

Fully heavy multiquarks in neural-network quantum states

Wen-min Li,^{1,2,3} Zhenyu Zhang^{1,2,3,4,5,†} and Qian Wang^{1,3,6,*}

¹State Key Laboratory of Nuclear Physics and Technology, Institute of Quantum Matter,
South China Normal University, Guangzhou 510006, China

²Key Laboratory of Atomic and Subatomic Structure and Quantum Control (MOE), Guangdong-Hong
Kong Joint Laboratory of Quantum Matter, Guangzhou 510006, China

³Guangdong Basic Research Center of Excellence for Structure and Fundamental Interactions of Matter,
Guangdong Provincial Key Laboratory of Nuclear Science, Guangzhou 510006, China

⁴Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

⁵China Center of Advanced Science and Technology, Beijing 100190, China

⁶Southern Center for Nuclear-Science Theory (SCNT), Institute of Modern Physics,
Chinese Academy of Sciences, Huizhou 516000, Guangdong Province, China



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Exotic hadrons beyond the conventional quark model provide a direct window into the dynamics of strong interaction. However, extracting the multiquark spectroscopy has to face the quantum many-body problem, which is still a theoretical challenge. In this case, diquark-antidiquark model is proposed as an approximation. Although this model can describe the spectroscopy roughly, it cannot describe the detailed dynamics. Furthermore, the methods aiming at dealing with many-body problem, e.g., the Gaussian expansion method and diffusion Monte Carlo, are proposed, but face severe computational bottlenecks. In this work, we introduce the neural-network quantum state (NNQS) approach to investigate the spectra of fully heavy multiquark states within the nonrelativistic potential quark model. By employing deep neural networks to represent the complex many-body spatial wave function, and constructing the color-spin part exactly from group theory to enforce fermionic antisymmetry, our approach effectively overcomes the dimensionality obstacles inherent in traditional methods. The results are compared with various model calculations, demonstrating that NNQS offers superior accuracy and flexibility, particularly in treating high-dimensional correlations. This work establishes NNQS as a promising tool for exploring the spectroscopy of exotic hadrons.

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I. INTRODUCTION

Hadron spectroscopy is one of the most direct ways to shed light on the dynamics of the strong interaction. Due to color confinement in quantum chromodynamics (QCD), any color-neutral object is allowed—not only the conventional mesons ($q\bar{q}$) and baryons (qqq) described by the quark model [1,2]. Consequently, the search for exotic hadrons beyond the conventional quark model has become one of the most important frontiers in hadron physics. Since the first discovery of the $X(3872)$ by the Belle Collaboration in 2003 [3], a large number of exotic hadron candidates have been observed experimentally, including

the $T_{cc}^+(3875)$ [4,5], $Z_c(3900)$ [6,7], P_c [8–10], P_{cs} [11], and $T_{cc\bar{c}\bar{c}}(6900)$ [12]. Several interpretations have been proposed to understand their internal structures [13–19], among which loosely bound hadronic molecules [13,16] and compact multiquark states [14–16,18,20,21] are the most intensively discussed. The former, having a larger size, corresponds to a bound state formed by the color-neutral residual strong force, while the latter, with a smaller size, is a bound state formed directly by the fundamental color force.

Solving the quantum many-body problem for multiquark states presents significant theoretical challenges. For an N -quark system, the SU(3) color degree of freedom makes the system more complex than electron or nucleon systems. In previous studies, physical approximations such as the diquark-antidiquark model have been adopted to reduce the complexity of the system [15,16,18,20–27]. Although this approximation can significantly reduce the system's degrees of freedom, it artificially restricts the wave function to a specific configuration, ignoring the many-body correlation effects between (anti)quarks. Such configurations in

*Contact author: qianwang@m.scnu.edu.cn

†These author contributed equally to this work.

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wave function may lead to systematic errors and deviate from physical reality.

To overcome the above restricted configurations problem, more rigorous numerical methods are performed to directly solve multiquark systems. Currently, numerical approaches such as diffusion Monte Carlo (DMC) [28–30] and basis expansion methods, including the Gaussian expansion method (GEM) [31] and the explicitly correlated Gaussian (ECG) [32,33] method, have been widely applied to solve multiquark systems. However, these methods face computational bottlenecks when dealing with multiquark systems. For basis expansion methods, the number of basis grows exponentially with the increasing number of quarks, making the precise solution of complex systems highly challenging. And the DMC method inevitably suffers from the fermion sign problem during imaginary time evolution, severely limiting its applicability to strongly correlated multiquark systems. Furthermore, wave function cusps [34] arising from the short-range color Coulomb interaction further increase the difficulty of convergence for traditional basis expansion methods.

Recently, machine learning techniques have provided a new approach to solving the quantum many-body problem. Motivated by their exceptional capacity to approximate high-dimensional functions [35], neural-network quantum states (NNQS) offer a flexible wave function representation capable of capturing complex many-body correlations efficiently [36]. This neural network based variational Monte Carlo (VMC) framework was implemented in quantum spin systems [37] and condensed matter physics [38,39], as well as ab-initio chemistry problems [34,40,41]. Furthermore, this method has been effectively extended to nuclear physics [42–47]. In hadron physics, machine learning techniques have demonstrated exceptional predictive power for the mass spectra and decay widths of exotic hadrons [48–51]. However, directly solving the quantum many-body problem in hadron physics remains in the exploratory stage. Recently, the DeepQuark framework [52] was proposed, which marks the first successful implementation of the deep neural networks (DNNs) based VMC method in multiquark systems. These recent developments imply the feasibility of extending this method to multiquark systems.

In this work, we introduce NNQS approach to investigate the mass spectra of fully heavy multiquark states within the nonrelativistic potential quark model, with a particular focus on its advantages over the GEM. For the color-spin wave function, we construct it based on group theory and symmetry, ensuring that the trial wave function exactly satisfies the fermionic antisymmetry constraint. For the complex many-body spatial wave function, we entirely employ DNNs for high-dimensional fitting. This approach effectively overcomes the computational bottlenecks faced by traditional methods in solving high-dimensional spatial

many-body correlations, thereby providing more accurate theoretical predictions for the mass spectra of fully heavy multiquark systems. This paper is organized as follows. In Sec. II, we introduce the nonrelativistic Hamiltonian of the system. The configurations of the multiquark states are constructed in Sec. III. In Sec. IV, we detail the architecture of the neural-network wave function and the optimization procedure. Finally, the numerical results and discussions are presented in Sec. V.

II. HAMILTONIAN

In this work, we adopt the nonrelativistic quark potential model (NRQPM) to describe fully heavy multiquark states. The Hamiltonian is given by

$$H = \sum_i^n (m_i + T_i) + \sum_{i<j}^n V_{ij}(r_{ij}), \quad (1)$$

where m_i and T_i denote the mass and kinetic energy of the i th (anti)quark, respectively. The term $V_{ij}(r_{ij})$ represents the effective potential between the i th and j th (anti)quarks, which depends on their relative distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. The effective potential $V_{ij}(r_{ij})$ consists of a one-gluon exchange (OGE) potential and a linear confinement potential [53,54], written as $V_{ij}(r_{ij}) = V_{ij}^{\text{OGE}}(r_{ij}) + V_{ij}^{\text{Conf}}(r_{ij})$. The forms of V_{ij}^{OGE} and V_{ij}^{Conf} are given by

$$V_{ij}^{\text{OGE}} = \frac{\alpha_{ij}}{4} (\lambda_i \cdot \lambda_j) \left[\frac{1}{r_{ij}} - \frac{\pi \sigma_{ij}^3 e^{-\sigma_{ij}^2 r_{ij}^2}}{2 \pi^{3/2}} \frac{4}{3 m_i m_j} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \right],$$

$$V_{ij}^{\text{Conf}} = -\frac{3}{16} (\lambda_i \cdot \lambda_j) b r_{ij}, \quad (2)$$

where λ_i is the Gell-Mann matrix acting on the i th quark (replaced by $-\lambda^*$ for antiquarks), and $\boldsymbol{\sigma}_i$ represents the Pauli matrix. The parameters α_{ij} and σ_{ij} are the strong coupling strength and the regulator of the spin-spin interaction, respectively. b is the strength of the linear confinement potential. The parameters of model are given in Table I, which are well determined by fitting the mass spectra of charmonium, bottomonium, and B_c mesons [53,54]. The parameters and the potential are identical to those used in the GEM of Refs. [53–55].

TABLE I. Parameters of model used in this work [53,54].

m_c/m_b (GeV)	1.483/4.852
$\alpha_{cc}/\alpha_{bc}/\alpha_{bb}$	0.5461/0.5021/0.4311
$\sigma_{cc}/\sigma_{bc}/\sigma_{bb}$ (GeV)	1.1384/1.3000/2.3200
b (GeV ²)	0.1425

III. THE CONFIGURATION OF MULTIQUARKS

The total wave function of multi-quark can be expressed as a direct product of the flavor, spatial, spin, and color wave functions

$$\Psi_{\text{total}} = \Psi_{\text{spatial}} \otimes \Psi_{\text{spin}} \otimes \Psi_{\text{color}} \otimes \Psi_{\text{flavor}}. \quad (3)$$

In this work, the spin and color wave functions are constructed via $SU(3) \otimes SU(2)$ symmetry, and the spatial wave function is parametrized by DNNs. Additionally, by considering only multi-quark with identical flavors, the flavor wave function is symmetric.

