DeepQuark: a deep-neural-network approach to multiquark bound states

Wei-Lin Wu (吴伟霖)

Peking University

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Coauthors: Lu Meng (孟璐), Shi-Lin Zhu (朱世琳)

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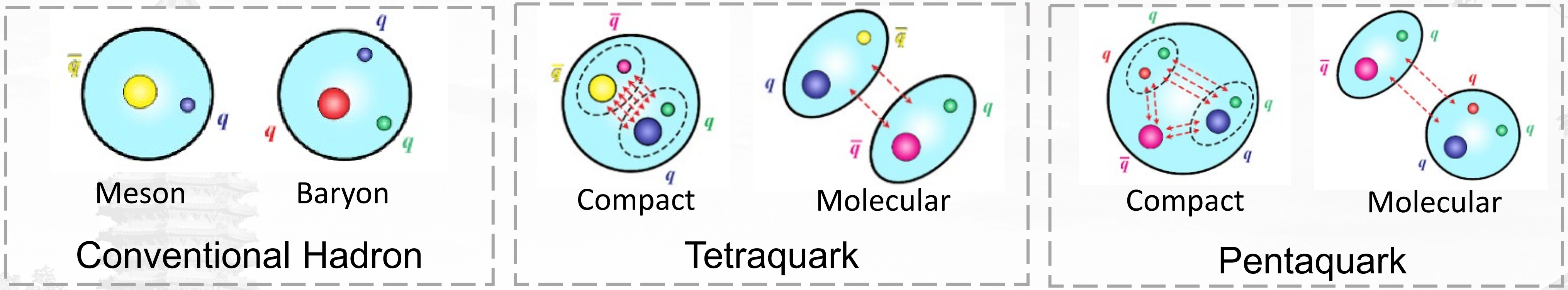
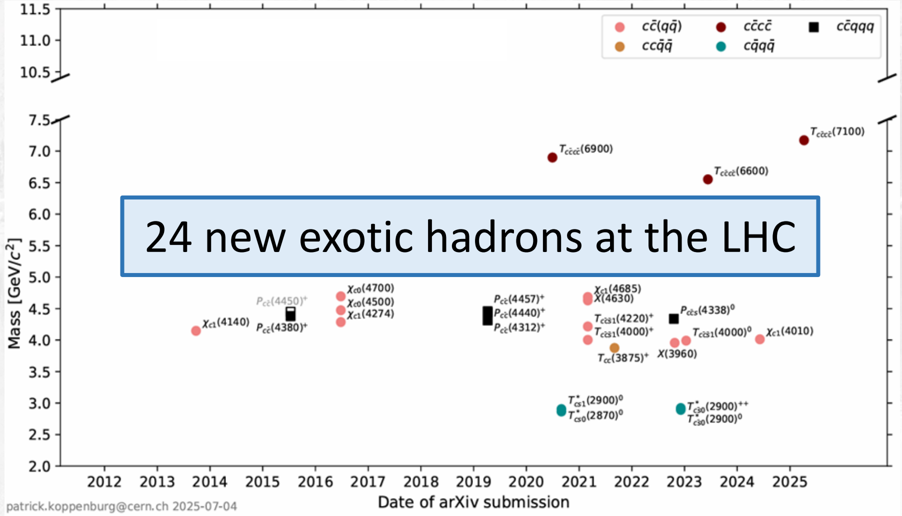
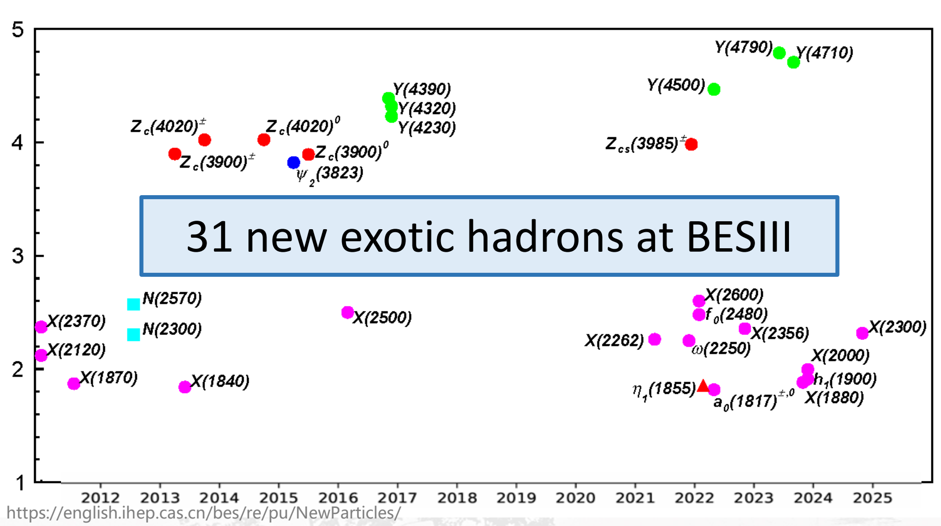
Multiquark States



- Numerous new hadron states as multiquark candidates





- Main questions in phenomenological descriptions:
  - ➢ pattern of mass spectra
  - ➢ clustering of quarks: compact / molecular / …

Quark Potential Model

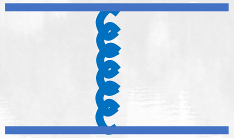
- QCD is nonperturbative at low energies → QCD-inspired models / EFT
- Quark potential model
  - ➢ Constituent quarks
  - ➢ Minimal potential model

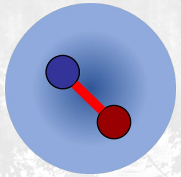
Cornell model: PRD 17,3090 (1978) ; BGS model: PRD 72,054026 (2005) , …

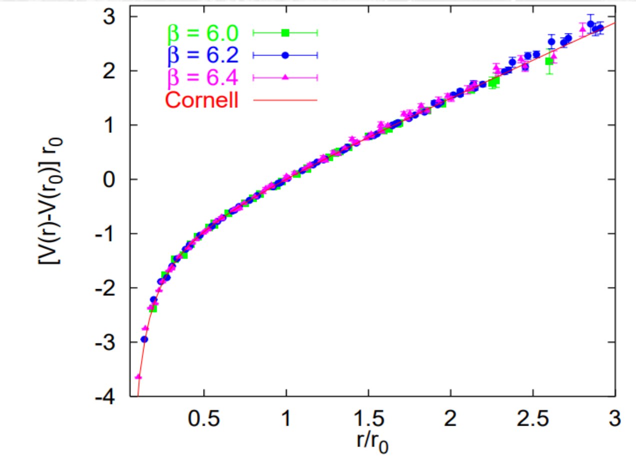
$$V_{ij}(r) = V_{ij}^{OGE} + V_{ij}^{conf.} = \left[\left(\frac{\alpha_s}{r} - \frac{8\pi\alpha_s}{3m_Q^2}\tilde{\delta}(\sigma;r)\boldsymbol{S}_i\cdot\boldsymbol{S}_j\right) + \left(-\frac{3}{4}br\right)\right]\frac{\lambda_i\cdot\lambda_j}{4}$$

