Learning Hadron Interactions From Lattice QCD

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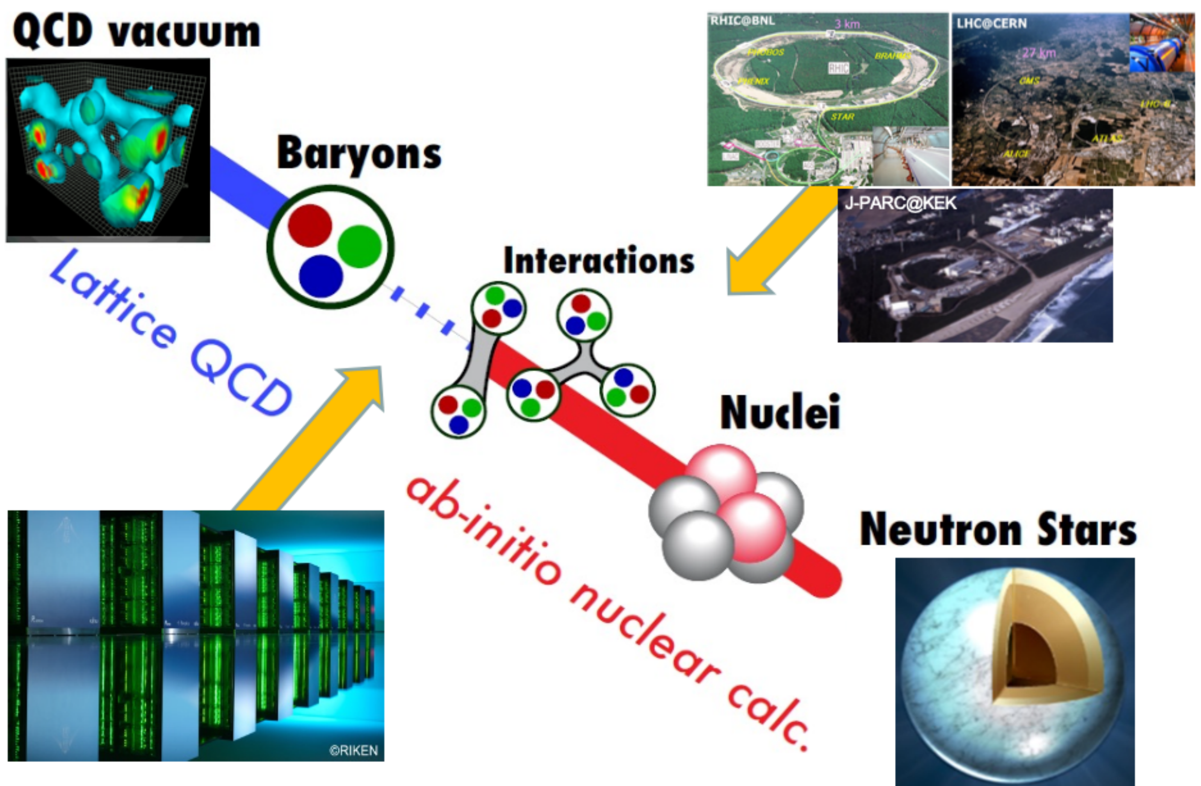
In preparation within HAL QCD collaboration (**Takumi Doi**, **Tetsuo Hatsuda**, **Yan Lyu**)

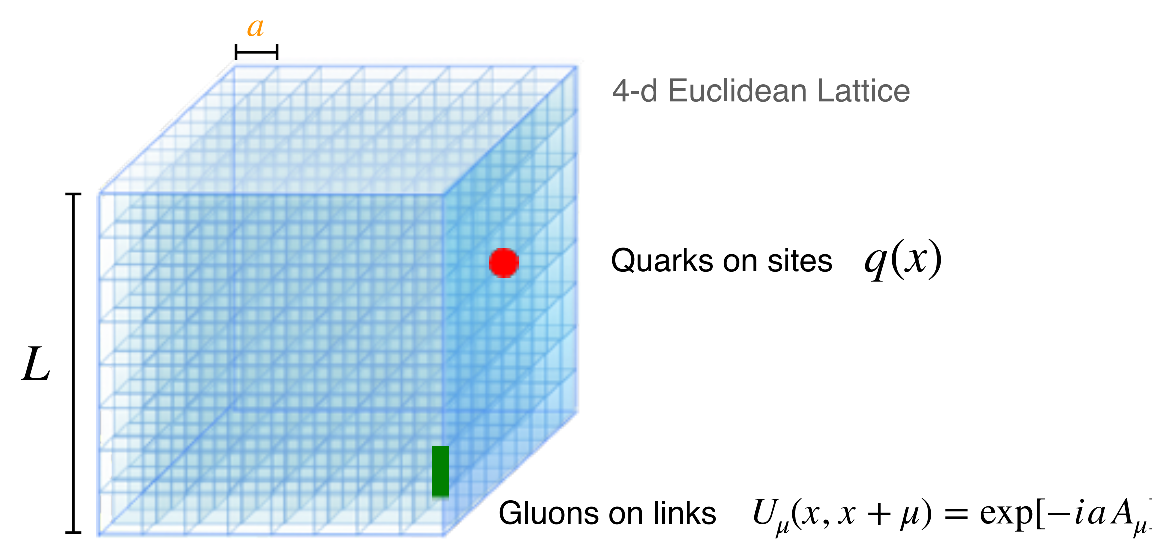
August 2, LATTICE 2024, the University of Liverpool, UK

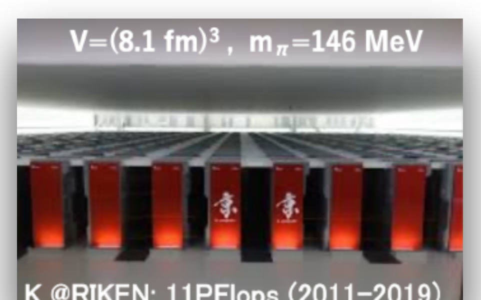
Hadron Forces

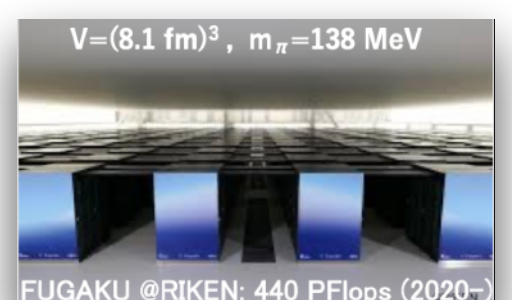


slides@T.Hatsuda

$$\mathscr{L} = -\frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a + \bar{q}\gamma^\mu(i\partial_\mu - g t^a A^a_\mu)q - m\bar{q}q$$







Huge integration variables

$\sim 10^{9-10}$ for 96^4 lattice, ~ 50 GB/config

Importance Sampling

Hybrid MC = MD + Metropolis

Continuum & Thermodynamic Limits

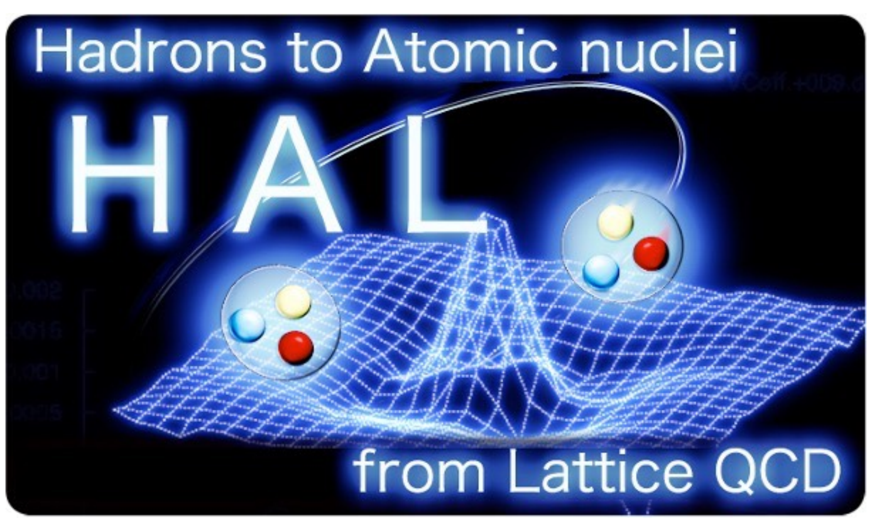
$a \to 0, L \to \infty$

HAL QCD

K(2011-2019)

Fugaku(2020-)

Hadrons to Atomic nuclei from Lattice QCD
(HAL QCD Collaboration)

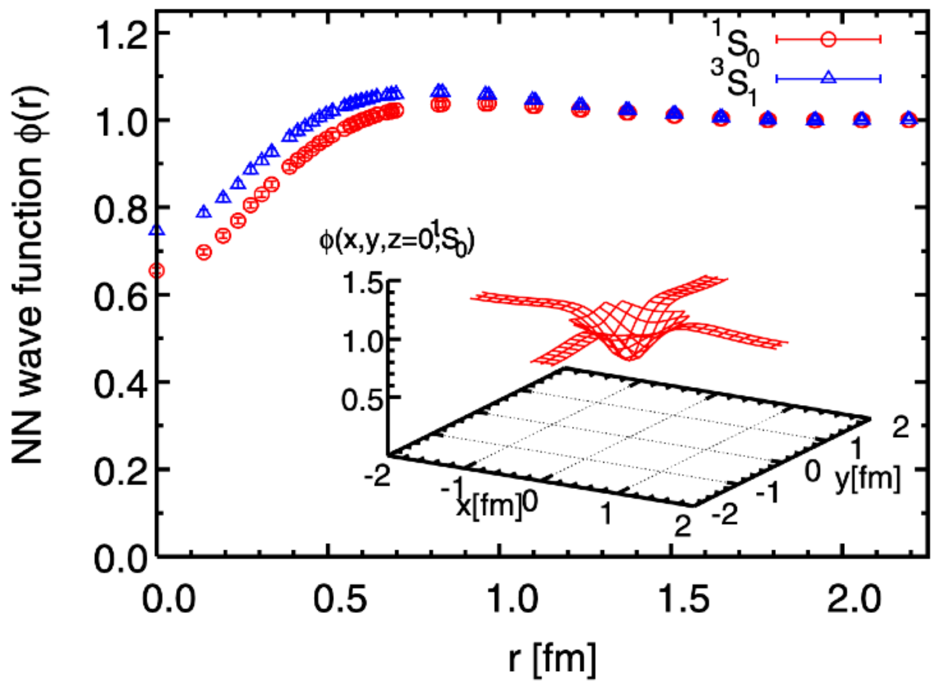


S. Aoki, T. M. Doi, E. Itou (Kyoto U.)
T. Aoyama (ISSP)
T. Doi, T. Hatsuda, Y. Lyu, L. Wang,
R. Yamada, L. Zhang (RIKEN)
F. Etminan (U. of Birjand)
Y. Ikeda, N. Ishii, P. Junnarkar, H. Nemura,
K. Sasaki(Osaka U.)
T. Inoue (Nihon U.)
K. Murakami (TITech)
K. Murase (Tokyo Metropolitan U.)
T. Sugiura (Rissho U.)
H. Tong (U. of Bonn)

HAL QCD Method

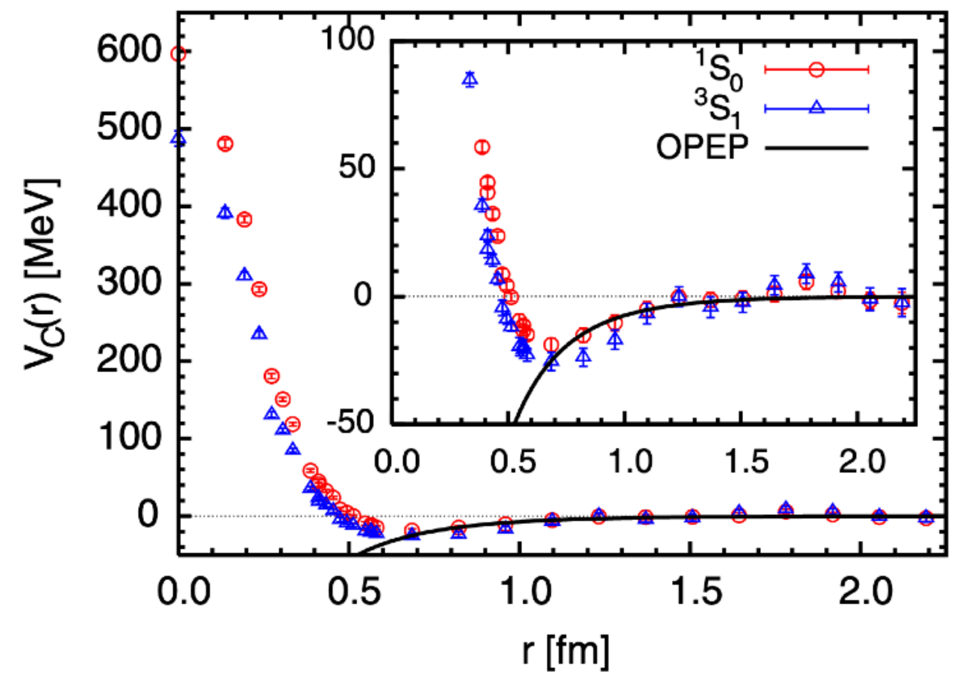
Rebuild Potential

N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007)
S. Aoki, T. Hatsuda, and N. Ishii, Prog. Theor. Phys. 123, 89 (2010)
Aoki, S., Doi, T., Front. in Phys. 8, 307 (2020)
S. Aoki and T. Doi, in Handbook of Nuclear Physics(2023), pp. 1–31



Nambu-Bethe-Salpeter (NBS) wave function

Local Approx. Gradient Expansion



Nulcear Force

$$\psi_{NBS}(\vec{r}) = \langle 0|N(\vec{r})N(\vec{0})|N(\vec{k})N(-\vec{k}), in\rangle$$
$$\simeq e^{i\delta_l(k)}\sin(kr - l\pi/2 + \delta_l(k))/(kr)$$

