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DeepQuark: Deep-Neural-Network Approach to Multiquark Bound States

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Hadron Physics Workshop 2025

Outline

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1. Introduction

Why Exotic Hadrons Matter

QCD: The Unsolved Theory

- Strong force governs nuclear matter
- Confinement remains poorly understood
- Quarks never observed in isolation — why?

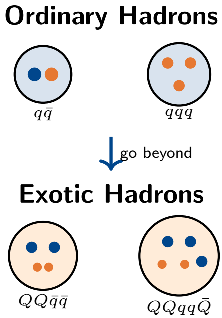
Exotic Hadrons as Probes:

- States beyond $q\bar{q}$ mesons and qqq baryons
- Directly probe **how color forces work**
- Test our understanding of nonperturbative QCD

The Central Question:

How do multiple quarks arrange themselves?

- Compact multiquark cluster?
- Loosely bound hadronic molecule?
- Dynamical mixture of configurations?



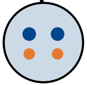
Understanding exotics $\Rightarrow$ insights into confinement

The Multiquark Zoo: Experimental Discoveries

Key Experimental Milestones:

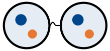
- **2003**: $X(3872)$ at Belle — first exotic candidate
- **2015**: P_c pentaquarks at LHCb ($uudc\bar{c}$)
- **2020**: $T_{4c}(6900)$ at LHCb — fully heavy $cc\bar{c}\bar{c}$
- **2021**: $T_{cc}(3875)^+$ at LHCb — doubly charmed $cc\bar{u}\bar{d}$
- **2024**: CMS reports $J^{PC} = 2^{++}$ T_{4c} states

Compact?



or

Molecule?



DeepQuark answers this!

> **This Work:** Study T_{cc}, T_{bb}, T_{4c}, T_{4b}, and triply heavy pentaquarks $QQqq\bar{Q}$

Computational Challenges in Multiquark Systems

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Exponential Complexity:

- Wave function dimension scales exponentially
- Extra SU(3) color degree of freedom
- Multiple quantum numbers: S, I, J^{PC}, color

Strong Correlations:

- Single-particle approximation fails
- No shell structure (unlike atoms/nuclei)
- Full multi-channel dynamics required

Limitations of Existing Methods:

Gaussian Expansion Method (GEM):

- Exponential growth of basis states
- Incomplete for 5+ quarks

Diffusion Monte Carlo (DMC):

- Notorious sign problem
- Limited for strongly correlated systems

Previous Pentaquark Studies:

- Approximations in spatial configurations
- $\Rightarrow$ Unknown systematic errors

2. Deep Learning Background

What is Machine Learning?

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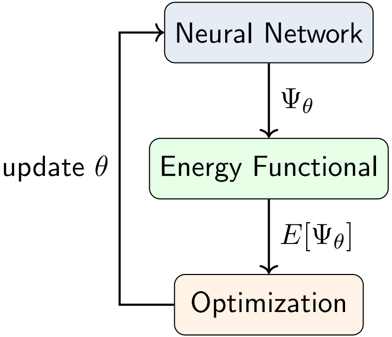
Core Idea:

Learn patterns from data without explicit programming

Types of Learning:

- **Supervised:** Learn from labeled examples
- **Unsupervised:** Find hidden structure
- **Variational:** Optimize a target functional $\Leftarrow$ What we use!

> **Universal Approximation Theorem:**
> Neural networks can approximate *any* continuous function to arbitrary accuracy



Variational Learning

Single Neuron:

$$y = \sigma(\mathbf{W}\mathbf{x} + \mathbf{c})$$

where $\sigma = \tanh$ (activation function)

Physics Analogy: Basis Expansion

Traditional wave function:

$$\Psi(x) = \sum_i c_i \phi_i(x)$$

Neural network:

$$\Psi(x) = \sum_i w_i \sigma\left(\sum_j W_{ij} x_j + c_j\right)$$

Key difference:

- Basis functions ϕ_i are *fixed* in traditional methods
- Neural network *learns* the optimal basis!
- Adaptive, data-driven representation

Variational Monte Carlo Optimization

Variational Principle:

$$E_{\boldsymbol{\theta}} = \frac{\langle \psi_{\boldsymbol{\theta}} | H | \psi_{\boldsymbol{\theta}} \rangle}{\langle \psi_{\boldsymbol{\theta}} | \psi_{\boldsymbol{\theta}} \rangle} \geq E_0$$

Minimize energy to find ground state!

