

A deep neural network approach to solve the Dirac equation

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We extend the method from [Naito, Naito, and Hashimoto, Phys. Rev. Research **5**, 033189 (2023)] to solve the Dirac equation not only for the ground state but also for low-lying excited states using a deep neural network and the unsupervised machine learning technique. The variational method fails because of the Dirac sea, which is avoided by introducing the inverse Hamiltonian method. For low-lying excited states, two methods are proposed, which have different performances and advantages. The validity of this method is verified by the calculations with the Coulomb and Woods-Saxon potentials.

I. INTRODUCTION

Nowadays, machine learning is being utilized in various fields of physics [1]. Among machine learning algorithms, the unsupervised machine learning is a powerful technique to optimize neural networks without training datasets. With the powerful optimization ability, it is an ideal tool to solve variational problems.

The key idea of applying the unsupervised machine learning to quantum mechanics is to find the loss function suitable for the system. By using the energy as the loss function, searching the minimum of the loss function is equivalent to finding the ground state of the system.

The pioneer work solved spin systems by using the Boltzmann machine [2]. The following work extended this method with a higher accuracy with introducing pair-wise ansatz [3] and deterministic time evolution [4]. The extension to the excited-state calculation with two different ansatz were proposed in Refs. [5, 6]. Other approaches to solve spin systems applied Jastrow-Slater wave function ansatz [7] and hidden-fermion one [8]. Reference [9] proposed a generalization model for spins, which is to take perceptrons as the transfer matrix of a spin-glass Hamiltonian.

For continuous systems, the design of the machine learning algorithm should be based on the (anti)symmetrization of the system. Several models of bosonic systems were solved with a fully connected deep neural network (DNN) in Ref. [10]. Reference [11] employed the Deep Sets neural-network architecture to solve periodic systems. For fermionic systems, from electrons to nucleons, the Jastrow-Slater ansatz was a successful application to consider the antisymmetrization [12–25]. Recent progress on this direction is summarized in Ref. [26]. Another application was based on the Jordan-Wigner mapping or similar mapping methods from the

fermionic system into a spin system and using the Boltzmann machine [27]. Reference [28] proposed a DNN model to solve the ground state and excited states in the coordinate space, which included symmetrization for bosons or antisymmetrization for fermions. Soon this method was extended with spin and isospin degrees of freedom by applying a non-fully connected DNN structure [29]. However, all these works focused on the non-relativistic case. The relativistic formulation using the Dirac equation is sometimes crucial to describe electronic structure of atoms [30], molecules [31], and nuclear systems [32]. However, the unsupervised machine learning has not been applied to the Dirac equation yet; one of the difficulties of the Dirac equation using a variational method is the so-called the variational collapse. Due to the existence of the Dirac sea, the ground state energy is not the lowest eigenvalue of a Dirac Hamiltonian. Therefore, minimizing the energy directly causes the loss function falling into the Dirac sea, which is the variational collapse.

In this paper, we propose an unsupervised DNN method to solve the Dirac equation, which is an extension of the method proposed in Ref. [28]. We apply the inverse Hamiltonian method [33] to avoid the variational collapse. To calculate low-lying excited states, we propose two methods: One is adjusting a parameter contained in the inverse Hamiltonian method, and the other is an extension based on the method in Ref. [28], which applies the orthonormal condition to eliminate components of the lower excited states and the ground state in the DNN output. Throughout our test, both two methods are capable of generating precise energies and wave functions, while the inverse Hamiltonian method is easier to use and the orthonormal method converges faster.

This paper is organized as follows: In Sec. II, we discuss the Dirac equation with spherical symmetry, and introduce the inverse Hamiltonian method to solve the ground state, where the excited states are solved by both the inverse Hamiltonian and the orthonormal method. In Sec. III, we introduce our DNN model. The results of Coulomb and Wood-Saxon potential calculations are shown in Secs. IV and V, respectively. Section VI is the

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summary of our work.