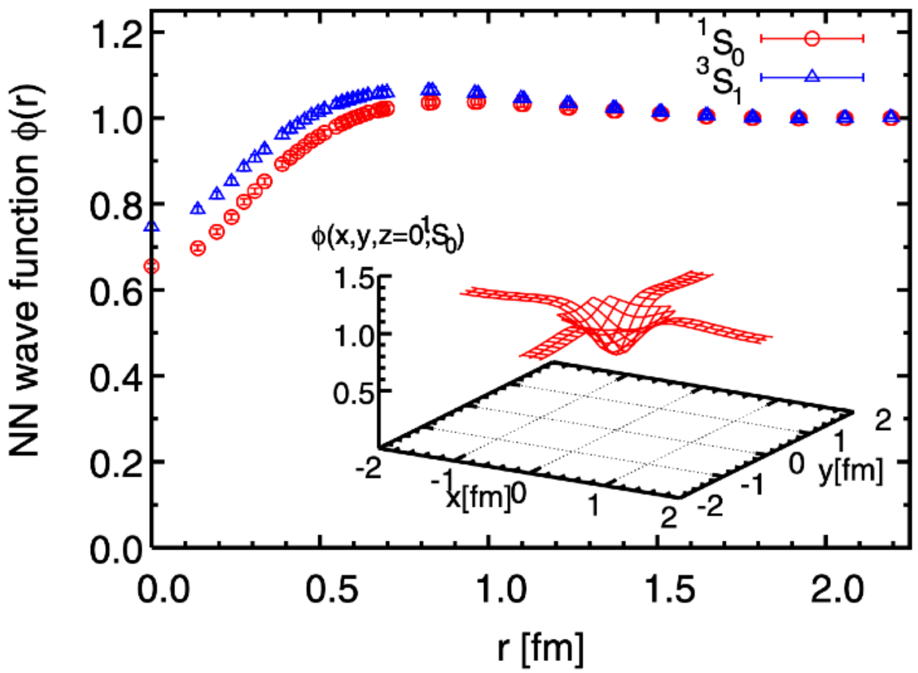
(at asymptotic region)

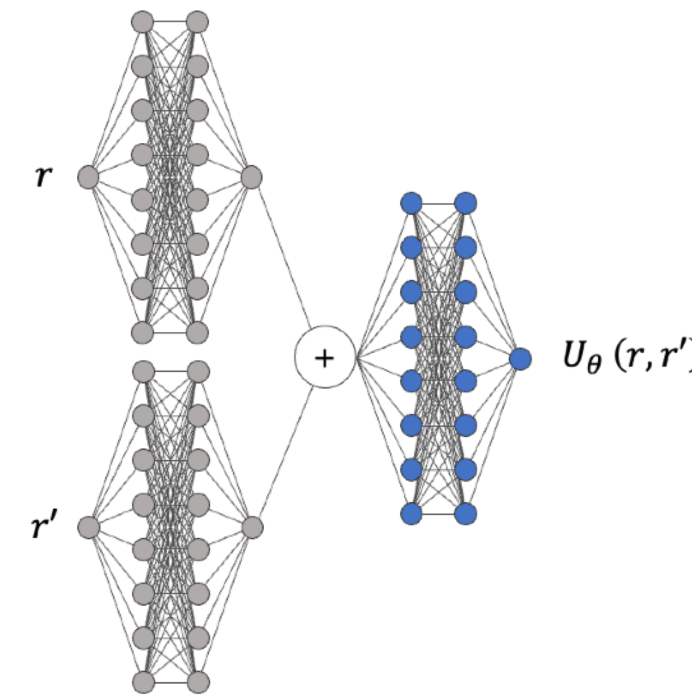
$$(k^2/m_N - H_0)\,\psi_{NBS}(\vec{r}) = \int d\vec{r}'\,U(\vec{r},\vec{r}')\psi_{NBS}(\vec{r}')$$

(Schrodinger eq.)

Learning Potential

Inverse Problem





Gradient Decent

NBS wave function → **Potential Function**

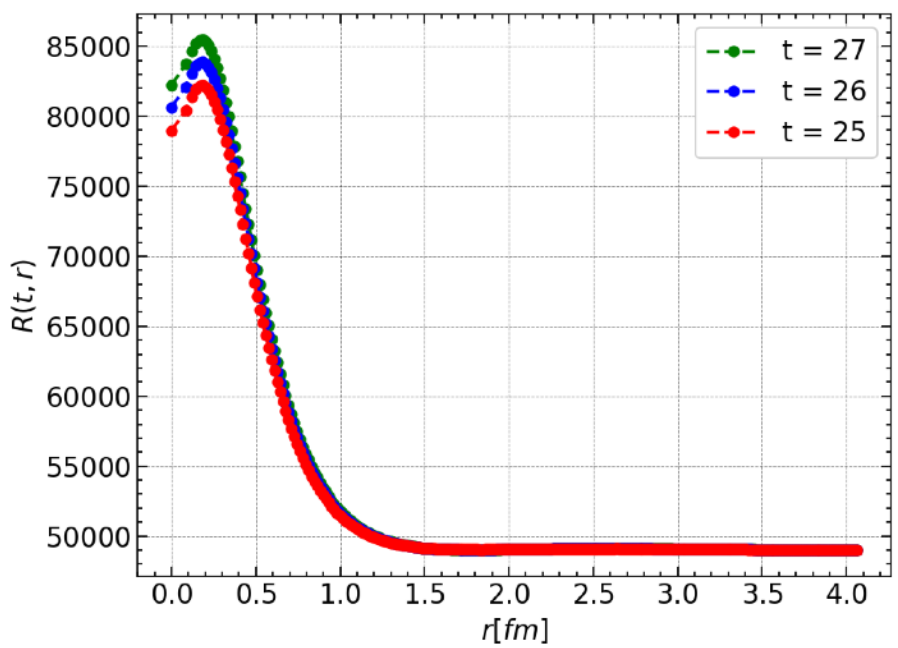
Data(Observations) ← Physics Properties

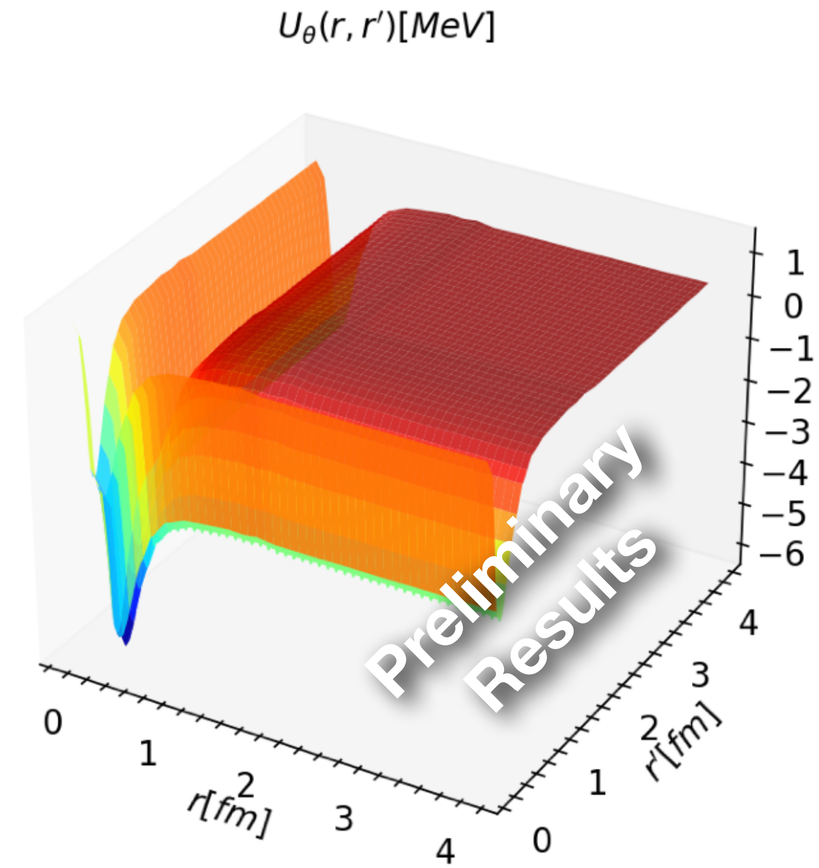
Maximize Likelihood Estimation

$$\min_\theta \mathcal{L} = \sum_k \int d^3\mathbf{r}\left[\left(E_k - H_0\right)\phi_\mathbf{k}(\mathbf{r}) - \int d^3\mathbf{r}'U_\theta(\mathbf{r},\mathbf{r}')\phi_\mathbf{k}(\mathbf{r}')\right]^2$$

Non-local Potential

Inverse Problem





NBS wave function → **Gradient Decent** → **Potential Function**

Maximize Likelihood Estimation

$$\min_\theta \mathscr{L} = \sum_k \int d^3\mathbf{r} \left[\left(E_k - H_0 \right) \phi_\mathbf{k}(\mathbf{r}) - \int d^3\mathbf{r}' U_\theta(\mathbf{r}, \mathbf{r}') \phi_\mathbf{k}(\mathbf{r}') \right]^2$$

Toy Model

In preparation within HAL QCD collaboration(Takumi Doi, Tetsuo Hatsuda, Yan Lyu)

Toy Model

Separable Potential

Aoki, S., Doi, T., Front. in Phys. 8, 307 (2020)

$$U(\mathbf{r}, \mathbf{r}') \equiv \omega \nu(\mathbf{r}) \nu(\mathbf{r}'), \quad \nu(\mathbf{r}) \equiv e^{-\mu r}$$

The S-wave solution of the Schrodinger equation with this potential is given exactly by,

$$\phi_k^0(r) = \frac{e^{i\delta_0(k)}}{kr} \left[\sin\{kr + \delta_0(k)\} - \sin\delta_0(k) e^{-\mu r} \left(1 + \frac{r(\mu^2 + k^2)}{2\mu} \right) \right],$$

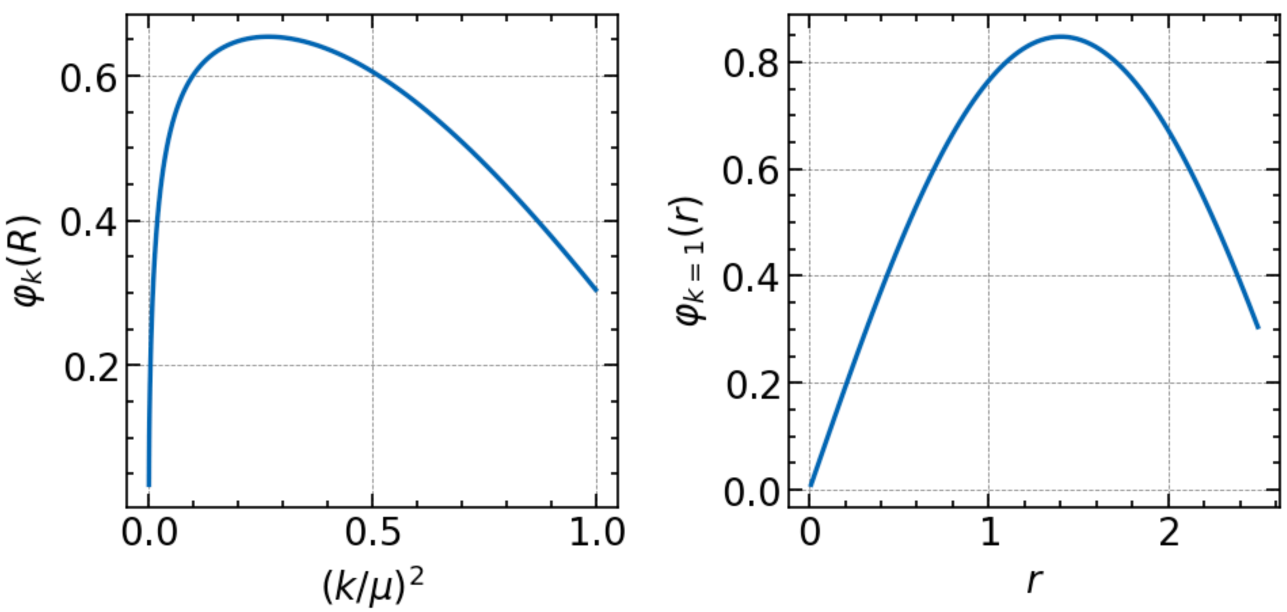
where,

$$k \cot \delta_0(k) = -\frac{1}{4\mu^2} \left[2\mu(\mu^2 - k^2) - \frac{3\mu^2 + k^2}{4\mu^3} (\mu^2 + k^2)^2 + \frac{(\mu^2 + k^2)^4}{8\pi m \omega} \right]$$

As a numerical example, we take $\mu = 1.0, \omega = -0.017\mu^4, m = 3.30\mu, R = 2.5/\mu$

Toy Model

Separable Potential



?

$$\phi_k^0(r) = \frac{e^{i\delta_0(k)}}{kr}\left[\sin\{kr + \delta_0(k)\} - \sin\delta_0(k) e^{-\mu r}\left(1 + \frac{r(\mu^2 + k^2)}{2\mu}\right)\right]$$

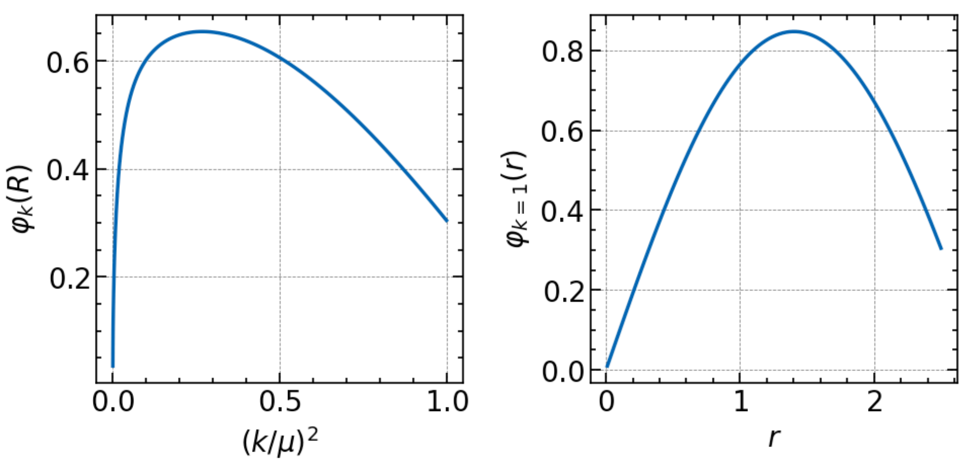
$$U(\mathbf{r}, \mathbf{r}') \equiv \omega \nu(\mathbf{r}) \nu(\mathbf{r}'), \quad \nu(\mathbf{r}) \equiv e^{-\mu r}$$

