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

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Hadron Physics Workshop 2025

arXiv:2506.20555

The Multiquark Zoo

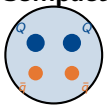
Timeline of Exotic Discoveries:

- **2003**: $X(3872)$ at Belle — first exotic candidate
- **2013**: $Z_c(3900)^+$ at BESIII — manifestly exotic $(c\bar{c}u\bar{d})$
- **2015**: P_c pentaquarks at LHCb
- **2020**: $T_{4c}(6900)$ at LHCb — fully heavy tetraquark
- **2021**: $T_{cc}(3875)^+$ at LHCb — doubly charmed tetraquark

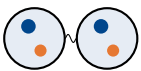
Central Question:
What is the internal structure?

- Compact tetraquark/pentaquark?
- Loosely bound hadronic molecule?
- Mixture of configurations?

Compact



Molecule



Computational Challenges in Multiquark Systems

Exponential Complexity:

- Wave function dimension scales exponentially with particle number
- 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 calculations for 5+ quarks

Diffusion Monte Carlo (DMC):

- Notorious **sign problem**
- Limited applicability to strongly correlated systems

Previous Pentaquark Studies:

- Approximations in spatial configurations
- Simplified color degree of freedom
- $\Rightarrow$ Unknown systematic errors

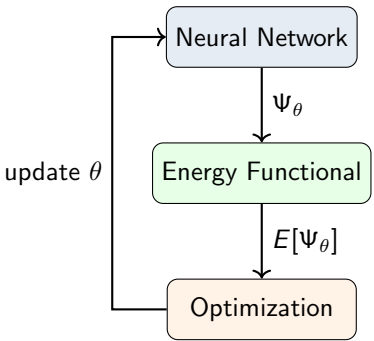
What is Machine Learning?

Core Idea:
Learn patterns from data without explicit programming

Types of Learning:

- **Supervised:** Learn from labeled examples (classification, regression)
- **Unsupervised:** Find hidden structure (clustering, dimensionality reduction)
- **Variational:** Optimize a target functional $\Leftarrow$ **What we use!**

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



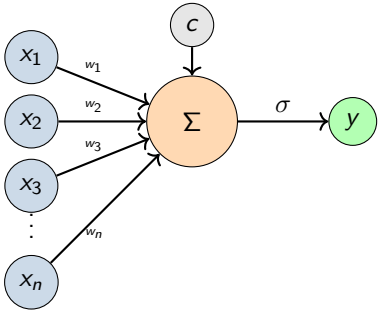
Variational Learning

Neural Networks: The Basic Building Block

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

Deep Neural Networks: Stacking Layers

From Shallow to Deep:

- Multiple hidden layers between input and output
- Each layer transforms features progressively
- Deeper networks $\Rightarrow$ more complex functions

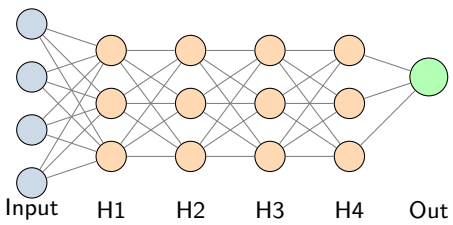
DeepQuark Architecture:

- **4 fully connected hidden layers**
- Layer sizes: $(32\text{–}40, 16\text{–}20, 16\text{–}20, 16\text{–}20)$
- $\sim$**1000–3000 parameters**
- Activation: $\sigma = \tanh$

Why "Deep"?

- Efficiently captures hierarchical correlations
- Exponentially more expressive than shallow networks

Deep Neural Network



Neural Network Quantum States (NNQS)

Key Insight: Use neural networks to represent quantum wave functions

$$\Psi(\mathbf{x}) = f_{\text{NN}}(\mathbf{x}; \theta)$$

Pioneering Work:

- **Carleo & Troyer (2017):** Quantum spin systems with Restricted Boltzmann Machines
- **FermiNet (2020):** Ab initio molecular chemistry
- **PauliNet (2020):** Deep learning for quantum chemistry

Advantages:

- No fixed basis — adaptive representation
- Captures complex many-body correlations
- Scalable to larger systems

Applications:

- Atomic & molecular physics
- Condensed matter systems
- Nuclear physics (since 2020)
- **Multiquark systems (this work!)**

Why not applied to quarks before?

