Unified Extraction of In-Medium Heavy Quark Potentials from RHIC to LHC Energies via Deep Learning

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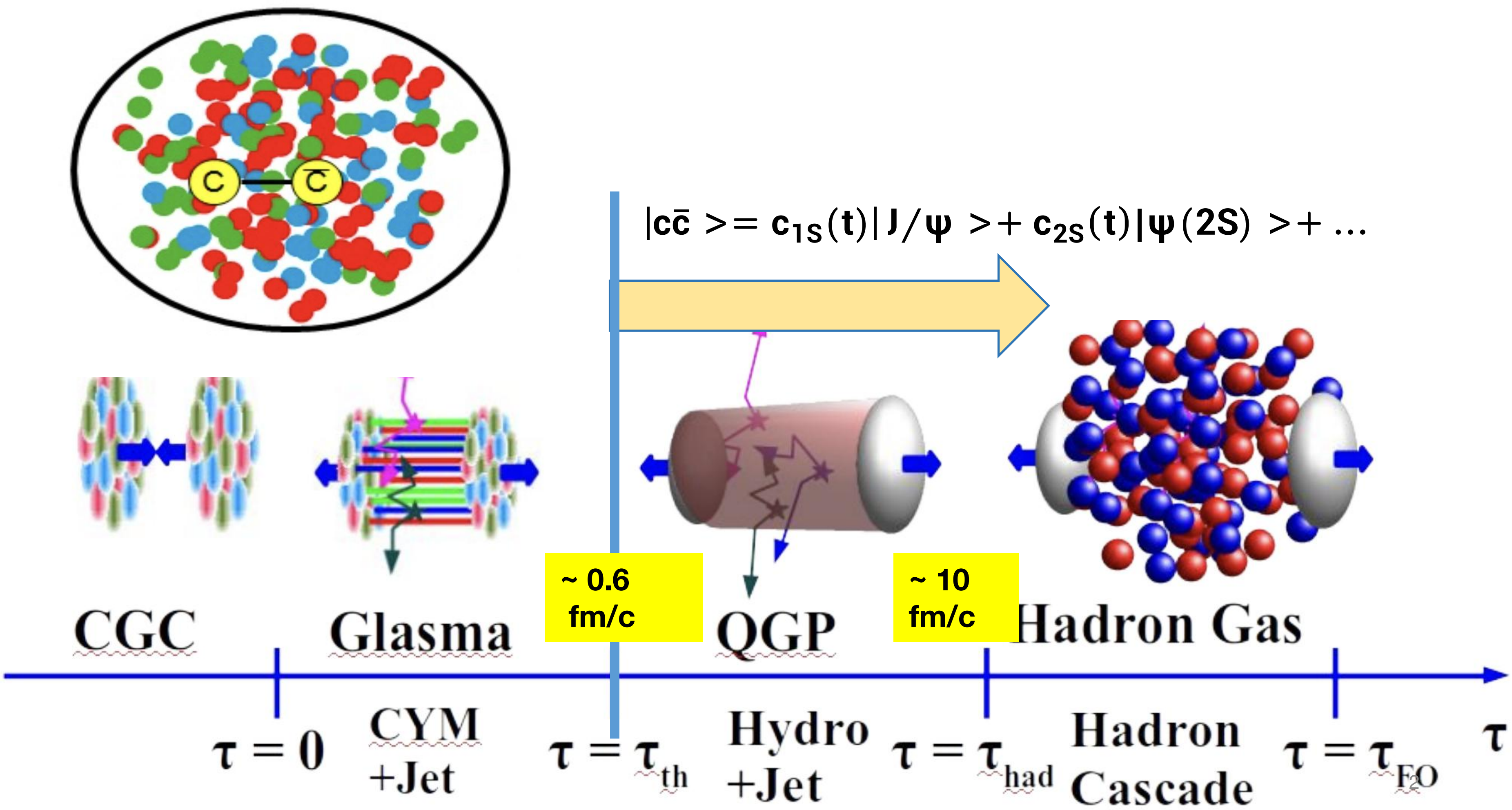
arXiv: 2604.09198	deep learning
Phys.Lett.B 839 (2023) 137774	AA collision
Chin.Phys.C 46 (2022) 114102	pA collision
Eur.Phys.J.C 84 (2024) 1193	pp collision

quarkonium in deconfined medium

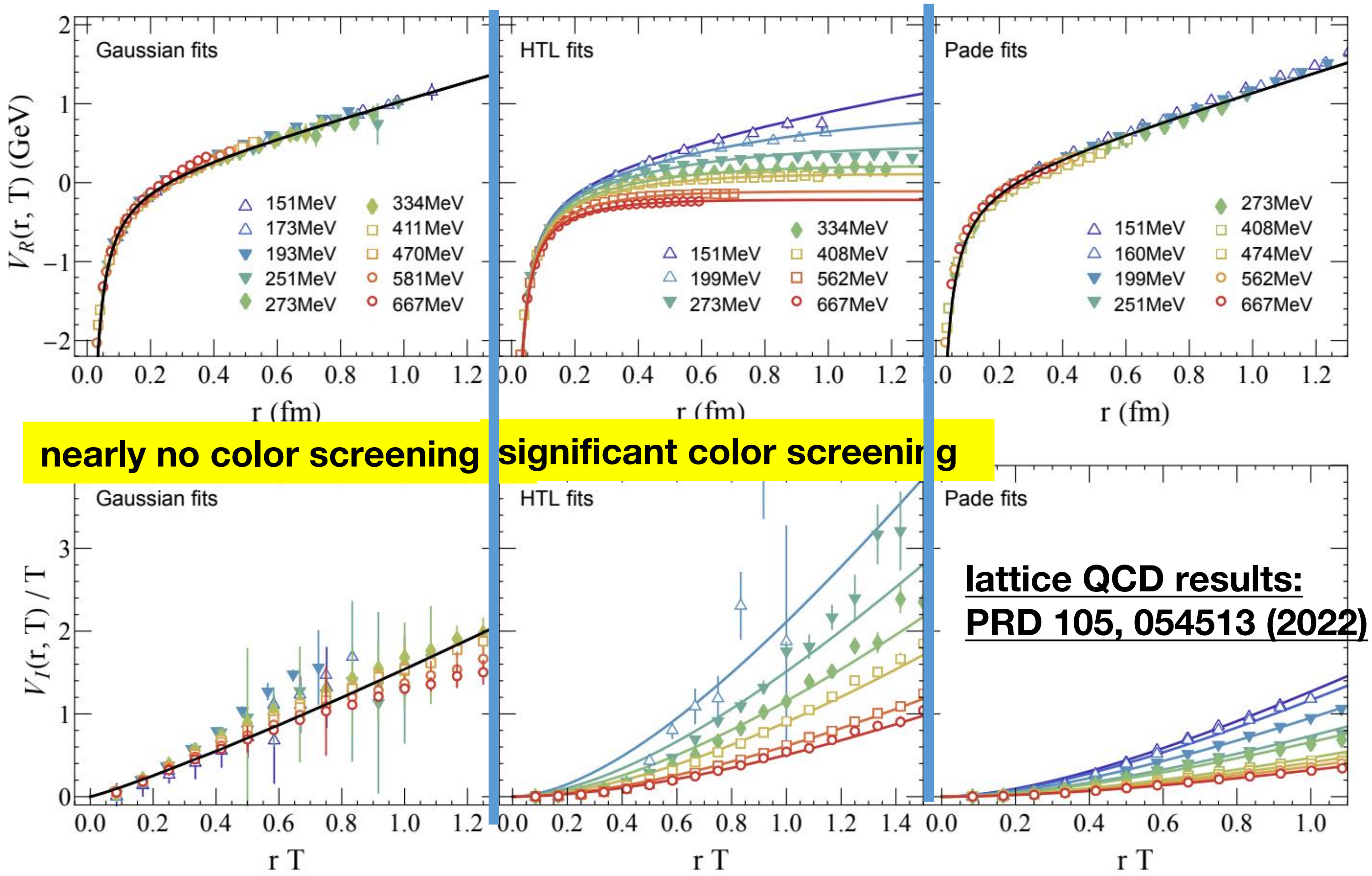
in-medium heavy quark potential:

(1) color screening ? reduced attractive potential of color-singlet states

(2) parton inelastic scattering ? transitions between singlets and octets, etc



complex potential from lattice QCD



lines: our fit in EPJC 84 (2024) 8, 869

- **Gaussian, HTL, Pade fits:**
  Three methods give very different complex heavy quark potentails
  necessary to extract V(T,r) from heavy quarkonium observables !

a strong potential is needed

In 2011 PLB,

RHIC energy

Tsinghua Transport model has explained well the bottomonium data at RHIC with strong potential (V=U),

Physics Letters B 697 (2011) 32–36

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Υ production as a probe for early state dynamics in high energy nuclear collisions at RHIC

Yunpeng Liu [a,*], Baoyi Chen [a], Nu Xu [b], Pengfei Zhuang [a]

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[b] Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

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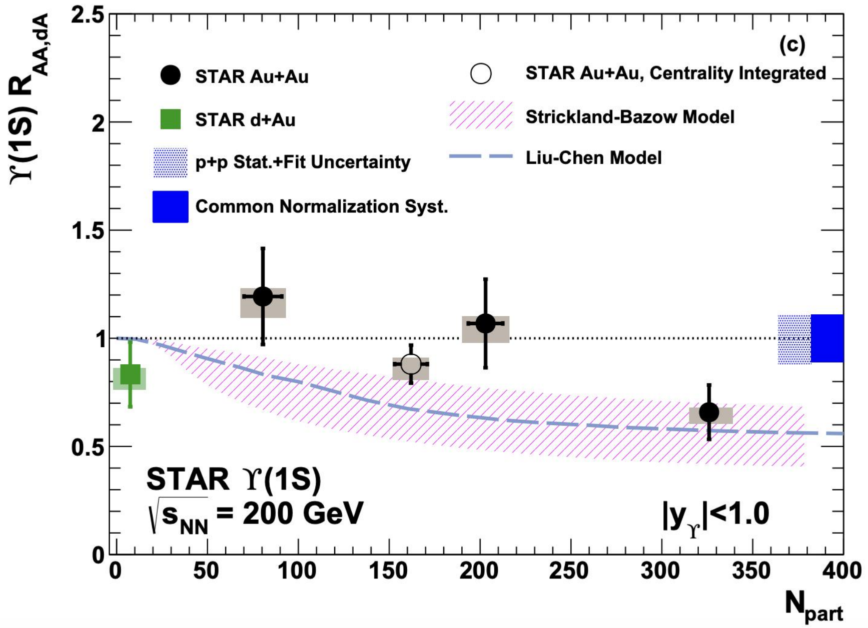
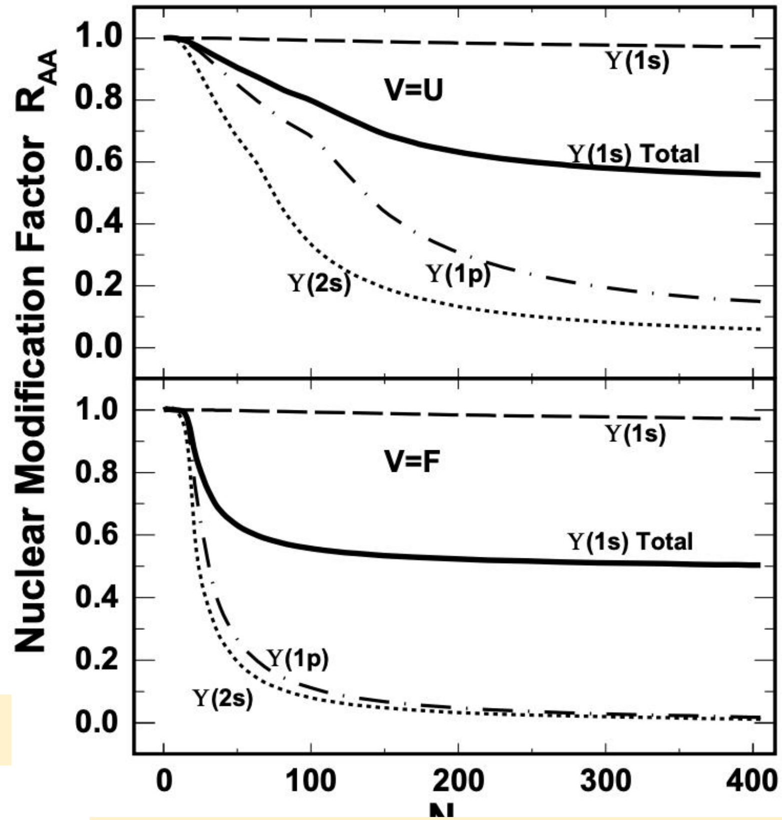