Monte Carlo Evaluation:

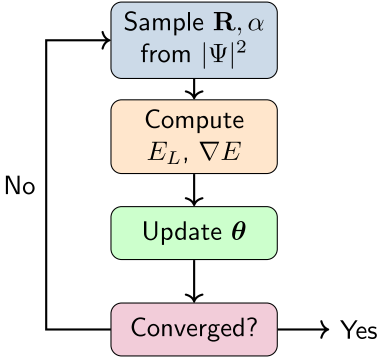
$$E_{\boldsymbol{\theta}} \approx \frac{1}{N} \sum_{n=1}^{N} E_L(\mathbf{R}_n, \alpha_n)$$

Sample from $|\Psi(\mathbf{R}, \alpha)|^2$

Stochastic Reconfiguration:

$$\boldsymbol{\theta}^{i+1} = \boldsymbol{\theta}^{i} - \eta (S + \epsilon I)^{-1} \nabla E$$

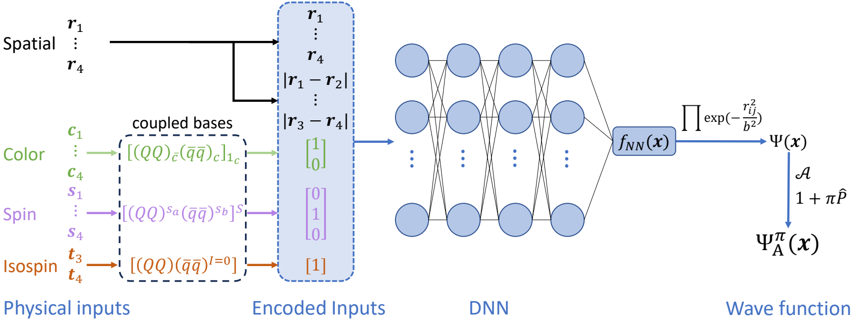
VMC Loop



Key advantage: No sign problem (unlike DMC)!

3. DeepQuark Framework

DeepQuark Architecture



Four types of input: Spatial coordinates $\mathbf{r}_i$, $|\mathbf{r}_i - \mathbf{r}_j|$ + Color α_c + Spin α_s + Isospin α_t

DeepQuark Wave Function

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Full wave function with built-in symmetries:

$$\Psi^{\pi}_{\mathsf{A}}(\boldsymbol{x}) = (1+\pi\hat{P})\mathcal{A}\left[f_{NN}(\boldsymbol{x})\prod_{i<j}\exp\left(-\frac{r_{ij}^2}{b^2}\right)\right]$$

Key Components:

- $f_{NN}(\boldsymbol{x})$: Neural network amplitude
- $\mathcal{A}[\cdots]$: Antisymmetrization (Fermi-Dirac)
- $(1+\pi\hat{P})$: Parity projection $(\pi=\pm1)$
- $e^{-r_{ij}^2/b^2}$: Gaussian boundary $(b\sim 2\text{–}4$ fm)

Input Features:

Coupled Basis Approach:

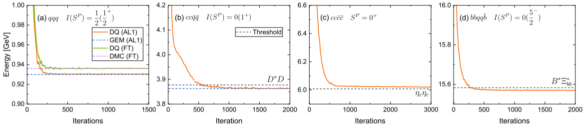
- Color-spin-isospin bases
- Example for $QQ\bar{q}\bar{q}$: $\bar{3}_c\otimes 3_c$ and $6_c\otimes\bar{6}_c$
- Network learns mixing automatically

Why This Works:

- No *a priori* structure assumption
- Same ansatz $\Rightarrow$ molecular or compact

4. Results

Benchmarks: DeepQuark Performance



(a) nucleon, (b) T_{cc}, (c) T_{4c}, (d) pentaquark

Key Performance Metrics:

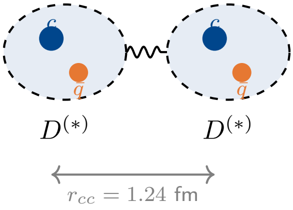
- Matches GEM/DMC to < 0.1 MeV
- Converges in $\sim$1000–3000 iterations
- $\sim$1000–3000 parameters (compact!)

Unique Capability:

- Handles flux-tube confinement
- GEM cannot do this efficiently!

Same accuracy, handles complex interactions

Molecular Structure



Ground State Properties:

- Binding energy: $\Delta E = -\mathbf{15}$ MeV
- **Color mixing:**
  $\chi_{\bar{3}\times 3} : \chi_{6\times\bar{6}} = 55\% : 45\%$
- Significant mixing of both configurations!

RMS Radii (Molecular Structure):

$r_{c\bar{q}}$	1.06 fm
r_{cc}	1.24 fm
$r_{\bar{q}\bar{q}}$	1.41 fm

$r_{cc}, r_{\bar{q}\bar{q}} > r_{c\bar{q}} \Rightarrow$ Molecular D^*D

Consistent with LHCb $T_{cc}(3875)^+$ discovery!

Doubly Bottom Tetraquark T_{bb}: Compact Diquark

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Ground State Properties:

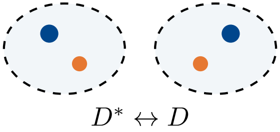
- Binding energy: $\Delta E = -153$ MeV
- **Color:** $\chi_{\bar{3}\times 3} : \chi_{6\times\bar{6}} = 97\% : 3\%$
- Dominated by $\bar{3}_c \otimes 3_c$ configuration!