II. THEORETICAL FRAMEWORK

A. The Dirac equation with spherical symmetry

The Dirac equation reads [34]

$$H_D \phi = E \phi, \quad (1)$$

where an eigenvalue E includes the rest mass mc^2 . We define the internal energy ε by

$$\varepsilon = E - mc^2. \quad (2)$$

The one-body Dirac Hamiltonian H_D in the coordinate space reads

$$H_D = c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta (mc^2 + S(\mathbf{r})) + V(\mathbf{r}), \quad (3)$$

where \mathbf{p} denotes the momentum operator, and $S(\mathbf{r})$ and $V(\mathbf{r})$ denote the scalar and vector potentials, respectively. The $\boldsymbol{\alpha}$ and β are the Dirac matrices, which are

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad (i = x, y, z), \quad (4a)$$

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \quad (4b)$$

with the Pauli matrices σ_i and the 2×2 identity matrix I_2 . We define H'_D by

$$\begin{aligned} H'_D &= H_D - mc^2 \\ &= \boldsymbol{\alpha} \cdot \mathbf{p} + \beta (mc^2 + S(\mathbf{r})) + V(\mathbf{r}) - mc^2, \end{aligned} \quad (5)$$

where the eigenvalue of H'_D is the internal energy ε .

We assume that the potentials are spherically symmetric, i.e., $V(\mathbf{r}) = V(r)$ and $S(\mathbf{r}) = S(r)$. Then, eigenfunctions of H'_D can be written as

$$\phi_{n\kappa j_z}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} F_{n\kappa}(r) \mathcal{Y}_{j_z}^A(\theta, \psi) \\ iG_{n\kappa}(r) \mathcal{Y}_{j_z}^B(\theta, \psi) \end{pmatrix} \quad (\kappa = -j - 1/2), \quad (6a)$$

$$\phi_{n\kappa j_z}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} F_{n\kappa}(r) \mathcal{Y}_{j_z}^B(\theta, \psi) \\ iG_{n\kappa}(r) \mathcal{Y}_{j_z}^A(\theta, \psi) \end{pmatrix} \quad (\kappa = j + 1/2), \quad (6b)$$

where $F_{n\kappa}(r)$ and $G_{n\kappa}(r)$ denote the large and small components of a radial wave function, respectively. The subscripts n and j_z , respectively, denote the principal quantum number the z -projection of the total angular momentum j . For a given j , $\kappa = j + 1/2$ if the orbital angular momentum l satisfies $l = j + 1/2$, and $\kappa = -j - 1/2$ if l satisfies $l = j - 1/2$. The detailed forms of the tensor spherical harmonics are given by

$$\mathcal{Y}_{j_z}^A(\theta, \psi) = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l+m+1} Y_{l,l_z}(\theta, \psi) \\ \sqrt{l-m} Y_{l,l_z+1}(\theta, \psi) \end{pmatrix}, \quad (7a)$$

$$\mathcal{Y}_{j_z}^B(\theta, \psi) = \frac{1}{\sqrt{2l+3}} \begin{pmatrix} -\sqrt{l-m+1} Y_{l+1,l_z}(\theta, \psi) \\ \sqrt{l+m+1} Y_{l+1,l_z+1}(\theta, \psi) \end{pmatrix}, \quad (7b)$$

respectively, where $Y_{l,l_z}(\theta, \psi)$ is a spherical harmonics with l_z denoting the z -projection of l .

