\partial J}{\partial \theta_i} = \sum_{\mathrm{x} \in \text{data set}} (\tilde{\mathrm{y}}(\boldsymbol{\theta}, \mathrm{x}) - \mathrm{y}(\mathrm{x})) \cdot \frac{\partial \tilde{\mathrm{y}}(\boldsymbol{\theta}, \mathrm{x})}{\partial \theta_i} + \lambda \theta_i$$

$$z_i^{(l)} = b_i^{(1)} + \sum_j W_{ij}^{(l)} a_j^{(l-1)}, \quad a_i^{(l)} = \sigma^{(l)}\left(z_i^{(l)}\right)$$

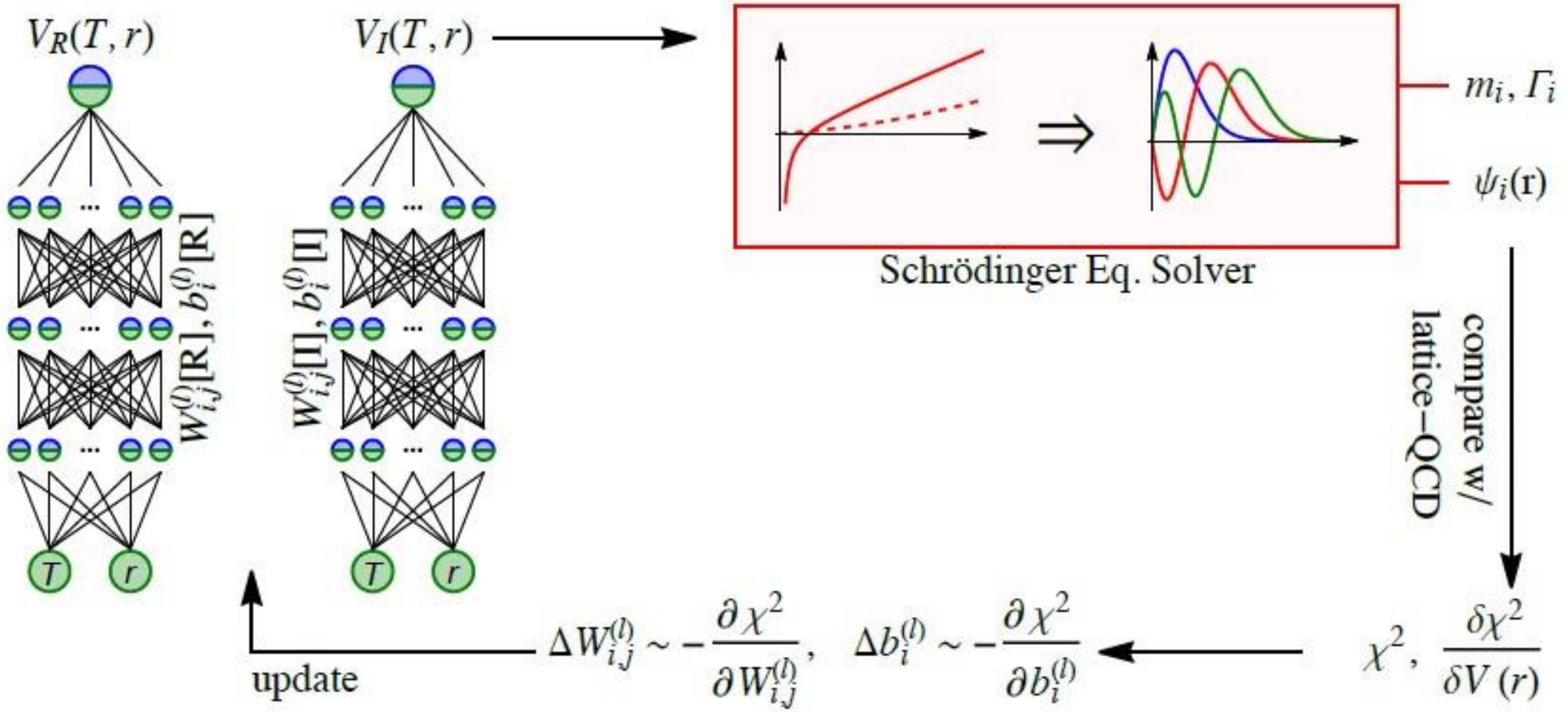
Fp

$$\longrightarrow \quad \frac{\partial J}{\partial w_{ij}^{[l]}} = a_j^{[l-1]} \frac{\partial J}{\partial z_i^{[l]}} \qquad \frac{\partial J}{\partial b_i^{[l]}} = \frac{\partial J}{\partial z_i^{[l]}}$$

$$\frac{\partial J}{\partial z_i^{[l]}} = \sigma'\left(z_i^{[l]}\right) \sum_j W_{ji}^{[l+1]} \frac{\partial J}{\partial z_j^{[l+1]}}$$

Bp

Cost function for 'DNN+ Shrödinger Eq.'



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

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

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

$i \in \{1S, 2S, 3S, 1P, 2P\}$

Perturbation treatment for Shrödinger Eq.

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

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

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

Hellmann-Feynman theorem

Phys. Rev. (1939)

Perturbation treatment for Shrödinger Eq.