one-gluon-exchange

linear confinement



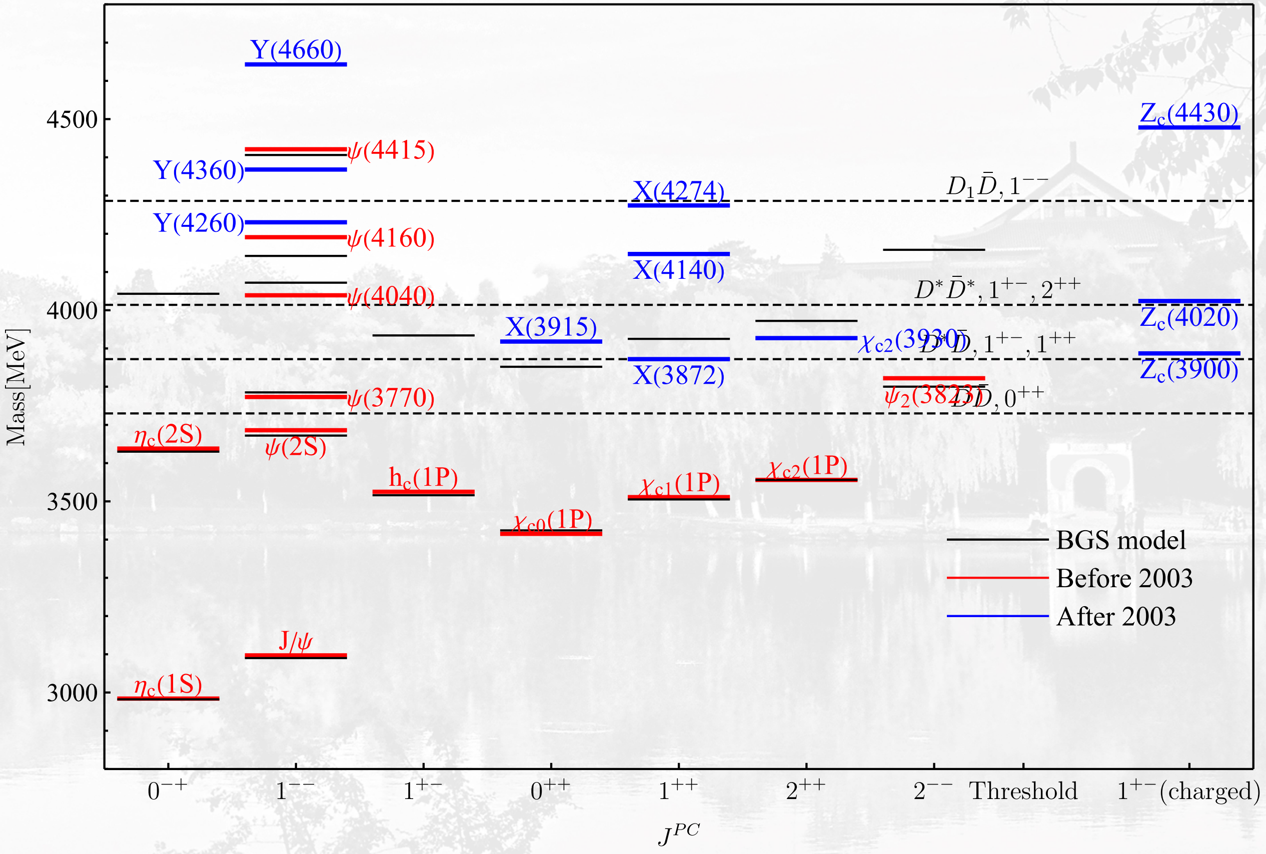




Phys.Rept. 343, 1-136 (2001)

Quark Potential Model

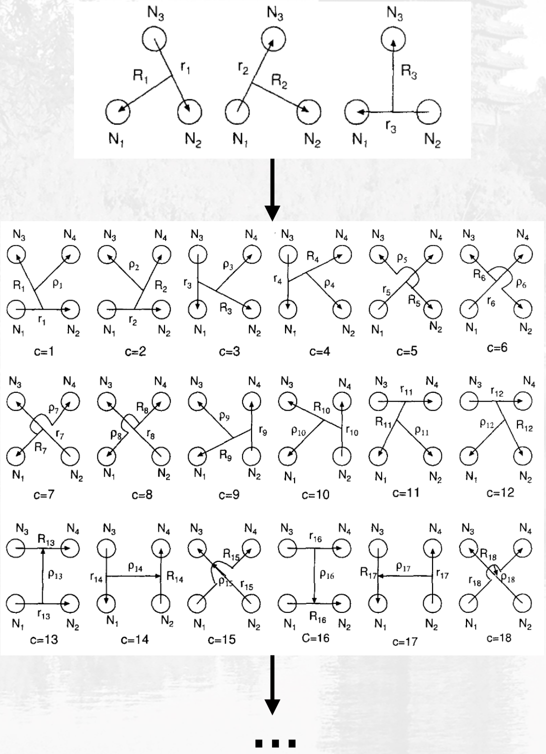
- Great success in conventional hadrons
- Charmonia: PRD 72, 054026 (2005)
  - NRQM with only 4 params
  - Well describe low-lying states below open-flavor thresholds
  - EM transitions, open flavor strong decays
  - Inconsistent above the thresholds, multiquarks ($c\bar{c}q\bar{q}$) involved

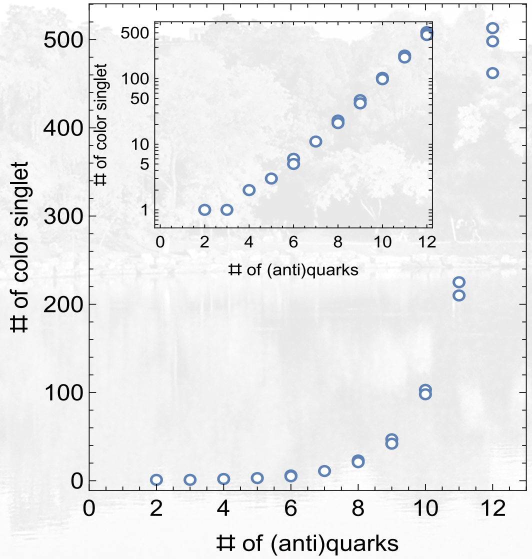


Solving multiquark states in QM

Dimensionality curse

- Basis construction: spatial ⊗ spin ⊗ flavor ⊗ color
- Exponential growth of basis

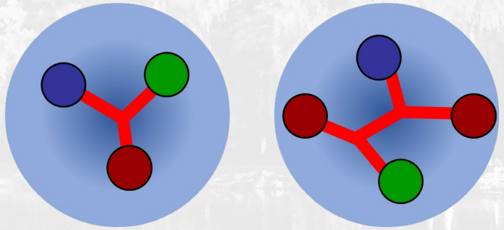




Confinement interaction

- Exp. tetraquark results ⇒ confinement pictures

- Flux-tube interaction is supported by lattice QCD



PRL 86, 18 (2001) ;
PRD 72, 014505 (2005) ;
PRD 96, 074508 (2017)