- Extra SU(3) color degree of freedom
- Strong correlations (no shell structure)
- Complex confinement interactions

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

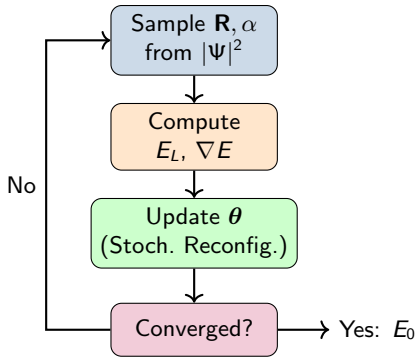
Stochastic Reconfiguration:

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

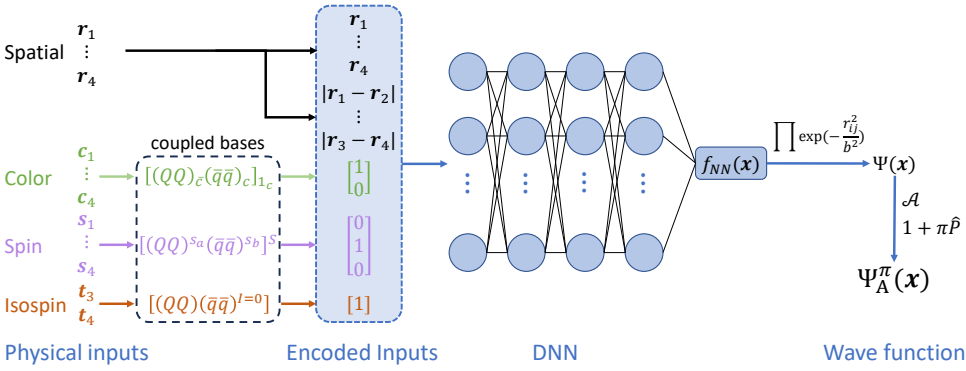
where S is the quantum Fisher information matrix

Key advantage: No sign problem (unlike DMC)!

VMC Loop



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

Encoding Quantum Numbers

Coupled Basis Representation:
Color-spin-isospin bases for tetraquark $QQ\bar{q}\bar{q}$:

$$\chi_{\bar{3}_c\otimes 3_c}\phi^{s_a,s_b}\xi^{I=0} = \left[(QQ)^{s_a}_{\bar{3}_c}(\bar{q}\bar{q})^{s_b,I=0}_{3_c}\right]^{S=1}_{1_c}$$

$$\chi_{6_c\otimes\bar{6}_c}\phi^{s_a,s_b}\xi^{I=0} = \left[(QQ)^{s_a}_{6_c}(\bar{q}\bar{q})^{s_b,I=0}_{\bar{6}_c}\right]^{S=1}_{1_c}$$

Why coupled bases?

- Automatically enforces symmetry
- Natural for strong correlations
- No single-particle approximation needed

One-Hot Encoding:
Map discrete quantum numbers to vectors

Example with 2 color bases:

$$\chi_{\bar{3}_c\otimes 3_c} \to \alpha_c = (1,0)$$
$$\chi_{6_c\otimes\bar{6}_c} \to \alpha_c = (0,1)$$

Key insight:
Standard basis vectors ensure no prejudiced correlation between different bases

Input features:

$$\mathbf{x} = (\mathbf{r}_i, |\mathbf{r}_i - \mathbf{r}_j|, \alpha_c, \alpha_s, \alpha_t)$$

Symmetry Enforcement

Full wave function with all symmetries:

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

Boundary Condition:

$$\prod_{i<j} e^{-r_{ij}^2/b^2}$$

- Confines system to localized space
- $b = 2$–4 fm (order of $\Lambda_{\mathrm{QCD}}^{-1}$)
- Ensures convergence from random initialization

Antisymmetrization:

$$\mathcal{A}[\cdots]$$

- Enforces Fermi-Dirac statistics
- Sum over permutations of identical particles
- Factorial complexity, but manageable for 3–4 identical quarks

Parity Projection:

$$(1 + \pi\hat{P})$$

- Projects onto definite parity $\pi = \pm 1$
- $\hat{P}$: spatial inversion operator
- Ground states: positive parity (tetraquark), negative parity (pentaquark)

Key Innovations of DeepQuark

1. Coupled Bases vs. Determinant Ansatz

- Previous NNQS (FermiNet, PauliNet): Slater determinants + Jastrow factors
- Originates from single-particle orbitals
- Works for weakly correlated systems

DeepQuark:

- Coupled color-spin-isospin bases
- No single-particle assumption
- Natural for strongly correlated hadrons

2. Unbiased Structure Description

- Same wave function ansatz describes:
  - Compact tetraquarks (T_{bb})
  - Hadronic molecules (T_{cc})
  - Scattering states
- No *a priori* assumption about structure
- Network *learns* the configuration!