STAR, Phys.Lett.B 735 (2014) 127-137



Y. Liu, B.Chen, N.Xu, P.Zhuang 2011, PLB

a strong potential is needed

In 2014,

LHC energy

Tsinghua Transport model also studied the bottomonium at LHC

ELSEVIER

Nuclear Physics A
Volume 931, November 2014, Pages 654-658

Υ production in heavy ion collisions at LHC

Kai Zhou [a], Nu Xu [b c], Pengfei Zhuang [a]

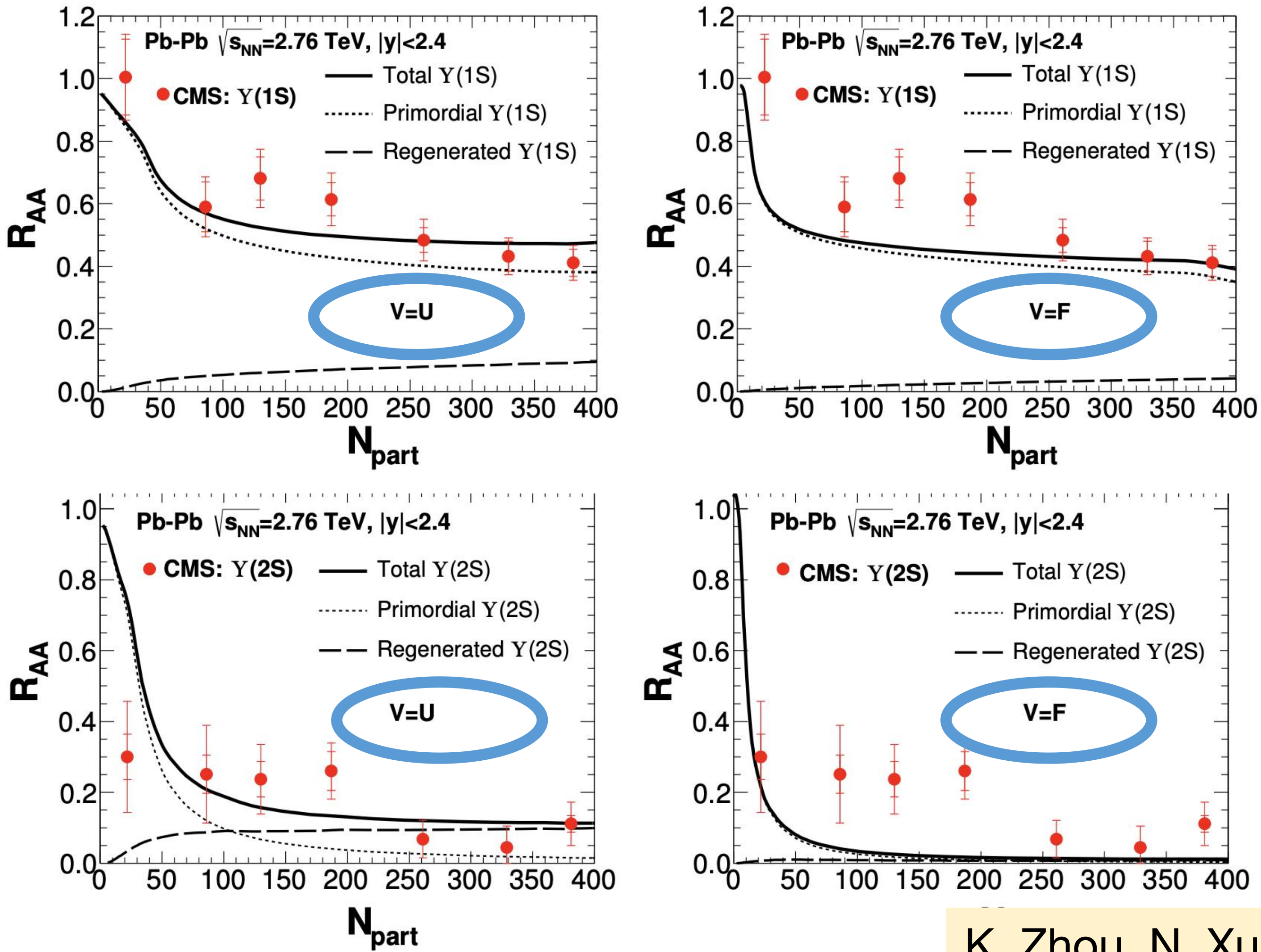
K. Zhou, N. Xu, P. Zhuang, 2014

a strong potential is needed

In 2014,

LHC energy

Tsinghua Transport model also studied the bottomonium at LHC



1S

2S

K. Zhou, N. Xu, P. Zhuang, 2021

potential-based models

- **X. Guo, S. Shi, P. Zhuang, et al**

Time-independent relativistic Schrodinger *Phys.Lett.B* 2012

- **S.Shi, J.Zhao, K. Zhou, P. Zhuang, et al**

Bayesian analysis and deep learning Phys.Rev.D 105 (2022) 014017; 2512.11536

- ***P. Gaussian, R. Katz, et al***

Schrodinger-Langevin equation *Annals Phys. 368 (2016) 267-295*

- ***A. Rothkopf, Y. Akamatsu, et al,*** *Phys.Rev.D 97 (2018) 1, 014003*

  Stochastic Schrodinger equation

- **Zuoxuan Xie, Baoyi Chen,** *Chin.Phys.C 47 (2023) 5, 054101*

- **M. Strickland et al,**

Time-dependent Schrodinger, with complex potential *Phys.Lett.B 2020*

- **J. Liu, S. Zheng, B. Chen, et al,** *Phys.Lett.B 2023*

- **Nora Brambilla, et al,**

Lindblad model with color-singlet and octet potentials, *JHEP 08 (2022) 303*

- **Xiaojun Yao, Yinru Xu, Weiyao Ke, et al**

Coupled transport model, *JHEP 01 (2021) 046*

- **Ralf Rapp, Min He, Xiaojian Du, et al**

transport model, *PRC 96 (2017) 5, 054901* And other references…….

Time-dependent Schrodinger equation

In 2015 summer, Prof. Pengfei Zhuang and Prof. Ralf Rapp started a project about heavy quarkonium in heavy ion collisions:
Xiaojian come to Tsinghua; Baoyi come to TAMU.

$$i\hbar\frac{\partial}{\partial t}\psi(r,t)=\left(-\frac{\hbar^2}{2m_\mu}\frac{\partial^2}{\partial r^2}+V(r,T)+\frac{L(L+1)\hbar^2}{2m_\mu r^2}\right)\psi(r,t)$$

r: relative distance between c and $\bar{c}$

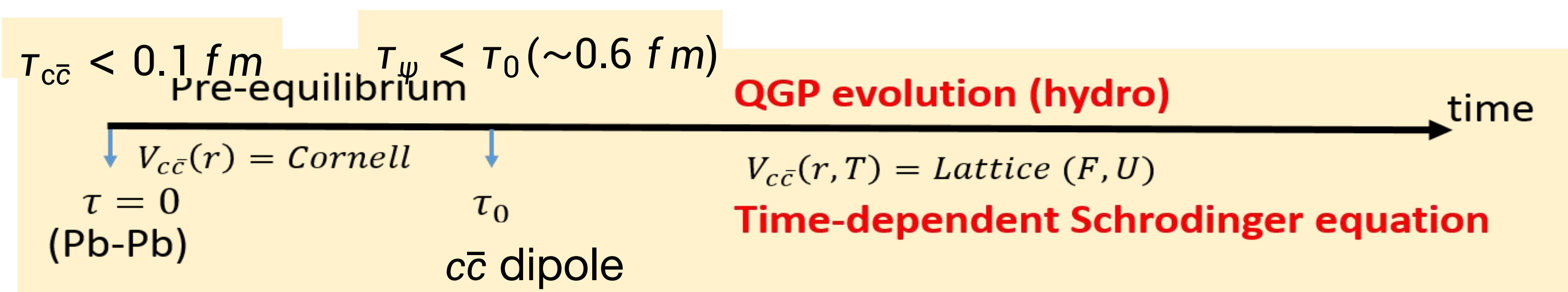
$m_\mu = m_c/2$: scaling mass

$$\Psi_{klm}(\vec{r}) = R_{kl}(r)Y_{lm}(\theta,\varphi)$$

color-singlet states

- **mS eigenstate components** in one dipole:

$$c_{mS}(t)=\langle R_{mS}(r)|\frac{\psi(r,t)}{r}\rangle=\int R_{mS}(r)\psi(r,t)\cdot r dr$$



Initial conditions in HIC

1. $c\bar{c}$ internal Initial wavefunction:

Taken as quarkonium eigenstates
(neglect the pre-equilibrium effect)

$$\psi_{c\bar{c}}(\tau = \tau_0) = \phi_{1S,2S}(\mathbf{r})$$

Initial direct yields: charmonium

$$f_{pp}^{J/\psi} : f_{pp}^{\chi_c} : f_{pp}^{\psi(2S)} = 0.68 : 1 : 0.19$$

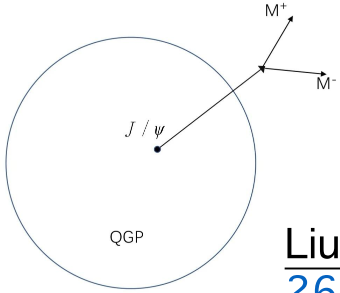
bottomonium

State	$\Upsilon(1s)$	$\chi_b(1p)$	$\Upsilon(2s)$	$\chi_b(2p)$	$\Upsilon(3s)$
$\sigma_{\exp}(nb)$	57.6	33.51	19	29.42	6.8
$\sigma_{\text{direct}}(nb)$	37.97	44.2	18.27	37.68	8.21

2. The initial momentum and spatial distribution of the center of $c\bar{c}$ dipole

$$f_\Psi(\mathbf{p},\mathbf{x}|\mathbf{b}) = (2\pi)^3\delta(z)T_{\rm p}(\mathbf{x}_T)T_{\rm A}(\mathbf{x}_T - \mathbf{b}) \times \mathcal{R}_{\rm g}(x_g,\mu_{\rm F},\mathbf{x}_{\rm T} - \mathbf{b})\frac{d\bar{\sigma}_{pp}^{\Psi}}{d^3\mathbf{p}},$$

Shadowing effect from EPS09 NLO



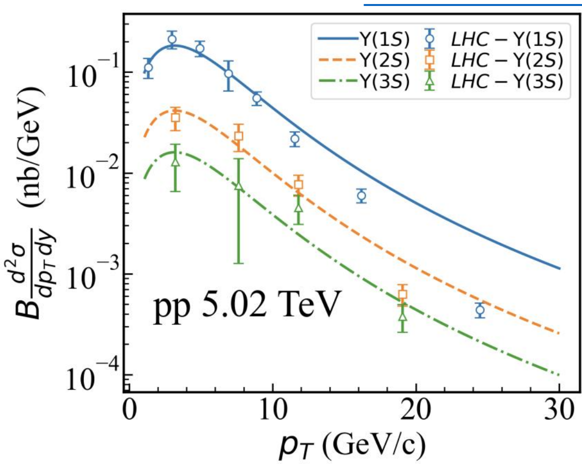
Liu,Zhou,BC, 2604.09198

The initial momentum of $c\bar{c}$ dipoles in pp,

$$\frac{dN_{J/\psi}}{2\pi p_T dp_T} = \frac{(n-1)}{\pi(n-2)\langle p_T^2\rangle_{pp}}\left[1 + \frac{p_T^2}{(n-2)\langle p_T^2\rangle_{pp}}\right]^{-n}$$

n = 3.2 $\quad \langle p_T^2\rangle(y) = \langle p_T^2\rangle(y=0)[1 - (\frac{y}{ymax})^2]$

$ymax = \ln(\sqrt{s_{NN}}/m_\Psi)$



nuclear modification factor

- **The initial yields of charmonium eigenstates**

$$n_{mS}^{t=0}(\mathbf{x}_T, p_T|\mathbf{b}, y) = n_{c\bar{c}}(\mathbf{x}_T, p_T|\mathbf{b}) \times |\langle R_{mS}(r)|\phi_0(r)\rangle|^2$$

$$|c_{mS}(t=0|\mathbf{b})|^2 = \int d\mathbf{x}_T \int_{p_{T1}}^{p_{T2}} dp_T \; n_{mS}(\mathbf{x}_T, p_T|\mathbf{b})$$

- **Charmonium direct R_{AA} with hot medium effects,**

$$R_{pA}^{\rm direct}(nl) = \frac{\langle |c_{nl}(t)|^2\rangle_{\rm en}}{\langle |c_{nl}(t_0)|^2\rangle_{\rm en}} = \frac{\int d\mathbf{x}_\Psi d\mathbf{p}_\Psi |c_{nl}(t, \mathbf{x}_\Psi, \mathbf{p}_\Psi)|^2 \frac{dN_{pA}^\Psi}{d\mathbf{x}_\Psi d\mathbf{p}_\Psi}}{\int d\mathbf{x}_\Psi d\mathbf{p}_\Psi |c_{nl}(t_0, \mathbf{x}_0, \mathbf{p}_\Psi)|^2 \frac{dN_{pA}^\Psi}{d\mathbf{x}_\Psi d\mathbf{p}_\Psi}}$$