➢ Matrix elements no longer analytical

→ basis expansion intractable

AI4S enables a new framework for multiquark states

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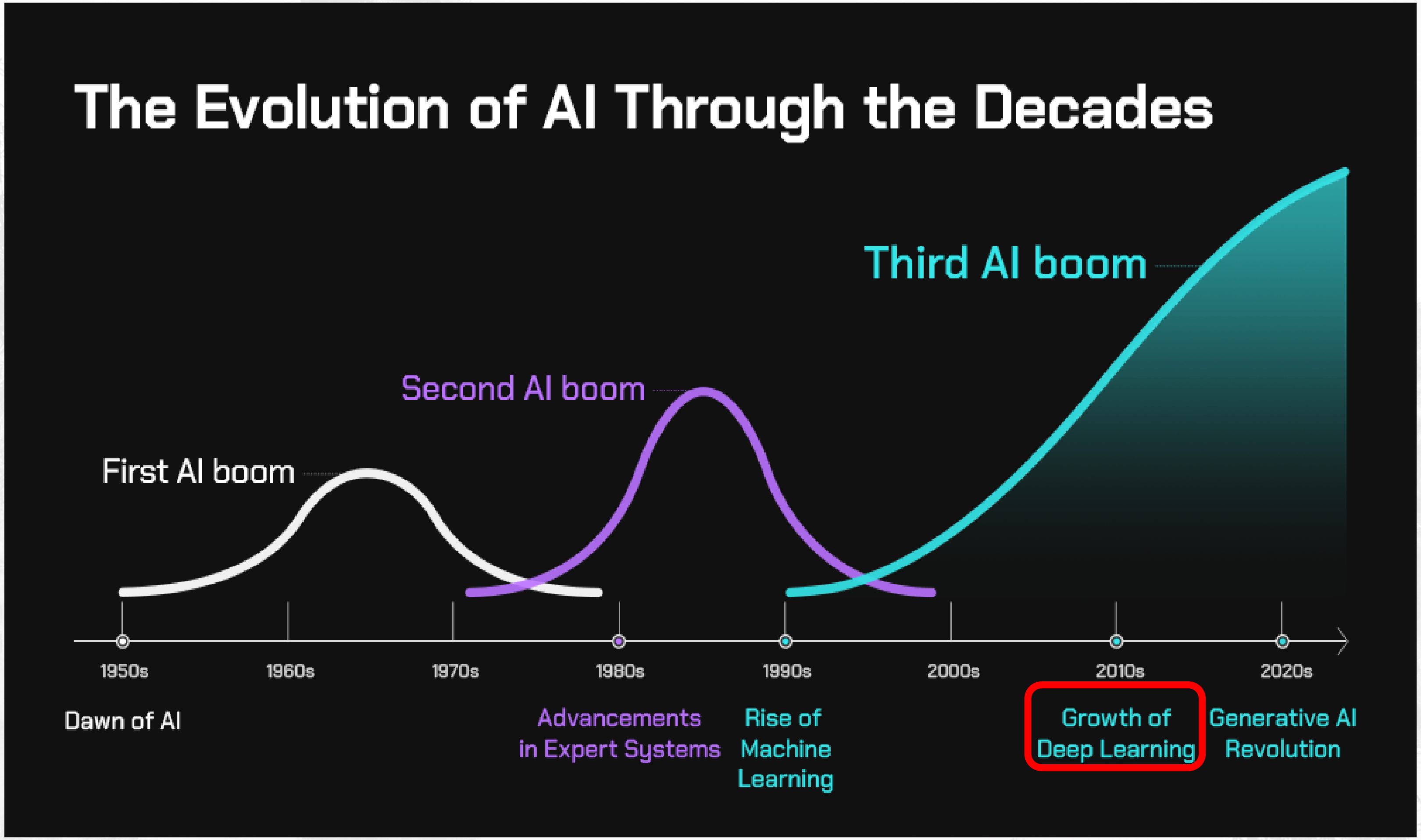
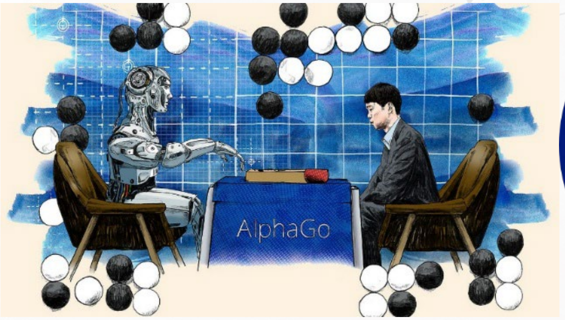
AI & DNN



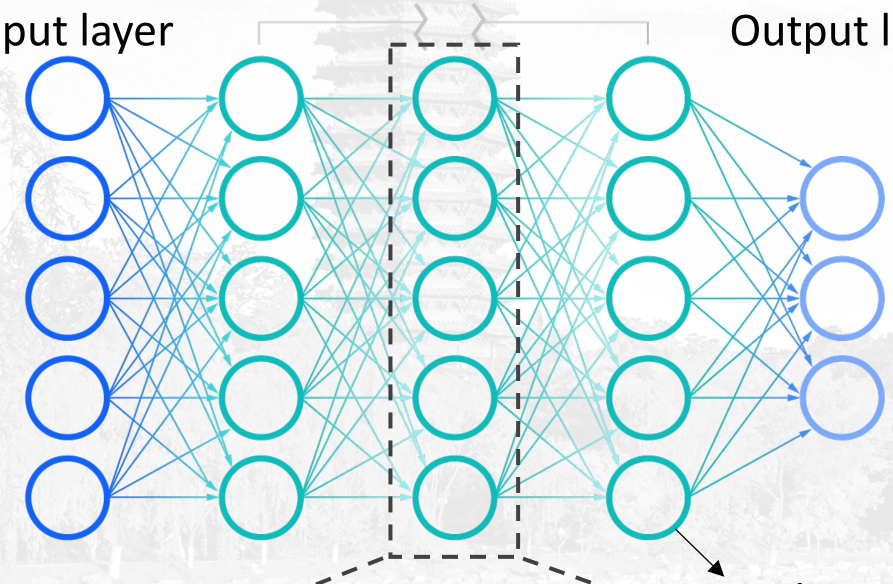


ChatGPT

deepseek

Deep Learning: Machine learning based on **Deep Neural Networks (DNN)**

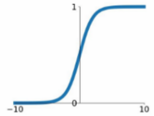
Deep Neural Network (DNN)



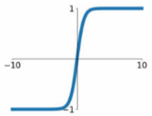
$$\vec{h}^{(i+1)} = \sigma\left(W^{(i)}\vec{h}^{(i)} + \vec{b}^{(i)}\right)$$

- Linear: Trainable parameters $W^{(i)}, \vec{b}^{(i)}$
- Nonlinear: Activation function $\sigma(x)$

Sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$



tanh $\tanh(x)$



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- Representation of high-dimensional function
- Training process:

  Minimize loss function by varying params
- Universal Approximation Theorem:

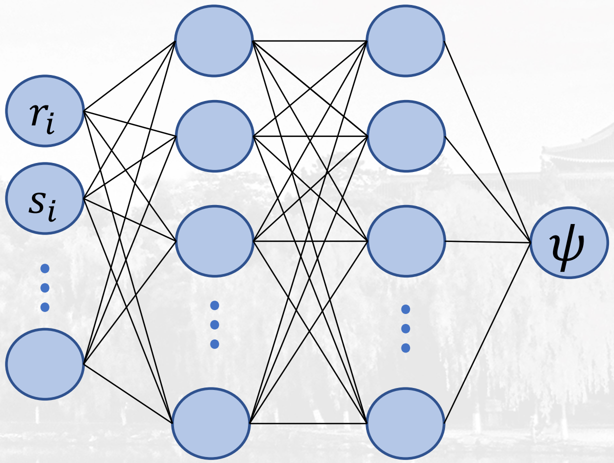
sufficiently wide or deep

> *Neural networks with a certain structure can, in principle, approximate **any continuous function** to **any desired accuracy***

Neural-network Quantum State (NQS)