After the separation of radial and angular parts, the radial Dirac equation is

$$H'_{Dr} \varphi_{n\kappa}(r) = \varepsilon_{n\kappa} \varphi_{n\kappa}(r), \quad (8)$$

where H'_{Dr} and $\varphi_{n\kappa}$, respectively, read

$$H'_{Dr} = \begin{pmatrix} V(r) + S(r) & -\frac{d}{dr} + \frac{\kappa}{r} \\ \frac{d}{dr} + \frac{\kappa}{r} & V(r) - S(r) - 2mc^2 \end{pmatrix}, \quad (9)$$

$$\varphi_{n\kappa}(r) = \begin{pmatrix} F_{n\kappa}(r) \\ G_{n\kappa}(r) \end{pmatrix}. \quad (10)$$

According to Eq. (8), $G_{n\kappa}(r)$ can be calculated by

$$G_{n\kappa}(r) = \frac{\frac{d}{dr} + \frac{\kappa}{r}}{\varepsilon_{n\kappa} - V(r) + S(r) + 2mc^2} F_{n\kappa}(r). \quad (11)$$

The normalization condition for the radial wave functions reads

$$\int_0^\infty [F_{n\kappa}^2(r) + G_{n\kappa}^2(r)] dr = 1. \quad (12)$$

B. The inverse Hamiltonian method

A Dirac Hamiltonian H_D has the positive and negative eigenvalues. The former and latter, respectively, correspond to the particle and anti-particle states. Because of the existence of the negative-energy states, the ground-state energy is no longer the lowest eigenvalue of H_D . Therefore, minimizing the energy naively leads to the variational collapse, i.e., the energy expectation value diverges into the negative infinite. We introduce the so-called inverse Hamiltonian method [33] to our DNN method in order to apply DNN for energy minimization to obtain the ground state.

The inverse Hamiltonian for given n and κ is defined by

$$H_{inv}^{n\kappa} = (\varepsilon'_{n\kappa} - H'_{Dr})^{-1}. \quad (13)$$

The ground state is $\kappa = -1$ and $n = 1$; thus, we choose an arbitrary value between the ground-state energy $\varepsilon_{1,-1}$ and the highest eigenvalue of negative energy states ($\varepsilon_{1,-1}^* - 2mc^2$) for $\varepsilon'_{1,-1}$, that is, $(\varepsilon_{1,-1}^* - 2mc^2) < \varepsilon'_{1,-1} < \varepsilon_{1,-1}$ to obtain the ground-state energy. The schematic figure of the spectrums of H'_D and $H_{inv}^{1,-1}$ is shown in Fig. 1. The lowest eigenstate of $H_{inv}^{1,-1}$ corresponds the ground state.

Another benefit of applying the inverse Hamiltonian method is that both the ground and low-lying excited states can be calculated by varying $\varepsilon'_{n\kappa}$. To calculate the state of quantum number $n + 1$ and κ , we set $\varepsilon'_{(n+1)\kappa}$ satisfying between

$$\varepsilon_{n\kappa} < \varepsilon'_{(n+1)\kappa} < \varepsilon_{(n+1)\kappa}. \quad (14)$$

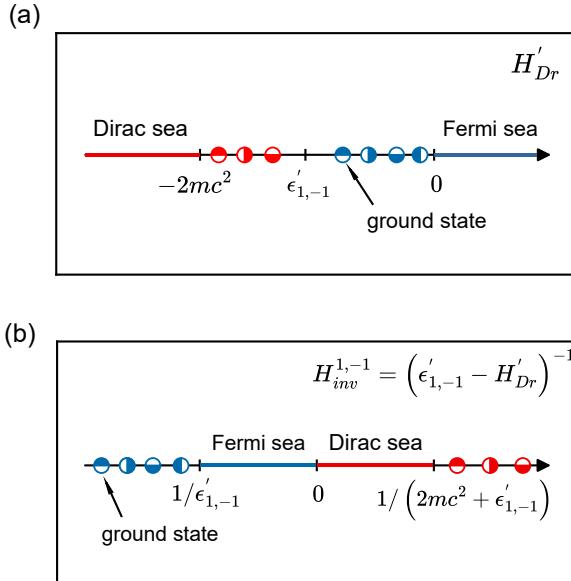


FIG. 1. (a) Spectrum of eigenstates of the Dirac Hamiltonian H'_{Dr} . The half-filled blue circles denote the ground state and low-lying excited states, while the blue line denotes positive continuum states. The half-filled red circles and red line denote the bound states and continuum states in the Dirac sea, respectively. (b) Spectrum of eigenstates of the inverse Hamiltonian $H'_{inv}^{1,-1}$ [33] for the ground state calculation. The continuum states are reversed in the middle between bound states. The order among the bound states in both the Fermi sea and the Dirac sea does not change, respectively. The ground state is the lowest state in the spectrum.