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$$\Big(\frac{\widehat{p}^2}{2m}+V(r)+\delta V(r)\Big)|\psi_i'\rangle = (E_i+\delta E_i)|\psi_i'\rangle.$$

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

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

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

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

Gradients for the Cost

$$\chi^2 = \sum_{T,i,j} \Big(R_{ij}^{(T)} \Delta m_{T,i} \Delta m_{T,j} + I_{ij}^{(T)} \Delta\Gamma_{T,i} \Delta\Gamma_{T,j} + 2M_{ij}^{(T)} \Delta m_{T,i} \Delta\Gamma_{T,j} \Big) ,$$

$$\frac{\partial\chi^2}{\partial\theta_{R,n}} = \sum_{T,i,k} \frac{\partial\chi^2}{\partial m_{T,i}} \frac{\partial V_R(T,r_k)}{\partial\theta_{R,n}} |\psi_i(T,r_k)|^2 \mathrm{d}r ,$$

$$\frac{\partial\chi^2}{\partial\theta_{I,n}} = -\sum_{T,i,k} \frac{\partial\chi^2}{\partial\Gamma_{T,i}} \frac{\partial V_I(T,r_k)}{\partial\theta_{I,n}} |\psi_i(T,r_k)|^2 \mathrm{d}r ,$$

$$\frac{\partial J}{\partial\theta_{R,n}} = \sum_{T,i} \Big\{ \Big[\sum_k \frac{\partial V_R(T,r_k)}{\partial\theta_{R,n}} |\psi_i(T,r_k)|^2 \mathrm{d}r \Big] \times \sum_j \Big[R_{i,j}^{(T)} \Delta m_{T,j} + M_{ij}^{(T)} \Delta\Gamma_{T,j} \Big] \Big\} + \lambda\theta_{R,n} ,$$

$$\frac{\partial J}{\partial\theta_{I,n}} = -\sum_{T,i} \Big\{ \Big[\sum_k \frac{\partial V_I(T,r_k)}{\partial\theta_{I,n}} |\psi_i(T,r_k)|^2 \mathrm{d}r \Big] \times \sum_j \Big[I_{i,j}^{(T)} \Delta\Gamma_{T,j} + M_{ij}^{(T)} \Delta m_{T,j} \Big] \Big\} + \lambda\theta_{I,n} ,$$

Bayesian Inference for Uncertainty Estimation

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

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

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

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

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

Reference Sampler ~

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

$$\Sigma^{-1}_{ab} \equiv \frac{\partial^2 J(\boldsymbol{\theta})}{\partial\theta_a\partial\theta_b}$$

re-weighting with :
$\omega(\theta) = p\left(V_\theta(T,r)\right)/\tilde{p}\,(\theta)$ to grantee posterior sampling