For conventional mesons and baryons, the construction of their color-spin configurations is well established. For multi-quark, the configurations become more complex. The absence of one-light-meson exchanges makes fully heavy systems highly favorable to form genuine compact multi-quark configurations rather than conventional hadronic molecules [53,54]. To describe such compact states, we adopt the $\{Q_1 Q_2\} \{\bar{Q}_3 \bar{Q}_4\}$ configuration for fully heavy tetraquarks,¹ which includes the following systems: $cc\bar{c}\bar{c}$, $bb\bar{b}\bar{b}$, and $bb\bar{c}\bar{c}$. In the color space, there exist two color-singlet bases for the tetraquark system, whose explicit forms are

$$\mathcal{C}_1 = |(Q_1 Q_2)^6 (\bar{Q}_3 \bar{Q}_4)^{\bar{6}}\rangle, \quad (4)$$

$$\mathcal{C}_2 = |(Q_1 Q_2)^3 (\bar{Q}_3 \bar{Q}_4)^3\rangle. \quad (5)$$

Here, the superscripts denote the irreducible representations of the $SU(3)$ color group for the diquark and antidiquark, respectively. Based on the $SU(3)$ Clebsch-Gordan (CG) coefficients, the explicit forms of the color wave functions can be written as follows [53,56–59]:

$$\begin{aligned} \mathcal{C}_1 = \frac{1}{2\sqrt{6}} & [(rb + br)(\bar{b}\bar{r} + \bar{r}\bar{b}) + (gr + rg)(\bar{g}\bar{r} + \bar{r}\bar{g}) \\ & + (gb + bg)(\bar{b}\bar{g} + \bar{g}\bar{b}) + 2(rr)(\bar{r}\bar{r}) + 2(gg)(\bar{g}\bar{g}) \\ & + 2(bb)(\bar{b}\bar{b})], \end{aligned} \quad (6)$$

$$\begin{aligned} \mathcal{C}_2 = \frac{1}{2\sqrt{3}} & [(br - rb)(\bar{b}\bar{r} - \bar{r}\bar{b}) - (rg - gr)(\bar{g}\bar{r} - \bar{r}\bar{g}) \\ & + (bg - gb)(\bar{b}\bar{g} - \bar{g}\bar{b})]. \end{aligned} \quad (7)$$

With the color wave functions, the matrix elements $\langle \lambda_i \cdot \lambda_j \rangle$ can be evaluated [60], and the results are summarized in Table II.

In the spin space, the total spin of the system can take values of $J = 0, 1$, and 2 , are represented as follows:

$$\mathcal{S}_1 = |(Q_1 Q_2)_0 (\bar{Q}_3 \bar{Q}_4)_0\rangle_0, \quad (8)$$

¹Note that this does not mean a diquark-antidiquark approximation, but a way to combine to a color neutral object.

TABLE II. Color matrix elements of the tetraquarks.

$\hat{O}$	$\lambda_1 \cdot \lambda_2$	$\lambda_1 \cdot \lambda_3$	$\lambda_1 \cdot \lambda_4$	$\lambda_2 \cdot \lambda_3$	$\lambda_2 \cdot \lambda_4$	$\lambda_3 \cdot \lambda_4$
$\langle \mathcal{C}_1 \hat{O} \mathcal{C}_1 \rangle$	4/3	-10/3	-10/3	-10/3	-10/3	4/3
$\langle \mathcal{C}_2 \hat{O} \mathcal{C}_2 \rangle$	-8/3	-4/3	-4/3	-4/3	-4/3	-8/3
$\langle \mathcal{C}_1 \hat{O} \mathcal{C}_2 \rangle$	0	$-2\sqrt{2}$	$2\sqrt{2}$	$2\sqrt{2}$	$-2\sqrt{2}$	0

$$\mathcal{S}_2 = |(Q_1 Q_2)_1 (\bar{Q}_3 \bar{Q}_4)_1\rangle_0, \quad (9)$$

$$\mathcal{S}_3 = |(Q_1 Q_2)_0 (\bar{Q}_3 \bar{Q}_4)_1\rangle_1, \quad (10)$$

$$\mathcal{S}_4 = |(Q_1 Q_2)_1 (\bar{Q}_3 \bar{Q}_4)_0\rangle_1, \quad (11)$$

$$\mathcal{S}_5 = |(Q_1 Q_2)_1 (\bar{Q}_3 \bar{Q}_4)_1\rangle_1, \quad (12)$$

$$\mathcal{S}_6 = |(Q_1 Q_2)_1 (\bar{Q}_3 \bar{Q}_4)_1\rangle_2. \quad (13)$$

Here, the subscript denotes spin quantum number. Based on the $SU(2)$ CG coefficients, the explicit forms of the spin wave functions can be written as follows [53]:

$$\mathcal{S}_1 = \frac{1}{2}(\uparrow\downarrow\uparrow\downarrow - \uparrow\downarrow\downarrow\uparrow - \downarrow\uparrow\uparrow\downarrow + \downarrow\uparrow\downarrow\uparrow), \quad (14)$$

$$\begin{aligned} \mathcal{S}_2 = \sqrt{\frac{1}{12}} & (2\uparrow\uparrow\downarrow\downarrow - \uparrow\downarrow\uparrow\downarrow - \uparrow\downarrow\downarrow\uparrow \\ & - \downarrow\uparrow\uparrow\downarrow - \downarrow\uparrow\downarrow\uparrow + 2\downarrow\downarrow\uparrow\uparrow), \end{aligned} \quad (15)$$

$$\mathcal{S}_3 = \sqrt{\frac{1}{2}}(\uparrow\downarrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow), \quad (16)$$

$$\mathcal{S}_4 = \sqrt{\frac{1}{2}}(\uparrow\uparrow\uparrow\downarrow - \uparrow\uparrow\downarrow\uparrow), \quad (17)$$

$$\mathcal{S}_5 = \frac{1}{2}(\uparrow\uparrow\uparrow\downarrow + \uparrow\uparrow\downarrow\uparrow - \uparrow\downarrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow), \quad (18)$$

$$\mathcal{S}_6 = \uparrow\uparrow\uparrow\uparrow. \quad (19)$$

With the spin wave functions, the matrix elements $\langle \sigma_i \cdot \sigma_j \rangle$ can be evaluated [60], and the results are summarized in Table III.

TABLE III. Spin matrix elements of the tetraquarks.

$\hat{O}$	$\sigma_1 \cdot \sigma_2$	$\sigma_1 \cdot \sigma_3$	$\sigma_1 \cdot \sigma_4$	$\sigma_2 \cdot \sigma_3$	$\sigma_2 \cdot \sigma_4$	$\sigma_3 \cdot \sigma_4$
$\langle \mathcal{S}_1 \hat{O} \mathcal{S}_1 \rangle$	-3	0	0	0	0	-3
$\langle \mathcal{S}_2 \hat{O} \mathcal{S}_2 \rangle$	1	-2	-2	-2	-2	1
$\langle \mathcal{S}_1 \hat{O} \mathcal{S}_2 \rangle$	0	$-\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$-\sqrt{3}$	0
$\langle \mathcal{S}_3 \hat{O} \mathcal{S}_3 \rangle$	-3	0	0	0	0	1
$\langle \mathcal{S}_4 \hat{O} \mathcal{S}_4 \rangle$	1	0	0	0	0	-3
$\langle \mathcal{S}_5 \hat{O} \mathcal{S}_5 \rangle$	1	-1	-1	-1	-1	1
$\langle \mathcal{S}_6 \hat{O} \mathcal{S}_6 \rangle$	1	1	1	1	1	1

For simplicity, we consider the $\{Q_1 Q_2 Q_3 Q_4\} \bar{Q}_5$ configuration for fully heavy pentaquarks, where the four quarks are identical flavors, which includes the following systems: $cccc\bar{c}$, $cccc\bar{b}$, $bbbb\bar{b}$, and $bbbb\bar{c}$. In the color space, three color-singlet states can be constructed via the SU(3) group theory. Its Young tableau representation is given by [61]

$$C_1 = \begin{array}{|c|c|} \hline 1 & 4 \\ \hline 2 & \\ \hline 3 & \\ \hline \end{array} \otimes (5)_{\bar{3}}, \quad C_2 = \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline 4 & \\ \hline \end{array} \otimes (5)_{\bar{3}}, \quad C_3 = \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \hline 4 & \\ \hline \end{array} \otimes (5)_{\bar{3}}. \quad (20)$$