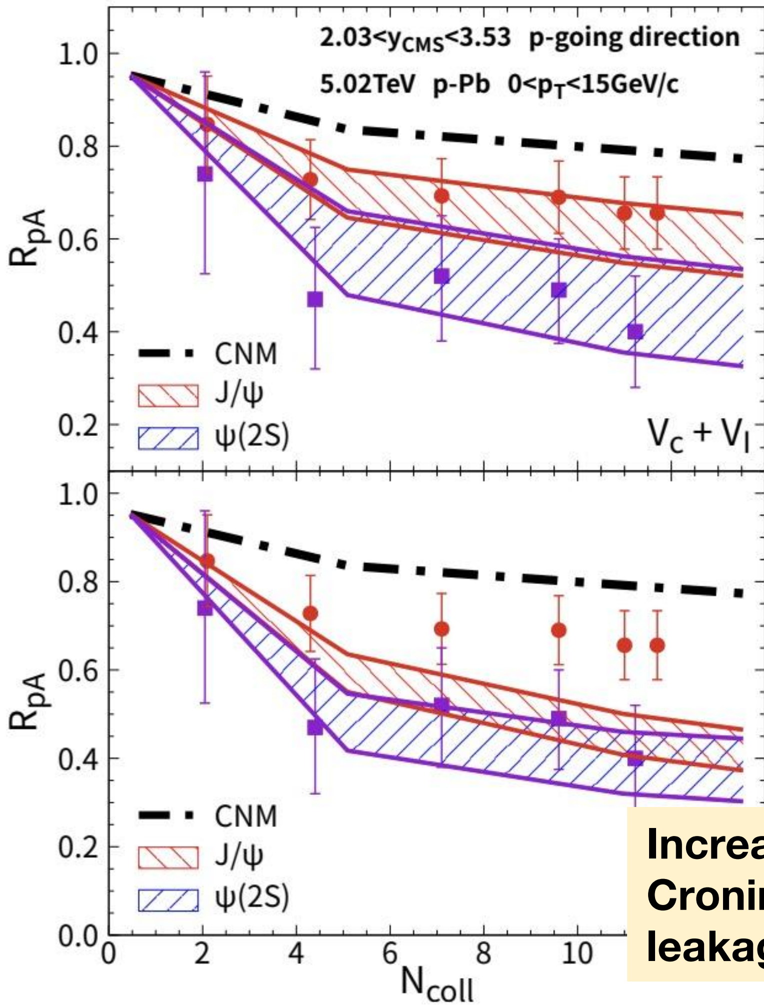
$$R_{pA}(J/\psi) = \frac{\sum_{nl}\langle |c_{nl}(t)|^2\rangle_{\rm en} f_{pp}^{nl}\mathcal{B}_{nl\to J/\psi}}{\sum_{nl}\langle |c_{nl}(t_0)||\rangle^2\rangle_{\rm en} f_{pp}^{nl}\mathcal{B}_{nl\to J/\psi}}$$

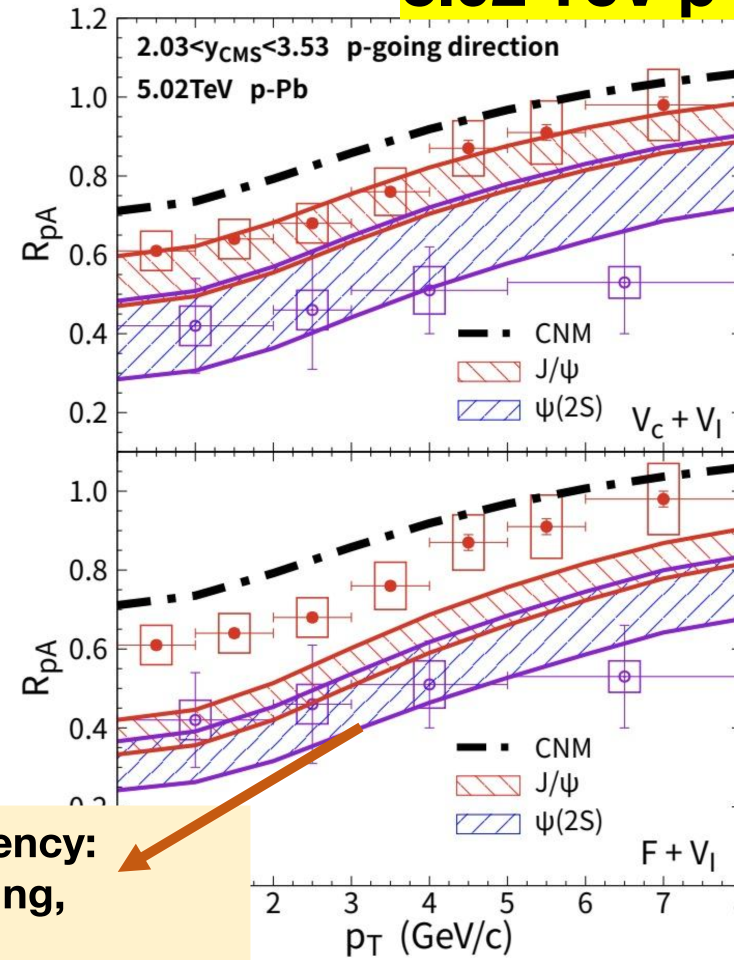
$c\bar{c}$ dipoles move inside QGP

$$\mathbf{R}_{c\bar{c}}(\tau+\Delta\tau) = \mathbf{R}_{c\bar{c}} + \mathbf{v}_{c\bar{c}}\cdot\Delta\tau$$

Quarkonium in p-Pb collisions

5.02 TeV p-Pb





Increasing tendency: Cronin, shadowing, leakage effects

Band comes from the uncertainty in V_l

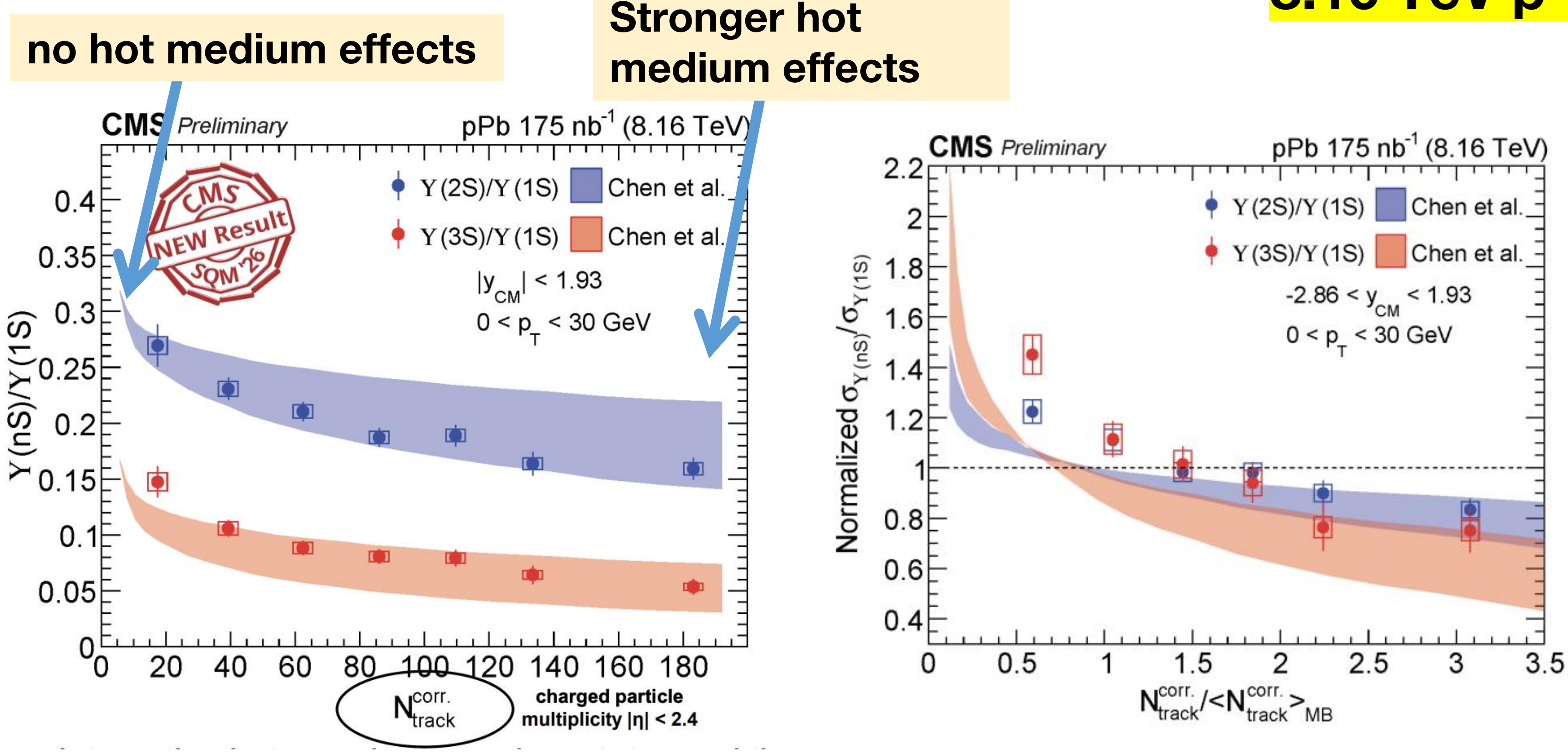
Wen, Shi, Du, BC, CPC 46 (2022) 114102

- R_{pA} as a function of N_{coll}
- R_{pA} as a function of p_T

weak in-medium potential **V=F(T,r)**
Strong in-medium potential **V=Vc(r)**

Quarkonium in p-Pb collisions

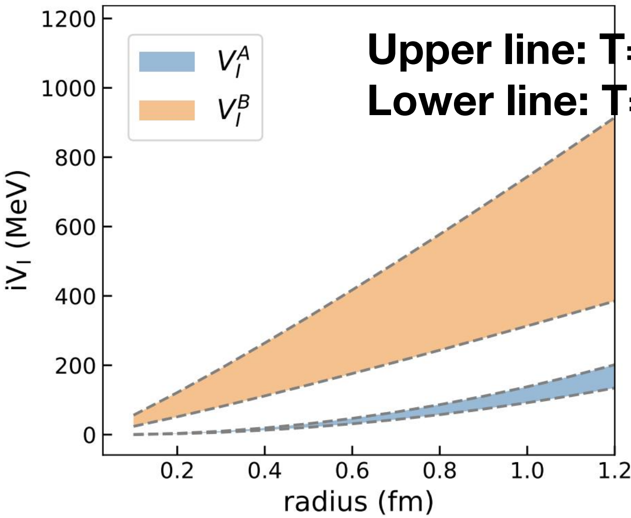
8.16 TeV p-Pb



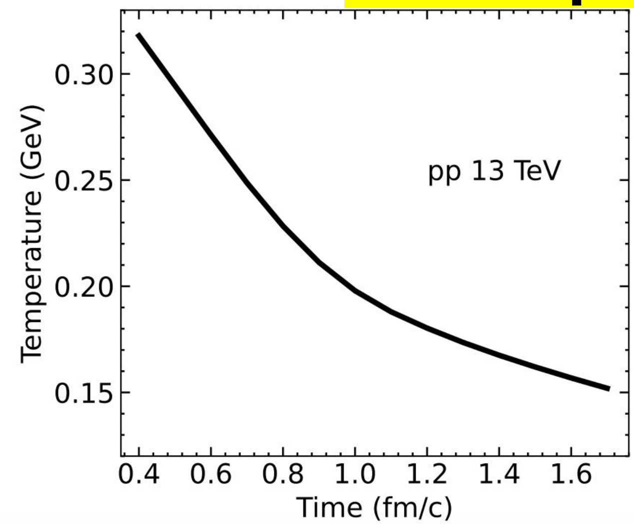
- **Bottomonium yield ratios nS/1S:** **decreasing tendency induced by the final-state-interactions,** not the initial conditions
- Normalized cross section: similar as the yield ratio
- Band: induced by the uncertainty of the imaginary potential