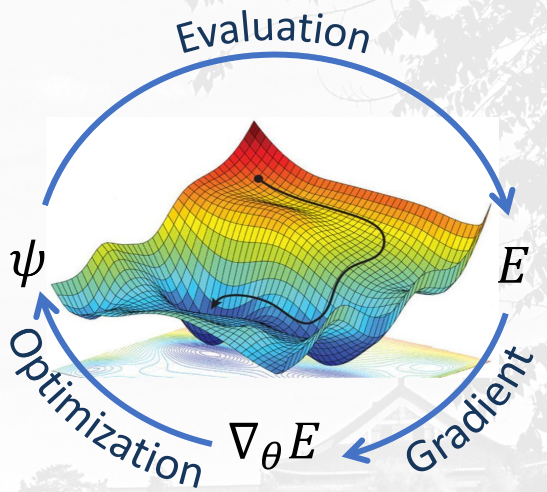
- Input: many-body configuration $(r_i, s_i, \dots)$
- Output: wave function amplitude $\psi(r_i, s_i, \dots)$
- Physical symmetry constraints

  (antisymmetry, quantum number projection)



- Advantages:
  - Polynomial scaling with N
  - Flexible and unbiased representation: describing various configurations
- Unsupervised learning: no additional data, trained by physical equation

Variational Monte Carlo (VMC)



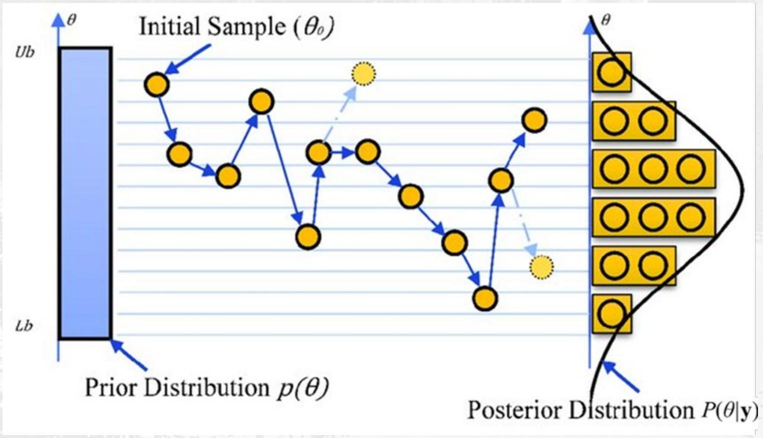
Variational Principle. $E[\theta] = \langle \psi_\theta | H | \psi_\theta \rangle / \langle \psi_\theta | \psi_\theta \rangle \geq E_0$

- Minimizing $E[\theta]$ approaches ground state
- Traditional ansatz: based on *a priori* knowledge, limited expressiveness
- **NQS: a universal, flexible ansatz**

Monte Carlo Estimation. High-dim integral via importance sampling:

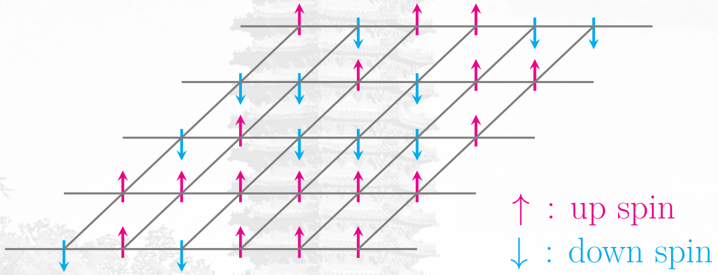
$$E[\theta] = \frac{\int |\psi_\theta(r)|^2 \frac{H\psi(r)}{\psi(r)} dr}{\int |\psi_\theta(r)|^2 dr} \approx \frac{1}{N} \sum_i E_L(r_i) \qquad E_L(r) = \frac{H\psi(r)}{\psi(r)} = \frac{T\psi(r)}{\psi(r)} + V(r)$$

- Samples $r_i \sim |\psi_\theta|^2$ generated by Metropolis-Hastings algorithm
- Efficient evaluation with statistical error $\sim 1/\sqrt{N}$
- easily handles complicated potentials, only needs $V(r_i)$



Applications in many-body physics

Spin Model



Science 355, 602 (2017).

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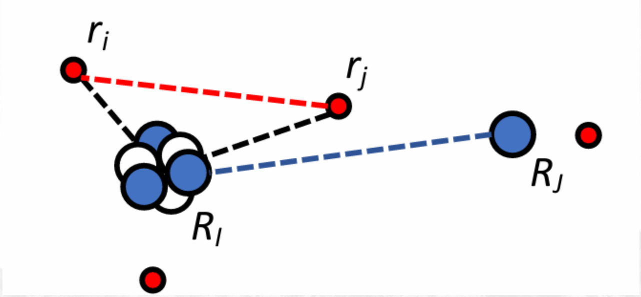
Atomic & Molecular Systems



FermiNet: Phys. Rev. Res. 2, 033429 (2020).

PauliNet: Nat. Chem. 12, 891 (2020).

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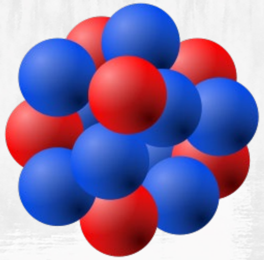
Nuclear Physics



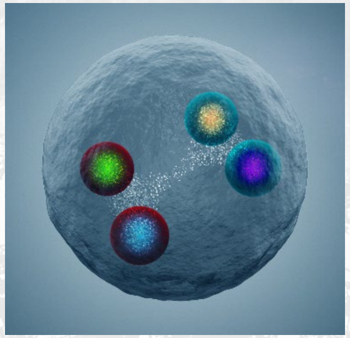
Deuteron: PLB 809, 135743 (2020).

$A \leq 4$: PRL 127, 022502 (2021).

Neutron-α scattering: PRL 135, 172502 (2025) .

…

Hadron Physics: a new frontier



DeepQuark: PRL 136, 071901 (2026)

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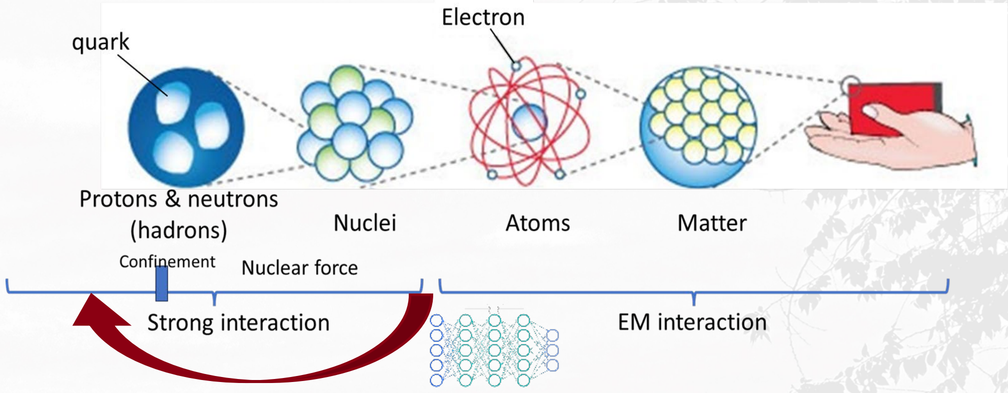
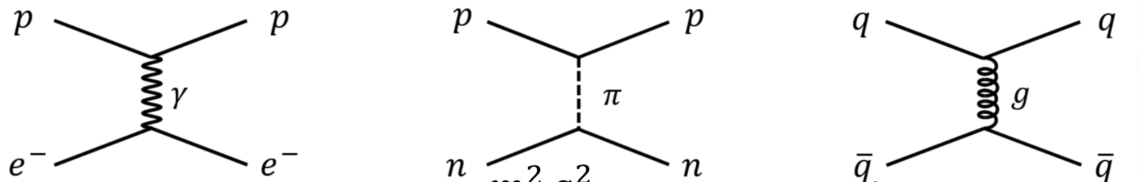
Challenges in multiquark systems