and calculate by Eq. (13)

$$\varepsilon_{(n+1)\kappa} = \varepsilon'_{(n+1)\kappa} - \left(\min \frac{\langle \varphi | H_{inv}^{(n+1)\kappa} | \varphi \rangle}{\langle \varphi | \varphi \rangle} \right)^{-1}. \quad (15)$$

Practically, ε' is chosen slightly smaller than zero. If the trial with another parameter ε'' which is much smaller than ε' returns the same eigenvalue, we can safely assume the obtained state is the ground state. If the test with ε'' returns a lower eigenvalue, then we repeat the process until we obtain the ground state with two different trial parameters with a large gap. In the case with spherical symmetry, a more direct strategy is to count the number of nodes in the big component of wave functions, which is equal to n . Then, in a recursive approach, the state of quantum number $n+1$ and κ can be obtained by setting $\varepsilon'_{(n+1)\kappa}$ slightly greater than the n -th eigenvalue $\varepsilon_{n\kappa}$.

C. The orthonormal method

Besides the inverse Hamiltonian method, we also extend the method to calculate low-lying excited states proposed in Ref. [28] to obtain excited states of the Dirac equation. The eigenfunctions satisfy the orthonormal condition

$$\langle \varphi_{i\kappa} | \varphi_{n\kappa} \rangle = \delta_{i,n}. \quad (16)$$

For arbitrary states $|\varphi\rangle$ with a given κ , we can construct a state $|\varphi'\rangle$ that is orthonormal to the eigenstates $|\varphi_{i\kappa}\rangle$ with $i = n_{\min}, n_{\min} + 1, \dots, n$

$$|\varphi'\rangle = |\varphi\rangle - \sum_{i=n_{\min}}^n \langle \varphi_{i\kappa} | \varphi \rangle |\varphi_{i\kappa}\rangle. \quad (17)$$

Because the state $|\varphi'\rangle$ is orthonormal to eigenstates $|\varphi_{i\kappa}\rangle$ with lower principle quantum numbers from n_{\min} to n , the state of principle quantum number $n+1$ is obtained by minimizing the energy variational

$$\varepsilon_{(n+1)\kappa} = \varepsilon'_{n_{\min}\kappa} - \left(\min \frac{\langle \varphi' | H_{inv}^{n_{\min}\kappa} | \varphi' \rangle}{\langle \varphi' | \varphi' \rangle} \right)^{-1}. \quad (18)$$

Note that $|\varphi'\rangle$ is constructed in a recursive way for a given κ , so that wave functions of the lowest state cannot be obtained in this method. Therefore, the lowest-energy state in Eq. (17) is obtained by the inverse Hamiltonian method.

III. NEURAL NETWORK MODELS

A. Discretization of the Dirac equation

We define a trial wave function $f_{n\kappa}$ by

$$f_{n\kappa}(r) = \frac{\tilde{f}_{n\kappa}(r)}{r} \quad (19)$$

to give an accurate description of the asymptotic behavior near the origin. The boundary condition reads $f_{n\kappa}(0) = f_{n\kappa}(\infty) = 0$.