Quarkonium in high-multiplicity pp

13 TeV p-p

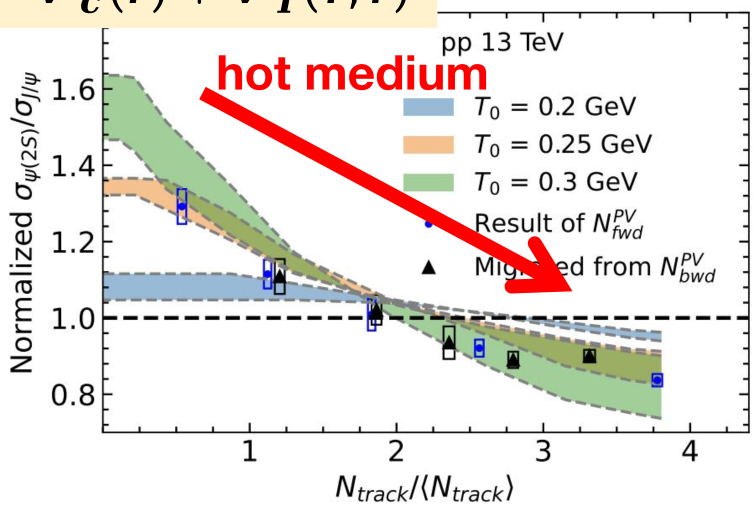


Upper line: T=300 MeV
Lower line: T=200 meV

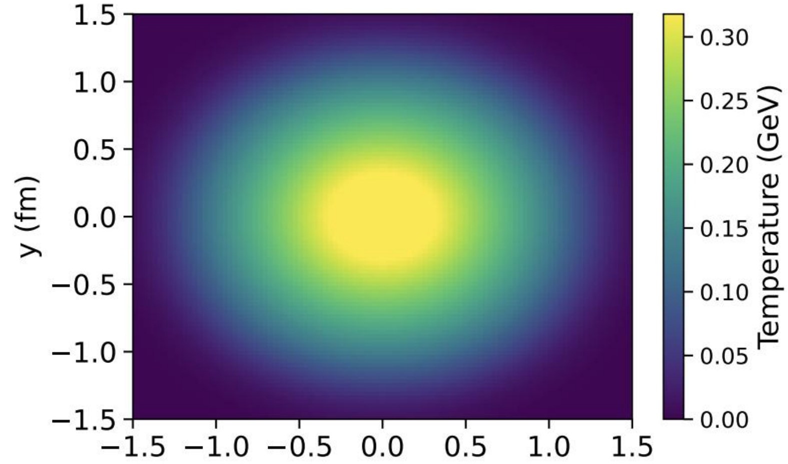


$$V = V_c(r) + V_I(T, r)$$

No color screening



Bulk medium evolution from MUSIC



Quarkonium suppression from imaginary potential

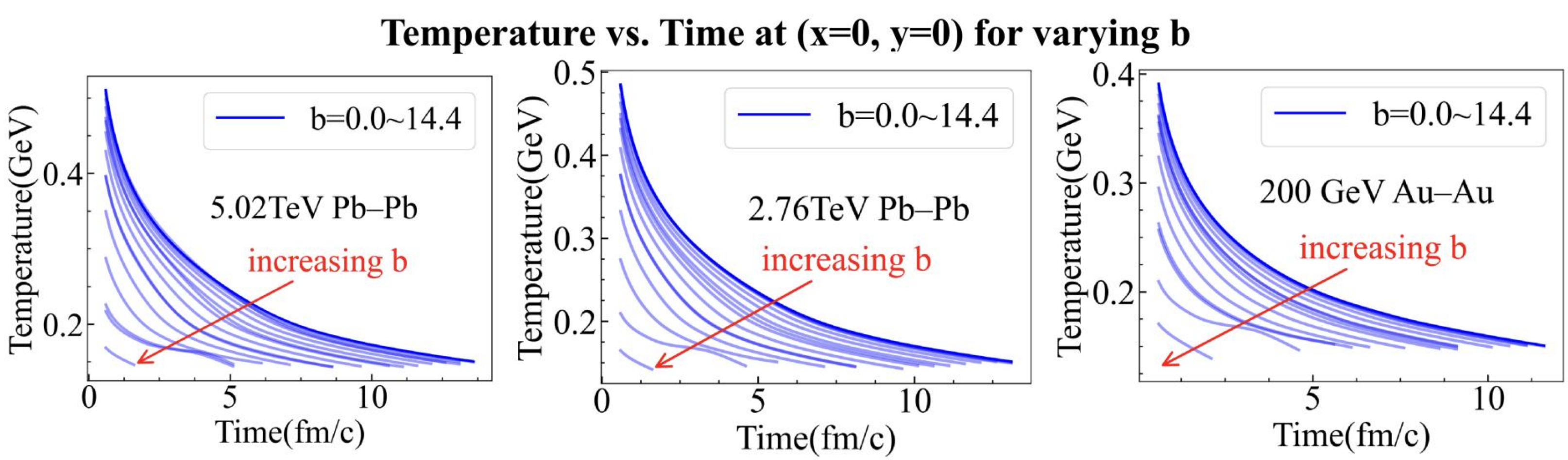
Y.Bai, BC, EPJC 84 (2024) 1193

Quarkonium in Pb-Pb

-

Collision System	t_0 (fm/c)	$T_0(x_T{=}0\|b=0)$ (MeV)
$\sqrt{s_{NN}} = 5.02$ TeV (Pb–Pb)	0.6	510
$\sqrt{s_{NN}} = 2.76$ TeV (Pb–Pb)	0.6	484
$\sqrt{s_{NN}} = 200$ GeV (Au–Au)	0.6	390

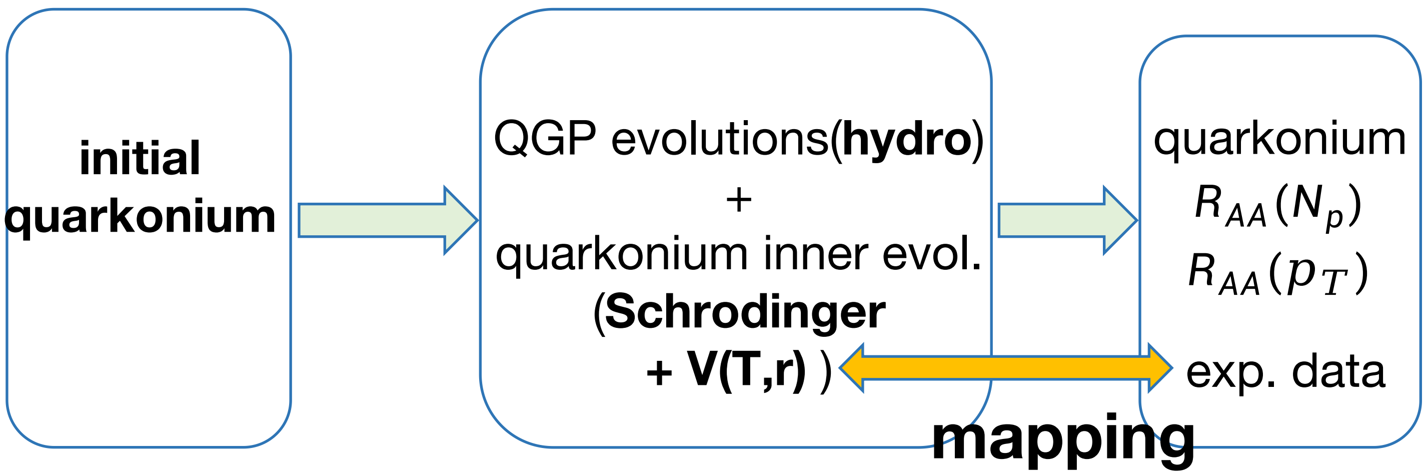
Maximal temperature of QGP at three systems



Medium temperatures from MUSIC

parametrization of V(T,r)

various phenomelogical studies in different systems indicate
a strong heavy quark potential at finite temperatures,
and quarkonium suppression is induced by the imaginary potential.
A systematic study is urgent.



in-medium HQ potential parametrization

$$V(T,r)=\begin{cases} V_R(T,r)+V_I(T,r), & T\geq T_{\rm sw} \\ V_c(r), & T< T_{\rm sw}\end{cases}$$

above this T, QGP effects dominant in quarkonium

parametrization of V(T,r)

Real part of the potential:

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

Debye mass: $\mu_D = a_4 T\sqrt{4\pi N_c\left(1+\frac{N_f}{6}\right)\frac{\alpha}{3}}.$

Imaginary part of the potential:

$$V_I = -iT^{a_0}\left(a_1 r + a_2 r^{a_3}\right)$$

parameter ranges:

Parameter	Sampling Range
a_0	$[1.0,\ 2.0]$
a_1	$[0.0,\ 0.5]$
a_2	$[0.2,\ 0.7]$
a_3	$[2.0,\ 3.0]$
a_4	$[0.1,\ 1.0]$
$T_{\rm sw}$	$[0.17,\ 0.25]$

parametrization of V(T,r)

Real part of the potential:

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

Debye mass:

$$\mu_D = a_4 T\sqrt{4\pi N_c\left(1+\frac{N_f}{6}\right)\frac{\alpha}{3}}$$

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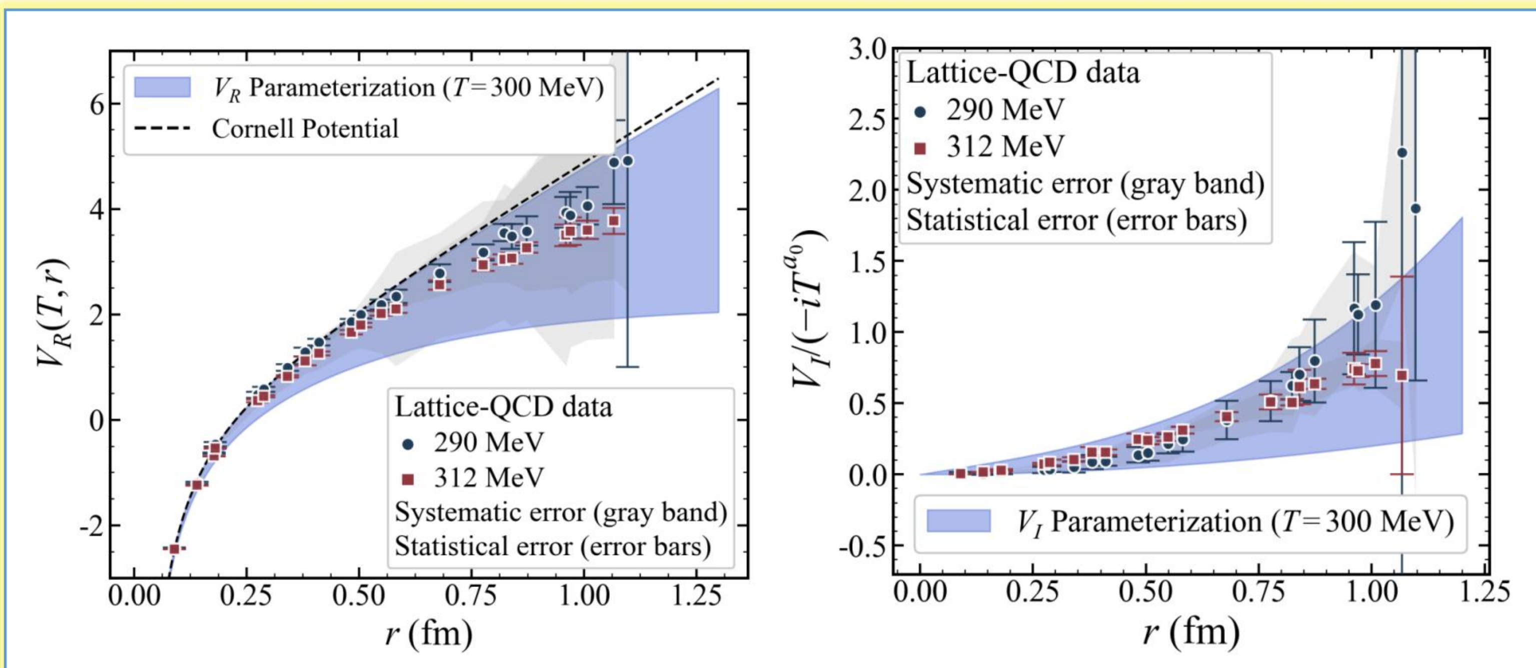
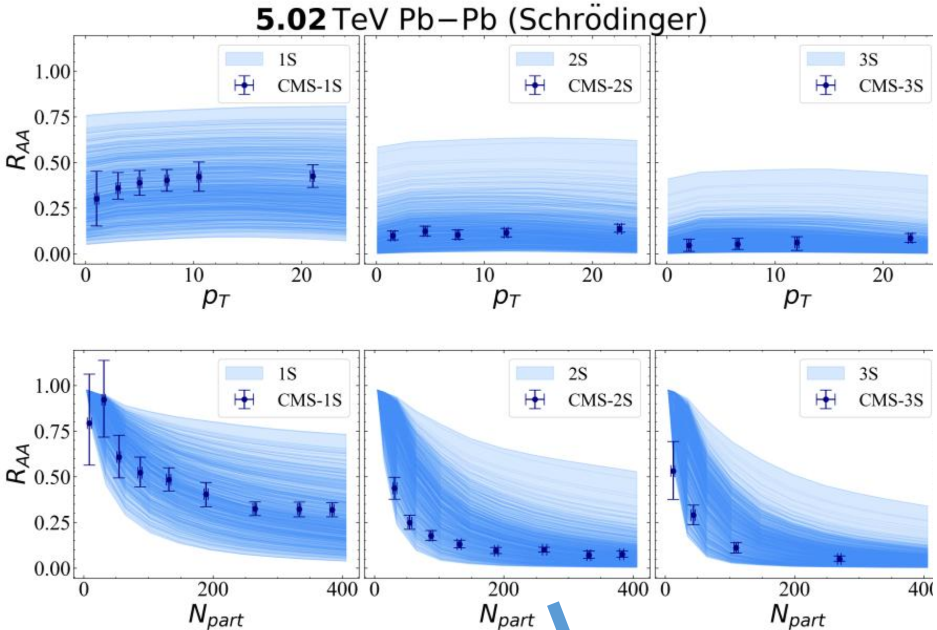
arXiv: 2604.09198