As a numerical example, we take $\mu = 1.0$, $\omega = -0.017\mu^4, m = 3.30\mu, R = 2.5/\mu$

Warm-Up

Two parameters

$$U_{\theta}(\mathbf{r},\mathbf{r}') = \omega \exp(-\theta_1 r)\exp(-\theta_2 r')$$



$$\phi_k^0(r) = \frac{e^{i\delta_0(k)}}{kr}\left[\sin\{kr+\delta_0(k)\} - \sin\delta_0(k)e^{-\mu r}\left(1+\frac{r(\mu^2+k^2)}{2\mu}\right)\right]$$

A practical set-up for training,

$k = [0.01, 1.0], N_k = 20, r = R.$

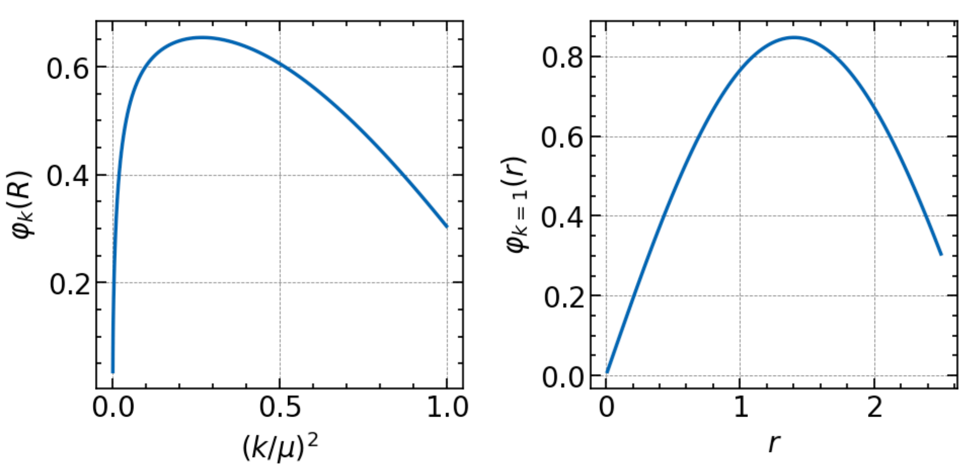
$$\mathrm{min}_{\theta}\mathscr{L} = \sum_k \left[\left(E_k - H_0\right)\phi_{\mathbf{k}}(r=R) - \int 4\pi dr'\, r' U_{\theta}(R,r')\phi_k(r')\right]^2$$

```
Epoch 0, Loss: 4.375710964202881, Theta1: 0.5099999904632568, Theta2: 0.49000000953674316
Epoch 200, Loss: 0.1396370679140091, Theta1: 0.950462281703949, Theta2: 0.39753425121307373
Epoch 400, Loss: 0.04474024847149849, Theta1: 1.14754319190979, Theta2: 0.510127604007721
Epoch 600, Loss: 0.01694628968834877, Theta1: 1.184393048286438, Theta2: 0.6280280947685242
Epoch 800, Loss: 0.009242076426744461, Theta1: 1.1597602367401123, Theta2: 0.6997004151344299
Epoch 1000, Loss: 0.005497976206243038, Theta1: 1.133785605430603, Theta2: 0.752680778503418
Epoch 1200, Loss: 0.0034021069295704365, Theta1: 1.1116809844970703, Theta2: 0.7952543497085571
Epoch 1400, Loss: 0.0021468503400683403, Theta1: 1.0929081439971924, Theta2: 0.8305171728134155
Epoch 1600, Loss: 0.0013651829212903976, Theta1: 1.0768871307373047, Theta2: 0.8601892590522766
Epoch 1800, Loss: 0.0008674096898175776, Theta1: 1.063176155090332, Theta2: 0.8853644728660583
Epoch 2000, Loss: 0.0005469319876283407, Theta1: 1.0514411926269531, Theta2: 0.9067927598953247
Epoch 2200, Loss: 0.00034017590223811567, Theta1: 1.041424036026001, Theta2: 0.9250178933143616
Epoch 2400, Loss: 0.00020751418196596205, Theta1: 1.0329188108444214, Theta2: 0.9404546618461609
Epoch 2600, Loss: 0.00012344479910098016, Theta1: 1.025755763053894, Theta2: 0.9534343481063843
Epoch 2800, Loss: 7.118881330825388e-05, Theta1: 1.019789695739746, Theta2: 0.9642329216003418
Epoch 3000, Loss: 3.954790372517891e-05, Theta1: 1.0148907899856567, Theta2: 0.9730932712554932
Epoch 3200, Loss: 2.1019024643464945e-05, Theta1: 1.0109381675720215, Theta2: 0.980238676071167
Epoch 3400, Loss: 1.0608729098748881e-05, Theta1: 1.0078167915344238, Theta2: 0.9858796000480652
Epoch 3600, Loss: 5.043078999733552e-06, Theta1: 1.0054134130477905, Theta2: 0.9902217388153076
Epoch 3800, Loss: 2.2376170818461105e-06, Theta1: 1.003617763519287, Theta2: 0.993465781211853
Optimised Theta1: 1.0023272037506104
Optimised Theta2: 0.9957966208457947
```

Neural Network

Non-Local Potential

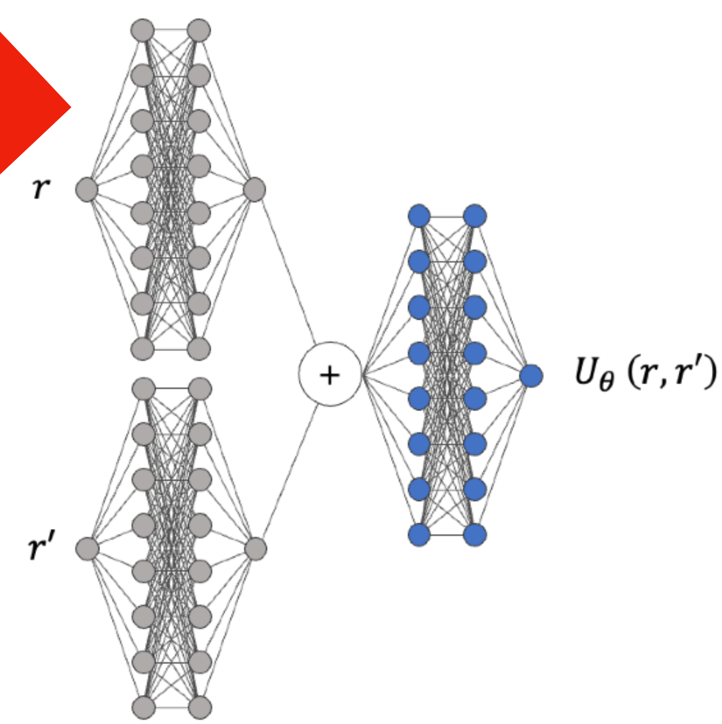
$$U_\theta(\mathbf{r}, \mathbf{r}') = \omega f_\theta(r, r'), U_{\mathbf{NN}}(r, r') \equiv f_\theta(r, r')$$



$$\phi_k^0(r) = \frac{e^{i\delta_0(k)}}{kr}\left[\sin\{kr + \delta_0(k)\} - \sin\delta_0(k)e^{-\mu r}\left(1 + \frac{r(\mu^2 + k^2)}{2\mu}\right)\right]$$

$$\mathbf{min}_\theta \mathscr{L} = \sum_r \sum_k \left[\left(E_k - H_0\right)\phi_k(r) - \int 4\pi d\, r' r' U_\theta(r, r')\phi_k(r')\right]^2$$

Adding Physics!



Symmetricly Sharing Parameters

A practical set-up for training,

$k = [0.01, 1.0], N_k = 10,$

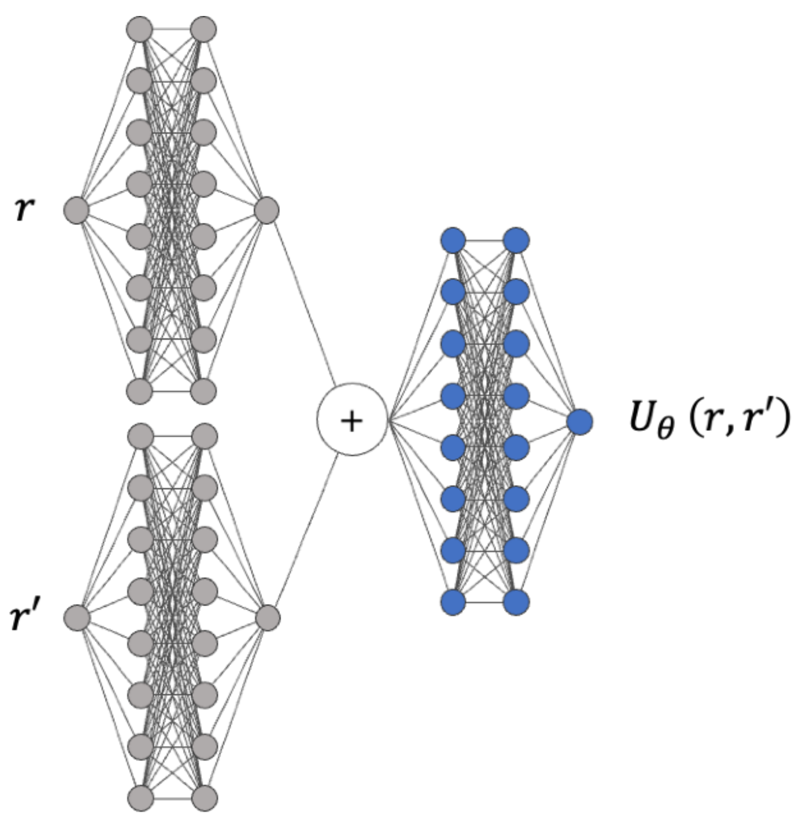
$r = [0.01, 5R], N_r = 100.$

Neural Network

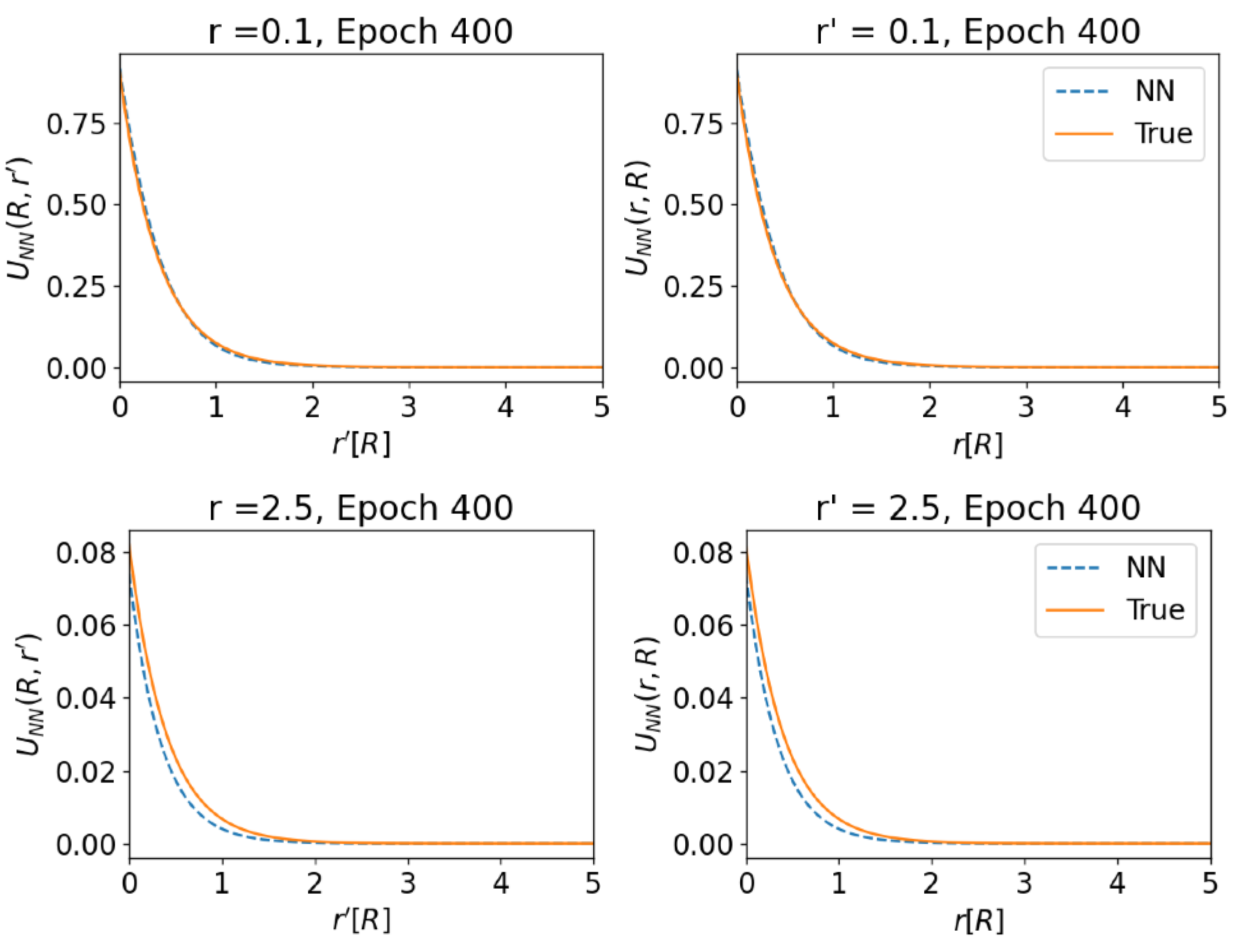
Non-Local Potential

$$U_\theta(\mathbf{r}, \mathbf{r}') = \omega f_\theta(r, r'), U_{\mathbf{NN}}(r, r') \equiv f_\theta(r, r')$$

$$\mathbf{min}_\theta \mathscr{L} = \sum_r \sum_k \left[\left(E_k - H_0\right) \phi_k(r) - \int 4\pi d\, r' r' U_\theta(r, r') \phi_k(r') \right]^2$$