Using the SU(3) CG coefficients [58], the explicit forms of the color wave functions for the pentaquark can be written as follows [62]:

$$C_1 = \frac{1}{3\sqrt{2}} (grbb - rgbb + rgbg - brgb + bgrb - gbrb) \bar{b} \\ + (grbr - rgbr + rbgr - brgr + bgrr - gbr) \bar{r} \\ + (grbg - rbgg + rbgr - brgg + bgrg - gbrg) \bar{g}, \quad (21)$$

$$C_2 = \frac{1}{4\sqrt{3}} (2bbgr - 2bbg + gbrb - gbbr + bgrb - bgr \\ - rgbg + rbbg - brgb + brbg) \bar{b} + (2rrbg - 2rrg \\ + rgrb - rgbr + grrb - grbr + rbgr - rbrg + bgr \\ - brrg) \bar{r} + (2ggrb - 2ggbr - rggb + rbgg - grgb \\ + grbg + gbgr - gbrg + bggr - bgrg) \bar{g}, \quad (22)$$

$$C_3 = \frac{1}{12} (3bgbr - 3gbbr - 3brbg + 3rbbg - rgbg - 2rgbb \\ + 2grbb + brgb + gbrb - bgrb) \bar{b} + (3grrb - 3grb \\ - 3brrg + 3rbgr - rbgr - 2gbrr + 2bgrr - grbr \\ + rgrb + bgr) \bar{r} + (3grgb - 3rggb + 3bggr - 3gbgr \\ - grbg + rbgg + 2rbgg - 2brgg + bgrg - bgrg) \bar{g}. \quad (23)$$

In the spin space, based on the SU(2) coupling rules, the total spin of the system can take values of $J = 5/2, 3/2,$

and $1/2$, and their corresponding Young tableaux are represented as follows:

$$J = \frac{5}{2} : \quad S_1 = \begin{array}{|c|c|c|c|c|} \hline 1 & 2 & 3 & 4 & 5 \\ \hline \end{array}. \quad (24)$$

$$J = \frac{3}{2} : \quad S_2 = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 5 & & & \\ \hline \end{array}, \quad S_3 = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 5 \\ \hline 4 & & & \\ \hline \end{array}, \\ S_4 = \begin{array}{|c|c|c|c|} \hline 1 & 3 & 4 & 5 \\ \hline 2 & & & \\ \hline \end{array}, \quad S_5 = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 4 & 5 \\ \hline 3 & & & \\ \hline \end{array}. \quad (25)$$

$$J = \frac{1}{2} : \quad S_6 = \begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline 4 & 5 & \\ \hline \end{array}, \quad S_7 = \begin{array}{|c|c|c|} \hline 1 & 3 & 4 \\ \hline 2 & 5 & \\ \hline \end{array}, \quad S_8 = \begin{array}{|c|c|c|} \hline 1 & 2 & 4 \\ \hline 3 & 5 & \\ \hline \end{array}, \\ S_9 = \begin{array}{|c|c|c|} \hline 1 & 2 & 5 \\ \hline 3 & 4 & \\ \hline \end{array}, \quad S_{10} = \begin{array}{|c|c|c|} \hline 1 & 3 & 5 \\ \hline 2 & 4 & \\ \hline \end{array}. \quad (26)$$

Incorporating the SU(2) CG coefficients, the explicit forms of the pentaquark spin wave functions can be derived

$$S_1 = \uparrow\uparrow\uparrow\uparrow\uparrow, \quad (27)$$

$$S_2 = \frac{1}{2\sqrt{5}} (4\uparrow\uparrow\uparrow\uparrow\downarrow - \uparrow\uparrow\uparrow\downarrow\uparrow \\ - \uparrow\uparrow\downarrow\uparrow\uparrow - \uparrow\downarrow\uparrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow\uparrow), \quad (28)$$

$$S_3 = \frac{1}{2\sqrt{3}} (3\uparrow\uparrow\uparrow\downarrow\uparrow - \uparrow\uparrow\downarrow\uparrow\uparrow - \uparrow\downarrow\uparrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow\uparrow), \quad (29)$$

$$S_4 = \frac{1}{\sqrt{2}} (\uparrow\downarrow\uparrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow\uparrow), \quad (30)$$

$$S_5 = \frac{1}{\sqrt{6}} (2\uparrow\uparrow\downarrow\uparrow\uparrow - \uparrow\downarrow\uparrow\uparrow\uparrow - \downarrow\uparrow\uparrow\uparrow\uparrow), \quad (31)$$

$$S_6 = \frac{1}{3\sqrt{2}} (3\uparrow\uparrow\uparrow\downarrow\downarrow - \uparrow\uparrow\downarrow\uparrow\downarrow - \uparrow\downarrow\uparrow\uparrow\downarrow - \downarrow\uparrow\uparrow\uparrow\downarrow - \uparrow\uparrow\downarrow\downarrow\uparrow - \uparrow\downarrow\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow\downarrow\uparrow + \uparrow\downarrow\downarrow\uparrow\uparrow + \downarrow\uparrow\downarrow\uparrow\uparrow + \downarrow\downarrow\uparrow\uparrow\uparrow), \quad (32)$$

$$S_7 = \frac{1}{2\sqrt{3}} (2\uparrow\downarrow\uparrow\uparrow\downarrow - 2\downarrow\uparrow\uparrow\uparrow\downarrow - \uparrow\downarrow\downarrow\uparrow\uparrow + \downarrow\uparrow\downarrow\uparrow\uparrow - \uparrow\downarrow\uparrow\downarrow\uparrow + \downarrow\uparrow\uparrow\downarrow\uparrow), \quad (33)$$

$$S_8 = \frac{1}{6}(4\uparrow\uparrow\downarrow\uparrow\downarrow - 2\uparrow\downarrow\uparrow\uparrow\downarrow - 2\downarrow\uparrow\uparrow\uparrow\downarrow - 2\uparrow\uparrow\downarrow\downarrow\uparrow + 2\downarrow\downarrow\uparrow\uparrow\uparrow + \uparrow\downarrow\uparrow\downarrow\uparrow + \downarrow\uparrow\uparrow\downarrow\uparrow - \uparrow\downarrow\downarrow\uparrow\uparrow - \downarrow\uparrow\downarrow\uparrow\uparrow), \quad (34)$$

$$S_9 = \frac{1}{2\sqrt{3}}(2\uparrow\uparrow\downarrow\downarrow\uparrow + 2\downarrow\downarrow\uparrow\uparrow\uparrow - \uparrow\downarrow\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow\downarrow\uparrow - \uparrow\downarrow\downarrow\uparrow\uparrow - \downarrow\uparrow\downarrow\uparrow\uparrow), \quad (35)$$

$$S_{10} = \frac{1}{2}(\uparrow\downarrow\uparrow\downarrow\uparrow - \uparrow\downarrow\downarrow\uparrow\uparrow - \downarrow\uparrow\uparrow\downarrow\uparrow + \downarrow\uparrow\downarrow\uparrow\uparrow). \quad (36)$$

By combining the color and spin wave functions with the CG coefficients of the S_4 permutation group [63], the color-spin wave functions Ψ^{CS} can be constructed as follows. For the S -wave pentaquark system with the $\{Q_1 Q_2 Q_3 Q_4\} \bar{Q}_5$ configuration, there are two wave functions corresponding to $J^P = 3/2^-$ and $1/2^-$:

$$\Psi_{3/2^-}^{\text{CS}} = \frac{1}{\sqrt{3}}(C_1 S_3 + C_2 S_4 - C_3 S_5), \quad (37)$$

$$\Psi_{1/2^-}^{\text{CS}} = \frac{1}{\sqrt{3}}(C_1 S_6 + C_2 S_7 - C_3 S_8). \quad (38)$$

One notices that there is no $J^P = 5/2^-$ pentaquark in this configuration, as it violates Fermi-Dirac statistics. It is worth mentioning that since both the spatial and flavor wave functions of the $\{Q_1 Q_2 Q_3 Q_4\}$ identical quarks are symmetric, the Pauli principle dictates that their color-spin wave function must be totally antisymmetric. States with a total spin of $J^P = 5/2^-$ are forbidden for such pentaquark configurations.

Based on the color-spin wave functions, one can evaluate the interactions within pentaquarks. Because the potential of V^{Conf} term depends on color interactions, it yields only diagonal matrix elements due to the orthogonality of the wave functions. The term V^{OGE} contains color-spin interactions, both diagonal and off-diagonal elements are evaluated. The calculated results are summarized in Table IV, where the subscript of the color-spin interactions,

TABLE IV. Color and spin interaction for the pentaquarks.

(i, j)	$\langle \lambda_i \cdot \lambda_j \rangle$	$\langle (\lambda_i \cdot \lambda_j)(\sigma_i \cdot \sigma_j) \rangle_{\frac{3}{2}^-}$	$\langle (\lambda_i \cdot \lambda_j)(\sigma_i \cdot \sigma_j) \rangle_{\frac{1}{2}^-}$
(1, 2)	-4/3	-28/9	-28/9
(1, 3)	-4/3	-28/9	-28/9
(1, 4)	-4/3	-28/9	-28/9
(1, 5)	-4/3	4/3	-8/3
(2, 3)	-4/3	-28/9	-28/9
(2, 4)	-4/3	-28/9	-28/9
(2, 5)	-4/3	4/3	-8/3
(3, 4)	-4/3	-28/9	-28/9
(3, 5)	-4/3	4/3	-8/3
(4, 5)	-4/3	4/3	-8/3

$\langle \cdots \rangle_{\frac{3}{2}^-}$ and $\langle \cdots \rangle_{\frac{1}{2}^-}$, indicate that the operator acts on different color-spin wave functions.