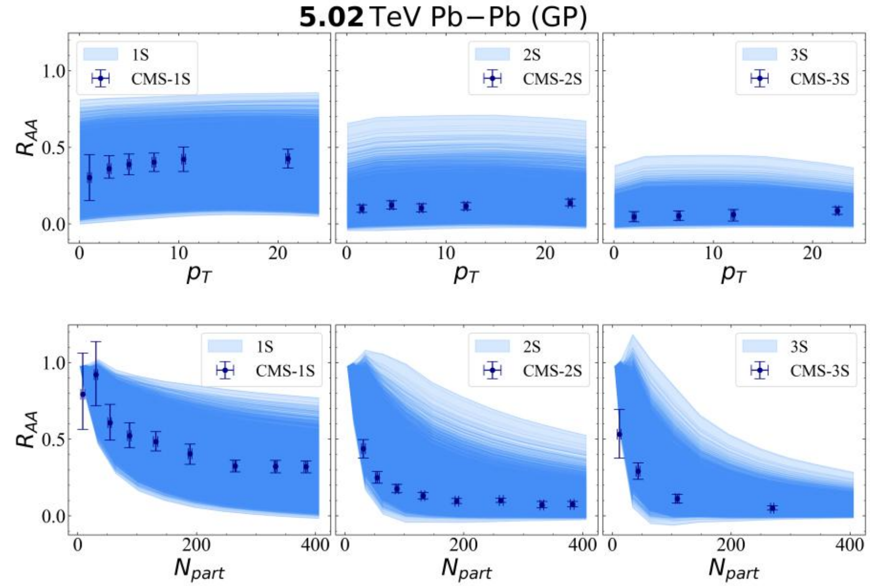


dataset generation

Schrodinger model



Gaussian process emulator



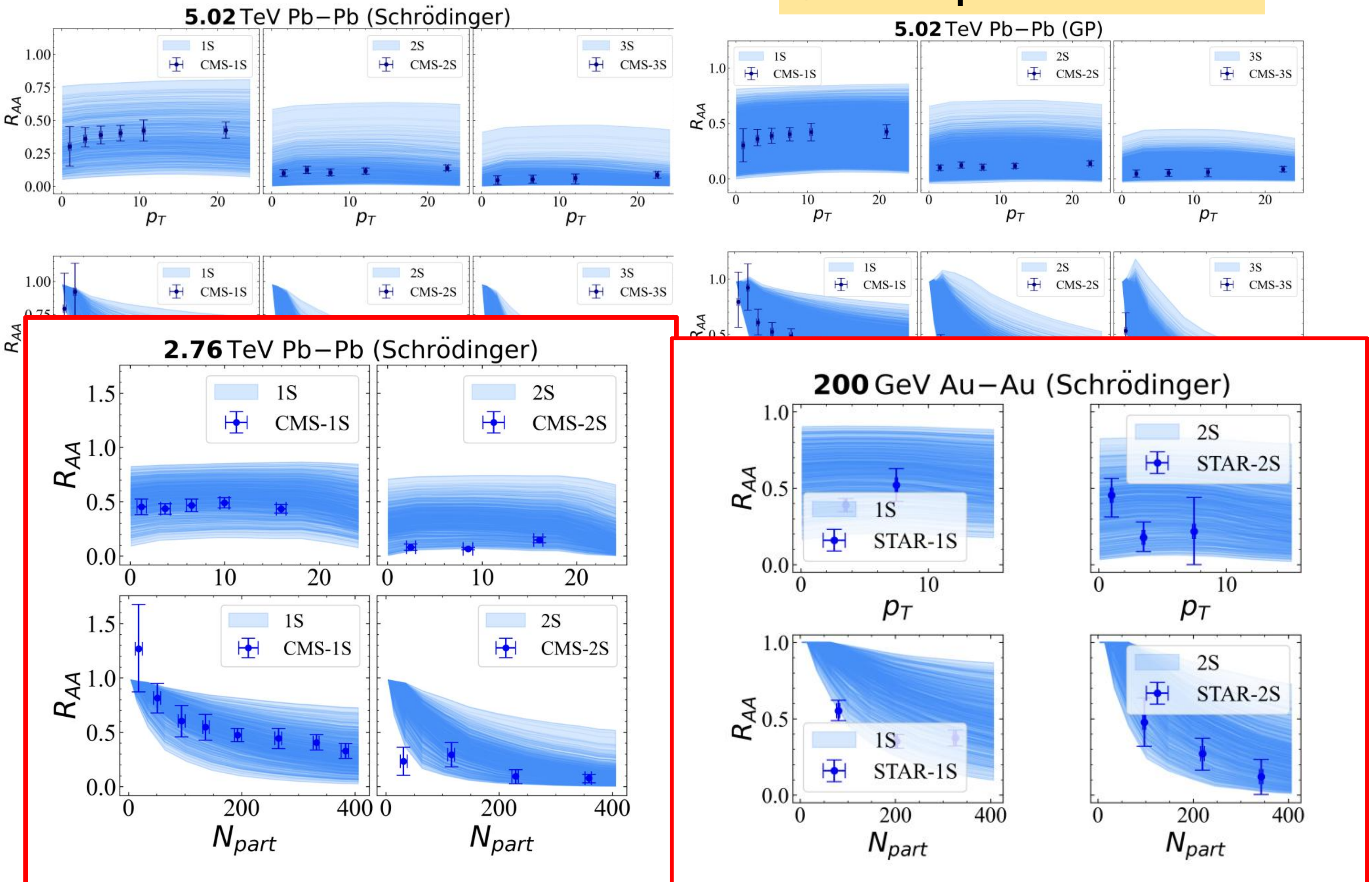
generate N=1000 samples **of V(T,r),** take into Schrodinger equation model coupled with the corresponding QGP profiles.

take 80% of original events from Schrodinger model into **Principal Component Analysis and Gaussian Process** emulator to generate a larger dataset, **10, 000 samples**.

dataset generation

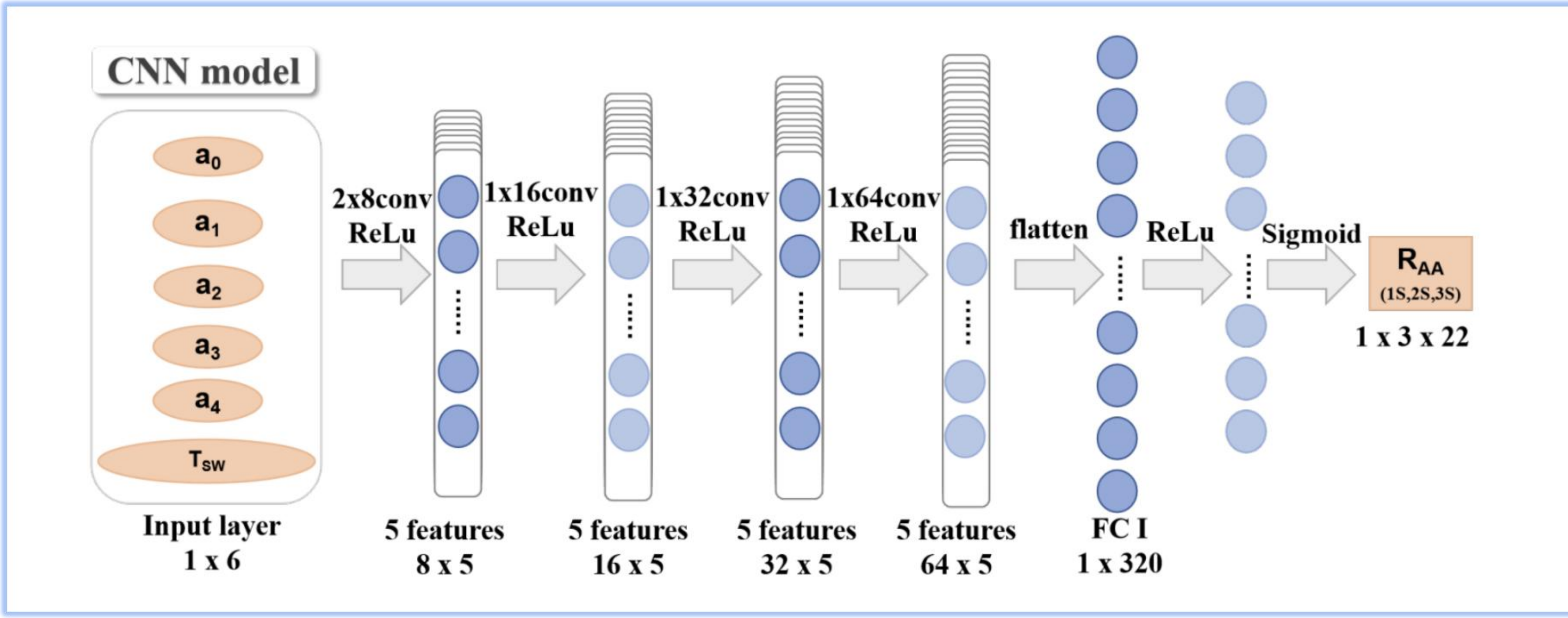
Schrodinger model

Gaussian process emulator



CNN framework

A convolutional Neural network is contructed to learn the mapping between V(T,r) and quarkonium observables



$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N_e} \frac{\left[y_{\mathrm{obs},i} - y_{\mathrm{CNN},i}(\boldsymbol{\theta})\right]^2}{\sigma_i^2}$$

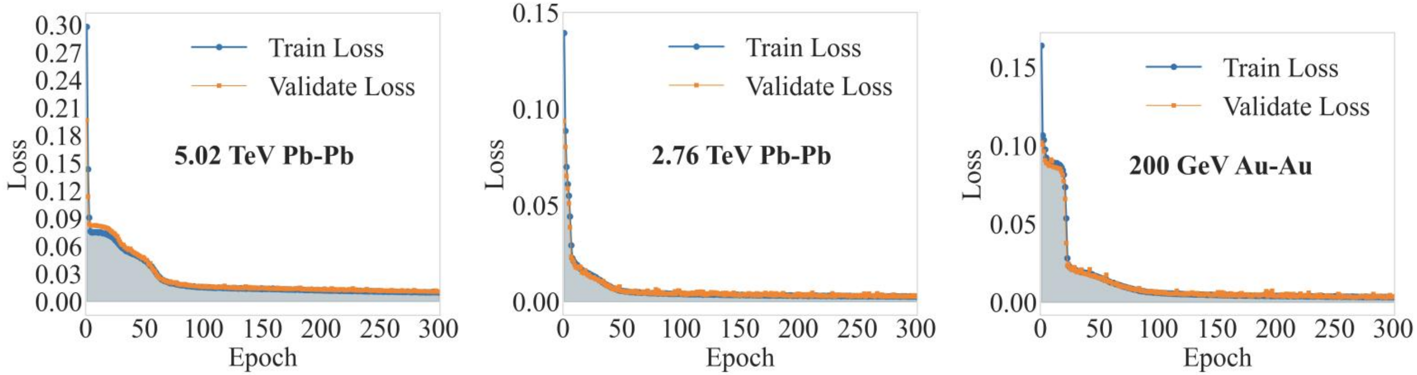
$$\mathbf{y}^{(g)}_{\mathrm{CNN}\to\mathrm{obs}}(\boldsymbol{\theta}) = \mathcal{I}_g\,\mathbf{y}_{\mathrm{CNN}}(\boldsymbol{\theta})$$