Symmetricly Sharing Parameters

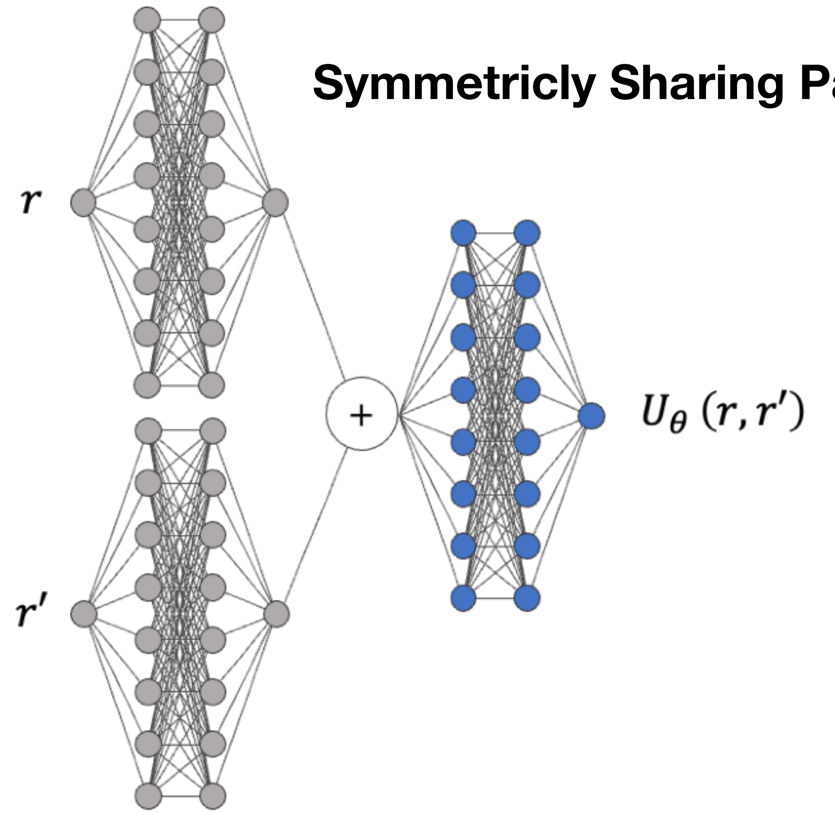


Neural Network

Non-Local Potential: More Physics Priors

$$U_\theta(\mathbf{r}, \mathbf{r}') = \omega f_\theta(r, r'), U_{\mathbf{NN}}(r, r') \equiv f_\theta(r, r')$$

$$\min_\theta \mathscr{L} = \sum_r \sum_k \left[\left(E_k - H_0\right) \phi_k(r) - \int 4\pi d\, r' r' U_\theta(r, r') \phi_k(r') \right]^2$$



Symmetricly Sharing Parameters

+

Asymptotic Behaviour as Regulator

$$\lim_{\mathbf{r}>R, \mathbf{r}'>R} U(\mathbf{r}, \mathbf{r}') \to 0$$

Neural Network

Non-Local Potential: More Physics Priors

$$U_\theta(\mathbf{r},\mathbf{r}') = \omega f_\theta(r,r'), U_{\text{NN}}(r,r') \equiv f_\theta(r,r')$$

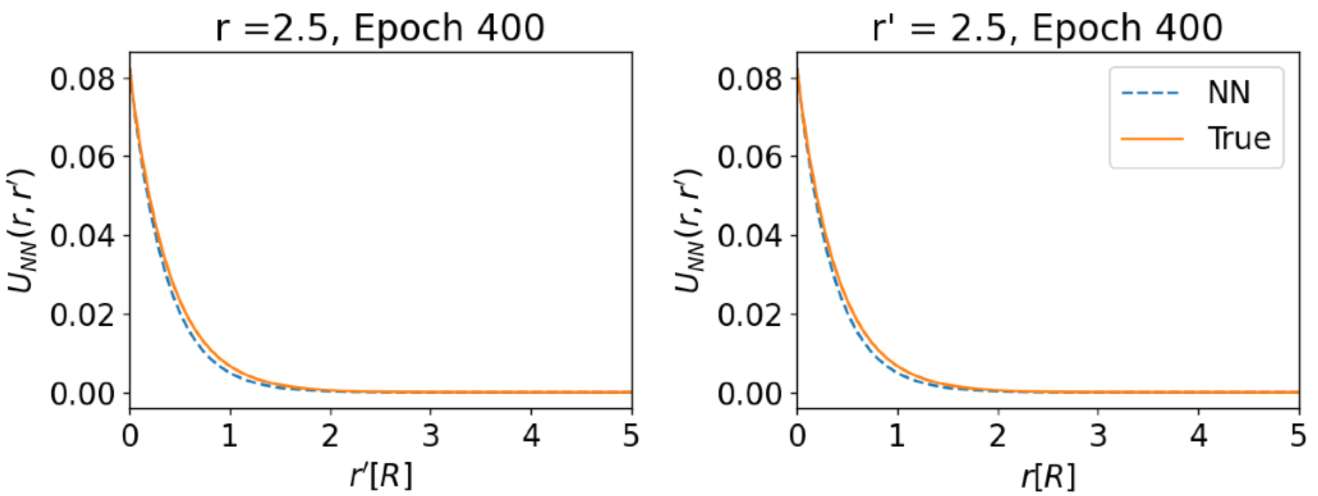
$$\text{min}_\theta \mathscr{L} = \sum_r \sum_k \left[\left(E_k - H_0\right) \phi_k(r) - \int 4\pi d\, r' r' U_\theta(r,r')\phi_k(r') \right]^2$$

Symmetricly Sharing Parameters

+

Asymptotic Behaviour as Regulator

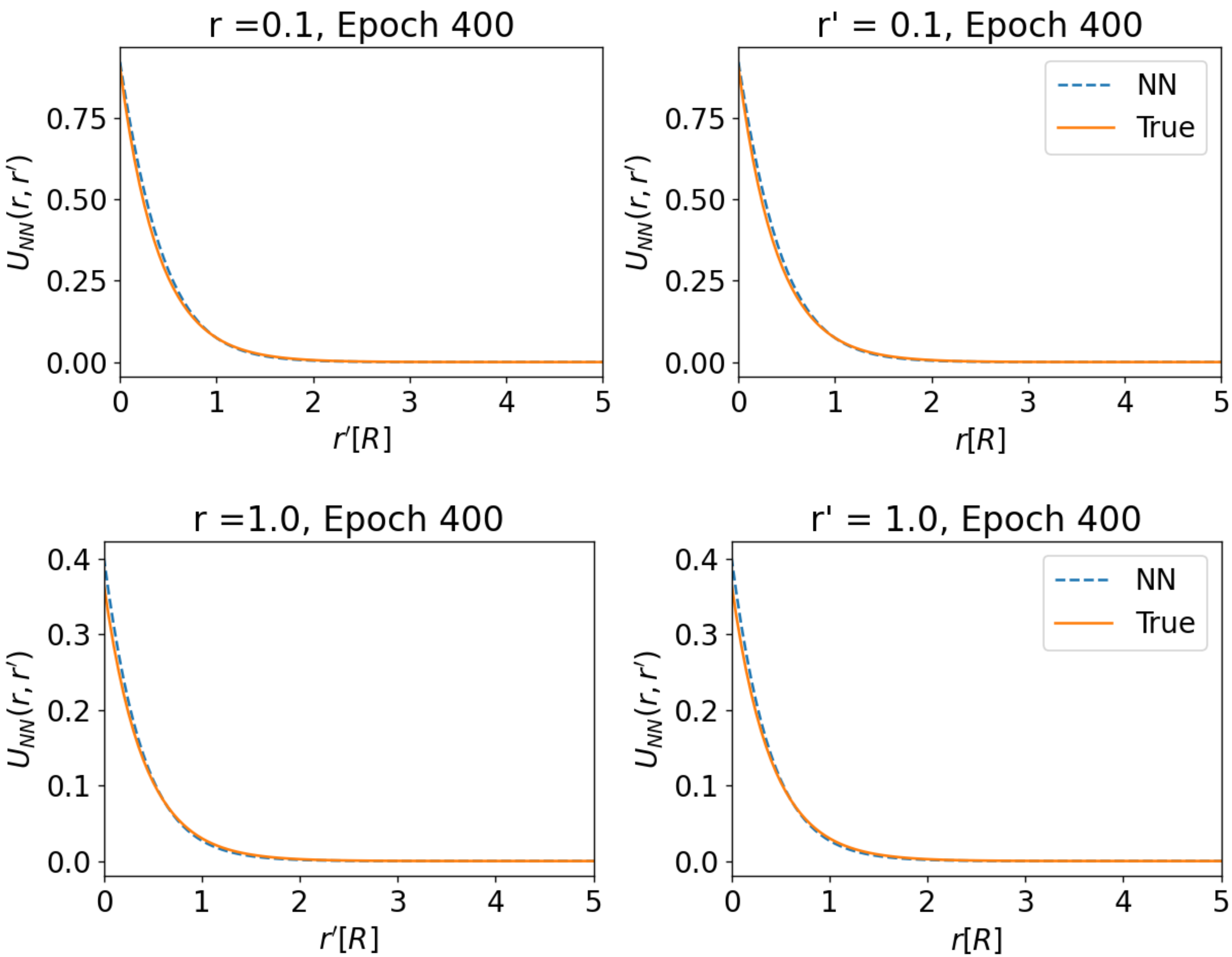
$$\lim_{\mathbf{r}>R,\mathbf{r}'>R} U(\mathbf{r},\mathbf{r}') \rightarrow 0$$



A practical set-up for training, $r_j \in [4R,\ 5R], N_{reg} = 100$, $\mathscr{L}_{\text{reg}} = \sum_i^{N_{reg}} \sum_j^{N_{reg}} (U_{\text{NN}}(r_i, r_j) - 0)^2$

Neural Network

Non-Local Potential: More Physics Priors



Case study:

$$\Omega_{ccc}\Omega_{ccc}({}^1S_0)$$

In preparation within HAL QCD collaboration(Takumi Doi, Tetsuo Hatsuda, Yan Lyu)

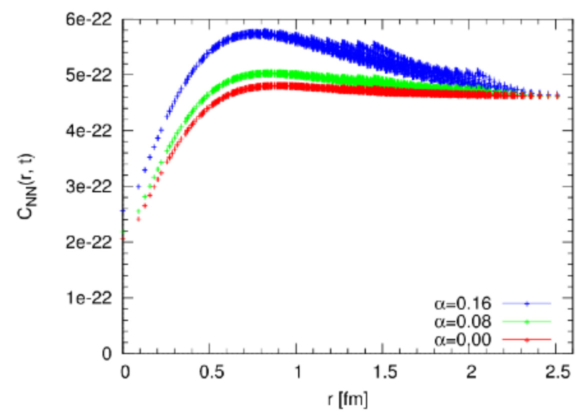
Real World

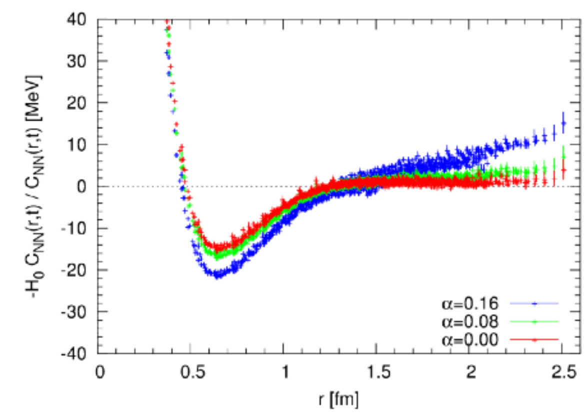
Time-Dependent HAL QCD

N. Ishii, etc., Phys. Lett. B 712, 437 (2012)

Normalized *NN* correlation function

$$R(t,\vec{r}) \equiv C_{NN}(\vec{r},t)/\left(e^{-m_N t}\right)^2$$

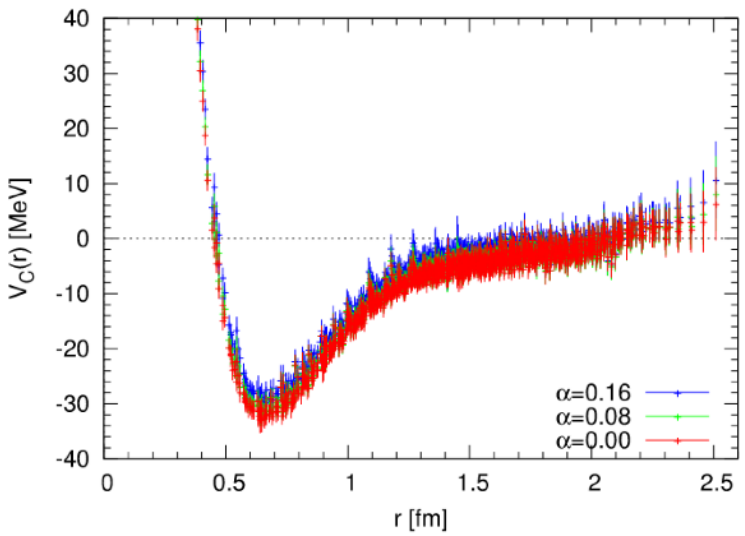




"Time-Dependent" Schrödinger-like Equation

$$\left\{\frac{1}{4m_N}\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0\right\} R(t,\vec{r}) = \int d^3r'\, U(\vec{r},\vec{r}\,')R(t,\vec{r}\,')$$

Alleviate the Ground State Saturation



Neural Networks

Time-Dependent HAL QCD

$$\left\{ \frac{1}{4m_N}\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right\} R(t,\vec{r}) = \int d^3r'\, U(\vec{r},\vec{r}')R(t,\vec{r}')$$