IV. NEURAL-NETWORK WAVE FUNCTION

For the spatial wave function of multi-quarks, it is determined by solving the many-body Schrödinger equation. Exactly solving the Schrödinger equation for multi-quarks is a high-dimensional quantum many-body problem. To investigate the ground state properties of the system, we employ the variational method, the parameters of the trial wave function Ψ_θ are optimized by minimizing the value of energy expectation.

$$E_\theta = \frac{\langle \Psi_\theta | H | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \geq E_0. \quad (39)$$

We employ DNNs to parametrize Ψ_{spatial} . We introduce the three-dimensional coordinates of all quarks $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n$, which constitute a $3n$ -dimensional vector. To remove the kinetic energy contribution from the center of mass motion [64], we define the internal coordinates $\bar{\mathbf{r}}_1, \bar{\mathbf{r}}_2, \dots, \bar{\mathbf{r}}_n$ as the neural network input, where $\bar{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}_{\text{CM}}$, $\mathbf{R}_{\text{CM}}$ is the center of mass coordinate of the system. The scalar output of the network is $\ln(\Psi_{\text{spatial}})$. This logarithmic representation is adopted to prevent numerical instabilities during the Monte Carlo sampling. To ensure the symmetry of the spatial wave function, we symmetrize the neural network wave function. Furthermore, we added a Gaussian function $-\alpha \sum_{i=1}^n |\bar{\mathbf{r}}_i|^2$ to confine the particle within a finite volume [42], where the parameter $\alpha = 0.05 \text{ fm}^{-2}$.

We employ a fully connected neural network for this work. Each hidden layer applies a linear function to its inputs, followed by a nonlinear activation function

$$\bar{\mathbf{r}}^{(l+1)} = f(\omega^{(l)} \bar{\mathbf{r}}^{(l)} + b^{(l)}), \quad (40)$$

where $\omega^{(l)}$ and $b^{(l)}$ denote the weights and biases of the l th layer, respectively, and f is the activation function. We employ the Sigmoid linear unit (SiLU) as the activation function in this work. Its specific form is expressed as

$$\text{SiLU}(x) = \frac{x}{1 + e^{-x}}. \quad (41)$$

For meson and baryon systems, the network consists of 4 hidden layers with 24 nodes per layer. For tetraquark and

pentaquark systems, the network has 6 hidden layers with 32 nodes each. This design ensures sufficient expressive power while preserving computational feasibility. See Appendix for more details.

To obtain the optimal parameters θ that minimize the energy expectation value E_θ , we employ the stochastic reconfiguration (SR) algorithm to optimize the variational parameters [65,66]. The SR algorithm is equivalent to performing imaginary-time evolution in the variational manifold and is closely related to the natural gradient descent method in unsupervised learning [42,67]. Compared to standard gradient descent, the SR approach enhances optimization stability. Specifically, at each iteration, we use Metropolis-Hastings Monte Carlo sampling [68,69] generates a large coordinate samples, which distributed as $|\Psi_\theta|^2$. During the sampling process, a cutoff is introduced to resolve the issue of potential singularities in Eq. (2). Therefore, no cusp condition is implemented in the present algorithm. Furthermore, the neural-network wave function includes contributions from all orbital angular momentum, the variational method leads the wave function to converge to the S -wave ground state in the optimization process [52]. From these samples, the energy expectation E_θ and its gradients $\nabla_\theta E_\theta$ are evaluated. The $\nabla_\theta E_\theta$ is calculated using the following formula:

$$\nabla_\theta E_\theta = 2 \left(\frac{\langle \partial \psi_\theta | H | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} - E_\theta \frac{\langle \partial \psi_\theta | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} \right), \quad (42)$$

where $|\partial \psi_\theta\rangle \equiv \partial |\psi_\theta\rangle / \partial \theta$, S matrix denotes the quantum Fisher information matrix, which is defined as

$$S_{ab} = \frac{\langle \partial_a \psi_\theta | \partial_b \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} - \frac{\langle \partial_a \psi_\theta | \psi_\theta \rangle \langle \psi_\theta | \partial_b \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle^2}. \quad (43)$$

By calculating $\nabla_\theta E_\theta$ and the S matrix, the parameters of the neural network can be updated through the parameter update rule, which is given by

$$\theta^{i+1} = \theta^i - \eta (S + \epsilon I)^{-1} \nabla_{\theta^i} E_{\theta^i}, \quad (44)$$

where i is the iteration step, η is the learning rate, ϵ is a small regularization constant set between 10^{-3} and 10^{-4} introduced to ensure matrix invertibility and I is the identity matrix. After hundreds of iterations, the energy expectation value converges to a minimum, yielding a neural-network wave function that approximates the ground state.

To accelerate the optimization process, we use a small batch size during the early stage. As optimization enters the final 30 steps, we increase the batch size from 2000 to 80,000 to reduce statistical errors. Throughout iterations, the learning rate decayed from 10^{-1} to 10^{-5} . To describe the random error of the SR algorithm, we employ a multistep averaging scheme in the final stage of optimization. Specifically, we take the average of the masses from the

final 10 iterations as our final result. Consequently, the total error δ_{tot} is obtained by combining the Monte Carlo statistical error δ_{MC} and the neural network error δ_{NN} , the δ_{tot} is given by

$$\delta_{\text{tot}} = \sqrt{\delta_{\text{MC}}^2 + \delta_{\text{NN}}^2}, \quad (45)$$

where δ_{NN} is the standard deviation of the last ten iterations. All of the above calculations were carried out within the PYTORCH [70] framework.

V. RESULTS AND DISCUSSION

In this section, we present the mass spectra of fully heavy multi-quark systems calculated via NNQS. All numerical calculations in this work focus exclusively on the S -wave ground states. Before applying the NNQS method to fully heavy multi-quark, we first tested it on conventional mesons and baryons. The results are summarized in Table V. For meson, the results show that the masses using our method agree with those from the GEM [53,54], which utilize Gaussian basis functions expanded in standard rearrangement channels as shown in Table V. This shows that the neural-network wave function is capable of effectively describing the spatial correlations of the two-body system. When the number of (anti)quarks increases to three, i.e., baryons, the superiority of the NNQS method becomes prominent. The masses of baryons in this work are lower about 4 to 13 MeV than those in Ref. [54], implying that our variational method produces results very close to the exact values. This suggests that the neural-network wave function has stronger expressive power than trial wave function constructed with predefined Gaussian bases in Ref. [54]. The reason is that the spatial wave function of many-body systems is complex. The neural network, as a universal function approximator without the need for

TABLE V. The masses (MeV) of meson and baryon. Our results are compared with GEM results by Liu and Ling *et al.* [53,54] and experimental data [71].

State	J^P	This work	GEM	Exp.
η_c	0^-	2983.7(10)	2983	2984
J/ψ	1^-	3097.2(8)	3097	3097
B_c	0^-	6270.7(9)	6271	6274
B_c^*	1^-	6326.3(10)	6328	...
η_b	0^-	9389.4(18)	9390	9399
Υ	1^-	9460.0(12)	9460	9460
Ω_{ccc}	$3/2^+$	4816.1(5)	4823	...
Ω_{bbb}	$3/2^+$	14408.0(9)	14421	...
Ω_{ccb}	$1/2^+$	8025.3(7)	8034	...
Ω_{ccb}^*	$3/2^+$	8050.3(6)	8057	...
Ω_{cbb}	$1/2^+$	11217.6(8)	11222	...
Ω_{cbb}^*	$3/2^+$	11246.1(7)	11250	...

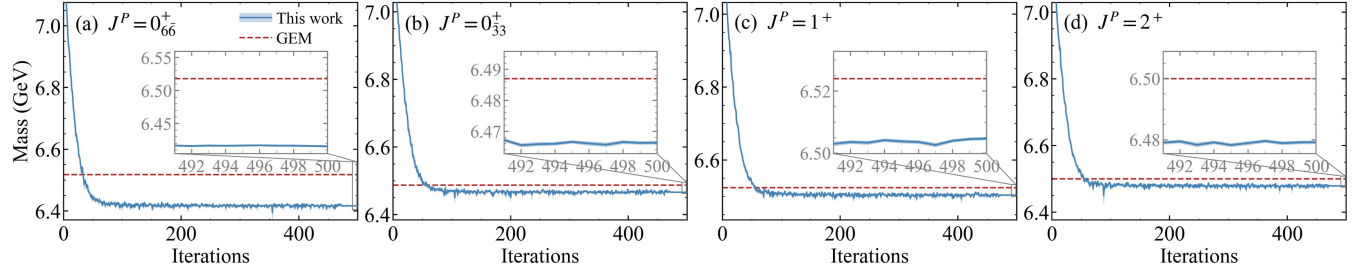


FIG. 1. The mass estimate as a function of iteration steps for $cc\bar{c}\bar{c}$ tetraquark configurations (a) $|\{cc\}_0^6\{\bar{c}\bar{c}\}_0^6\rangle_0^0$, (b) $|\{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$, (c) $|\{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$ and (d) $|\{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_2^0$ in the optimization progress. The Monte Carlo statistical errors of the masses are shown by the blue shaded area, and red dashed line represents the GEM prediction by Liu *et al.* [53]. The insets in each subplot magnifies the final optimization stage.

predefined functional forms, can capture the internal spatial distribution of three-body and more complex systems.