- Stronger interactions among quarks



$e^2 = 0.1$ $\quad \frac{m_\pi^2 g_A^2}{16\pi f_\pi^2} \sim 0.1$ $\quad \frac{4}{3}\alpha_s(m_c) \sim 0.4$

  - significant correlation effects
  - no evidence of shell structure in multiquarks
  - Slater-type wave function is not a good ansatz

$$\sum_{\mathcal{P}} \mathrm{sign}(\mathcal{P}) \prod_i \phi_i^k(\mathbf{x}_{\mathcal{P}_i}) = \begin{vmatrix} \phi_1^k(\mathbf{x}_1) & \dots & \phi_1^k(\mathbf{x}_n) \\ \vdots & & \vdots \\ \phi_n^k(\mathbf{x}_1) & \dots & \phi_n^k(\mathbf{x}_n) \end{vmatrix}$$

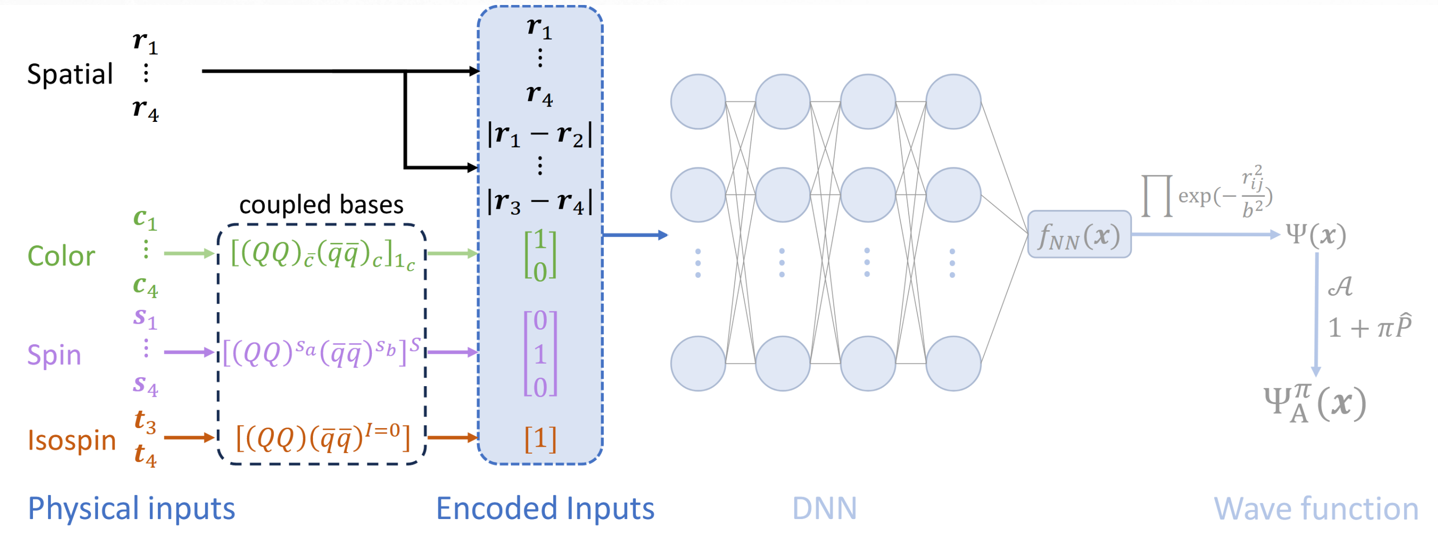
$$= \det\left[\phi_i^k(\mathbf{x}_j)\right] = \det[\mathbf{\Phi}^k],$$

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n) = \sum_k \omega_k \det[\mathbf{\Phi}^k],$$

- Symmetry constraints
  - color projection to ensure SU(3) singlet
  - spin projection to target states of interest

    $[cc\bar{q}\bar{q}]_{S=0}$: DD threshold, $[cc\bar{q}\bar{q}]_{S=1}$: T_{cc} state

DeepQuark Architecture



Empowered by NetKet
https://github.com/netket

Spatial Input

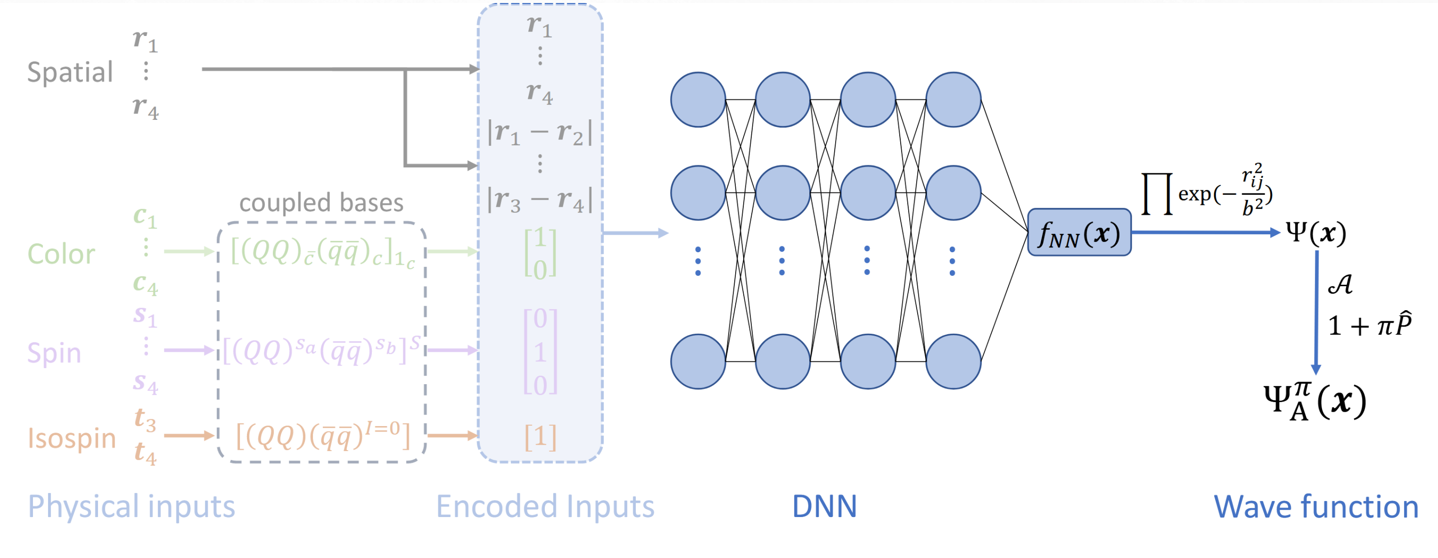
- Quark coordinates in c.m. frame
- Interparticle distances
  - ➢ encapsulate interparticle correlations
  - ➢ better describe wave function cusps

PRR 2, 033429 (2020)

Discrete Input

- Coupled bases instead of single particle (s_i, t_i, c_i)
  - ➢ satisfy discrete symmetry
  - ➢ describe multichannel coupling
- One-hot encoding
  - ➢ no prejudiced correlations between bases