Compact Structure:

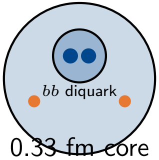
r_{bb}	0.33 fm (compact diquark!)
$r_{b\bar{q}}$	0.69 fm
$r_{\bar{q}\bar{q}}$	0.78 fm

Heavy bb diquark acts like $\bar{3}_c$ antiquark

T_{cc}: **Molecular**



T_{bb}: **Compact**



Same ansatz describes both molecular and compact structures!

T_{4c}: A Laboratory for Confinement

Why T_{4c} Is Special:

- **Pure QCD system** — no light quark chiral effects
- Short-range gluon exchange dominates
- Ideal testbed for confinement mechanisms

Experimental Motivation:

- LHCb (2020): $T_{4c}(6900)$ resonance
- CMS (2024): Three states with $J^{PC} = 2^{++}$
- ATLAS: Confirmation of structures

"A clear platform to investigate short-range gluon exchange and confinement"

Why DeepQuark Can Calculate It:

Challenge: Flux-tube confinement

- Many-body interaction (not pairwise)
- "Computationally intractable" for GEM
- Requires exponentially many basis states

DeepQuark Solution:

- VMC handles complex many-body forces
- No basis expansion needed
- Monte Carlo sampling is efficient
- No sign problem (unlike DMC)

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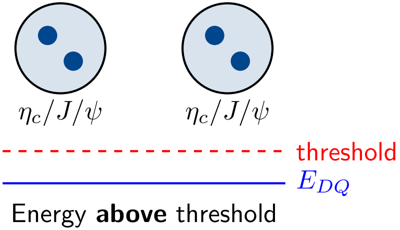
No Bound State



Results:

System	S^P	Bound?
$cc\bar{c}\bar{c}$	$0^+, 1^+, 2^+$	No
$bb\bar{b}\bar{b}$	$0^+, 1^+, 2^+$	No

Color proportion: $\chi_{\bar{3}\times 3} : \chi_{6\times\bar{6}} \approx 1 : 2$

$\Rightarrow$ Consistent with meson-meson scattering

Experimental context:

- LHCb (2020): $T_{4c}(6900)$ resonance
- CMS (2025): Three T_{4c} with $J^{PC} = 2^{++}$

$\Rightarrow$ Observed structures are resonances, not bound states

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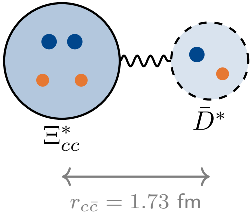
Molecular Structure



$\Delta E = -3$ MeV

Why $S = 5/2$ is special:

S-wave $S = \frac{3}{2}$ isoscalar baryon is forbidden by Fermi statistics!

$\Rightarrow$ Lowest threshold: $\bar{D}^*\Xi^*_{cc}$ (or $B^*\Xi^*_{bb}$)

Bound states found:

State	Mass	ΔE
$P_{cc\bar{c}}(5715)$	5715 MeV	$-\mathbf{3}$ MeV
$P_{bb\bar{b}}(15569)$	15569 MeV	$-\mathbf{14}$ MeV

Structure: Molecular $\bar{D}^*\Xi^*_{cc}$

- $r_{cc} = 0.50$ fm (compact Ξ^*_{cc})
- $r_{c\bar{c}} = 1.73$ fm (large separation)

5. Conclusions

Summary

DeepQuark: First DNN-based VMC for multiquark bound states

Method Achievements:

- Novel coupled color-spin-isospin bases
- Unbiased compact & molecular description
- Handles flux-tube confinement efficiently
- Competitive with GEM and DMC
- Scalable to larger systems

Physics Results:

- T_{cc}: Molecular, $\Delta E = -15$ MeV
- T_{bb}: Compact diquark, $\Delta E = -153$ MeV
- T_{4c}, T_{4b}: No bound states
- **New predictions:**
  - $P_{cc\bar{c}}(5715)$: -3 MeV
  - $P_{bb\bar{b}}(15569)$: -14 MeV

Experimental search: $P_{cc\bar{c}}(5715)$ in D-wave $J/\psi\,\Lambda_c$ at LHCb

Outlook: Toward Understanding Confinement

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Immediate Physics Goals:

- Other pentaquark systems (P_c, P_b)
- Hexaquarks (6 quarks, like d^*)
- Excited states and resonances

Probing Confinement:

- Flux-tube vs. pairwise confinement
- Many-body color interactions
- Connection to lattice QCD
- *Which mechanism governs multiquarks?*

DeepQuark is uniquely positioned to explore these questions!

Experimental Synergy:

- LHCb, CMS, ATLAS: more exotics coming
- BESIII: charm sector
- Belle II: B physics
- Predictions guide searches

The Big Picture:

- Exotics $\Rightarrow$ probe nonperturbative QCD
- Structure reveals color dynamics
- DeepQuark: first-principles predictions
- Deep learning enables previously intractable calculations

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