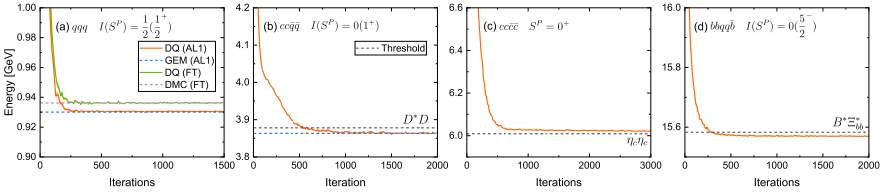
3. Complex Interactions:

- Handles flux-tube confinement
- No extra computational cost
- Opens door to many-body forces

Benchmark: Nucleon with Different Confinements

Confinement:
L: Pairwise

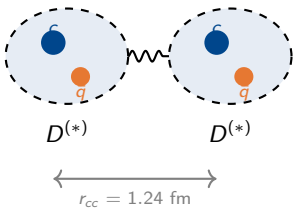
R: Flux-tube



(a) nucleon, (b) T_{cc}, (c) T_{4c}, (d) pentaquark — DeepQuark matches GEM/DMC

Doubly Charmed Tetraquark T_{cc}

Molecular Structure



See convergence plot: panel (b)

Ground State Properties:

- Binding energy: $\Delta E = -\mathbf{15}$ MeV (w.r.t. D^*D threshold)
- **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

Ground State Properties:

- Binding energy: $\Delta E = -153$ MeV (w.r.t. $\bar{B}^* \bar{B}$ threshold)
- **Color:** $\chi_{\bar{3}\times 3} : \chi_{6\times\bar{6}} = 97\% : 3\%$
- Dominated by $\bar{3}_c \otimes 3_c$ configuration!

Compact Structure:

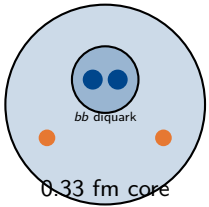
r_{bb}	**0.33 fm** (compact diquark!)
$r_{b\bar{q}}$	0.69 fm
$r_{\bar{q}\bar{q}}$	0.78 fm

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

T_{cc}: Molecular

$D^* \leftrightarrow D$

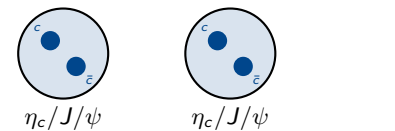
T_{bb}: Compact



Same ansatz describes both molecular and compact structures!

Fully Heavy Tetraquarks: T_{4c} and T_{4b}

No Bound State



Energy **above** threshold

See convergence plot: panel (c)

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

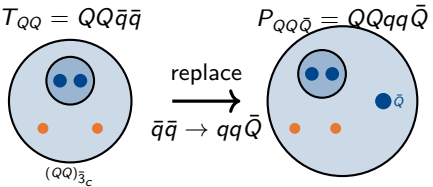
Experimental context:

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

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

Triply Heavy Pentaquarks: $QQqq\bar{Q}$

Diquark-Antiquark Analogy:
Heavy diquark $(QQ)_{\bar{3}_c}$ has same color as antiquark $\bar{Q}$



Color Bases for Pentaquark:

$$\chi_{\bar{3}\otimes\bar{3}} = \{[(QQ)_{\bar{3}}(qq)_{\bar{3}}]_3\bar{Q}\}_1$$
$$\chi_{\bar{3}\otimes 6} = \{[(QQ)_{\bar{3}}(qq)_{6}]_3\bar{Q}\}_1$$
$$\chi_{6\otimes\bar{3}} = \{[(QQ)_{6}(qq)_{\bar{3}}]_3\bar{Q}\}_1$$

Expectation:
If T_{QQ} is bound, perhaps $P_{QQ\bar{Q}}$ is too?

Complication:
$\bar{Q}$ can form quarkonium $(Q\bar{Q})_{1_c}$ with one of the heavy quarks — lower energy configuration!