Vacuum potential & B-quark mass Calibration

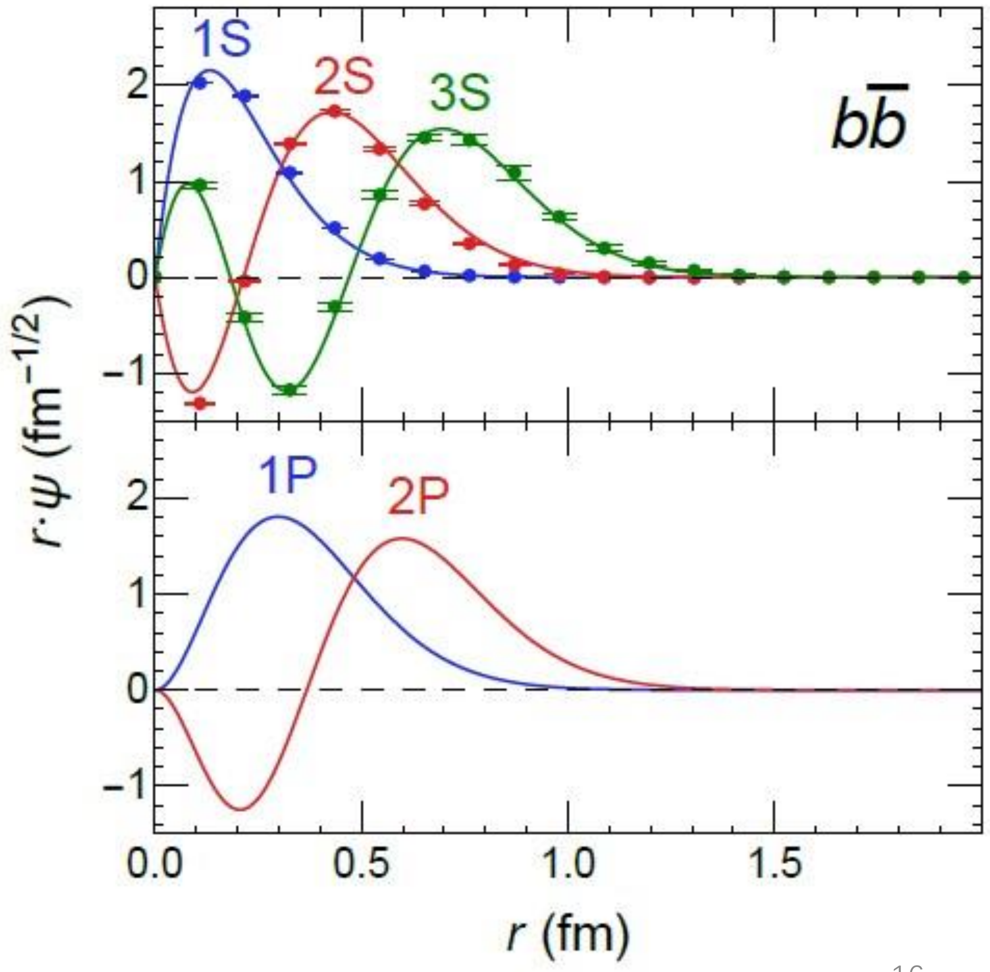
Cornell-Potential

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

$m_b = 6.00\ \mathrm{GeV}$ $\alpha = 0.406$

$\sigma = 0.221\ \mathrm{GeV}^2$ $B = -2.53\ \mathrm{GeV}$

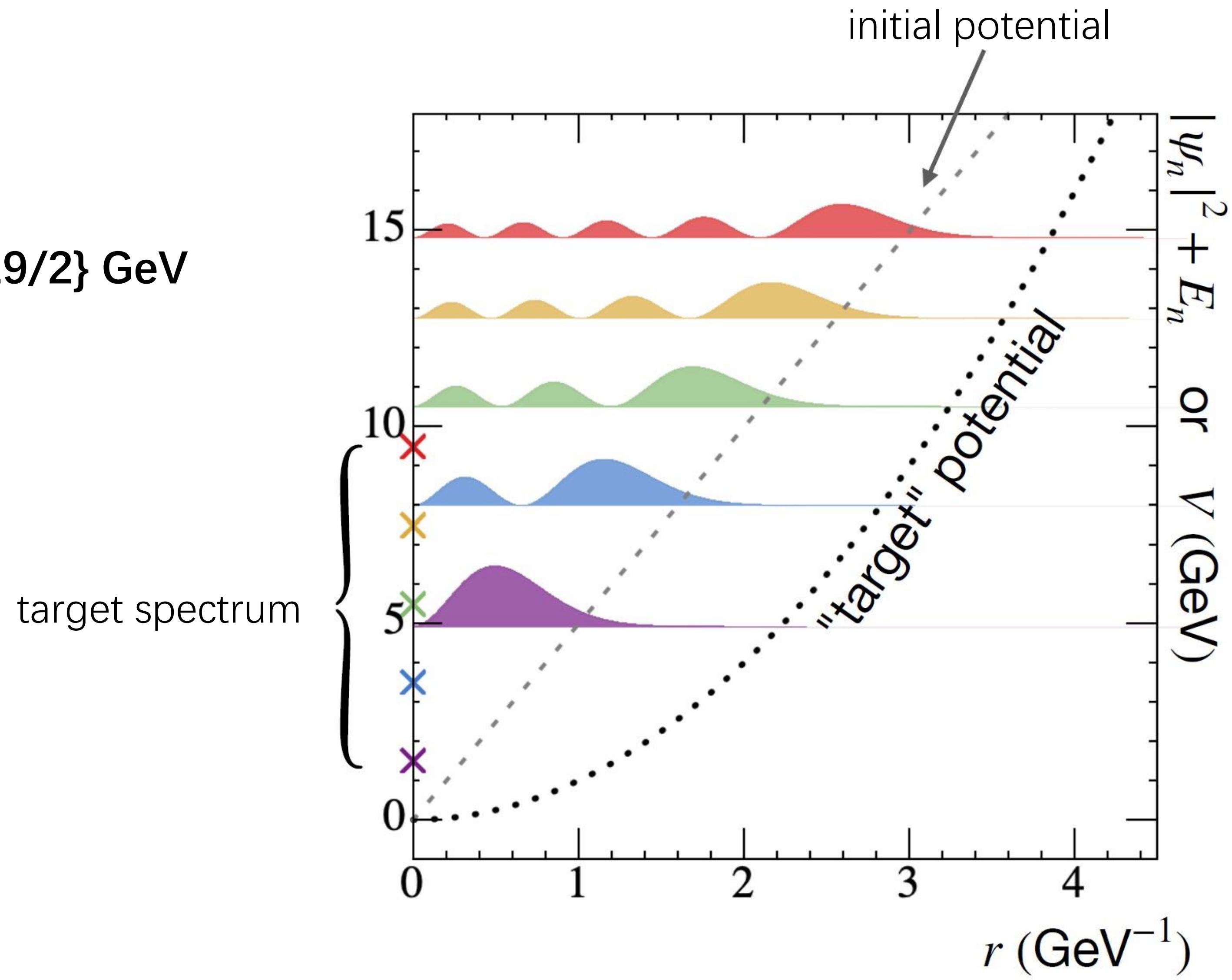
	1S	2S	3S	1P	2P
experiment (MeV)	9445	10017	10352	9891	10254
model (MeV)	9449	10003	10356	9893	10258
difference (MeV)	+4	−14	+4	+2	+4



Proof of Concept :