DeepQuark Architecture



Empowered by NetKet
https://github.com/netket

- 4 hidden layers with only $O(10^3)$ parameters

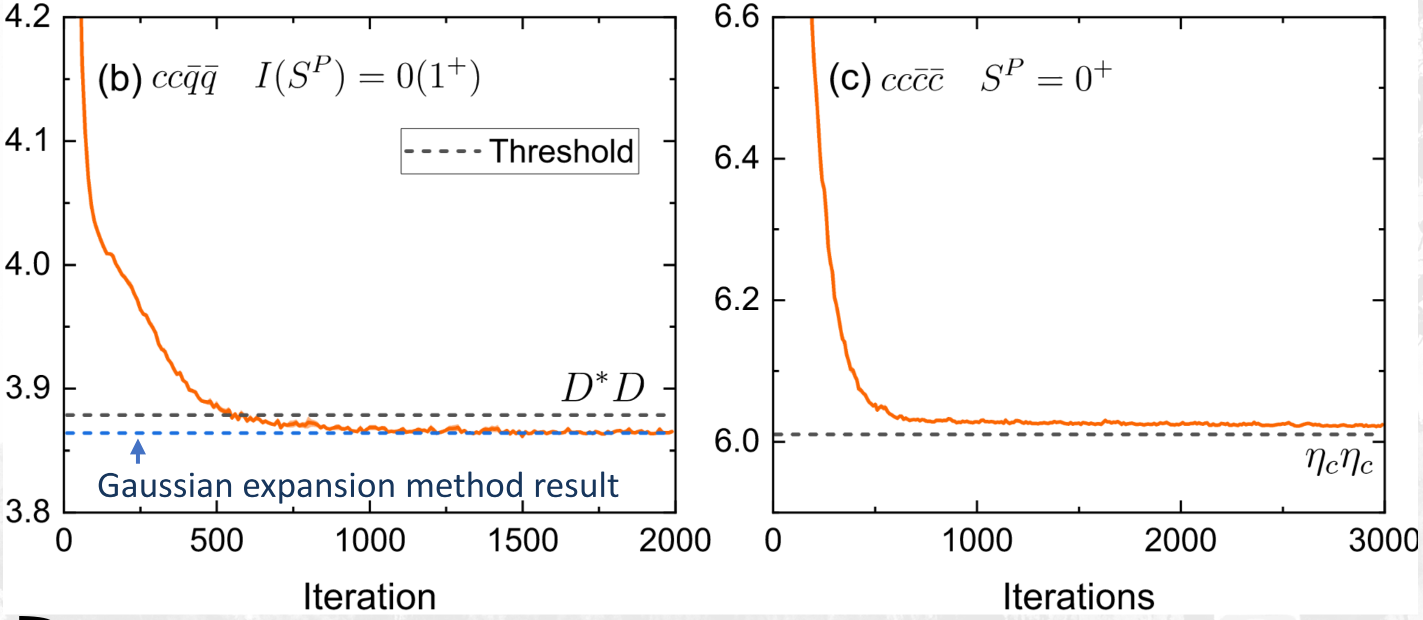
  vs. GEM for tetraquark: ~10^4 bases; $A \leq 4$ nuclei: ~10^4 paras

  PRL 127, 022502 (2021)

- Boundary condition $\exp(-r_{ij}^2/b^2)$
  - ➢ better initial state for faster convergence
- Antisymmetrization $\mathcal{A} = \sum_{\mathcal{P}}(-1)^{\mathcal{P}}\mathcal{P}$
  - ➢ $O(n!)$ for identical particles
  - ➢ the price for enforcing symmetry
- Parity projection $1 + \pi\hat{P}$

Tetraquarks with two-body interactions

- Convergence within 2000 iterations
- High accuracy competitive with Gaussian expansion method



- $cc\bar{q}\bar{q}$: molecular state, agree with exp.
- $bb\bar{q}\bar{q}$: compact tetraquark
- $QQ\bar{Q}\bar{Q}$: no bound states

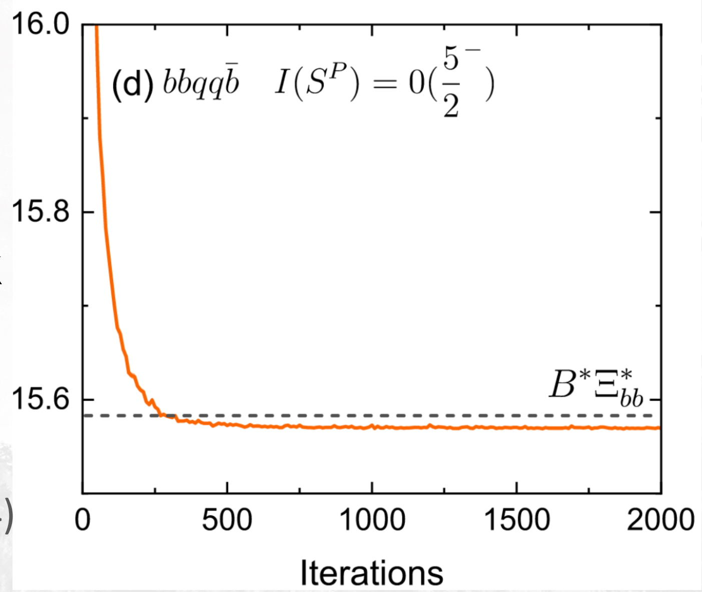
unified descriptions

	$I(S^P)$	Thresh.	ΔE	$P_{\bar{3}_c\otimes 3_c}$	$P_{6\otimes 6_c}$	r_{QQ}	$r_{\bar{q}\bar{q}}$	$r_{Q\bar{q}}$
$cc\bar{q}\bar{q}$	$0(1^+)$	DD^*	-15	55%	45%	1.24	1.41	1.06
$bb\bar{q}\bar{q}$	$0(1^+)$	$\bar{B}\bar{B}^*$	-153	97%	3%	0.33	0.78	0.69
$QQ\bar{Q}\bar{Q}$	$0(0^+)$ $0(1^+)$ $0(2^+)$	$\eta_c\eta_c$ $\eta_c J/\psi$ $J/\psi J/\psi$	Unbound					

Pentaquarks with two-body interactions

- Five-body dynamical calculations without approximations via DeepQuark
- Moderate increase in computational cost compared to tetraquark

  (2000 iters: ~40/60 mins on a A100 GPU for tetra/penta-quark)



- Possible bound pentaquark systems $QQ\bar{Q}qq$ PRD 88, 054014 (2013) PRD 110, 076014 (2024)
  - Heavy diquark-antiquark symmetry: $(QQ)_{\bar{3}_c} \to \bar{Q}$
  - $\bar{Q}\bar{Q}qq \to QQ\bar{Q}qq$
  - Given $\mathrm{M}_{\bar{Q}\bar{Q}qq} < M_{\bar{Q}q} + M_{\bar{Q}q}$, $\mathrm{M}_{QQ\bar{Q}qq} < M_{QQq} + M_{\bar{Q}q}$?