And then, we extend our method to fully heavy tetraquark. The optimization performance of NNQS in tetraquark is shown in Fig. 1, and we take different quantum number $cc\bar{c}\bar{c}$ systems as examples. The expected masses for the four configurations decrease rapidly during the initial optimization phase, converging stably below the GEM results presented by Liu *et al.* [53]. The Monte Carlo statistical uncertainties (blue shaded in Fig. 1) are limited and stable, confirming that the NNQS method provides a reliable prediction. All predicted mass spectra for the $cc\bar{c}\bar{c}$, $bb\bar{b}\bar{b}$, and $bb\bar{c}\bar{c}$ systems have been collected in Table VI. We label the two configurations of the $J^P = 0^+$ state $|\{QQ\}_0^6\{\bar{Q}\bar{Q}\}_0^6\rangle_0^0$ and $|\{QQ\}_1^3\{\bar{Q}\bar{Q}\}_1^3\rangle_1^0$ as 0_{66}^+ and 0_{33}^+ , respectively. The two physical 0^+ states are a mixture of 0_{66}^+ and 0_{33}^+ configurations. We first determine the two diagonal elements via neural network training. Furthermore, the off-diagonal elements are evaluated by the well trained network, i.e., using the wave functions determined by the training of the diagonal elements. With both diagonal and off-diagonal elements known, one can diagonalize the

matrix to extract the mass spectra. We found that the mass of the 0_{33}^+ state is slightly larger than that of 0_{66}^+ state. The mixing further pushes the lower state down and the higher state up, thereby enlarging their mass splitting. In all the tetraquark systems, this splitting between the two physical $J^P = 0^+$ states is from 70 to 110 MeV. The other two $J^P = 1^+$ and $J^P = 2^+$ fully charm tetraquarks are 6479.0 ± 0.7 MeV and 6503.8 ± 0.8 MeV, respectively, significantly lower than the values from Ref. [53]. The mass splitting between these two states is about 25 MeV. These masses and the mass splitting indicate that the observed $X(6900)$ cannot be an S -wave ground fully charmed tetraquark state.

In Fig. 2, we present the mass spectra of these tetraquark states and compare them with the GEM predictions from Refs. [53,55]. For the $cc\bar{c}\bar{c}$ system, in Fig. 2(a), the masses of states $J^P = 0_{33}^+$, $J^P = 1^+$ and $J^P = 2^+$ are approximately 20 MeV lower than the results in Ref. [53]. The mass of the $J^P = 0_{66}^+$ state is approximately 101 MeV lower. Due to the enlarged mass splitting induced by configuration mixing, the lower 0^+ state becomes 133 MeV lower than the results in Ref. [53], while the

TABLE VI. Predicted mass (MeV) spectra of tetraquarks for $cc\bar{c}\bar{c}$, $bb\bar{b}\bar{b}$, and $bb\bar{c}\bar{c}$ systems.

State	J^P	Configuration	$\langle H \rangle$	Mass
$cc\bar{c}\bar{c}$	0^+	$ \{cc\}_0^6\{\bar{c}\bar{c}\}_0^6\rangle_0^0$	$\begin{pmatrix} 6416.4(8) & -50.7(17) \\ -50.7(17) & 6466.2(7) \end{pmatrix}$	6384.8(16)
		$ \{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$		6497.8(16)
	1^+	$ \{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$	$(6479.0(7))$	6479.0(7)
	2^+	$ \{cc\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_2^0$	$(6503.8(8))$	6503.8(8)
$bb\bar{b}\bar{b}$	0^+	$ \{bb\}_0^6\{\bar{b}\bar{b}\}_0^6\rangle_0^0$	$\begin{pmatrix} 19209.1(11) & -27.6(23) \\ -27.6(23) & 19286.4(11) \end{pmatrix}$	19200.3(17)
		$ \{bb\}_1^3\{\bar{b}\bar{b}\}_1^3\rangle_1^0$		19295.2(17)
	1^+	$ \{bb\}_1^3\{\bar{b}\bar{b}\}_1^3\rangle_1^0$	$(19294.2(12))$	19294.2(12)
	2^+	$ \{bb\}_1^3\{\bar{b}\bar{b}\}_1^3\rangle_2^0$	$(19306.9(10))$	19306.9(10)
$bb\bar{c}\bar{c}$	0^+	$ \{bb\}_0^6\{\bar{c}\bar{c}\}_0^6\rangle_0^0$	$\begin{pmatrix} 12872.7(8) & -26.5(19) \\ -26.5(19) & 12919.6(7) \end{pmatrix}$	12860.8(16)
		$ \{bb\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$		12931.5(16)
	1^+	$ \{bb\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_1^0$	$(12926.2(9))$	12926.2(9)
	2^+	$ \{bb\}_1^3\{\bar{c}\bar{c}\}_1^3\rangle_2^0$	$(12939.6(8))$	12939.6(8)

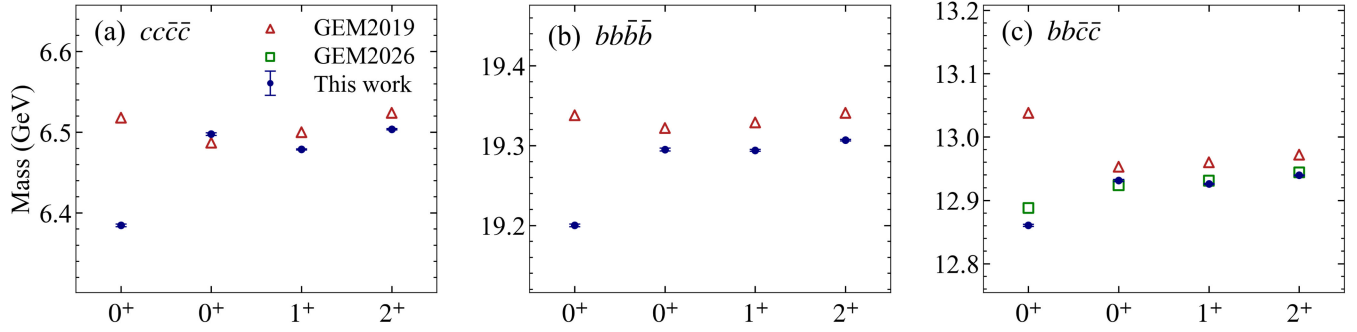


FIG. 2. A comparison of the predicted masses of the tetraquark states $cc\bar{c}\bar{c}$ (a), $bb\bar{b}\bar{b}$ (b), and $bb\bar{c}\bar{c}$ (c). The blue points, red triangles, and green squares represent this work predictions, the GEM predictions by Liu *et al.* in 2019 [53] and by Wang *et al.* in 2026 [55], respectively.

higher state becomes 10 MeV higher. For the $bb\bar{b}\bar{b}$ system in Fig. 2(b), the masses of states $J^P = 0^+_{33}$, $J^P = 1^+$ and $J^P = 2^+$ are approximately 35 MeV lower than the results in Ref. [53]. The $J^P = 0^+_{66}$ mass is approximately 128 MeV lower. The mixing scheme makes the two 0^+ masses lower than the results in Ref. [53] by 138 MeV and 27 MeV, respectively. The above results show that for tetraquarks, the expected masses from the NNQS are significantly lower than the GEM predictions in Ref. [53]. This shows that neural-network wave function has a stronger expressive power for the multi-quark wave function than the GEM used in Ref. [53], as indicated by the variational principle. This discrepancy originates from the difference in the expressive power of the multi-quark wave functions between the two methods. The GEM relies on predefined Gaussian bases, where the exponentially growing number of required basis in multi-quark needs to be truncated. In contrast, the neural networks, serving as a universal approximator of any functions, circumvents the need to predefine specific spatial wave function forms. This capability overcomes the bottleneck of conventional GEM, yielding a better variational upper bound for the ground state energy. Specifically, the pure $J^P = 0^+_{66}$ mass and the corresponding dominated state in NNQS predictions are quite different from the GEM predictions in Ref. [53]. This suggests that the color interactions between the two color-singlet bases $\mathcal{C}_1$ and $\mathcal{C}_2$ in Eq. (5) can affect the spatial wave function distribution. It suggests that in different color configurations, the Gaussian basis parameters in GEM need to be optimized separately to reflect how the color interactions impact the spatial wave function in each configuration.