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

Learn V(r) from 5 eigenvalues :
{ E_n } = {3/2, 7/2, 11/2, 15/12, 19/2} GeV



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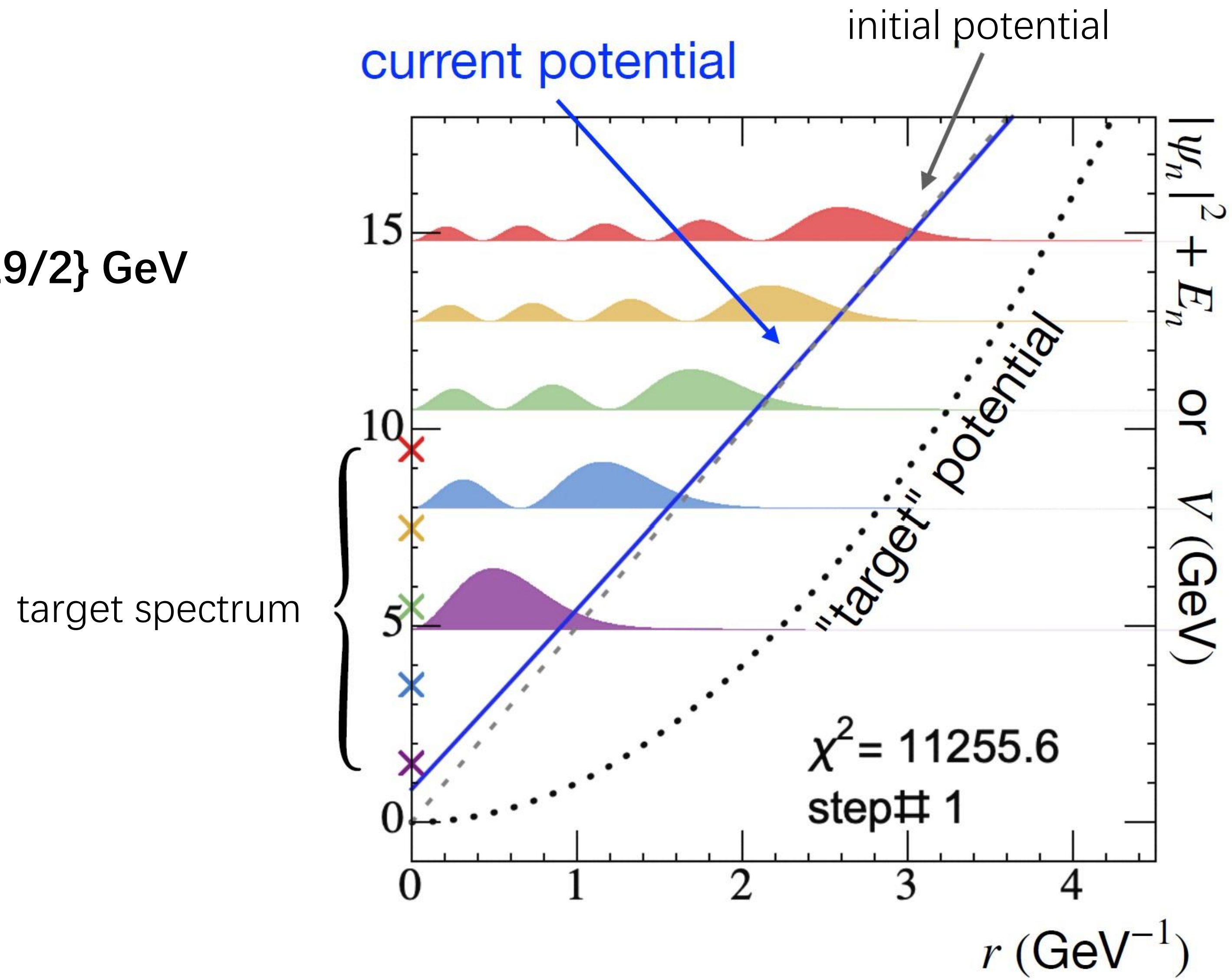

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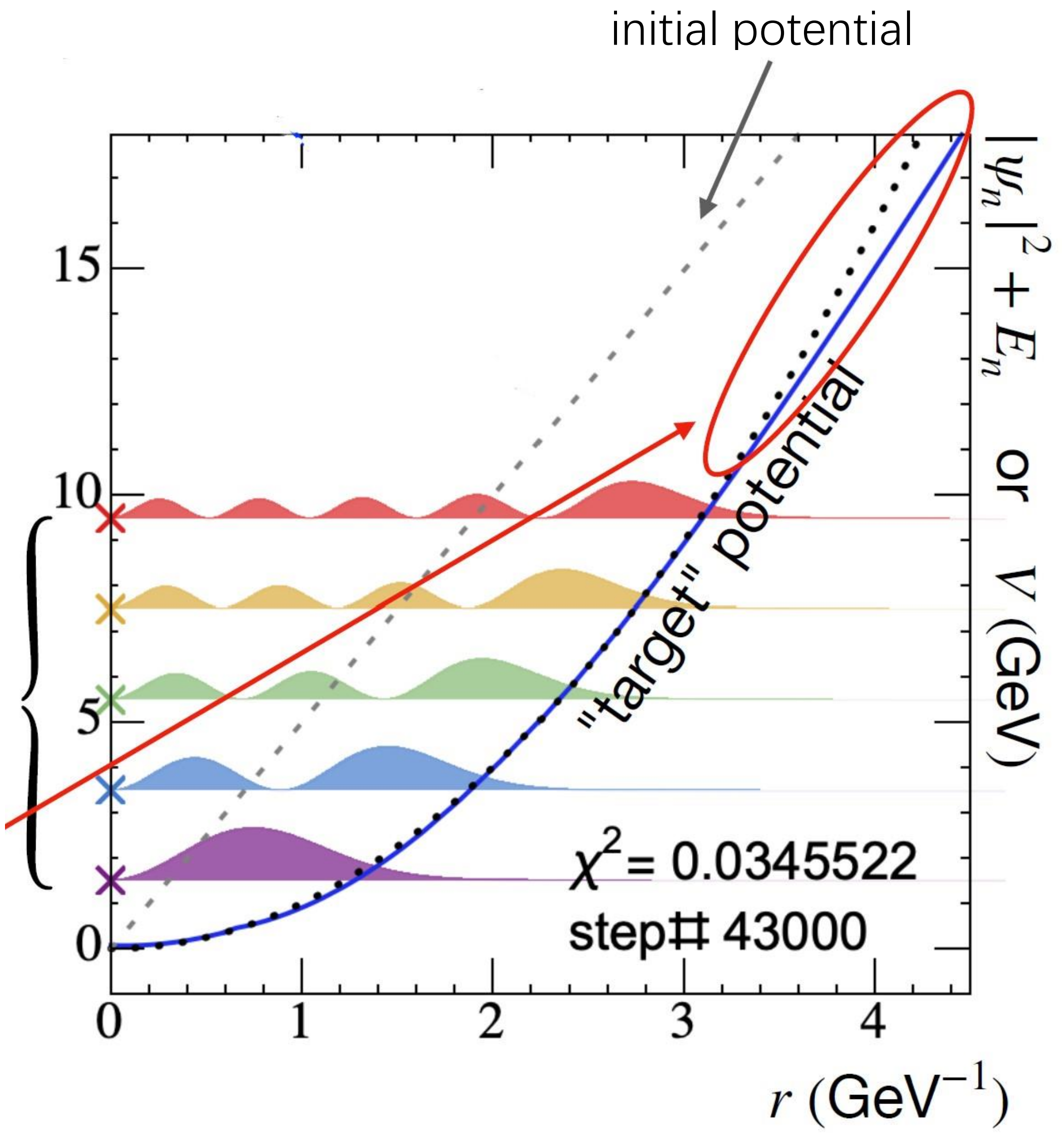