Maximize Likelihood Estimation

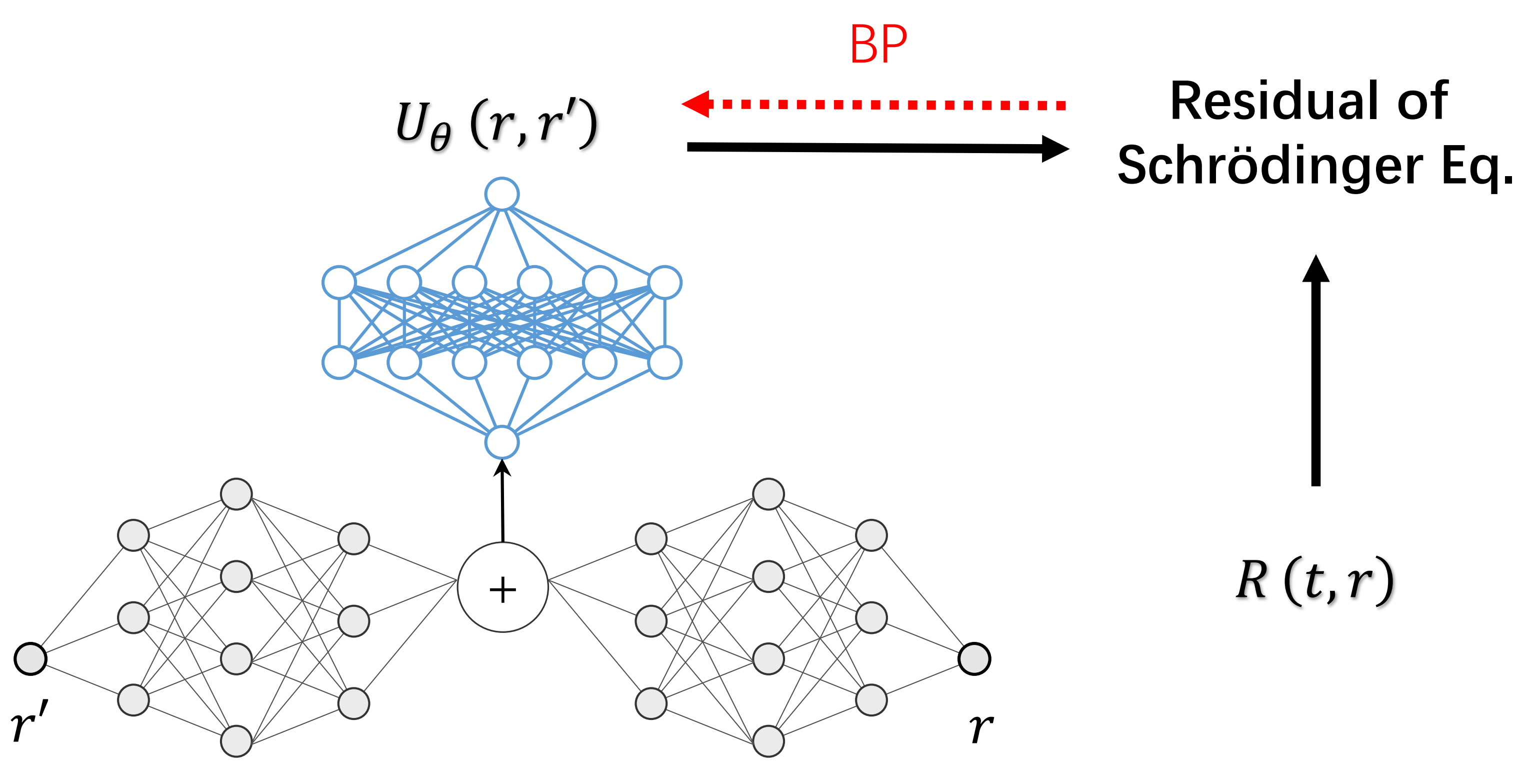
$$\textbf{min}_\theta \mathscr{L} = \sum_t \left\{ \frac{1}{4m_N} R_{tt}(t,r) - R_t(t,r) + \frac{1}{m_N} R_r(t,r) - \int 4\pi r'^2 dr'\, U_\theta(r,r') R(t,r') \right\}^2$$

$$R_{tt}(t,r) \equiv \partial_t^2 R(t,r), R_t(t,r) \equiv \partial_t R(t,r), R_r(t,r) \equiv \nabla^2 R(t,r)$$

Neural Networks

Time-Dependent HAL QCD

$$\mathbf{min}_\theta \mathscr{L} = \sum_t \left\{ \frac{1}{4m_N} R_{tt}(t,r) - R_t(t,r) + \frac{1}{m_N} R_r(t,r) - \int 4\pi r'^2 dr'\, U_\theta(r,r') R(t,r') \right\}^2$$

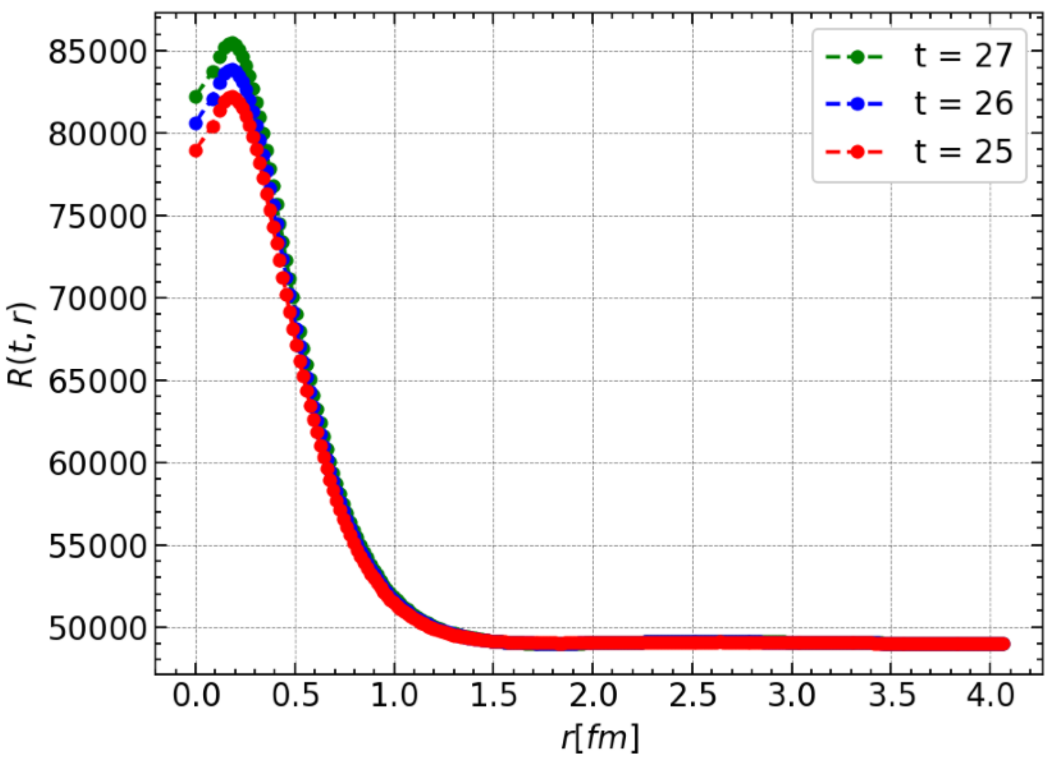


$$U_\theta(r,r') \equiv g(f(r) + f(r'))$$

$$\theta_{i+1} \to \theta_i + \frac{\partial \mathscr{L}}{\partial U_\theta(r,r')} \frac{\partial U_\theta(r,r')}{\partial \theta}$$

Neural Networks

Case study: $\Omega_{ccc}\Omega_{ccc}(^1S_0)$



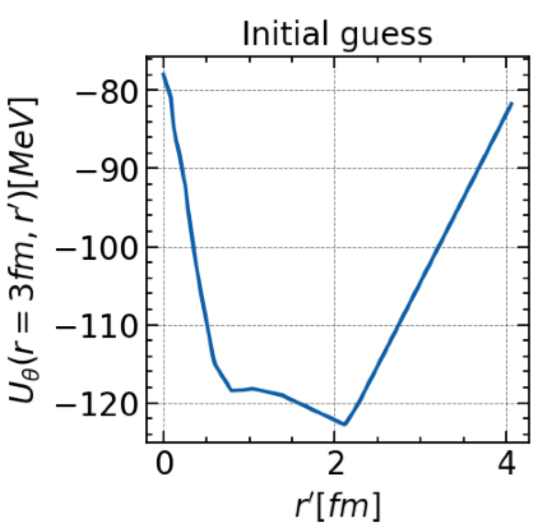
$$\mathscr{L}_t = \sum_t \left\{ \frac{1}{4m_N} R2(t,r) - R1(t,r) + \frac{1}{m_N} Rr(t,r) - \int dr'\, U_\theta(r,r') R(t,r') \right\}$$

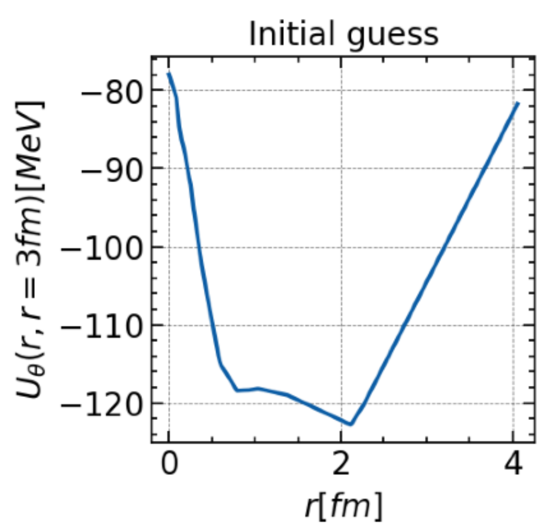
$$R2 = R_{t+1} - 2R_t + R_{t-1}, R1 = (R_{t+1} - R_{t-1})/2, Rr = \nabla^2 R(t,r)$$

$$\int dr' U_{NN}(r,r') R(t,r') \approx \sum_{r'} \Delta r'\, U_\theta(r,r') R(t,r')$$

Asymptotic Behaviour as Regulator

$$U_\theta(r > 3\mathbf{fm}, r' > 3\mathbf{fm}) \to 0$$





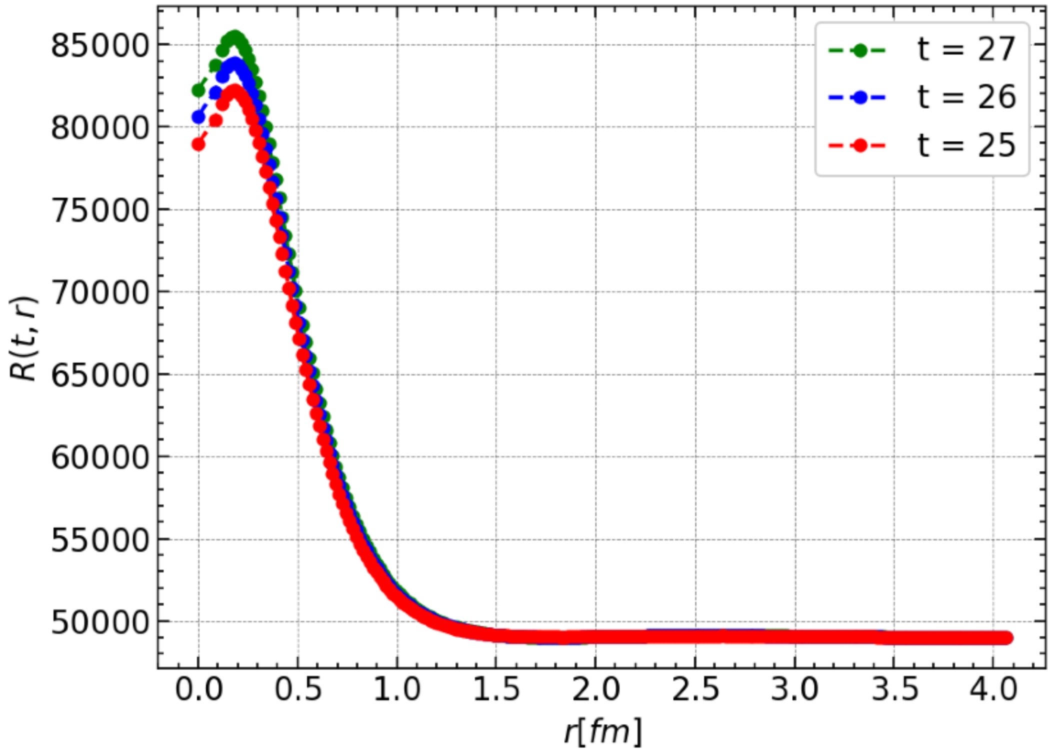
$$\mathscr{L}_r = \sum_{r=3fm}^{r_{max}} \sum_{r'=3fm}^{r_{max}} U_\theta(r,r')^2$$