It is worth mentioning that, for the $bb\bar{c}\bar{c}$ system in Fig. 2(c), the masses of the $J^P = 0^+_{33}$ -dominated physical state, $J^P = 1^+$ and $J^P = 2^+$ are lower than the GEM predictions by Liu *et al.* [53] in 2019 by approximately 20 to 30 MeV. The mass of the $J^P = 0^+_{66}$ -dominated physical state is lower by approximately 177 MeV. However, when we compare with their GEM predictions in 2026 [55], which utilized explicitly correlated Gaussian

basis functions, we found that the masses of the $J^P = 0^+_{33}$ -dominated physical state, $J^P = 1^+$ and $J^P = 2^+$ are very close, i.e., about 4 MeV lower. In addition, the mass of the $J^P = 0^+_{66}$ -dominated state is approximately 27 MeV lower. This indicates that our proposed method is a more favorable approach. At the same time, it suggests that the GEM and ECG prediction of the mass of the state $J^P = 0^+_{66}$ can continue to be improved.

To show how the color interactions between the two color-singlet bases $\mathcal{C}_1$ and $\mathcal{C}_2$ affect the spatial wave

TABLE VII. Our predicted masses(MeV) for the $cc\bar{c}\bar{c}$ system compared with others.

J^P	0^+	0^+	1^+	2^+
This work	6384.8(16)	6497.8(16)	6479.0(7)	6503.8(8)
Ref. [53]	6518	6487	6500	6524
Ref. [72]	6695	6477	6528	6573
Ref. [73]	6572	6469	6519	6545
Ref. [74]	7016	6797	6899	6956
Ref. [75]	6440–6820	6460–6470	6370–6510	6370–6510
Ref. [76]	6383	6437	6437	6437
Ref. [77]	6435	6542	6515	6543
Ref. [78]	6500	6411	6453	6475
Ref. [79]	6377	6425	6425	6432
Ref. [79]	6371	6483	6450	6479
Ref. [80]	...	6035	6139	6194
Ref. [80]	6407	...	6463	6486
Ref. [80]	6491	...	6580	6607
Ref. [30]	6351	...	6441	6471
Ref. [81]	6343	...	6439	6204
Ref. [23]	...	5883	6120	6246
Ref. [82]	...	6190	6271	6367
Ref. [83]	6346	6476	6441	6475
Ref. [84]	...	6200	...	...
Ref. [85]	...	6192	...	...
Ref. [86]	...	6038–6115	6101–6176	6172–6216
Ref. [87]	...	5990(80)	6050(80)	6090(80)
Ref. [22]	...	5969	6021	6115
Ref. [88]	...	5966	6051	6223
Ref. [89]	...	<6140	...	...

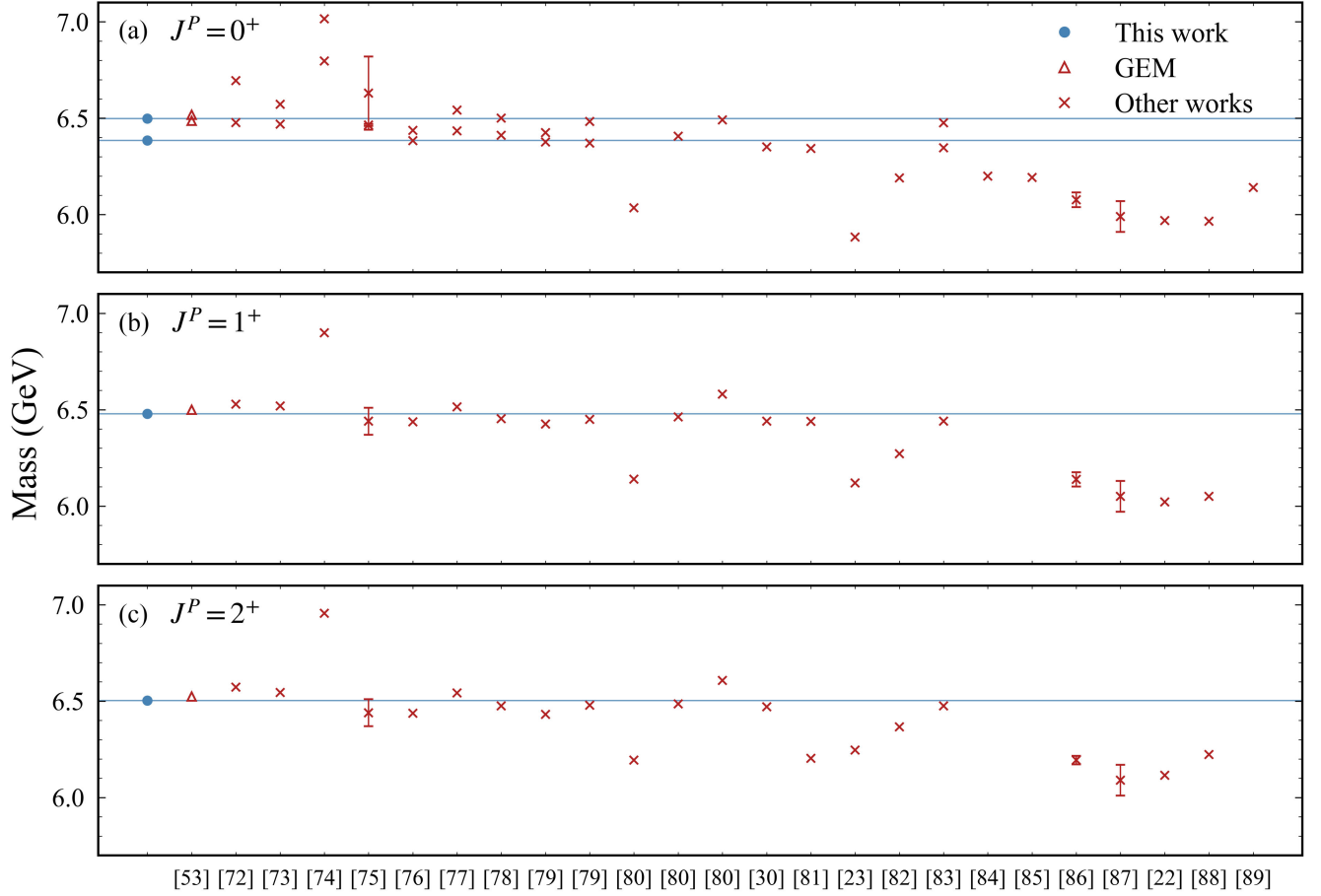


FIG. 3. A comparison of the predicted masses of the tetraquark state $cc\bar{c}\bar{c}$ with $J^P = 0^+$ (a), $J^P = 1^+$ (b), and $J^P = 2^+$ (c). The blue points (horizontal lines), red triangles and red crosses represent the predictions from this work, GEM by Liu *et al.* [53], and other works, respectively.

function distribution, we calculate the root-mean-square (RMS) radii R_{ij} for the 0_{66}^+ and 0_{33}^+ states of the $bb\bar{c}\bar{c}$ system, where $R_{ij} = \sqrt{\langle |\mathbf{r}_i - \mathbf{r}_j|^2 \rangle}$. For the 0_{66}^+ state, the RMS radii are $R_{bb} = 0.38$ fm, $R_{\bar{c}\bar{c}} = 0.49$ fm, and $R_{b\bar{c}} = 0.39$ fm. For the 0_{33}^+ state, the RMS radii are $R_{bb} = 0.28$ fm, $R_{\bar{c}\bar{c}} = 0.46$ fm, and $R_{b\bar{c}} = 0.41$ fm. This indicates that the 0_{66}^+ and 0_{33}^+ states have different spatial distribution structures. Furthermore, we define the point particle density [45],

$$\rho_{b/\bar{c}}(r) = \frac{1}{4\pi r^2} \frac{\langle \Psi | \sum_{i=1}^2 \delta(|\bar{\mathbf{r}}_i| - r) | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (46)$$

of the bottom and anti charm quarks. Taking $bb\bar{c}\bar{c}$ system as an example, in Fig. 4, we show the results of the calculation, where ρ_b and $\rho_{\bar{c}}$ represent the density of bottom and anti charm quarks, respectively. In both 0_{66}^+ and 0_{33}^+ states, the distribution of $\rho_{\bar{c}}$ is very close. However, the distribution of ρ_b in 0_{33}^+ state is clearly more compact than its distribution in 0_{66}^+ state. Our calculations show how the color configurations affect the spatial wave function.

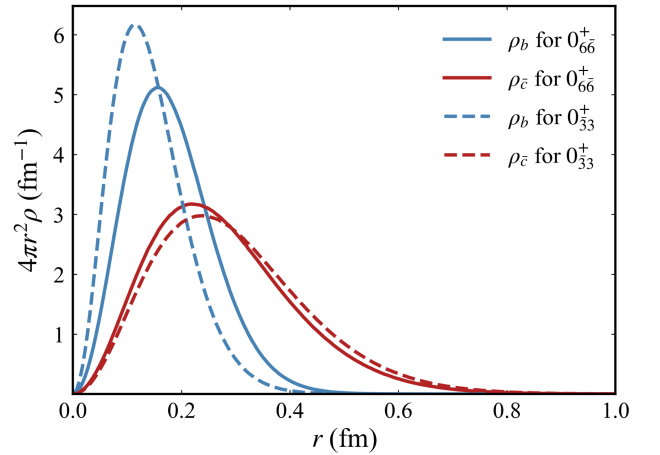


FIG. 4. Point particle densities [defined by Eq. (46)] of the $bb\bar{c}\bar{c}$ system for the 0_{66}^+ (solid lines) and 0_{33}^+ (dashed lines) states obtained with NNQS. The results for the bottom quark and anti charm quark are shown in blue and red, respectively.