Deviation happens where all given states' wavefunction vanishes

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

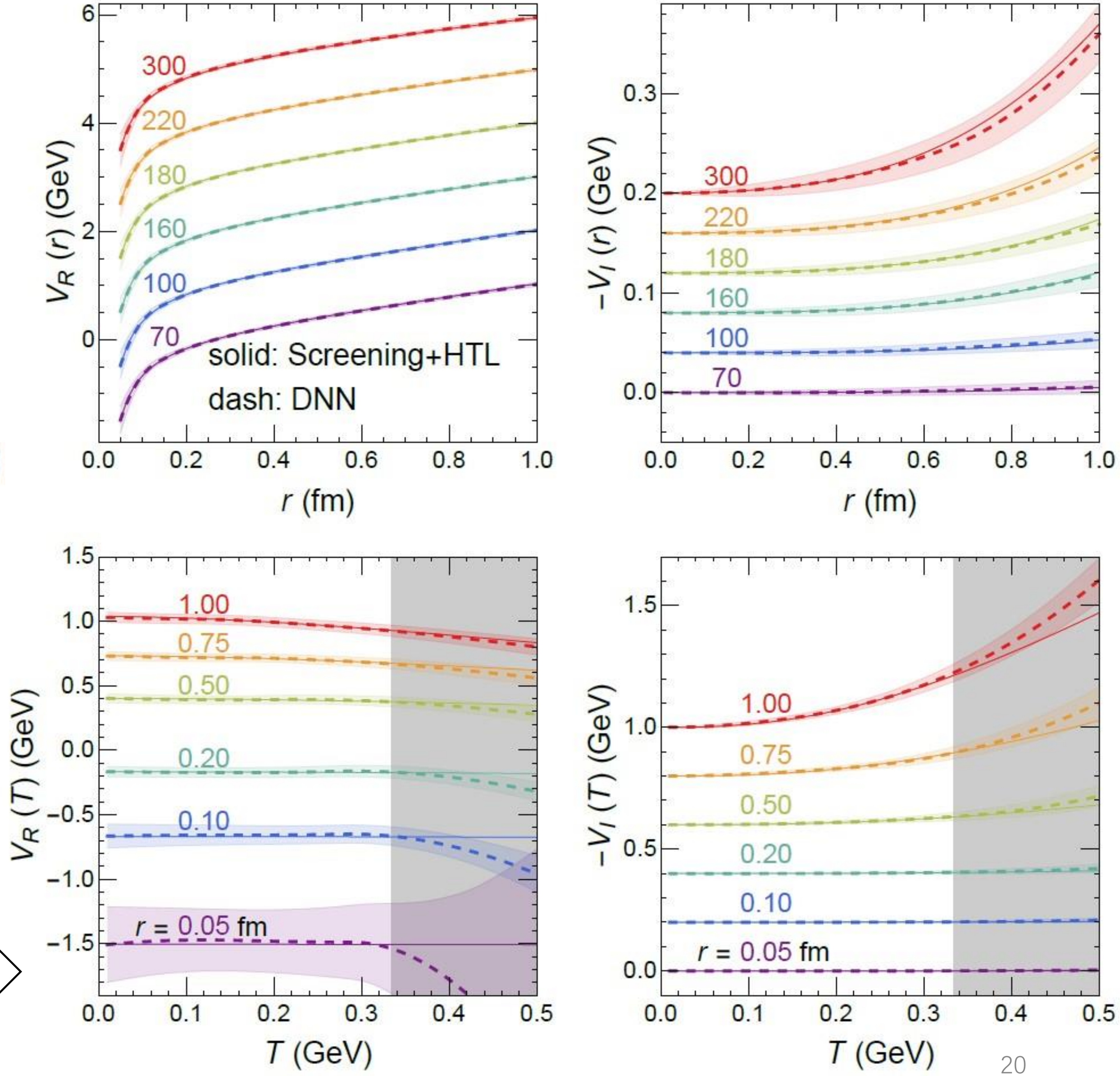
Closure Test

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

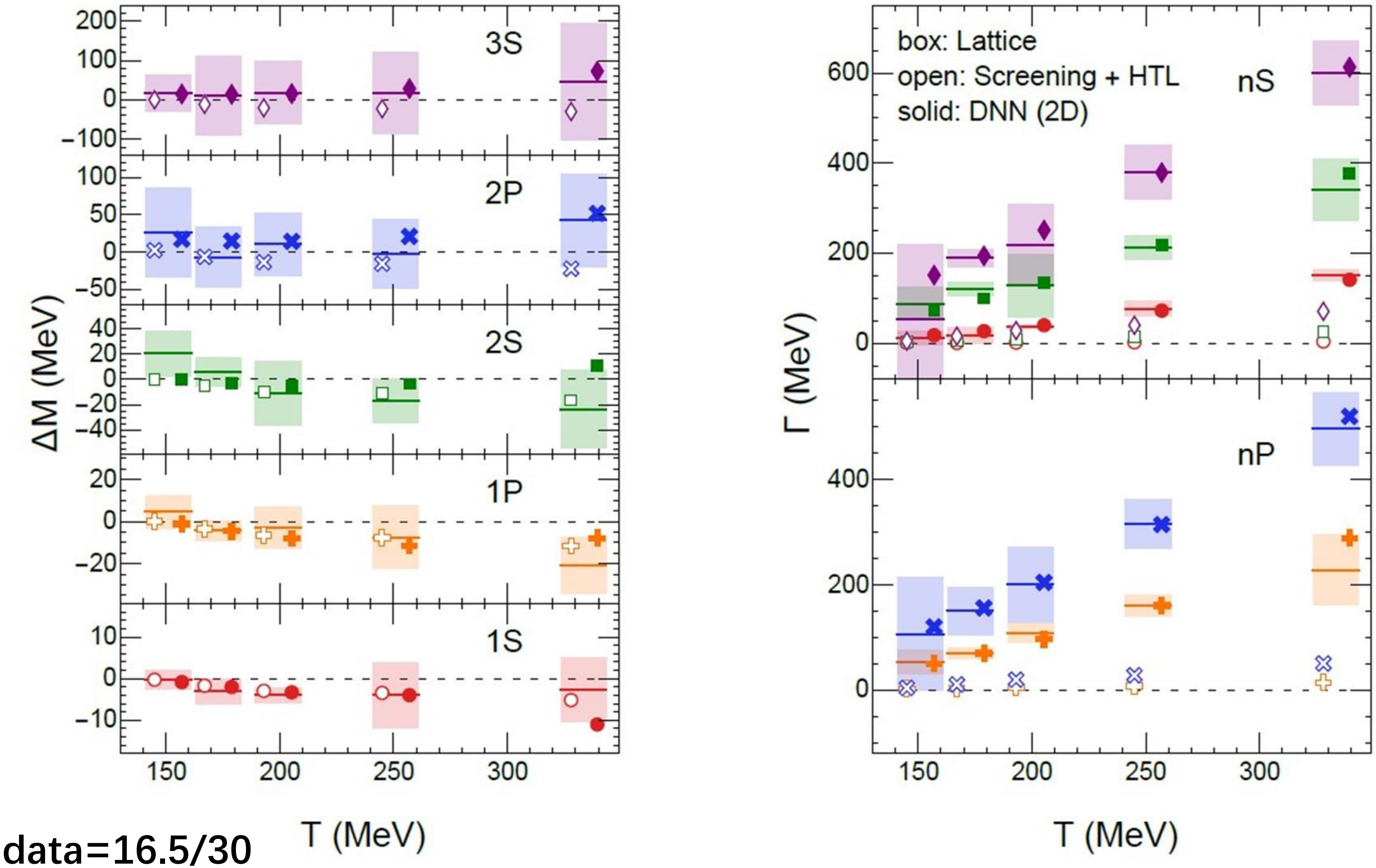
$$V_I(T,r) = -\frac{\sqrt{\pi}}{4}\mu_D T\sigma r^3 G^{2,2}_{2,4}\left(\begin{smallmatrix}-\frac{1}{2},-\frac{1}{2} \\ \frac{1}{2},\frac{1}{2},-\frac{3}{2},-1\end{smallmatrix}\middle|\frac{\mu_D^2 r^2}{4}\right) - \alpha T\,\phi(\mu_D r)\,,$$

$m_b = 4.676$ GeV, $\alpha = 0.39$,
$\sigma = 0.223$ 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 measured mass and width from : **HTL**(open symbols) and **DNNs** (solid symbols)