To perform numerical calculations, the radial coordinate $r \in [0, r_{\max}]$ is discretized with $M+1$ meshes. The Dirichlet boundary condition $f_{n\kappa}(0) = f_{n\kappa}(r_{\max}) = 0$ is imposed so that the actual number of mesh points used for DNN calculation is $M-1$. The discrete form of $f_{n\kappa}(r)$ is a $(M-1)$ -dimensional vector

$$f_{n\kappa}(r) \simeq \begin{pmatrix} \tilde{f}_{n\kappa 1} \\ \tilde{f}_{n\kappa 2} \\ \tilde{f}_{n\kappa 3} \\ \vdots \\ \tilde{f}_{n\kappa(M-3)} \\ \tilde{f}_{n\kappa(M-2)} \\ \tilde{f}_{n\kappa(M-1)} \end{pmatrix}. \quad (20)$$

Both the vector and scalar potentials are discretized as a $(M-1)$ -dimensional diagonal matrix:

$$V \pm S \simeq \begin{pmatrix} \tilde{V}_1 \pm \tilde{S}_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & \tilde{V}_2 \pm \tilde{S}_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \tilde{V}_3 \pm \tilde{S}_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \tilde{V}_{M-3} \pm \tilde{S}_{M-3} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \tilde{V}_{M-2} \pm \tilde{S}_{M-2} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \tilde{V}_{M-1} \pm \tilde{S}_{M-1} \end{pmatrix}, \quad (21)$$

where $\tilde{V}_i = V(r_i)$ and $\tilde{S}_i = S(r_i)$. The form of the differential operator depends on the distribution of mesh points, which will be discussed in Sec. IV B and Sec. V B. Then, the Dirac Hamiltonian H'_{Dr} is expressed by a $(2M-2)$ -dimensional matrix, which is used to construct the inverse Hamiltonian $H_{inv}^{n\kappa}$ numerically.

B. Design of the neural network

We construct a fully connected neural network for the trial wave function $f_{n\kappa}(r)$ on the TENSORFLOW [35]. Figure 2 shows the structure of the DNN, which contains one input unit and one output unit. It is confirmed that two hidden layers, each of which contains 16 units, are sufficient to generate faithful results, which is similar to our previous work [29]. The “softplus” function

$$\text{softplus}(x) = \log(1 + e^x) \quad (22)$$

is used as the activation function. The parameters of the DNN are updated by the ADAM optimizer [36].

Throughout the training process, all radial coordinates are treated as one batch sending into the DNN and the mini-batch technique is not used. The wave function $F_{n\kappa}$ is calculated by the DNN output $f_{n\kappa}$ by Eq. (19), and then it is used to calculate $G_{n\kappa}$ by Eq. (11). For the ground state, the loss function $\varepsilon_{n\kappa}$ is calculated by Eq. (15), while either Eq. (15) or (18) is used for excited states. According to Eq. (11), $\varepsilon_{n\kappa}$ is needed to calculate $G_{n\kappa}$. For the n -th epoch calculation, the $\varepsilon_{n\kappa}$ to calculate $G_{n\kappa}$ is from the $(n-1)$ -th epoch, while the initial $\varepsilon_{n\kappa}$ is set equal to $\varepsilon'_{n\kappa}$ for the first epoch.

IV. RESULTS OF THE HYDROGEN ATOM

A. The exact results

We apply our DNN method for the hydrogen atom. The scalar and vector potentials, respectively, read

$$V(r) = -\frac{1}{r}, \quad (23a)$$

$$S(r) = 0, \quad (23b)$$

where the Hartree atomic unit is used, i.e., $\hbar = 4\pi\varepsilon_0 = e^2 = m_e = 1$.

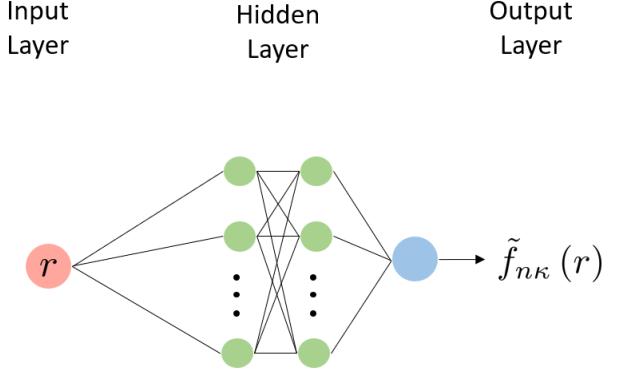


FIG. 2. Schematic figure of the DNN structure. The input layer contains one unit (red), where the input is the radial coordinate r . The output layer contains one unit (blue), where the output is $\tilde{f}_{n\kappa}(r)$. The hidden layers are composed of two fully connected layers, each of which contains 16 units (green).