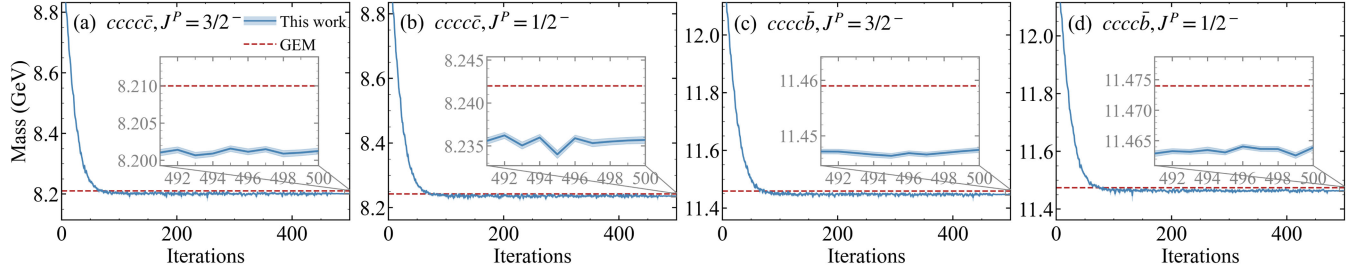


FIG. 5. The mass estimate as a function of iteration steps for (a) $J^P = 3/2^-$ $cccc\bar{c}$ pentaquark, (b) $J^P = 1/2^-$ $cccc\bar{c}$ pentaquark, (c) $J^P = 3/2^-$ $cccc\bar{b}$ pentaquark and (d) $J^P = 1/2^-$ $cccc\bar{b}$ pentaquark in the optimization progress. The Monte Carlo statistical errors of the masses are shown by the blue shaded area, and the red dashed line represents the GEM prediction by Liang *et al.* [54]. The insets in each subplot magnify the final optimization stage.

TABLE VIII. Predicted mass (MeV) spectra of pentaquarks for $cccc\bar{c}$, $cccc\bar{b}$, $bbbb\bar{b}$ and $bbbb\bar{c}$ systems.

State	J^P	Mass
$cccc\bar{c}$	$3/2^-$	8201.1(5)
	$1/2^-$	8235.5(7)
$cccc\bar{b}$	$3/2^-$	11446.9(6)
	$1/2^-$	11463.4(6)
$bbbb\bar{b}$	$3/2^-$	24217.8(9)
	$1/2^-$	24235.6(9)
$bbbb\bar{c}$	$3/2^-$	21038.2(5)
	$1/2^-$	21060.0(7)

Taking the $cc\bar{c}\bar{c}$ system as an example, we compare our results with other model calculations in Table VII and Fig. 3. Our predicted masses are slightly lower than those from the nonrelativistic quark models of Refs. [53,72], which explicitly treat both confining and Coulomb potentials. They are also lower than the MIT bag model result [73] and the diquark model with color-magnetic interactions [74]. In general, our results agree well with QCD sum rules [75] and several other potential model calculations [72,76–80]. However, our masses are higher than the DMC predictions [30] and the lattice-QCD predictions [81], and considerably higher than those reported in Refs. [22,23,80,82–89]. These differences arise partly from the use of different potential models [80,82,83] and partly

TABLE IX. Our predicted masses (MeV) for the $cccc\bar{c}$ and $cccc\bar{b}$ systems compared with others.

State	$cccc\bar{c}$		$cccc\bar{b}$	
	$3/2^-$	$1/2^-$	$3/2^-$	$1/2^-$
This work	8201.1(5)	8235.5(7)	11446.9(6)	11463.4(6)
Ref. [54]	8210	8242	11459	11474
Ref. [62]	8229	8262	11569	11582
Ref. [29]	8151	8194	11417	11437
Ref. [90]	8144.6	8193.2	11477.8	11501.5
Ref. [92]	8547.4	8537.4	11887.6	11867.7
Ref. [93]	8425.9(911)	8356.9(910)	...	...
Ref. [91]	8095	8045	...	...
Ref. [94]	7864	7949	11130	11177
Ref. [95]	...	7892.3(4)	...	...
Ref. [96]	...	7930(150)	...	...
Ref. [97]	7410 ⁺²⁷⁰ ₋₃₁₀	...	...	...
Ref. [98]	7628(112)	...	...	...

from the omission of explicit confining potentials in some of those studies [85,86,88,89].

In this work, we construct antisymmetric spin-color wave functions and symmetric spatial wave functions. This restriction makes our results above the dimeson threshold. It is worth mentioning that Wu *et al.* [52] construct the DeepQuark framework to formulate a more general wave function to ensure overall antisymmetry, with

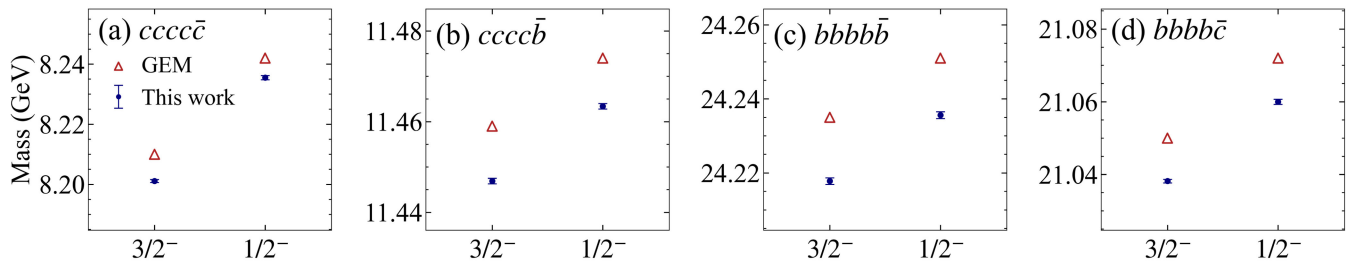


FIG. 6. A comparison of the predicted masses of the pentaquark states $cccc\bar{c}$ (a), $cccc\bar{b}$ (b), $bbbb\bar{b}$ (c), and $bbbb\bar{c}$ (d). The blue points, red triangles represent this work predictions and the GEM predictions by Liang *et al.* [54].

their calculated results for fully heavy tetraquark states approaching to the dimeson threshold.

Extending our method to fully heavy pentaquarks. The optimization performance of NNQS in pentaquark is shown in Fig. 5, and we take the $cccc\bar{c}$ and $cccc\bar{b}$ systems as examples. The mass expectation for the $cccc\bar{c}$ and $cccc\bar{b}$ pentaquarks decreases rapidly during the initial optimization phase, converging stably below the GEM results [54]. The Monte Carlo statistical uncertainties (blue shaded in Fig. 5) are limited and stable, confirming that the NNQS method provides a reliable prediction. All predicted mass spectra for the $cccc\bar{c}$, $cccc\bar{b}$, $bbbb\bar{b}$ and $bbbb\bar{c}$ systems have been given in Table VIII. We find that the mass of the $J^P = 1/2^-$ state is slightly larger than that of the

$J^P = 3/2^-$ state. In all pentaquark systems, the mass splitting between these two states is about 15 to 35 MeV.

In Fig. 6, we present the mass spectra of the pentaquark states and compare them with the results from the GEM calculated by Liang *et al.* in Ref. [54]. For the $cccc\bar{c}$ system, i.e., Fig. 6(a), the masses of the $J^P = 3/2^-$ and $J^P = 1/2^-$ states are approximately 6 to 9 MeV lower than those in Ref. [54]. For the $cccc\bar{b}$ system, i.e., Fig. 6(b), the masses of the $J^P = 3/2^-$ and $J^P = 1/2^-$ states are lower than those in Ref. [54] by approximately 10 to 12 MeV. For the $bbbb\bar{b}$ system, i.e., Fig. 6(c), the masses of the $J^P = 3/2^-$ and $J^P = 1/2^-$ are also lower than those predicted in Ref. [54] by approximately 15 to 17 MeV. For the $bbbb\bar{c}$ system, i.e., Fig. 6(d), the masses of the $J^P = 3/2^-$ and