$$\mathscr{L} \equiv \mathscr{L}_t + \lambda \mathscr{L}_r$$

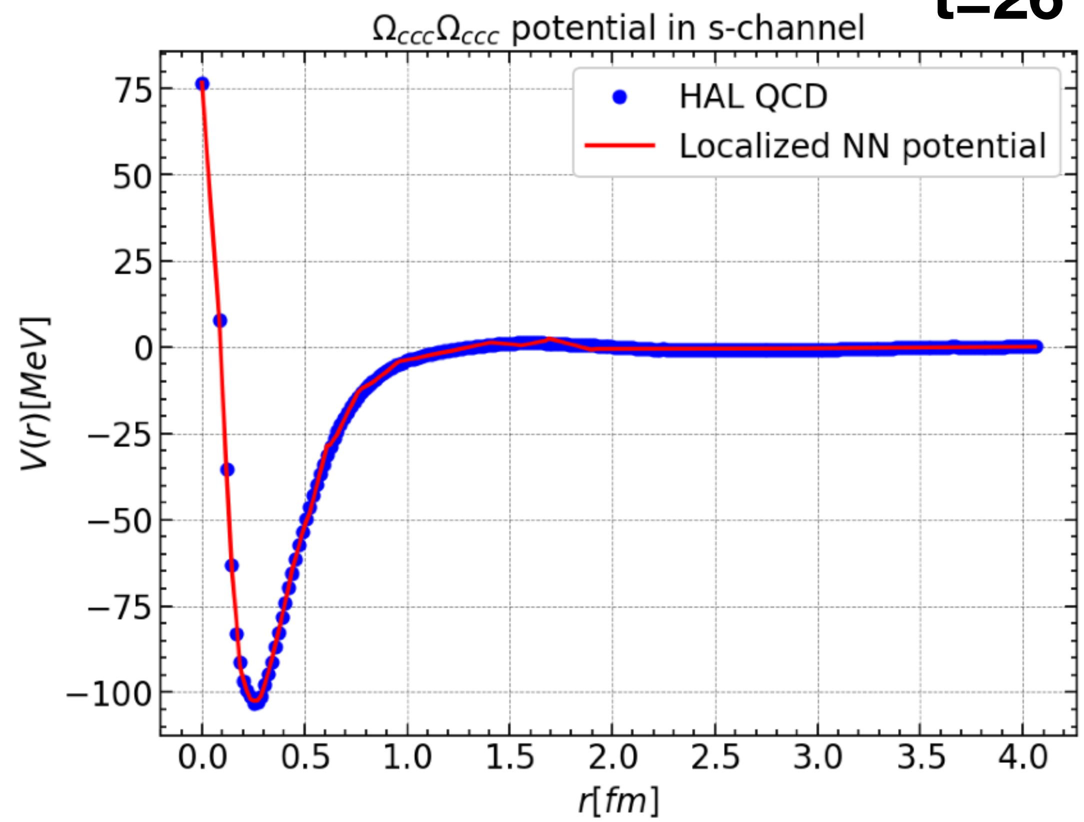
$$\lambda = 10^8$$

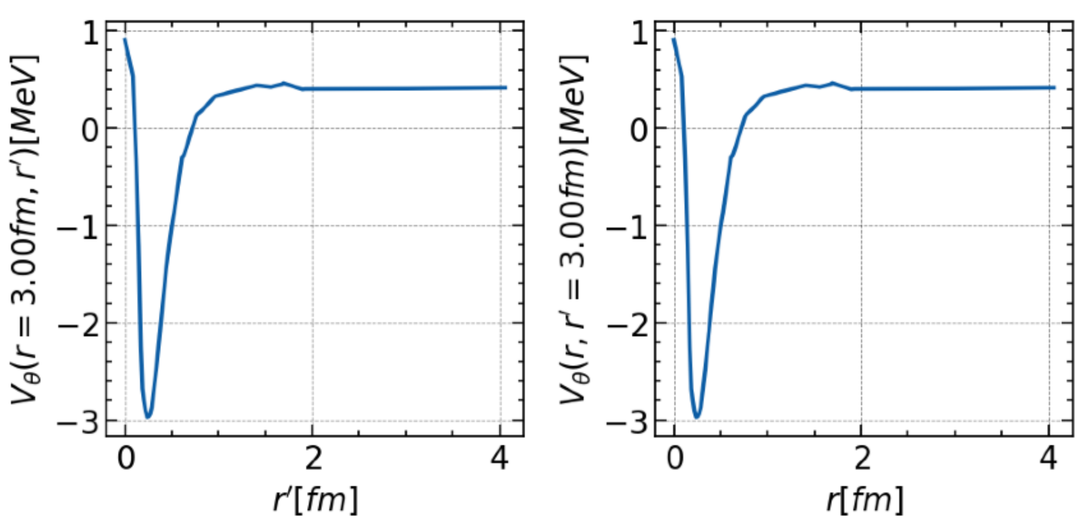
Neural Networks

Case study: $\Omega_{ccc}\Omega_{ccc}(^1S_0)$



t=26





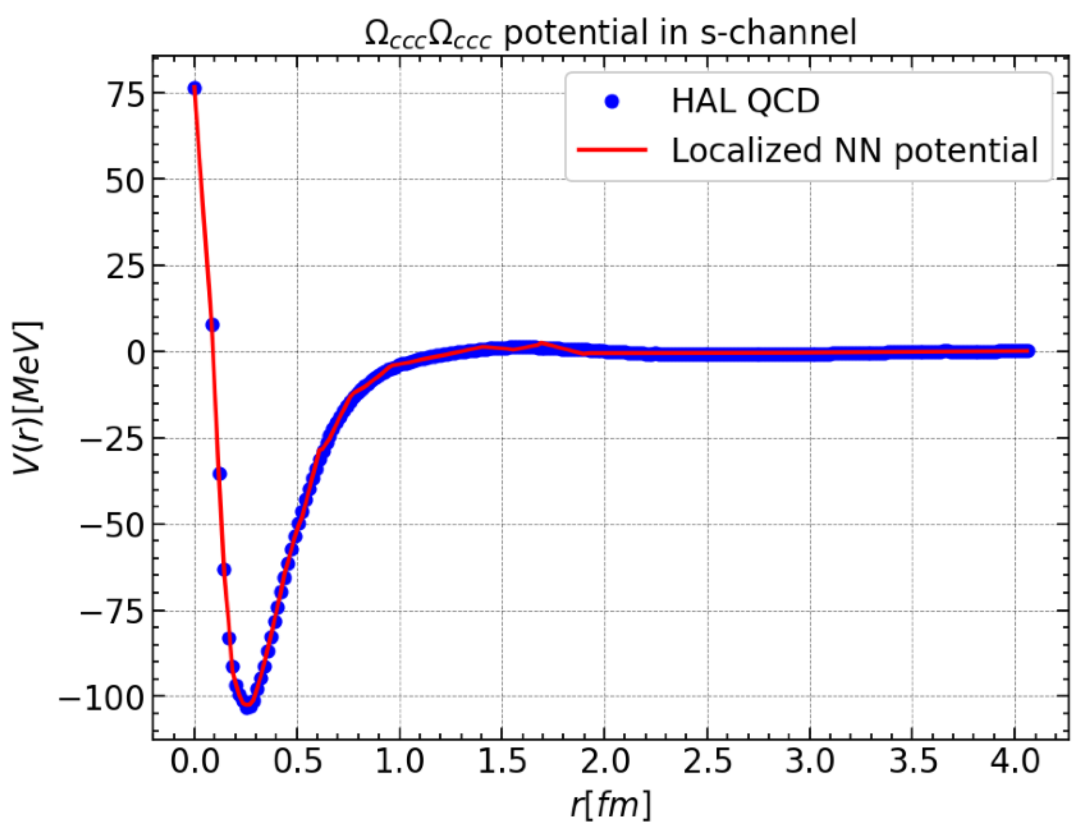
After 2000 epochs

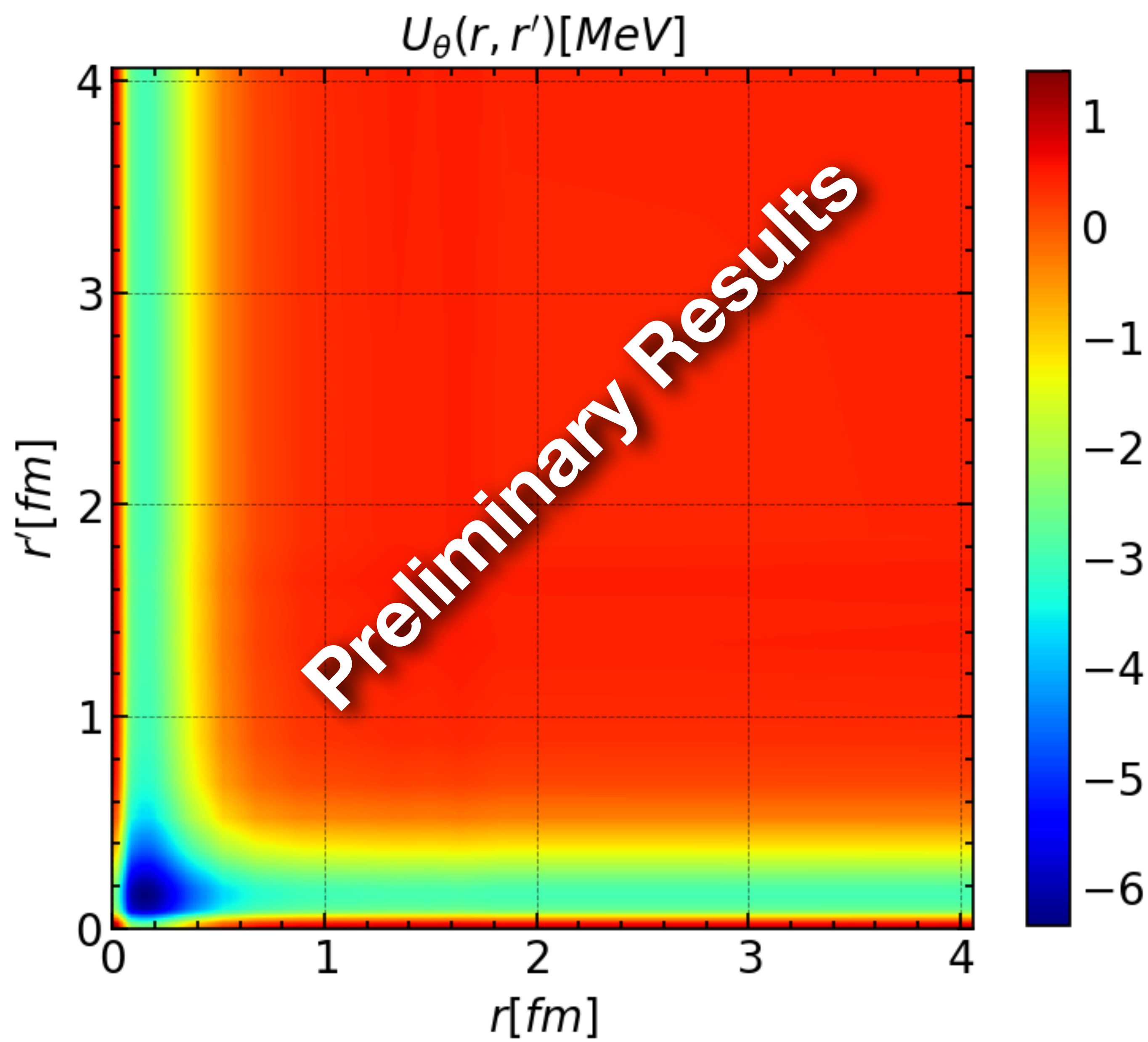
Localized NN Potential

$$V_\theta(r) \equiv \frac{\sum_{r'} \Delta r' \, U_\theta(r, r') R(t, r')}{R(t, r)}$$

Neural Networks

Case study: $\Omega_{ccc}\Omega_{ccc}(^1S_0)$

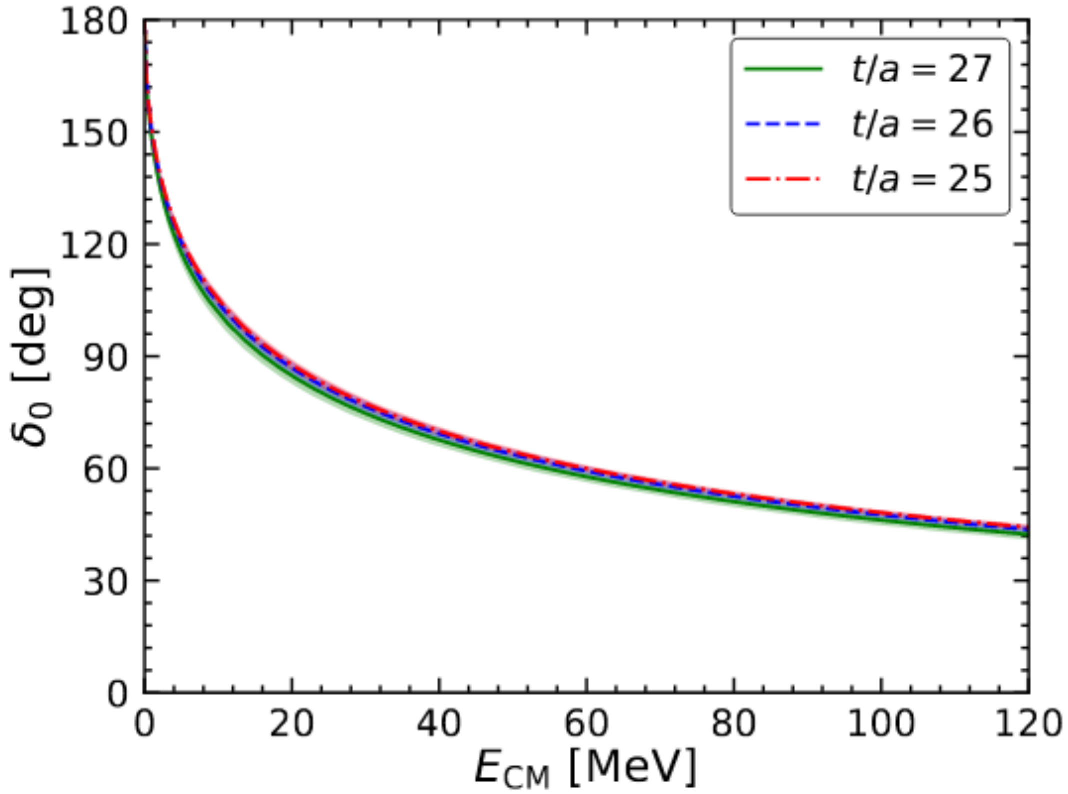




First time!
Non-local Potential!

Phase Shifts

To be calculated…



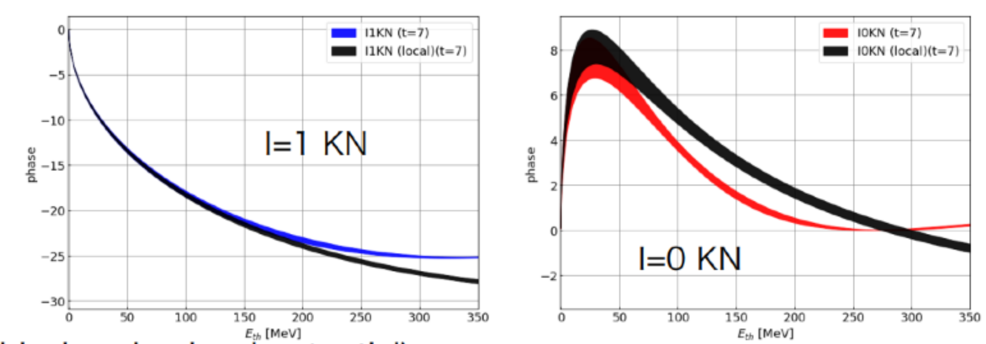
Y. Lyu, etc., Phys. Rev. Lett. 127, 072003 (2021)

Non-local potential matters!