Pentaquarks with $S = 1/2, 3/2$: No Binding

Results for $S = 1/2, 3/2$:

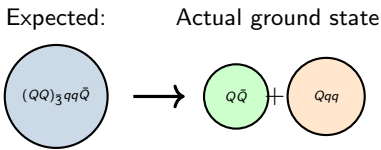
System	S^P	Bound?
$ccqq\bar{c}$	$\frac{1}{2}^-, \frac{3}{2}^-$	**No**
$bbqq\bar{b}$	$\frac{1}{2}^-, \frac{3}{2}^-$	**No**

Lowest thresholds:

- $ccqq\bar{c}$: $\eta_c\Lambda_c$ or $J/\psi\Lambda_c$
- $bbqq\bar{b}$: $\eta_b\Lambda_b$ or $\Upsilon\Lambda_b$

Why no binding?

The $\bar{Q}$ "steals" a heavy quark to form quarkonium:

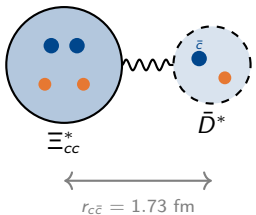


$(Q\bar{Q})_{1_c}$ quarkonium + (Qqq) baryon is more stable than $(QQ)_{\bar{3}_c}$ diquark configuration

$\Rightarrow$ Diquark-antiquark symmetry is **broken**

Novel Prediction: Bound $S = 5/2$ Pentaquarks

Molecular Structure



$\Delta E = -3$ MeV

See convergence plot: panel (d)

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)

$\Rightarrow$ Analogous to molecular T_{cc}!

Experimental Search for $P_{cc\bar{c}}(5715)$

Decay Channels:
$P_{cc\bar{c}}(5715)$ with $J^P = \frac{5}{2}^-$ can decay to lower-spin channels via spin-orbit coupling:

- Primary search channel: $\boxed{J/\psi\,\Lambda_c}$
- Requires **D-wave** decay (angular momentum barrier)

Expected Properties:

- **Narrow width** due to D-wave suppression
- Mass: ~ 5715 MeV
- Quantum numbers: $J^P = \frac{5}{2}^-$, $I = 0$

Production:
Similar to P_c pentaquarks at LHCb
$\Lambda_b \to J/\psi\,\Lambda_c\,K^-$ (or similar)

Properties of $P_{cc\bar{c}}(5715)$:

Property	Value
Mass	5715 MeV
ΔE	-3 MeV
J^P	$\frac{5}{2}^-$
Isospin	0
r_{QQ}	0.50 fm
r_{Qq}	1.39 fm
r_{qq}	1.90 fm
$r_{Q\bar{Q}}$	1.73 fm
$r_{q\bar{Q}}$	1.38 fm

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

Summary

DeepQuark: First DNN-based VMC for multiquark bound states

Method Achievements:

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

Physics Results:

- T_{cc}: Molecular, $\Delta E = -15$ MeV, 55:45 color mixing
- T_{bb}: Compact diquark, $\Delta E = -153$ MeV, 97% $\bar{3} \times 3$
- T_{4c}, T_{4b}: No bound states
- **New predictions:**
  - $P_{cc\bar{c}}(5715)$: -3 MeV
  - $P_{bb\bar{b}}(15569)$: -14 MeV
- Search in D-wave $J/\psi\,\Lambda_c$

Outlook and Future Directions

Immediate Extensions:

- Other pentaquark systems (P_c, P_b)
- **Hexaquarks** (6 quarks)
- Excited states and resonances
- Different quark model potentials

Confinement Physics:

- Flux-tube interactions in tetraquarks
- Many-body confinement mechanisms
- Connection to lattice QCD results

Methodological Improvements:

- More sophisticated network architectures
- Excited state methods (penalty, orthogonalization)
- Scattering state descriptions

Broader Impact:

- Forward-looking predictions for experiments
- Insights into nonperturbative QCD
- General quantum many-body physics
- Deep learning + physics integration

Acknowledgments

Collaborators:

- Wei-Lin Wu (Peking University)
- Shi-Lin Zhu (Peking University)

Helpful Discussions:

- Yao Ma, Yan-Ke Chen, Liang-Zhen Wen
- Yilong Yang, Pengwei Zhao

Funding:

- NSFC (No. 12475137)
- ERC NuclearTheory (Grant No. 885150)

Computing:
High-performance Computing Platform of Peking University
Software: NetKet package

Thank you!