The CNN is trained to minimize the loss function

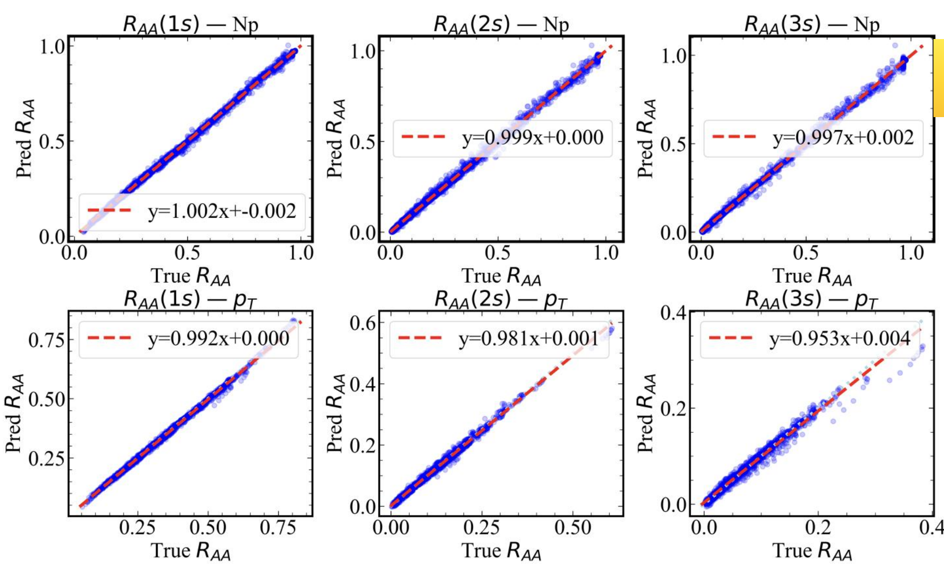
$$\mathcal{L}(\boldsymbol{\theta}) = -\log p(\mathbf{y}_{\mathrm{obs}} \mid \boldsymbol{\theta}) = \sum_g \sum_{i\in g} \frac{1}{2} \frac{\left(\mathbf{y}^{(g)}_{\mathrm{CNN}\to\mathrm{obs},i}(\boldsymbol{\theta}) - \mathbf{y}^{(g)}_{\mathrm{obs},i}\right)^2}{\sigma_i^2}$$

performance of CNN

loss function of three CNNs:



After 3 CNNs are well trained, use additional 20% of N=1000 events to test the CNN respectively.



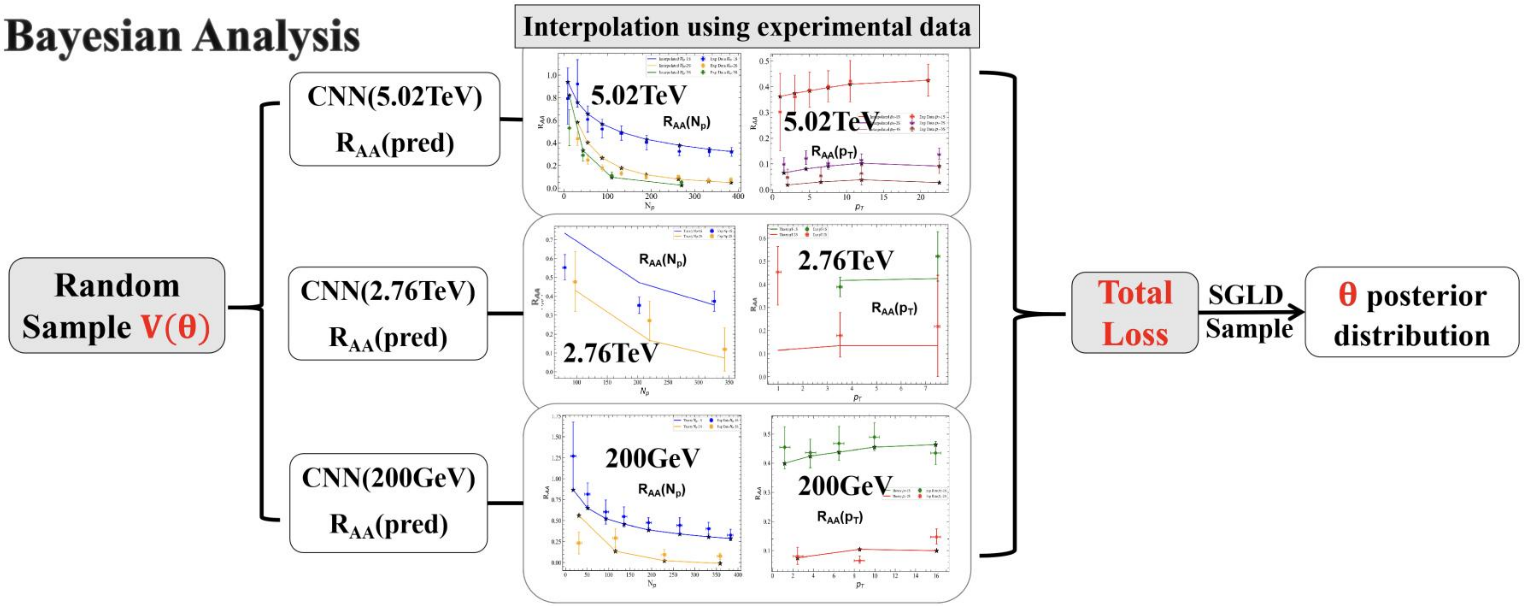
5.02 TeV Pb-Pb

x-axis: true value of R_{AA} from Schrodinger model

y-axis: predicted value of R_{AA} from CNN model

Similar for 2.76 TeV, 200 GeV

Extraction of V(T,r)

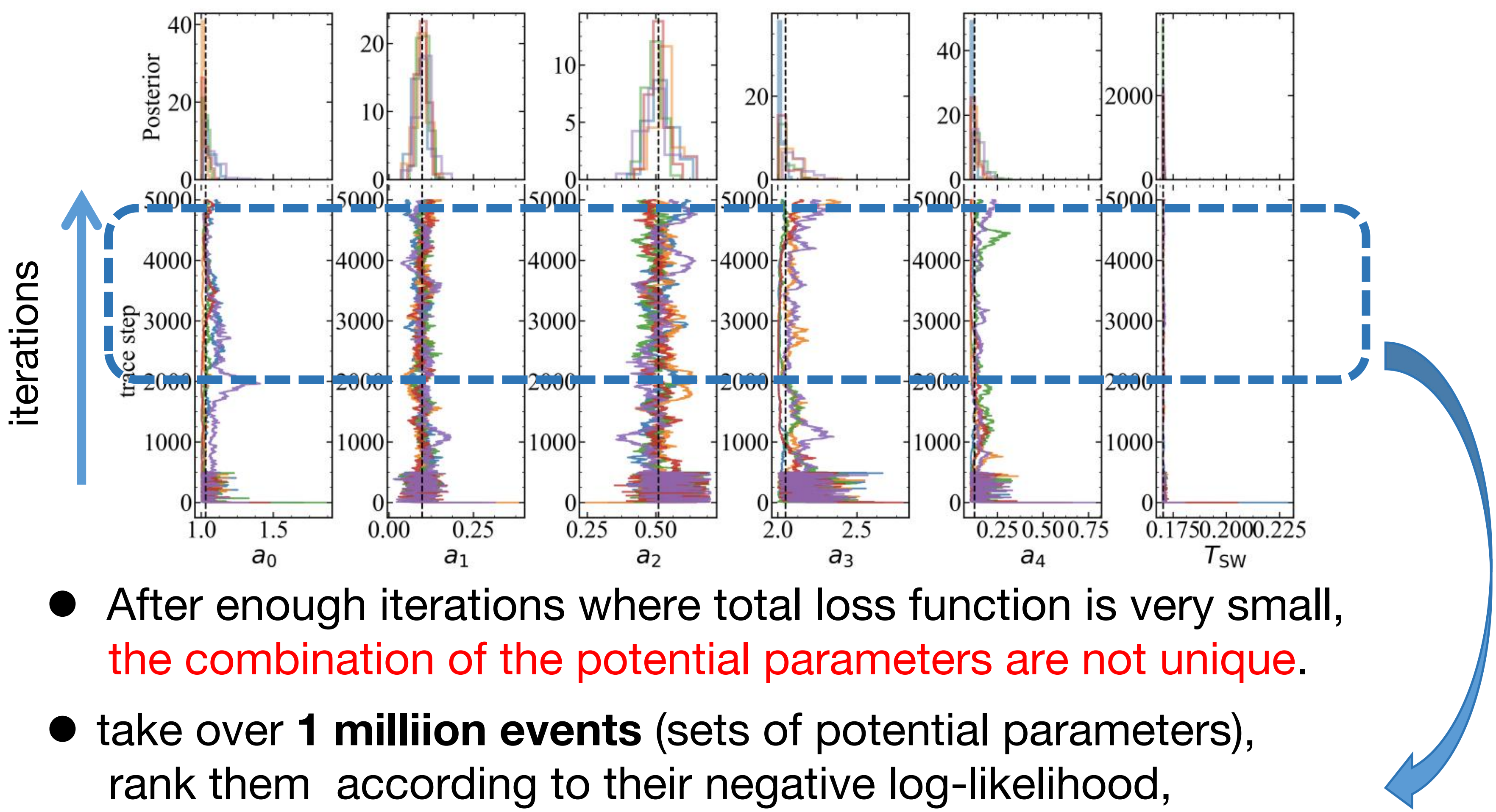


- **Now use the reverse process to extract V(T,r)** with quarkonium observables in all three systems **(5.02 TeV Pb-Pb, 2.76 TeV Pb-Pb, 200 GeV Au-Au)**

$$L_{tot} = L_{5.02TeV} + L_{2.76TeV} + L_{0.2TeV}$$

Take experimental data points of bottomonium, use **Stochastic Gradient Langevin Dynamics (SGLD)** algorithm to obtain the values of the potential parameters which gives **minimal total loss function**.

extraction of V(T,r)



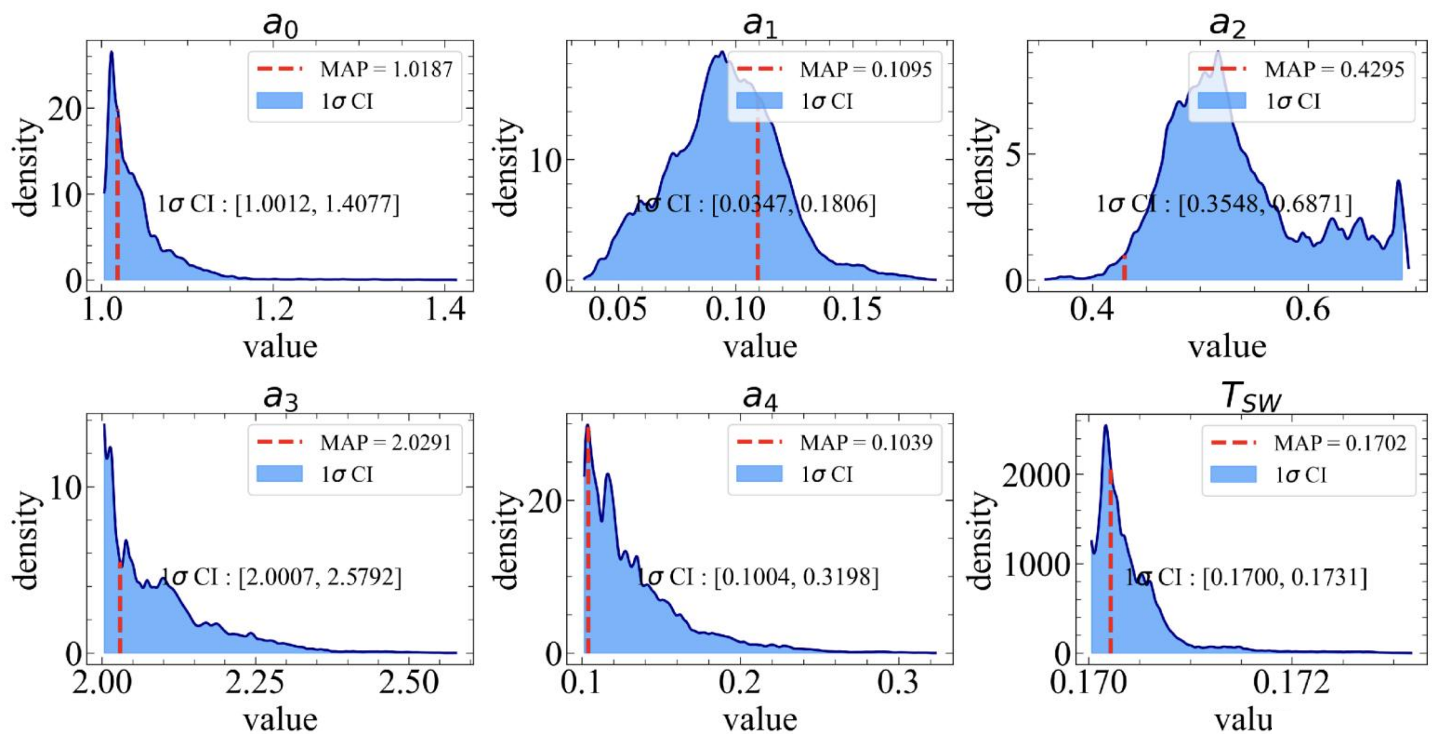
- After enough iterations where total loss function is very small, the combination of the potential parameters are not unique.
- take over **1 milliion events** (sets of potential parameters), rank them according to their negative log-likelihood, **in ascending order, get the first 68.27% of samples**

$$\mathcal{S}_\gamma = \{\boldsymbol{\theta}\} \qquad \gamma = 68.27\%$$

extraction of V(T,r)