	$I(S^P)$	Thresh.	ΔE	r_{QQ}	r_{Qq}	r_{qq}	$r_{Q\bar{Q}}$	$r_{q\bar{Q}}$
$cc\bar{c}qq$	$0(1/2^+, 3/2^+)$	$\eta_c\Lambda_c, J/\psi\Lambda_c$	Unbound					
	$0(5/2^+)$	$\bar{D}^*\Xi^*_{cc}$	-3	0.50	1.39	1.90	1.73	1.38
$bb\bar{b}qq$	$0(1/2^+, 3/2^+)$	$\eta_b\Lambda_b, \Upsilon\Lambda_b$	Unbound					
	$0(5/2^+)$	$B^*\Xi^*_{bb}$	-14	0.30	0.89	1.22	0.88	0.88

$\to J/\psi\Lambda_c$ (D-wave)

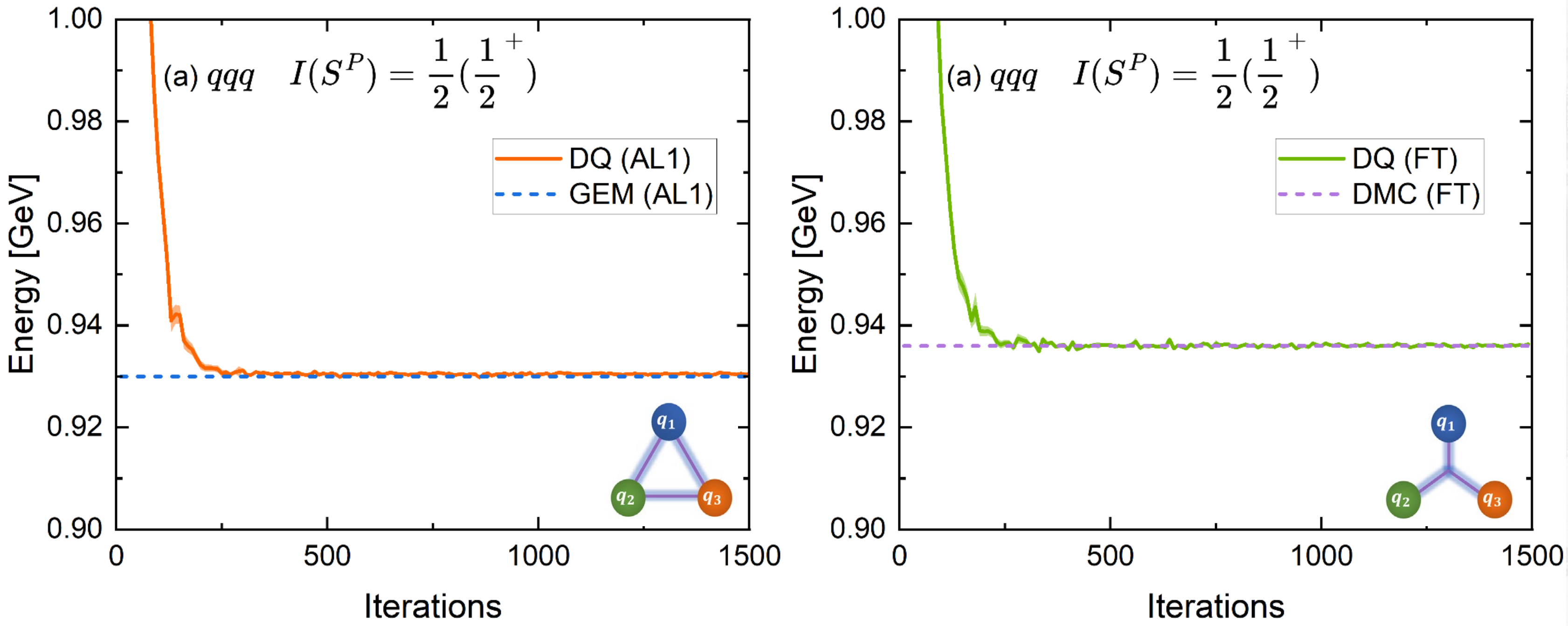
Baryons with flux-tube interactions

- Lattice QCD favors flux-tube confinement interactions for baryons PRL 86, 18-21 (2001)

$$V_{\text{conf}} = \sum_{i<j} \lambda r_{ij} \to \sigma L_{\min}$$

$$L_{\min} = \begin{cases} \left[\frac{1}{2}(a^2+b^2+c^2) + \frac{\sqrt{3}}{2}\sqrt{d(d-2a)(d-2b)(d-2c)}\right]^{1/2} & \max(\theta_a,\theta_b,\theta_c) < \frac{2\pi}{3}, \\ d - \max(a,b,c) & \max(\theta_a,\theta_b,\theta_c) > \frac{2\pi}{3}, \end{cases}$$

- DeepQuark efficiently incorporates flux-tube type interactions using VMC
- Ready for exploring different confinement mechanisms in tetraquarks



Summary & Outlooks

- DNN + VMC framework
  - DNN as many-body wave function: efficient, general, unbiased
  - VMC: solves ground state using variational principle; handles complicated interactions
- DeepQuark: Towards accurate solutions of multiquark Hamiltonians
  - Architecture for strongly correlated multiquark systems with symmetry constraints
  - Unbiased form: clustering behaviors (molecular / compact)
  - Outperforms traditional methods starting from pentaquarks
  - Capable of flux-tube interactions
- Outlooks:
  - Framework for exploring confinement mechanisms in multiquark states
  - DNN for scattering and resonances

Thanks for your attention!

Backup

Previous NQS

NQS in electronic / nuclear systems: Slater-Jastrow form

$$\Psi(\mathrm{x}) = e^{J}\,\det[\boldsymbol{\phi}]$$

Slater determinant

- Enforces fermionic antisymmetry
- Built from single-particle orbital
- Neural network:
  - generalize $\phi_i(x_j) \to \phi_i(x_j; x_1, \ldots, x_N)$
  - encode many-body correlations

Jastrow factor

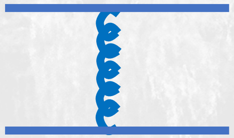
- Permutation invariant
- Captures correlations beyond mean field
- Cusps from short-range interactions
- Neural network:
  - generalize $J = \sum_{i<j} u(x_i, x_j) \to J(x_1, \ldots, x_N)$

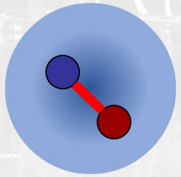
$x_i = (r_i, s_i, \ldots)$

AL1 model

$$H=\sum_i \frac{p_i^2}{2m_i}+\sum_{i<j} V_{\mathrm{OGE},ij}+V_{\mathrm{conf},ij}$$

- Minimal nonrelativistic model extended to multiquark sectors
- Pairwise interaction:
  - one-gluon-exchange $$V_{\mathrm{OGE},ij}=\frac{\lambda_i\cdot\lambda_j}{4}\left[\frac{\alpha_s}{r}-\frac{8\pi\alpha_s'}{3m_i m_j}\tilde{\delta}(\sigma;r)\boldsymbol{S}_i\cdot\boldsymbol{S}_j\right]$$
  - linear confinement $$V_{\mathrm{conf},ij}=\frac{\lambda_i\cdot\lambda_j}{4}\left(-\frac{3}{4}br+\Lambda\right)$$



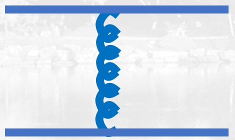


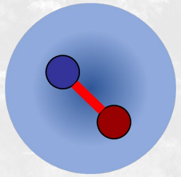
- Parameters fitted by meson spectra across all flavor sectors

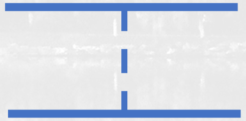
More models

TABLE SM-IV. Different ingredients in five different quark models.