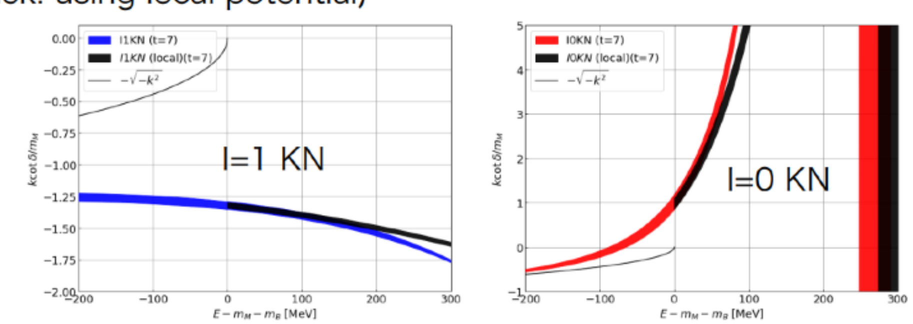
continuous function

$$\left(\frac{k^2}{m_N} - \frac{\nabla^2}{m_N}\right)\psi_k(r) = \int_0^\infty U_\theta(r, r')\psi_k(r')r'^2\, dr'$$

- phase shift (black: using local potential)



- $k \cot \delta$ (black: using local potential)



- same phase shifts up to ~100 MeV for I=1 KN while ~10 MeV for I=0 KN

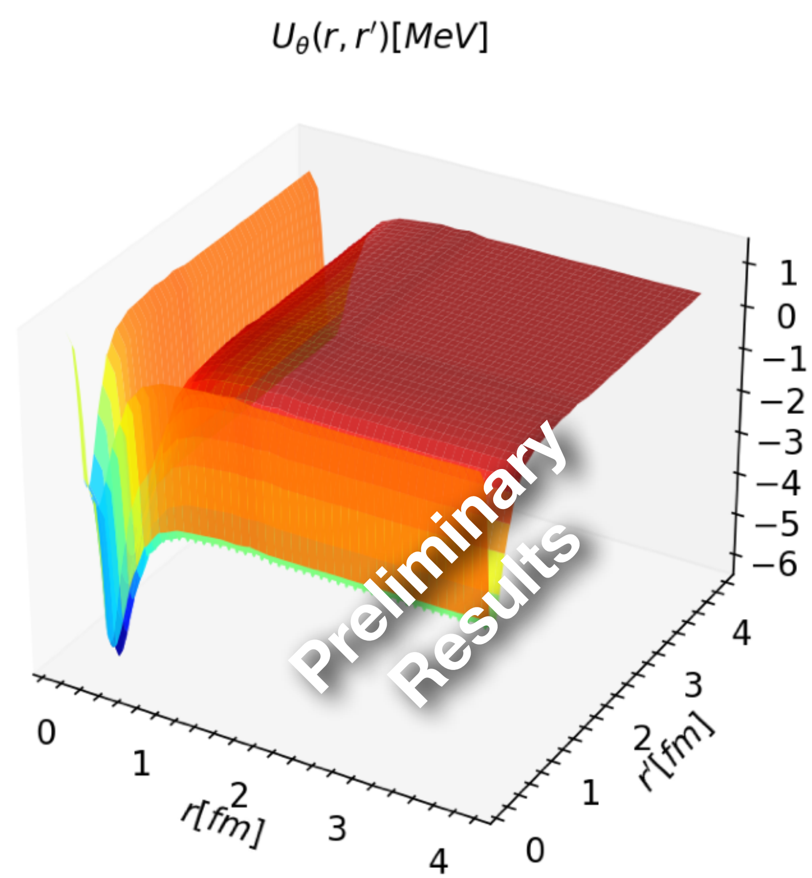
e.g., Separable Potential

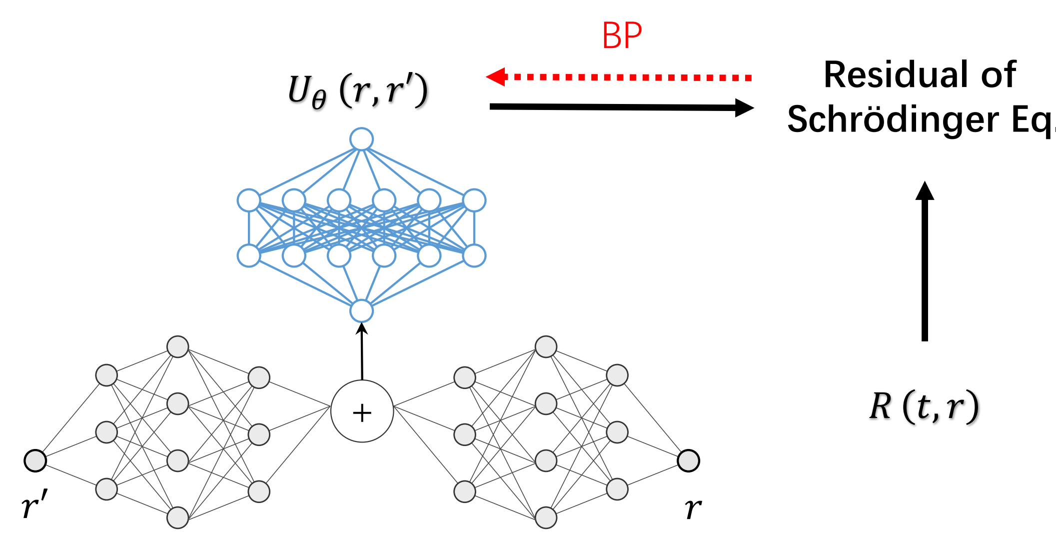
K. Murakami presents applications to Lambda(1405) @Lattice 2024, Aug 2, 2024, 12:55PM

Summary

Take-home messages

- **k-independent and non-local potential!**
- **Physics prior as regularization!**





Symmetricly Sharing Parameters

+

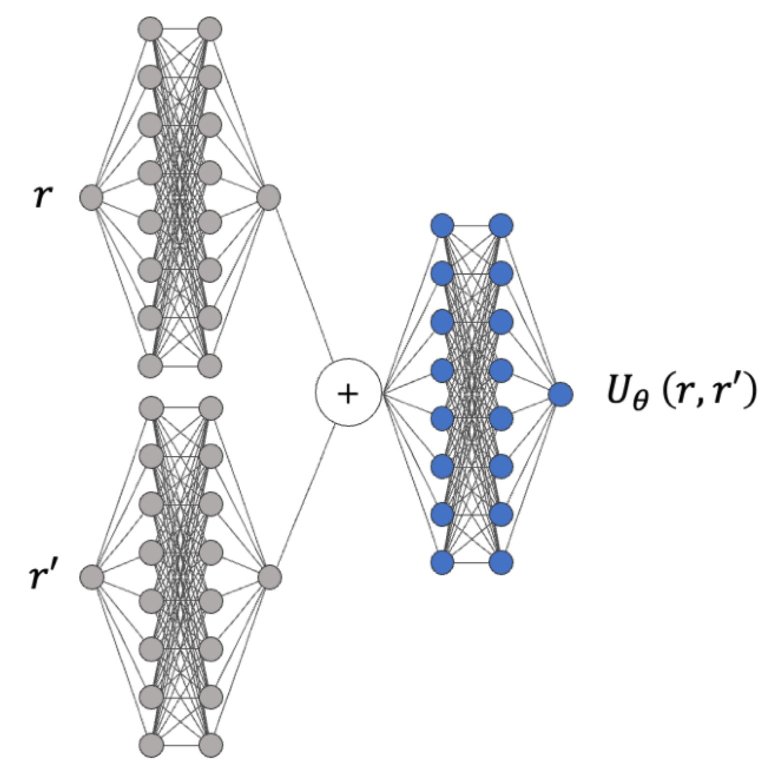
Asymptotic Behaviour as Regulator

$$\lim_{\mathbf{r}>R,\mathbf{r}'>R} U(\mathbf{r},\mathbf{r}') \to 0$$

Outlook

Roadmap

- Rebuild **Separable Potential**
  - Neural Network Non-Local Potential ✔
    - Exchange symmetry
    - Asympotoic behaviour
- t-HAL QCD method
  - **Omega-Omega(s-channel)** ✔
  - Non-local potential ✔
  - Phase Shifts 💪
- **Next Steps**
  - Full-t joint learning
  - More real cases
    (B-B, N-B, N-M, N-N, elastic scattering...)



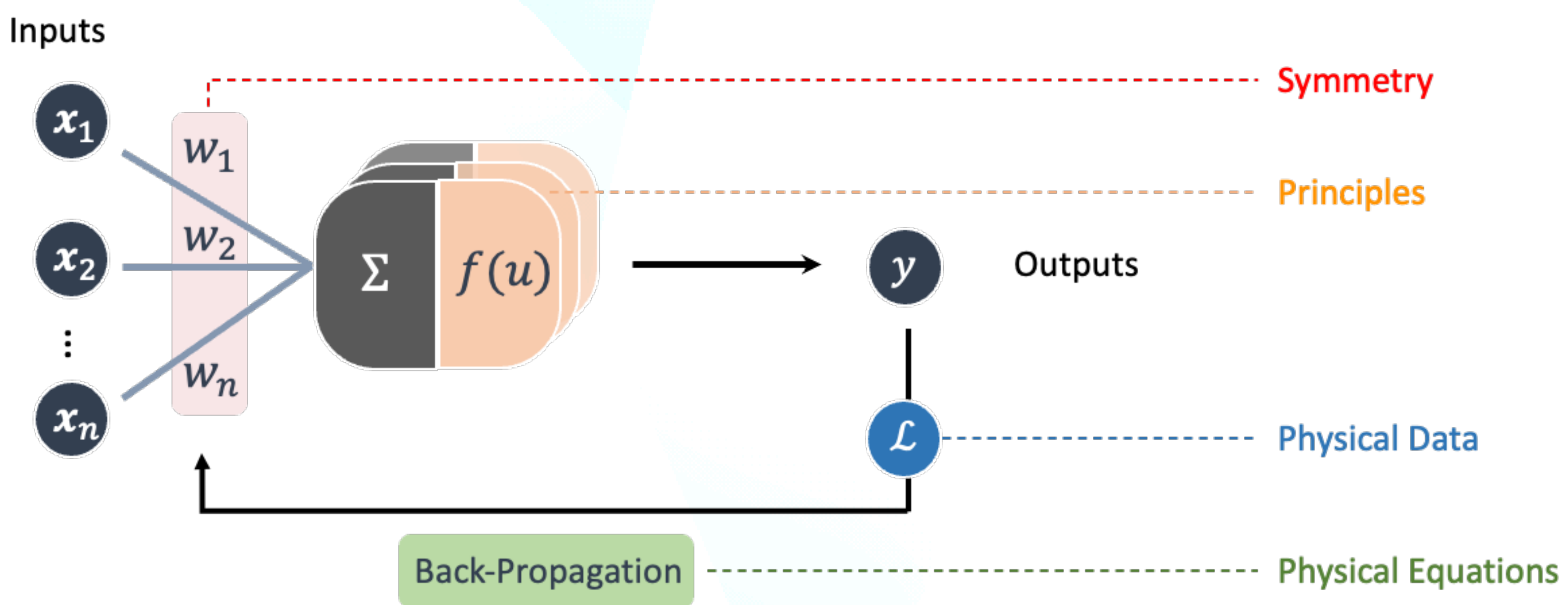
Symmetricly Sharing Parameters

+

Asymptotic Behaviour as Regulator

$$\lim_{\mathbf{r}>R, \mathbf{r}'>R} U(\mathbf{r}, \mathbf{r}') \to 0$$

Thank you!



Physics-Driven Deep Learning

DEEP-IN

iTHEMS 理化学研究所 数理創造プログラム
RIKEN Interdisciplinary Theoretical and Mathematical Sciences Program

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DEEP-IN Working Group

"DEEP learning for INverse problems (DEEP-IN) in Sciences" working group (April 1st, 2024 -)

Lattice Computations

Gert Aarts, Swansea U.
Takumi Doi, iTHEMS
Andreas Ipp, TU Wien
Tetsuo Hatsuda, iTHEMS
Yan Lyu, iTHEMS

Now mostly physicists -> **Future** more diverse scientists

BioPhysics: **Catherine Beauchemin,** iTHEMS
Condensed Matter Physics: **Steffen Backes,** iTHEMS
QCD Physics: **Kenji Fukushima,** UTokyo
Nuclear Physics: **Haozhao Liang,** UTokyo
Quantum Computing: **Enrico Rinaldi,** Quantinuum K.K./iTHEMS

Heavy-Ion Collisions

Long-Gang Pang, CCNU
Shuzhe Shi, THU
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Akira Harada, NIT-Ibaraki
Zhenyu Zhu, TDLI->RIT

Machine Learning

Akinori Tanaka, AIP/iTHEMS
Lingxiao Wang, iTHEMS

***in preparation* [Review]**

Physics-Driven Learning for Solving Inverse Problems towards QCD Physics

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ABSTRACT

The integration of deep learning techniques and physics-driven designs is reforming the way we address inverse problems, in which accurate physical properties are extracted from complex data sets. This is particularly relevant for quantum chromodynamics (QCD), the theory of strong interactions, with its inherent limitations in observational data and demanding computational approaches. This perspective highlights advances and potential of physics-driven learning methods, focusing on predictions of physical quantities towards QCD physics, and drawing connections to machine learning(ML). It is shown that the fusion of ML and physics can lead to more efficient and reliable problem-solving strategies. Key ideas of ML, methodology of embedding physics priors, and generative models as inverse modelling of physical probability distributions are introduced. Specific applications cover first-principle lattice calculations, and QCD physics of hadrons, neutron stars, and heavy-ion collisions. These examples provide a structured and concise overview of how incorporating prior knowledge such as symmetry, continuity and equations into deep learning designs can address diverse inverse problems across different physical sciences.