The wave functions and energy are analytically known as [37]

$$F_{n\kappa} = e^{-\rho}\rho^s \sum_{m=0}^{n-1/2-j} a_m \rho^m, \quad (24a)$$

$$G_{n\kappa} = e^{-\rho}\rho^s \sum_{m=0}^{n-1/2-j} b_m \rho^m, \quad (24b)$$

$$E_{n\kappa} = \sqrt{\frac{c^2}{1 + \frac{Z^2 \alpha^2}{\left(n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-Z^2 \alpha^2}\right)^2}}}, \quad (24c)$$

with

$$s = \sqrt{\kappa^2 - 1/c^2}, \quad (25a)$$

$$\rho = \frac{\sqrt{c^4 - E_{n\kappa}^2}}{c} r, \quad (25b)$$

$$\mu = \sqrt{\frac{c^2 - E_{n\kappa}^2}{c^2 + E_{n\kappa}^2}}, \quad (25c)$$

and the speed of light c . The normalization coefficients a_q and b_q are calculated by

$$C_q = \frac{a_q}{\frac{s+q-\kappa}{\mu} + \frac{1}{c}} = \frac{b_q}{s + q + \kappa - \frac{1}{c\mu}}, \quad (26)$$

where C_q satisfies the recurrence equation

$$C_q = \frac{2(q-n+j-\frac{1}{2})}{q(q+2s)} C_{q-1}. \quad (27)$$

B. Discrete representations with the log mesh

The Coulomb potential changes rapidly in the central region (small r). In order to calculate the central region

precisely, we define x by

$$r = e^x - e^{x_0}, \quad (28)$$

and x is discretized uniformly with the size Δx and x_0 as the small boundary point. Note that the term e^{x_0} is introduced to impose the boundary condition $f_{n\kappa}(r=0) = 0$ properly, as the following Eq. (30) requires $f_{n\kappa}(r(x_0)) = 0$. The first-order differential operator for the log mesh reads

$$\frac{\partial}{\partial r} = \frac{1}{e^x} \frac{\partial}{\partial x}, \quad (29)$$

where the corresponding derivative matrix reads

$$\frac{\partial}{\partial r} \simeq \frac{1}{2\Delta x} \begin{pmatrix} 0 & \frac{1}{e^{x_1}} & 0 & \cdots & 0 & 0 & 0 \\ -\frac{1}{e^{x_2}} & 0 & \frac{1}{e^{x_2}} & \cdots & 0 & 0 & 0 \\ 0 & -\frac{1}{e^{x_3}} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{1}{e^{x(M-3)}} & 0 \\ 0 & 0 & 0 & \cdots & -\frac{1}{e^{x(M-2)}} & 0 & \frac{1}{e^{x(M-2)}} \\ 0 & 0 & 0 & \cdots & 0 & -\frac{1}{e^{x(M-1)}} & 0 \end{pmatrix}. \quad (30)$$

C. DNN results

In this section, we use $M = 1700$ as the number of mesh points. For the orthonormal method, all states are calculated within a $e^{4.9} - e^{-10} \approx 100$ a.u. box to impose the orthonormal condition, while the box sizes of the inverse Hamiltonian are 20, 40, 40, 60, 90, 100 a.u. for states from $n = 1$ to 6, respectively.

The energies of the ground state and first five excited states for $\kappa = -1$ are listed in Table I. The inverse Hamiltonian method reaches at least 1×10^{-4} accuracy and the error does not depend on n except for $n = 1$. The relative error of the orthonormal method increases with the increase of n . This is because as n increases, more lower-energy states are used to construct $|\varphi'\rangle$ from Eq. (17), so that the error of lower-energy state data accumulates.