	One-gluon-exchange		Confinement		meson-exchange
	asymptotic freedom	Hyperfine	form	screening effect	
AL1	No	Gaussian	linear	No	No
AL2	Yes	Gaussian	linear	No	No
AP1	No	Gaussian	$p = 2/3$	No	No
AP2	Yes	Gaussian	$p = 2/3$	No	No
SLM	No	Yukawa	linear	Yes	Yes





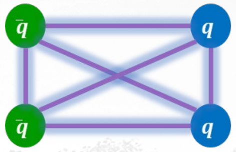


Potential	DQ		GEM [4]	
	E	ΔE	E	ΔE
AL1	10491	-153	10493	-152
AP1	10502	-176	10504	-175
AL2	10473	-151	10474	-151
AP2	10471	-174	10472	-174
SLM	10230	-362	10232	-360

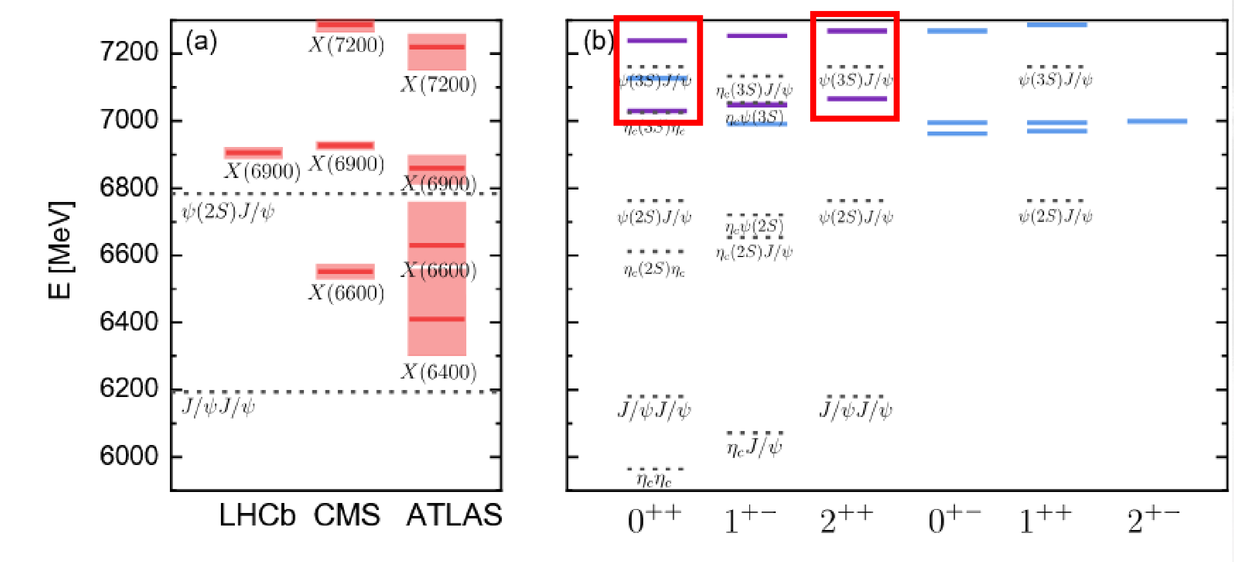
- Accommodate a wide variety of interactions
- Taking $bb\bar{q}\bar{q}$ as a testing system, all in agreement with GEM
- A flexible framework for spectroscopy studies

QM for tetraquark states

- Does QM work in multiquark sector?
- Previous tetraquark study:
  - Pairwise confinement interaction model

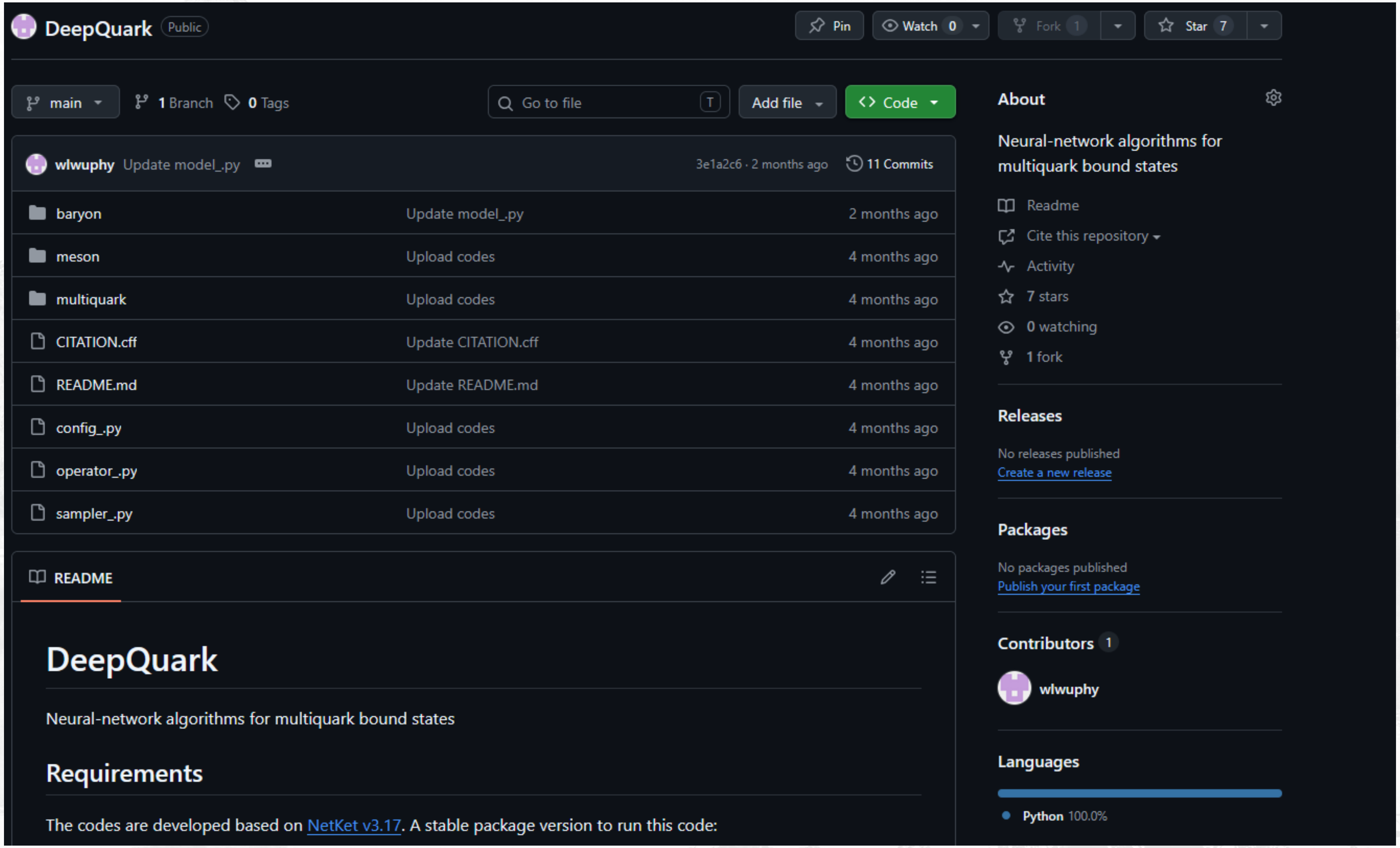


  - Gaussian expansion method (GEM) to solve 4-body problem PPNP 51, 223 (2003)
  - Bound and resonant states
    - ✓ $T_{cc}(3875)^+$ PLB 814, 136095 (2021)
    - ✓ $T_{cc\bar{c}\bar{c}}(6900), T_{cc\bar{c}\bar{c}}(7200)$ PRD 109, 054034 (2024)
    - ✓ $T^*_{cs0}(2870)^0$ PRD 109, 014010 (2024)



Experiment Theory

Code



Empowered by NetKet
https://github.com/netket

https://github.com/wlwuphy/DeepQuark