Paper:
arXiv:2506.20555

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Backup: AL1 Model Parameters

AL1 Quark Potential Model (Semay & Silvestre-Brac, 1996):

$$V_{ij} = V_{\text{OGE}} + V_{\text{conf}} = -\frac{3}{16}\boldsymbol{\lambda}_i \cdot \boldsymbol{\lambda}_j \left(-\frac{\kappa}{r_{ij}} - \Lambda + \frac{8\pi\kappa'}{3m_i m_j} \frac{e^{-r_{ij}^2/r_0^2}}{\pi^{3/2} r_0^3} \mathbf{s}_i \cdot \mathbf{s}_j + \lambda r_{ij} \right)$$

κ	λ (GeV^2)	Λ (GeV)	κ'	m_b (GeV)	m_c (GeV)
0.5069	0.1653	0.8321	1.8609	5.227	1.836

m_q (GeV)	r_0 (GeV^{-1})	A (GeV^{B-1})	B	C (GeV^4)
0.315	$A(2m_i m_j/(m_i + m_j))^{-B}$	1.6553	0.2204	2.02×10^{-3}

Backup: SU(3) Color Bases

Tetraquark $QQ\bar{q}\bar{q}$:

$$
\begin{aligned}
(QQ): &\quad 3 \otimes 3 = \bar{3} \oplus 6 \\
(\bar{q}\bar{q}): &\quad \bar{3} \otimes \bar{3} = 3 \oplus \bar{6} \\
\text{Color singlet}: &\quad \bar{3} \otimes 3 = 1 \quad \text{and} \quad 6 \otimes \bar{6} \supset 1
\end{aligned}
$$

Pentaquark $QQqq\bar{Q}$:

$$
\begin{aligned}
\chi_{\bar{3}\otimes\bar{3}} &= \{[(QQ)_{\bar{3}}(qq)_{\bar{3}}]_3 \bar{Q}\}_1 \\
\chi_{\bar{3}\otimes 6} &= \{[(QQ)_{\bar{3}}(qq)_6]_3 \bar{Q}\}_1 \\
\chi_{6\otimes\bar{3}} &= \{[(QQ)_6(qq)_{\bar{3}}]_3 \bar{Q}\}_1
\end{aligned}
$$

Note: $\chi_{6\otimes 6}$ does not contribute to color singlet

Backup: Optimization Details

Network Architecture:

System	S^P	Nodes	Parameters
qqq	$\frac{1}{2}^+$	$(16, 16, 16, 16)$	1105
$QQ\bar{q}\bar{q}$	1^+	$(32, 16, 16, 16)$	1889
$QQ\bar{Q}\bar{Q}$	$0^+, 1^+, 2^+$	$(32, 16, 16, 16)$	1793–1857
$QQqq\bar{Q}$	$\frac{1}{2}^-, \frac{3}{2}^-, \frac{5}{2}^-$	$(40, 20, 20, 20)$	2921–3081

Training:

- Initial: $N = 2 \times 10^4$ samples (fast exploration)
- Convergence: $N = 4$–8×10^4 samples (stable optimization)
- Final evaluation: $N \sim 10^6$ samples
- Learning rate η, regularization $\epsilon = 10^{-3}$
- Stochastic reconfiguration with quantum Fisher matrix

Backup: Electron System Benchmarks

Few-electron systems as QED counterparts:

System	DeepQuark (eV)	Reference (eV)	Difference
e^+e^- (Ps)	$-6.80301(16)$	-6.803 (exact)	$< 0.01\%$
$e^+e^-e^-$ (Ps^-)	$-7.12882(16)$	-7.130	0.02%
$e^+e^+e^-e^-$ (Ps_2)	$-14.0347(7)$	-14.04	0.04%

Comparison methods:

- Ps: Exact solution (hydrogen-like)
- Ps^-: Hylleraas-type variational (Ho, 1993)
- Ps_2: Explicitly correlated Gaussians (Kinghorn & Poshusta, 1993)

$\Rightarrow$ DeepQuark achieves $< 0.1\%$ accuracy on all benchmarks

Backup: DeepQuark vs. FermiNet/PauliNet

Feature	FermiNet/PauliNet	DeepQuark
Target systems	Atoms, molecules	Multiquark hadrons
Wave function	Slater determinants + Jastrow + backflow	Coupled bases
Basis assumption	Single-particle orbitals	None (fully correlated)
Color DOF	N/A	Full SU(3) treatment
Typical parameters	$\sim 10^5$–10^6	$\sim 10^3$
Correlations	Via backflow transform	Encoded in bases
Antisymmetry	Determinant structure	Explicit permutations

Key difference:

- FermiNet/PauliNet: Determinant ansatz from atomic/molecular physics
- DeepQuark: Coupled basis construction for strongly correlated hadrons