- use the values in $\mathcal{S}_\gamma = \{\boldsymbol{\theta}\}$ to plot the distributions of the potential parameters, which gives a small total loss function

- a small loss function indicates that These potentials can simultaneously explain well the exp. data in three collision systems.



$$\widehat{\boldsymbol{\theta}}_{\mathrm{MAP}} = \arg\min_{\boldsymbol{\theta}\in\Omega} \mathcal{L}(\boldsymbol{\theta})$$

The distributions of the potential parameters (dashed line: optimal value)

extraction of V(T,r)

1 sigma distributions of the potential parameters according to the samples extracted in the SGLD process

Parameters	1σ Uncertainties	MAP Value
a_0	$[1.001, 1.407]$	1.018 → linear T-dependence
a_1	$[0.034, 0.180]$	0.109
a_2	$[0.354, 0.687]$	0.429
a_3	$[2.000, 2.579]$	2.029
a_4	$[0.100, 0.319]$	0.103
T_{sw}	$[0.170, 0.173]$	0.170

Potential parametrization:

$$V_I = -\,i\,T^{a_0}\left(a_1 r + a_2 r^{a_3}\right)$$

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

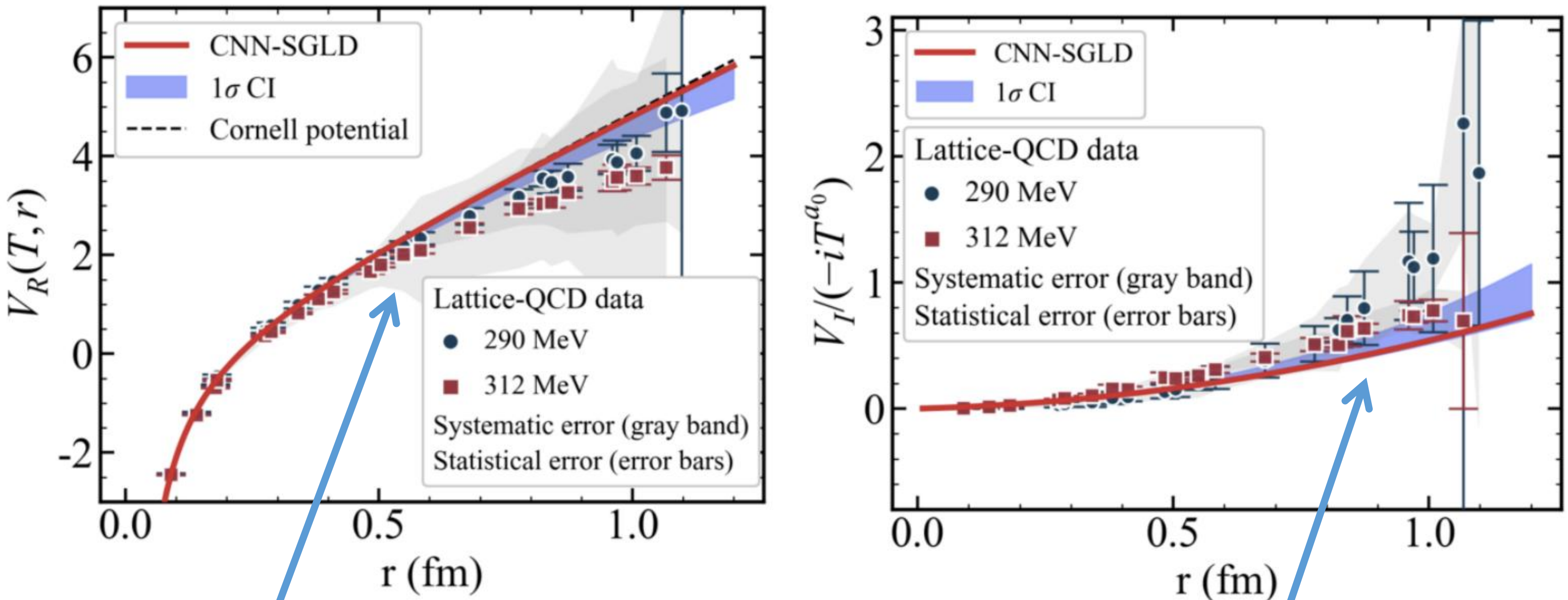
$$\text{with Debye mass } \mu_D = a_4 T\sqrt{\frac{4\pi N_c}{3}\left(1+\frac{N_f}{6}\right)\alpha}$$

✓ **small Debye mass -> small color screening effect**

extraction of V(T,r)

1 sigma distributions of the potential parameters according to the samples extracted in the SGLD process

Parameters	1σ Uncertainties	MAP Value



- **real potential:** very close to the vacuum case (see CNN-SGLD line)
- **Imaginary potential:** a bit smaller than the lattice QCD results.

Validation of the CNN-SGLD framework

① **randomly generate a set of potential parameters V(T,r)**

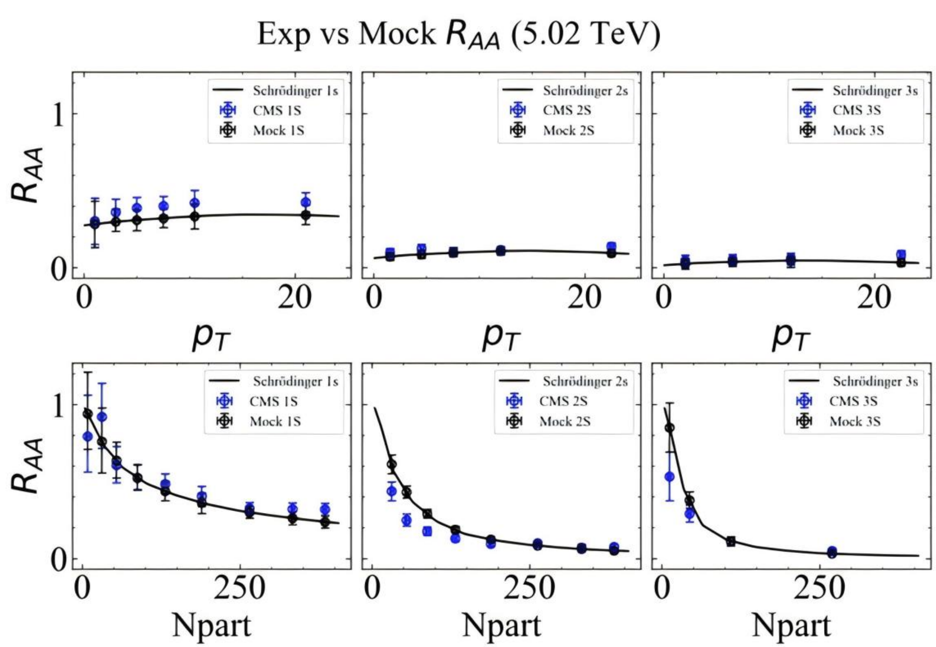
$$\theta^{\text{mock}} = (a_0, a_1, a_2, a_3, a_4, T_{\text{sw}}) = (1.6, , 0.2, , 0.3, , 2.7, , 0.3, , 0.18)$$

② **take into Schrodinger equation, to calculate the R_{AA}**

③ **We now know the relation:**

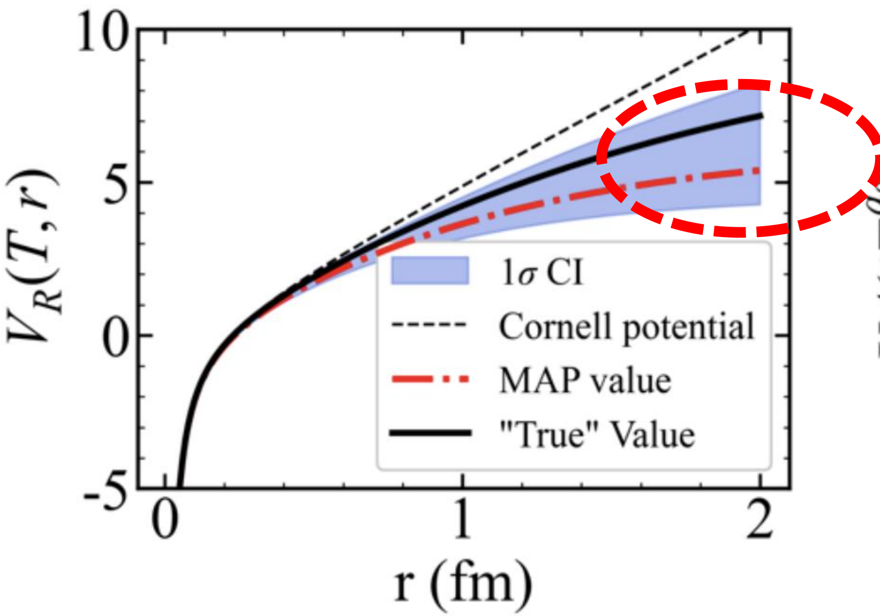
bottomonium R_{AA} ⟷ V(T,r)

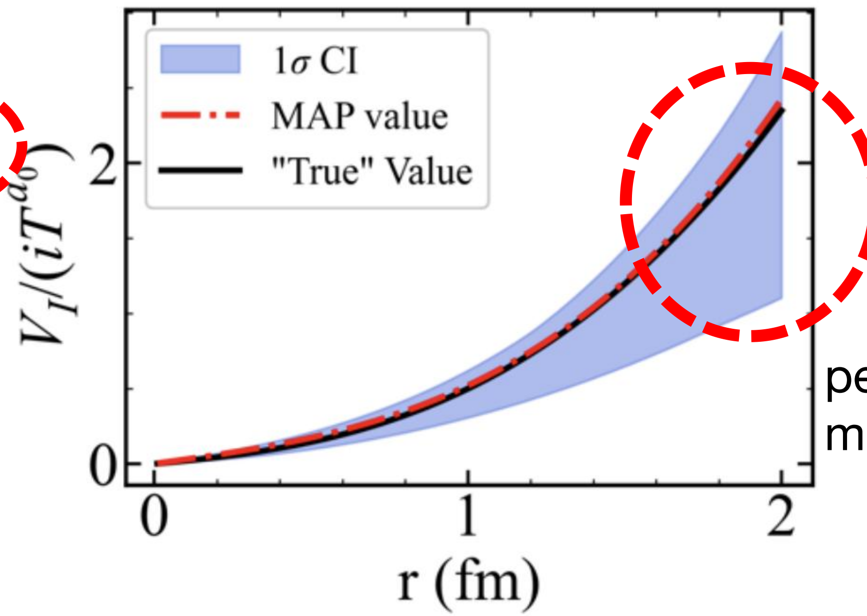
Take R_{AA} back into the CNN-SGLD framework



- Process the theoretical R_{AA} into the format of experimental data,
- it can then be fed into the CNN-SGLD framework.