Chi2-per-data=16.5/30

Consistency Check : with different parameterization

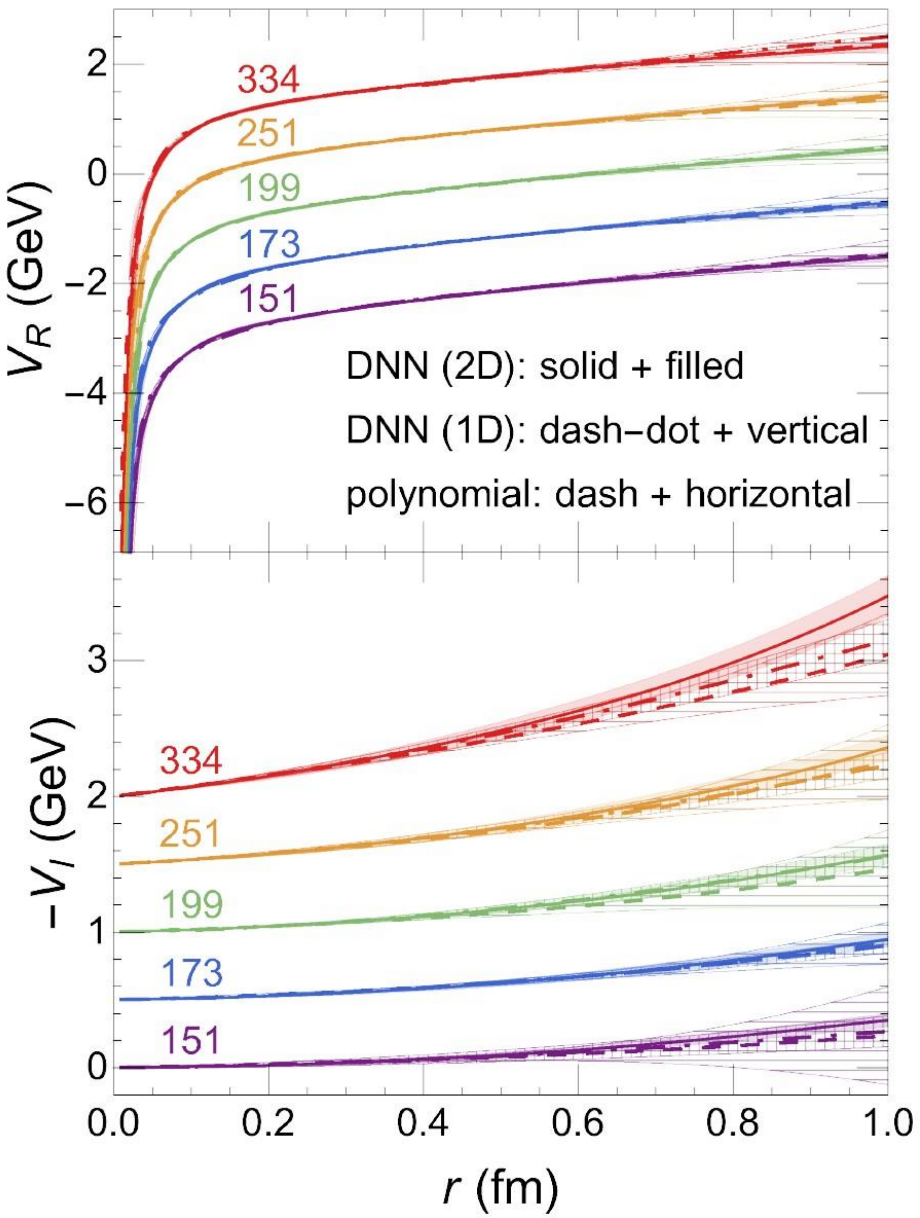
1, **DNN(2D)** :
T & r dependency

2, **DNN(1D)** :