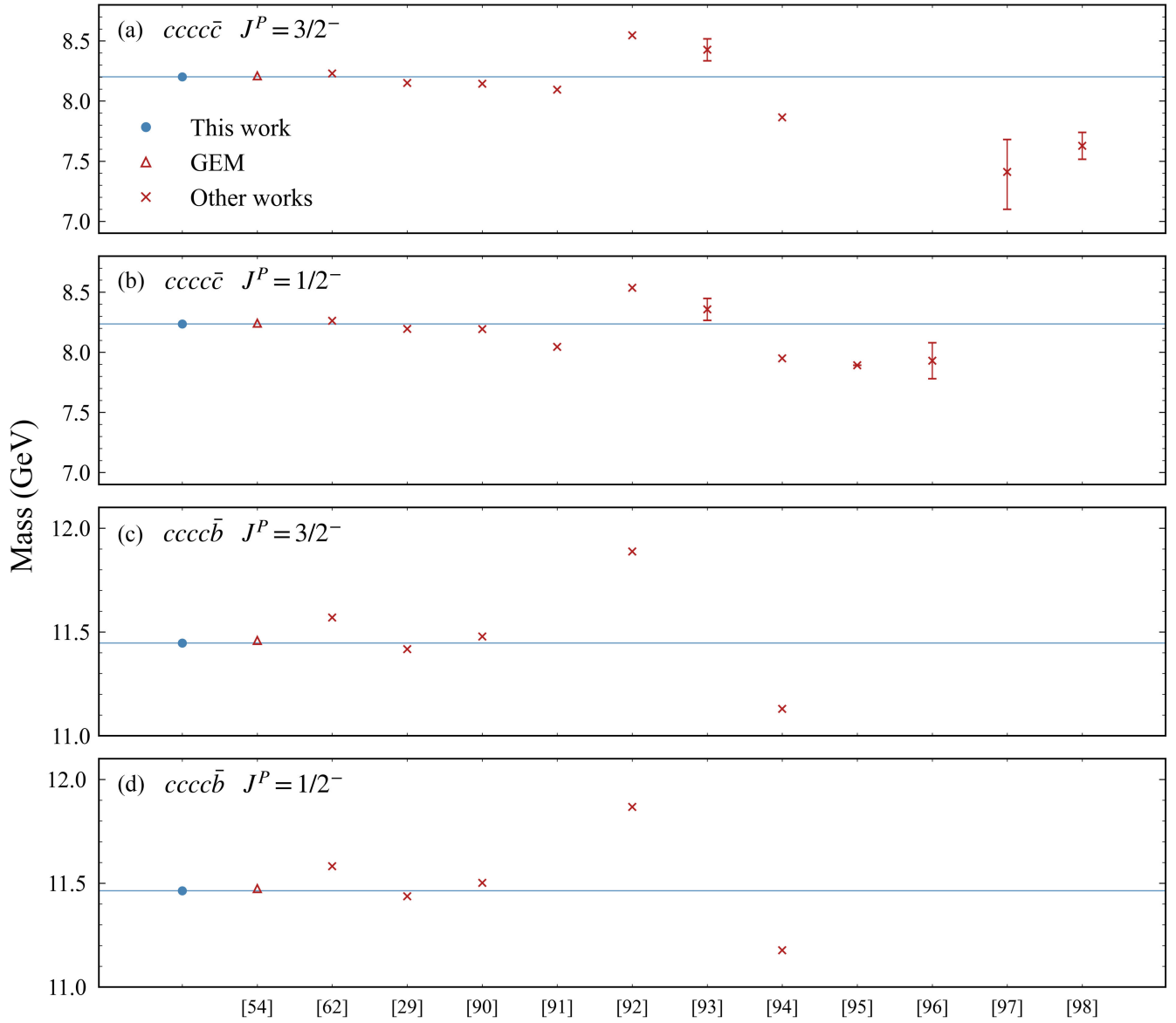


FIG. 7. A comparison of the predicted masses of the pentaquark states $cccc\bar{c}$ with $J^P = \frac{3}{2}^-$ (a) and $J^P = \frac{1}{2}^-$ (b), and $cccc\bar{b}$ with $J^P = \frac{3}{2}^-$ (c) and $J^P = \frac{1}{2}^-$ (d). The blue points (horizontal lines), red triangles and red crosses represent the predictions from this work, GEM by Liang *et al.* [54], and other works, respectively.

$J^P = 1/2^-$ states are approximately 12 MeV lower than those Ref. [54]. The above comparisons show that for pentaquarks, the mass expectations from the NNQS remain systematically lower than GEM predictions in Ref. [54]. In addition, the above comparison also illustrates that the deviations grow with the increasing quark masses, which means that the GEM in Ref. [54] performs better for charm systems than for bottom systems. It once again demonstrates that neural-network wave functions have stronger expressive power than GEM used in Ref. [54] on multi-quark wave functions.

Taking the $cccc\bar{c}$ and $cccc\bar{b}$ pentaquarks as examples, we compare our results with other model calculations in Table IX and Fig. 7. Our predicted masses are consistent with several recent calculations [29,54,62,90,91]. Specifically, they are slightly lower than the GEM results [54] and the MIT bag model [62], but slightly higher than those from the single Gaussian variational method [90], the DMC method [29], and the GEM combined with a complex-scaling approach [91]. In addition, our results are lower than the calculations based on the screened charge scheme [92] and the extended Gürsey-Radicati formalism [93]. On the other hand, our masses are significantly higher than those evaluated via the chromomagnetic interaction (CMI) model [94], the chiral quark model [95], and QCD sum rules [96–98]. These discrepancies largely originate from the different choices of the potentials employed in these models. Importantly, if the same potential were adopted, our variational approach would produce results closer to the true values, demonstrating its advantage in providing accurate predictions.

VI. SUMMARY

In this work, we propose a computational framework based on neural-network quantum states to calculate the mass spectra of fully heavy multi-quark systems within a nonrelativistic quark model. The color-spin wave functions are constructed exactly via $SU(3) \times SU(2)$ group theory to enforce fermionic antisymmetry, while the spatial part is parametrized by deep neural networks. After benchmarking on conventional mesons and baryons—where NNQS reproduces or improves upon the Gaussian expansion method results—we compute the S -wave ground-state masses of fully heavy tetraquarks and pentaquarks. Our approach consistently yields lower energies than GEM, a direct consequence of the variational principle, indicating that the neural network wave function offers greater expressive power by adaptively capturing nonperturbative many-body spatial correlations without relying on restrictive *a priori* assumptions. Compared with traditional methods, NNQS overcomes the exponential growth of basis size and avoids the fermion sign problem, making it particularly suitable for high-dimensional strongly correlated systems. Our results show good agreement with

various model calculations, and importantly, when the same potential is employed, NNQS produces values closer to the true ones, demonstrating its superior accuracy and reliability. This framework not only provides a robust tool for the spectroscopy of exotic hadrons but also offers a flexible continuous-space solver for investigating microscopic binding mechanisms. Future extensions to hexaquark and more complex systems are anticipated, which will further aid experimental searches for all-heavy multi-quark states.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: THE HYPERPARAMETERS USED IN OUR CALCULATIONS

In the Appendix, we explain and summarize the architecture of the neural network and the hyperparameters used in our calculations. We employ a fully connected neural network. Specifically, it is a fully connected neural network composed of an input layer, multiple hidden layers, and an output layer. The number of nodes corresponds to the number of neurons. The output of the previous layer serves directly as the input to the subsequent layer. Specifically, each hidden layer applies a nonlinear activation function

$$\bar{\mathbf{r}}^{(l+1)} = f(\omega^{(l)}\bar{\mathbf{r}}^{(l)} + b^{(l)}), \quad (\text{A1})$$

where $\omega^{(l)}$ and $b^{(l)}$ denote the weights and biases of the l th layer, respectively, and f is the activation function. We employ the SiLU as the activation function in this work. Its specific form is expressed as

$$\text{SiLU}(x) = \frac{x}{1 + e^{-x}}. \quad (\text{A2})$$

The number of hidden layer nodes and the number of layers control the expressive power of the neural network wave function. A higher number of nodes and layers yields a more expressive neural network, but incurs a higher computational cost. For meson and baryon systems, the network consists of four hidden layers with 24 nodes per layer. For tetraquark and pentaquark systems, the network

TABLE X. The hyperparameters used in our calculations.

Parameter	Value	Parameter	Value
Acceptance rate range	0.75–0.85	Regularization constant	$10^{-3} - 10^{-4}$
Acceptance rate factor	1.15	Batch size	2000
Steps	800	Large batch size	80000
Initial learning rate	0.04–0.05	Large batch iterations	30
Total iterations	500	Final average iterations	10

has six hidden layers with 32 nodes each. This design ensures sufficient expressive power while preserving computational feasibility. The hyperparameters for our calculations are summarized in Table X.

In the Metropolis-Hastings Monte Carlo sampling, a new position r' is randomly proposed and then accepted or rejected based on acceptance rate calculated by

$$P(r) = \frac{|\Psi(r)|^2}{\int dr |\Psi(r)|^2}, \quad (\text{A3})$$

$$P_{\text{accept}}(r \rightarrow r') = \min \left\{ 1, \frac{P(r')}{P(r)} \right\}. \quad (\text{A4})$$

To ensure an efficient and thorough exploration of the space, the sampling step size is adjusted. If the acceptance rate falls outside the acceptance rate range, the step size is multiplied or divided by the acceptance rate factor. The steps parameter refers to the number of random walk steps performed per neural network iteration. The total iterations parameter is the total number of training iterations for the neural network, and the regularization constant refers to the ϵ in Eq. (44). The batch size in our work is the number of Metropolis-Hastings samples. To reduce statistical uncertainty, during the last large batch iterations, we increase the sample size from batch size to the large batch size. Finally, we average the results over the final average iterations to obtain our final results.

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