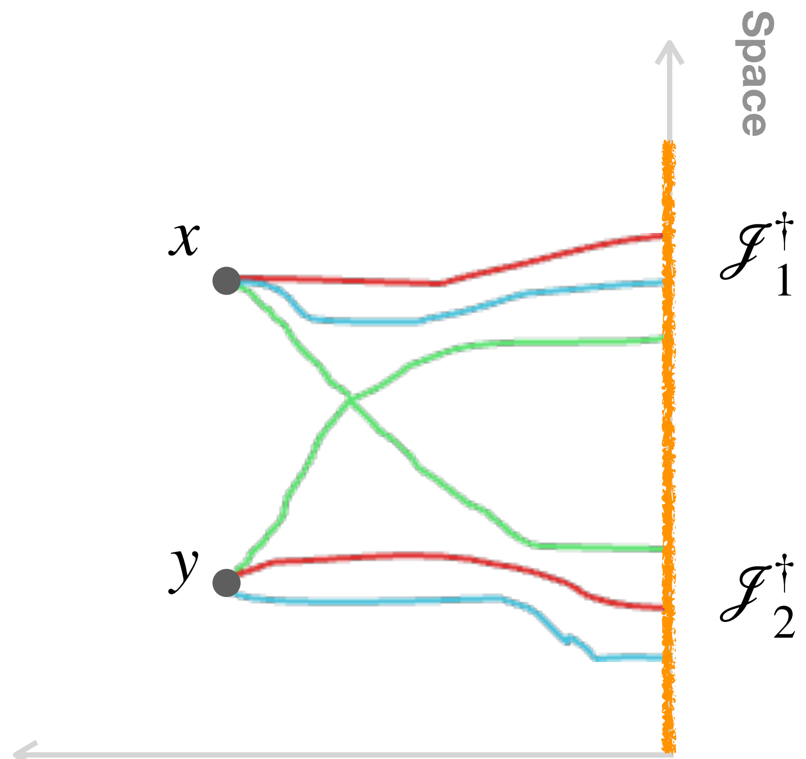
https://sites.google.com/view/deep-in-wg/homepage

Contact at lingxiao.wang@riken.jp

Backups

Scattering

N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007),
S. Aoki, T. Hatsuda, and N. Ishii, Prog. Theor. Phys. 123, 89 (2010).
N. Ishii, etc.(HAL QCD), Phys. Lett. B 712, 437 (2012)



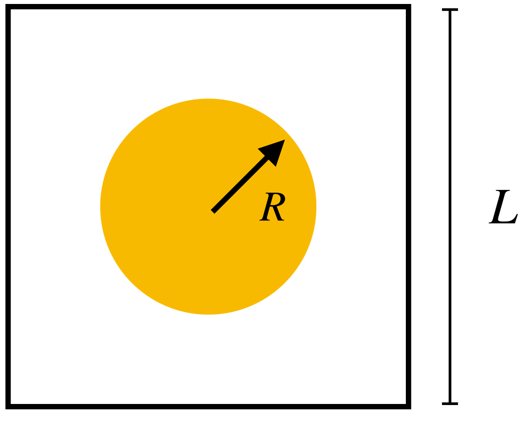
$$\langle N_1(\mathbf{x},t)N_2(\mathbf{y},t)\mathcal{J}_1^\dagger(0)\mathcal{J}_2^\dagger(0)\rangle$$

$$= \sum_n \langle 0|N_1(\mathbf{x})N_2(\mathbf{y})|n\rangle a_n e^{-E_n t}$$

$$\xrightarrow{t>t^*} \phi(\mathbf{r},t) = \sum_{n<n^*} b_n\phi_n(\mathbf{r})e^{-E_n t}$$

$\phi(\mathbf{r},t) \rightarrow$ **2 PI Kernel**

$$(E_k - H_0)\phi_{\mathbf{k}}(\mathbf{r}) = \int d^3r' U(\mathbf{r},\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}'), \quad r<R$$



Consider the wave function at "interacting region"
$\longrightarrow$Phase shift, Binding energy

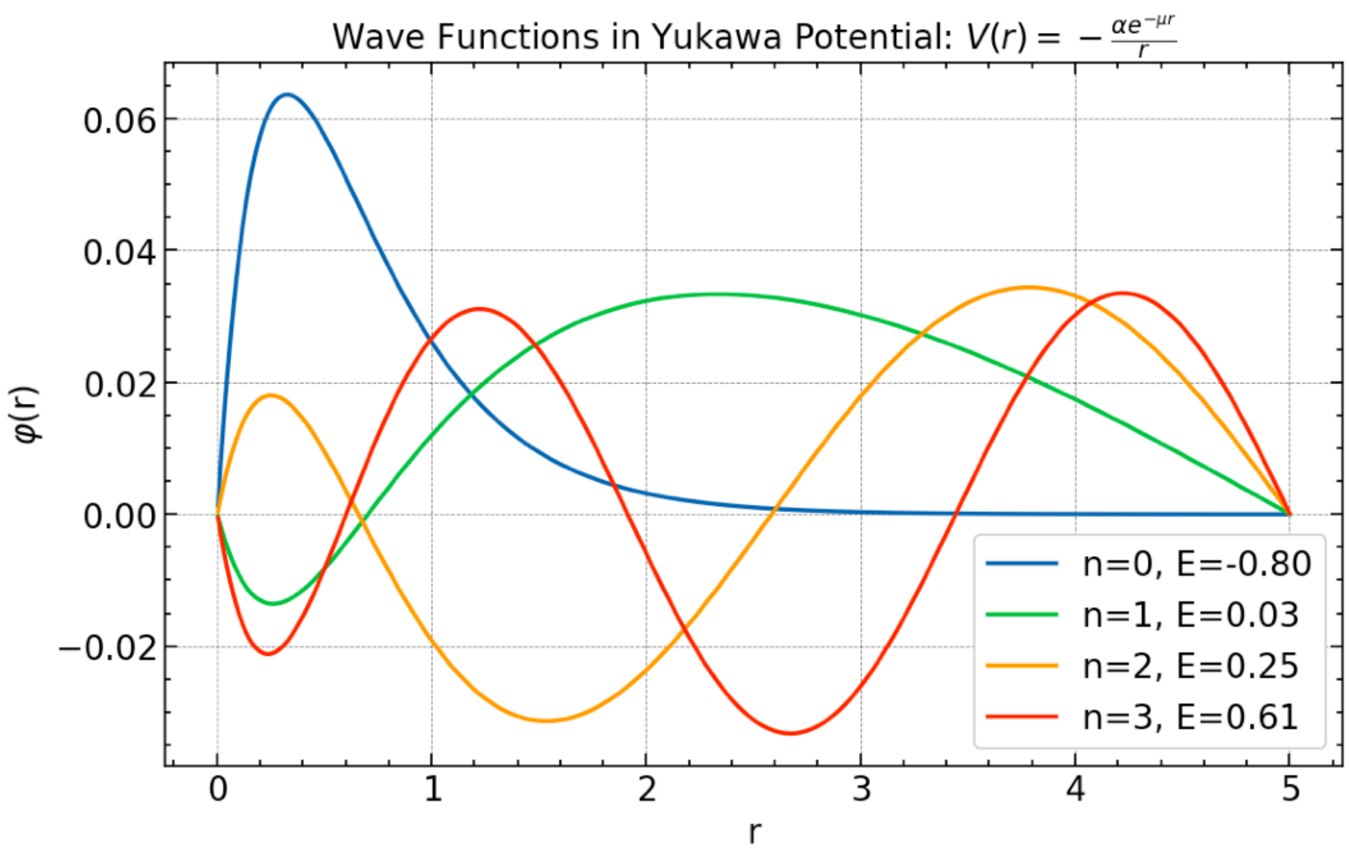
Toy Model-II

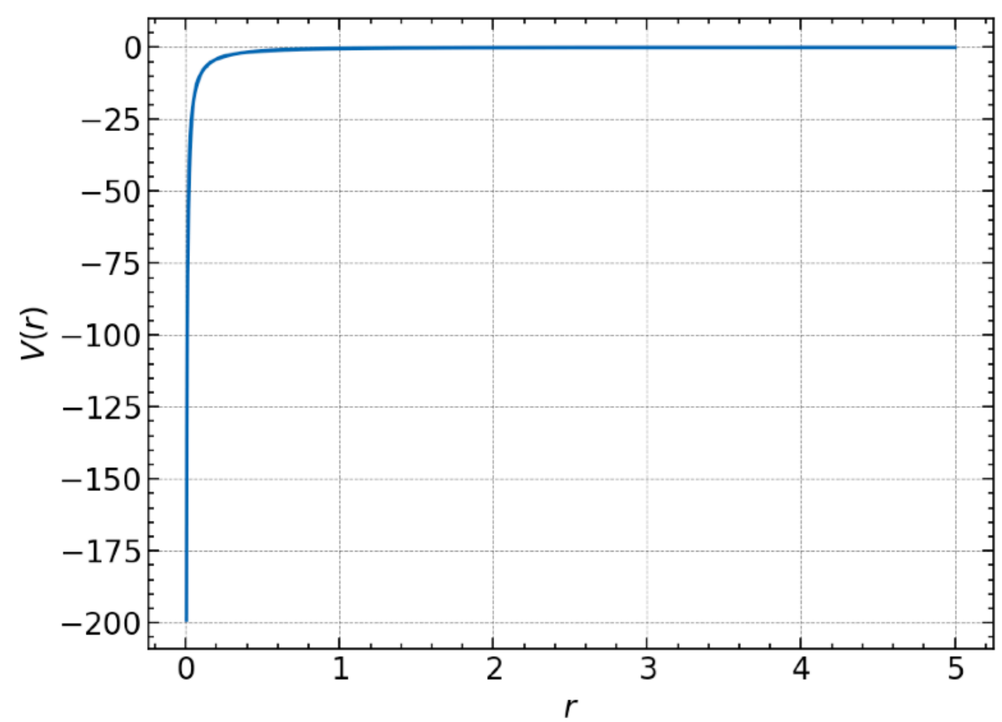
Yukawa Potential

Local potential approximation will give a Schordinger equation, $\left(-\frac{\nabla^2}{2m} + V(r)\right)\psi(r) = E\psi(r)$,

where $V(r) = -\alpha \frac{e^{-\mu r}}{r}$,

and α is the coupling(interaction) constant and μ is the mass of the exchanged particle.





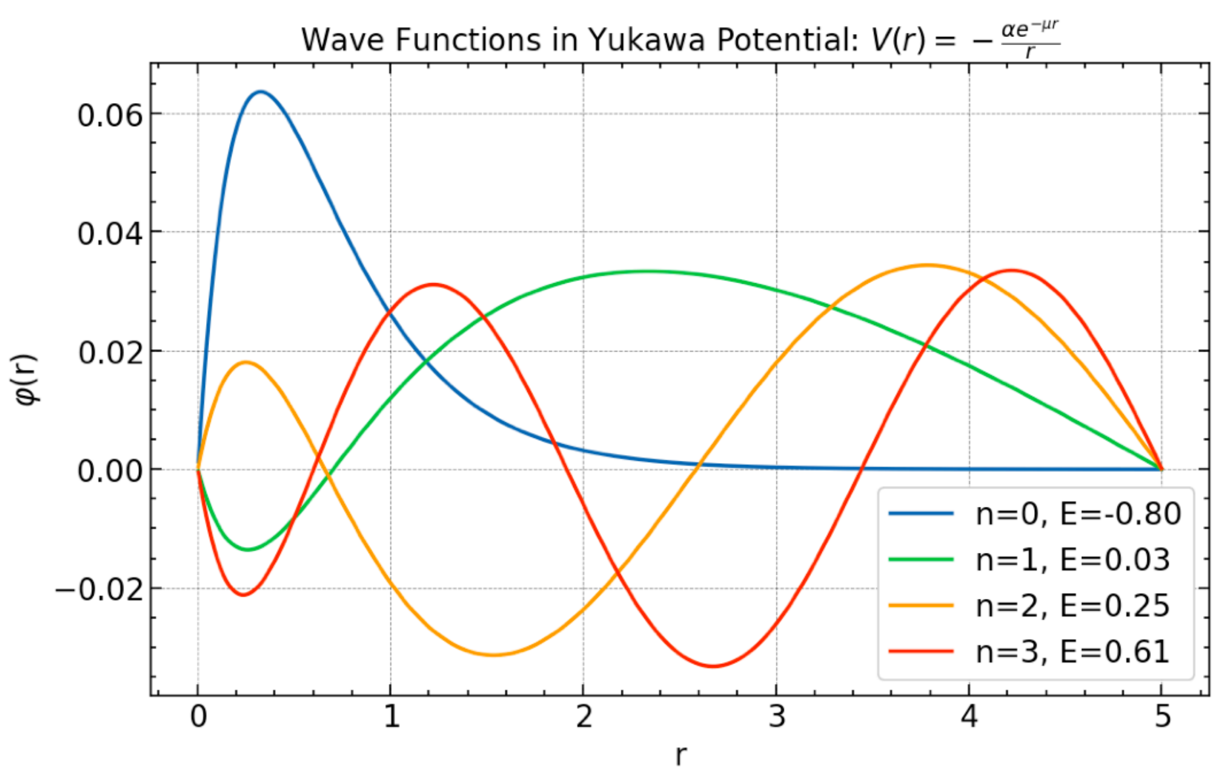
$$\mu = 1, \alpha = 2, m = 3.3\mu$$

Toy Model-II

Yukawa Potential

$$V_{\mathbf{NN}}(r) \equiv f_\theta(r)$$

$$\min_\theta \mathscr{L} = \sum_r \sum_k \left[\left(E_k - H_0\right) \phi_{\mathbf{k}}(r) - V_{\mathbf{NN}}(r)\phi_{\mathbf{k}}(r) \right]^2$$



A practical set-up for training,

$k = [0,1,2,3]$,

$r = [0.01, 5\mu], N_r = 2000.$