only r dependency

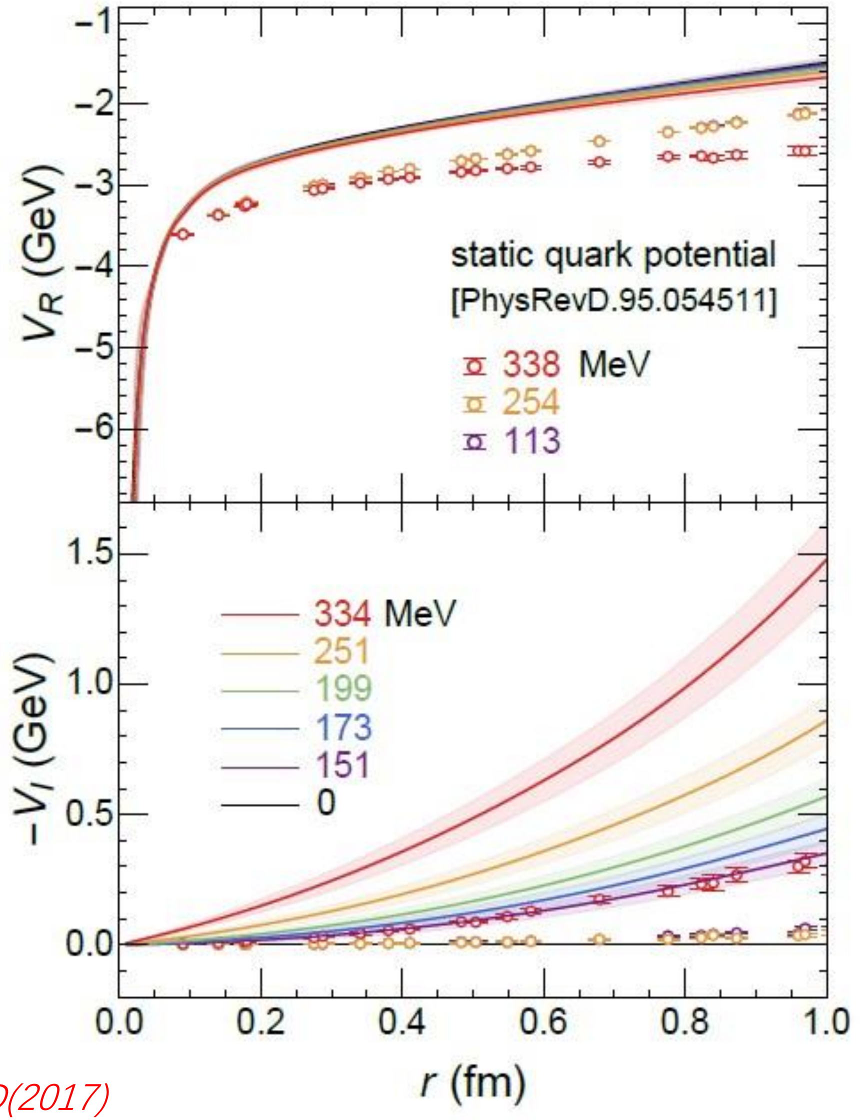
3, **Polynomial** :

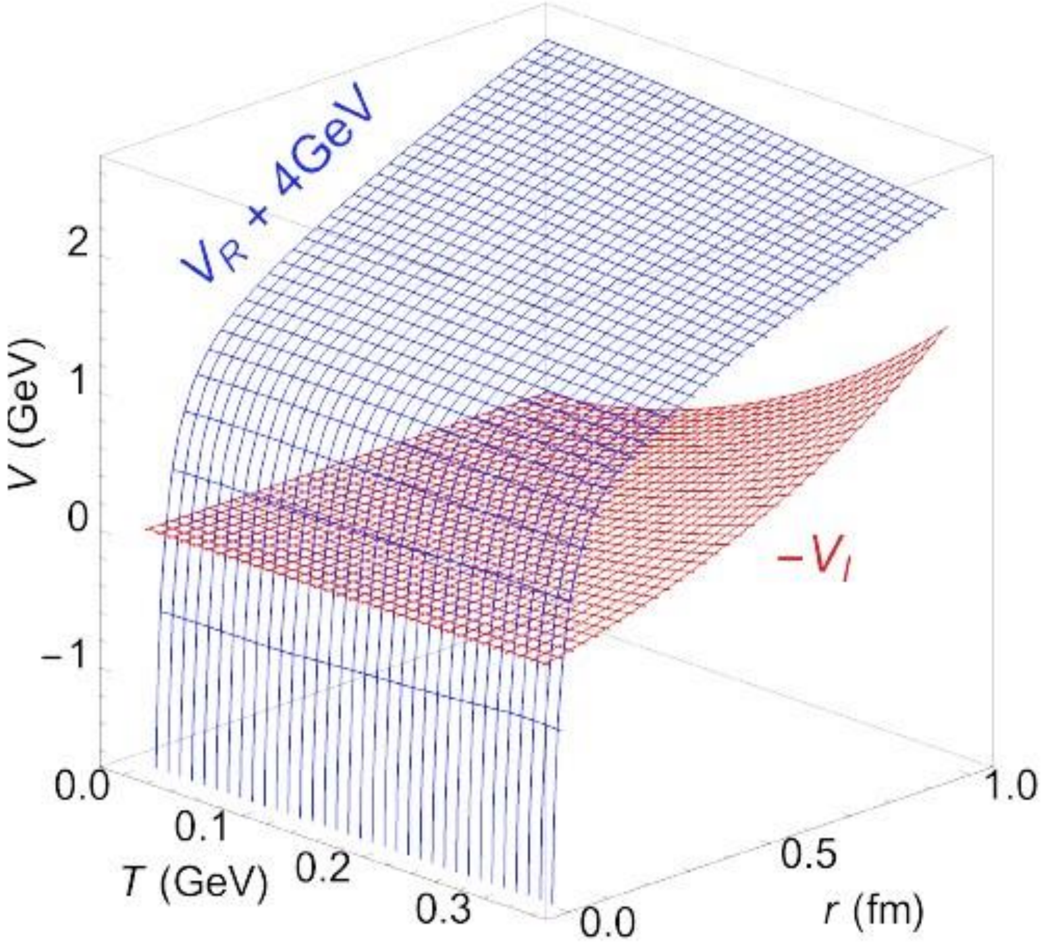
$$V_R(r) = \sum_{i=-1}^{3} c_{R,i}\, r^i,$$