Validation of the CNN-SGLD framework



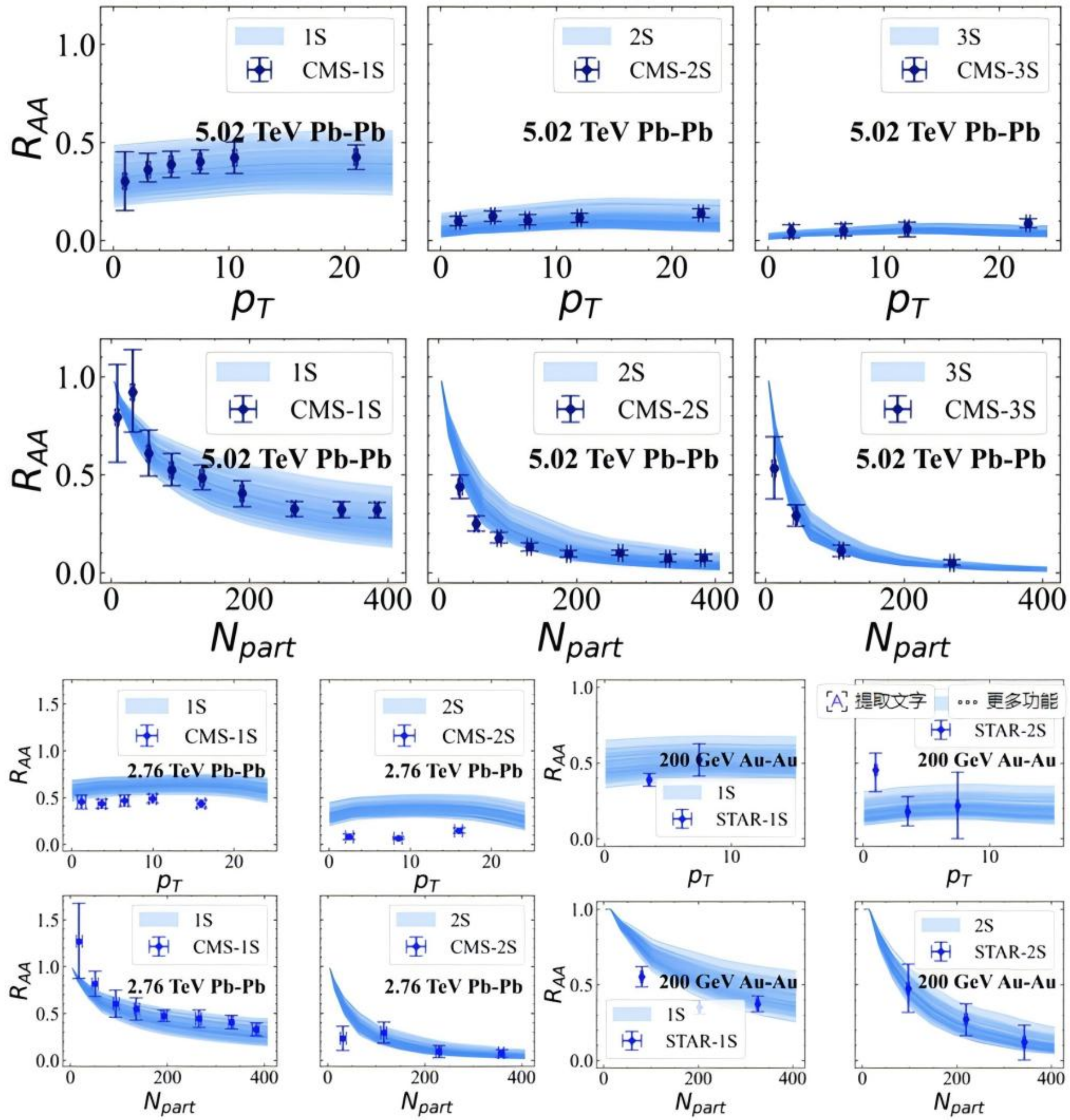


perfect match

- True value: potential of $\boldsymbol{\theta}^{\text{mock}} = (a_0, a_1, a_2, a_3, a_4, T_{\text{sw}}) = (1.6, , 0.2, , 0.3, , 2.7, , 0.3, , 0.18)$

- MAP value and the 1 sigma unvertanty: from **CNN-SGLD framework**
- **conclusion:**
  CNN-SGLD framework can correctly resconstruct the in-medium potential;

recalculate the RAA with the extracted V



5.02 TeV
1S, 2S, 3S

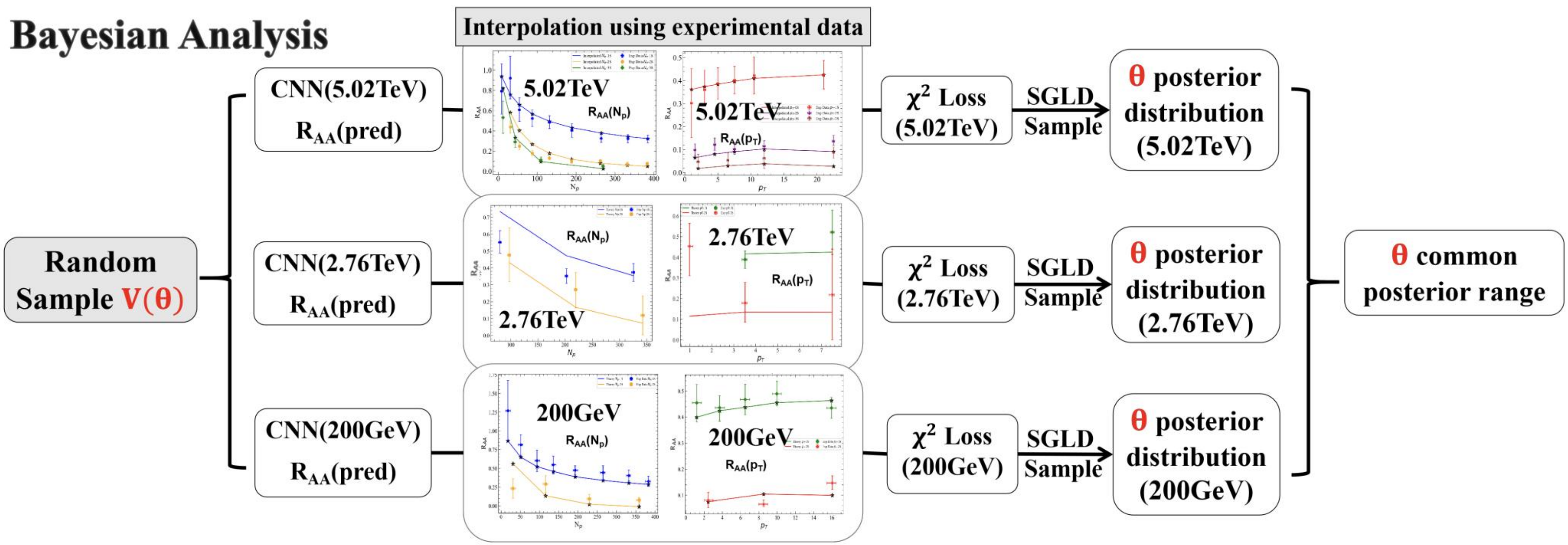
2.76 TeV
1S, 2S

200 GeV
1S, 2S

8

method 2: extract V(T,r) from each system

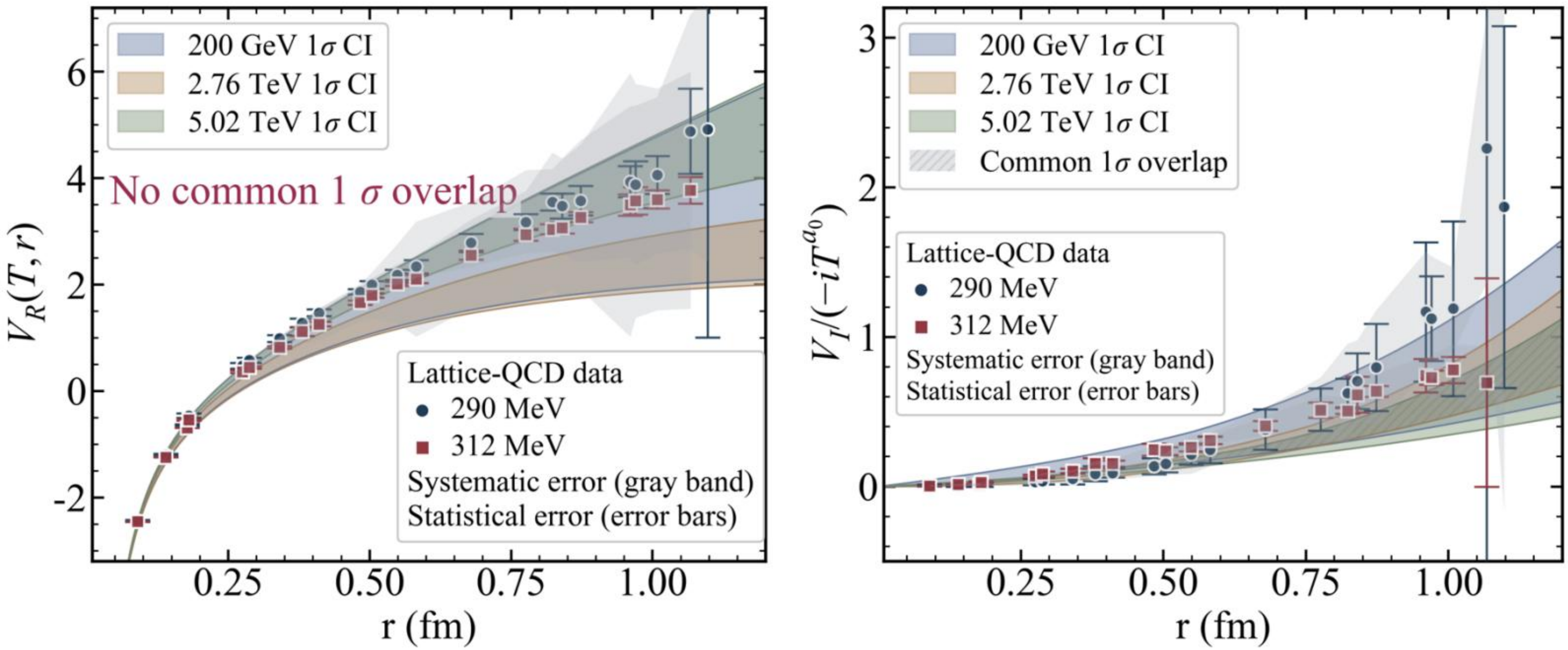
Another test



extract V(T,r) from each system

Another test

Parameter	5.02 TeV Pb–Pb	2.76 TeV Pb–Pb	200 GeV Au–Au	overlap
a_0	[1.005, 1.500]	[1.011, 1.941]	[1.039, 1.971]	[1.039, 1.500]
a_1	[0.051, 0.209]	[0.002, 0.132]	[0.122, 0.47]	[0.122, 0.132]
a_2	[0.221, 0.560]	[0.375, 0.698]	[0.201, 0.692]	[0.375, 0.560]
a_3	[2.012, 2.967]	[2.056, 2.983]	[2.01, 2.992]	[2.056, 2.967]
a_4	[0.100, 0.497]	[0.670, 1]	[0.120, 0.968]	None
T_{sw}	[0.170, 0.173]	[0.170, 0.174]	[0.170, 0.185]	[0.1701, 0.173]



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Summary

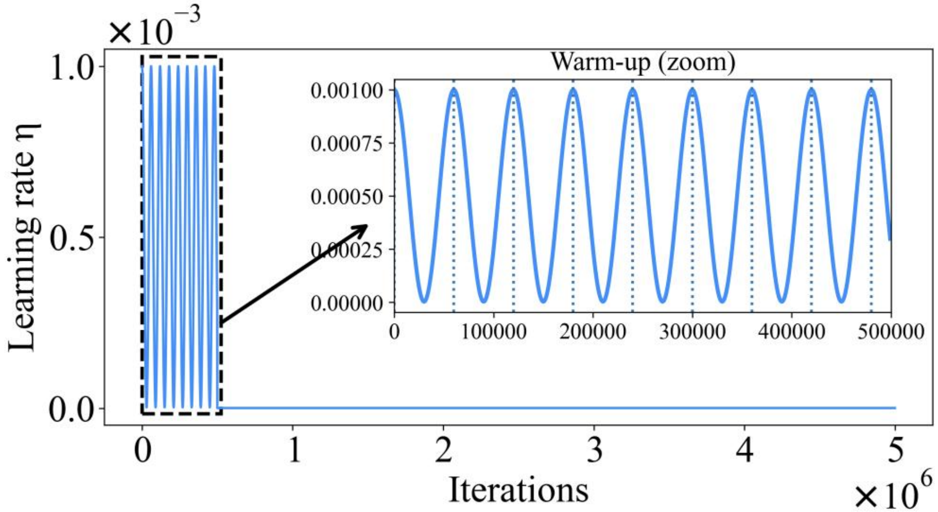
- **The Schrodinger model with the complex heavy quark potential** are introduced, applied in the high-multiplicity pp, p-Pb, and Pb-Pb collisions
  Phenomelogical studies about quarkonium indicate **a strong potential** in the medium from RHIC to LHC energies.

- A **CNN-SGLD framework is developed**. It extracts the in-medium heavy quark potential with the experimental data of quarkonium from (200 GeV Au-Au, 2.76 TeV Pb-Pb, 5.02 TeV Pb-Pb collisions).

- **A strong real part of the potential is obtained**, close to the Cornell potential, consistent with the lattice QCD results.
  Quarkonium suppression mainly induced by the imaginary part of the potential.

Extraction of V(T,r)

learning rate in the SGLD process,



$$\eta_{\max} = 10^{-3}$$

$$\eta_{\text{const}} = 1 \times 10^{-6}$$

$$\eta_t = \begin{cases} \eta_{\min} + \dfrac{\eta_{\max} - \eta_{\min}}{2}\left(1 + \cos\left(2\pi \dfrac{t \bmod P}{P}\right)\right), & 0 \le t < N_{\text{warm}}, \\ \eta_{\text{const}}, & t \ge N_{\text{warm}}. \end{cases}$$