$$V_I(r) = -\sum_{i=1}^{3} c_{I,i}\, r^i.$$



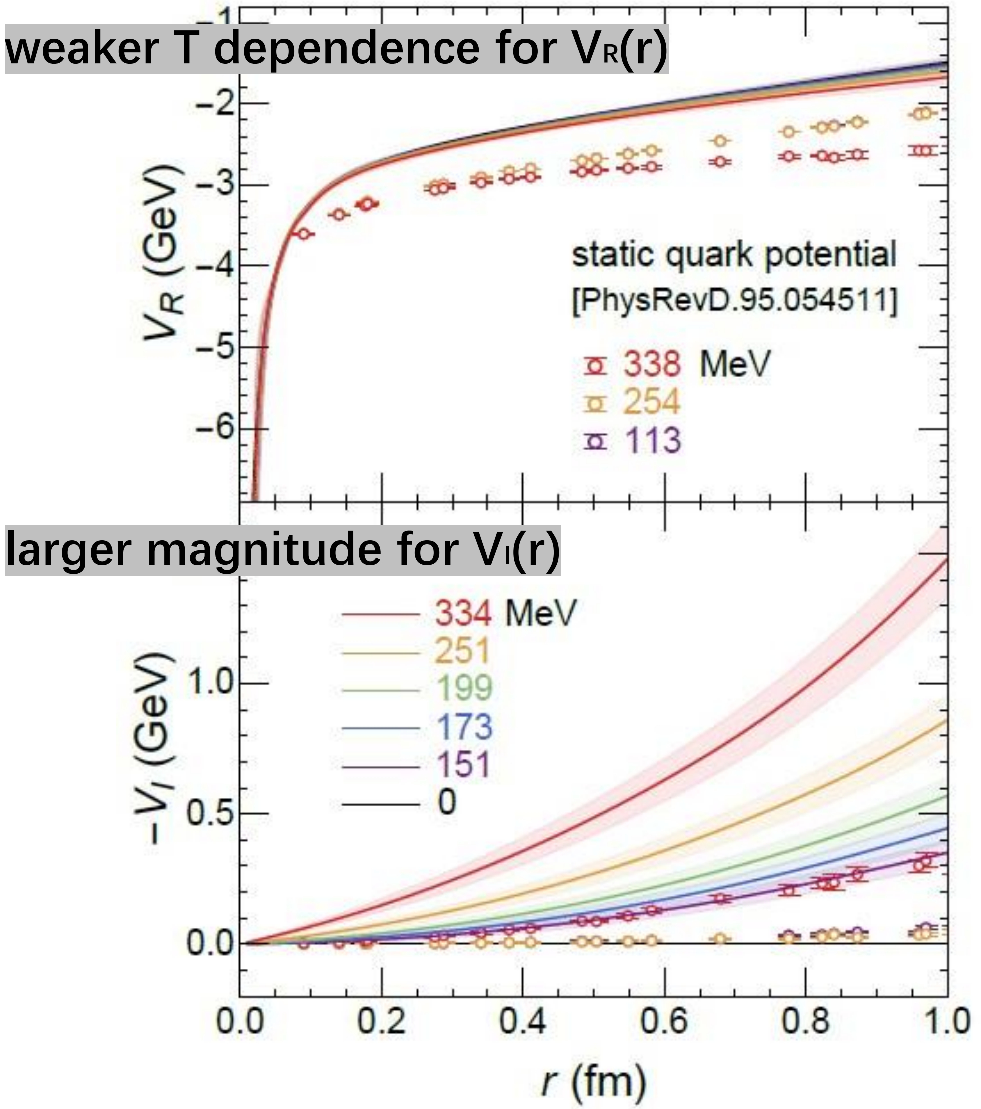
The reconstructed (B) interaction potentials





A.Rothkopf, PRD(2017)

Unconventional in-medium behavior



- Traditional picture,

V & F show **platform** at large r, and decrease in height with increase T, So : binding energy decrease, average size increase, until a **melting Temperature**

- New picture,

Im[V] induced thermal width are so significant (**continuous dynamic diss-ociation**), its enhancement compensates the vanishing of the melting effect (mild T-dependence of Re[V])

Summary

- Bias-free HQ complex interaction is reconstructed from our novel methodology **‘NN+perterb.+Bayesian’**
- Both T and r dependence of the interaction potential are captured via **network representation**
- We found mild T-dependent screening effect for Re[V], while the strength of the Im[V] increases significantly with T
- Color Screening melting to

  Continuous dynamic dissociation