The wave functions of the ground and first five excited states for $\kappa = -1$ are shown in Figs. 3 and 4. In general, both methods can reproduce the exact wave functions, except the peak of the $n = 6$ state at large r , since the 100 a.u. box size is too small for the $n = 6$ state. The relative errors between DNN wave functions and exact results are shown in Fig. 5. Except around the boundary, the DNN reproduces the exact wave functions. The precisions of wave functions are almost the same level for both methods. Note that due to the existence of nodes, the relative error diverges at the nodes.

The relative errors of the loss function to the exact energy as a function of epochs for both methods are shown in Fig. 6. As shown in Table I, the number of epochs to

converge for the orthonormal method is one order of magnitude less than the inverse Hamiltonian method, while the time per epoch of the orthonormal method is about twice longer than the inverse Hamiltonian method. The calculation cost of the inverse Hamiltonian method does not depend on n ; in contrast, larger n requires longer calculation due to the orthonormalization.

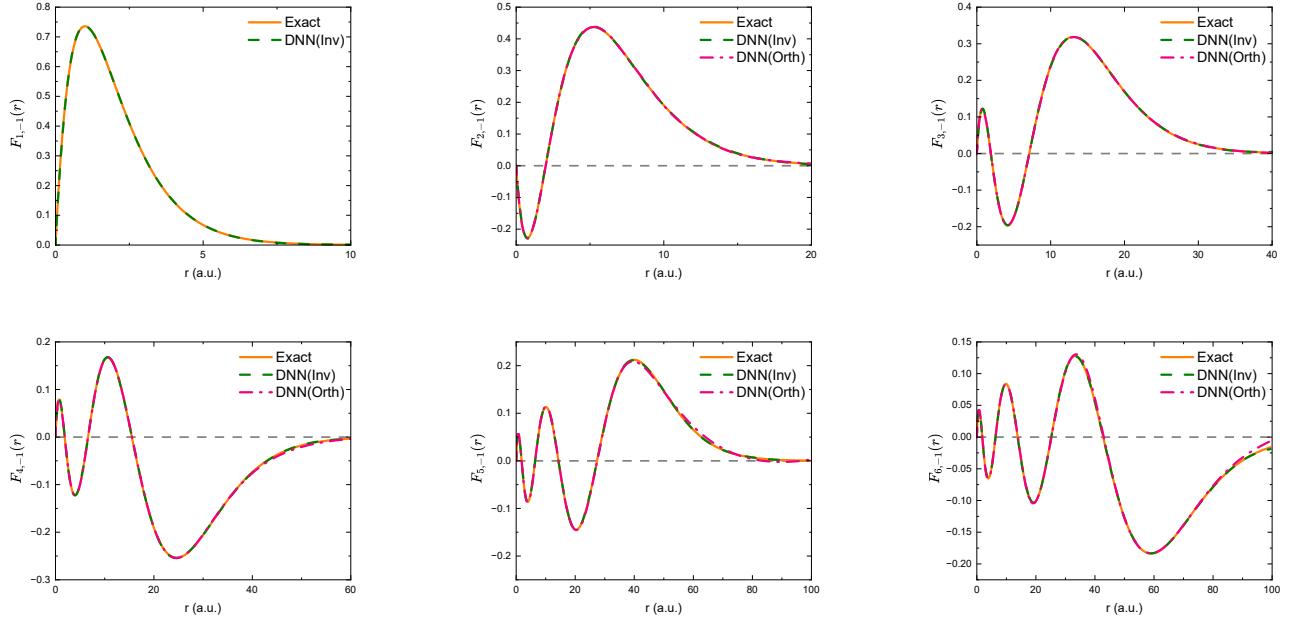


FIG. 3. The F -component of Dirac wave functions with $\kappa = -1$ of the hydrogen atom from $n = 1$ to 6. The DNN results from the inverse Hamiltonian method and the orthonormal one are shown as “DNN(Inv)” and “DNN(Orth)” in dash and dash-dotted lines, respectively. For comparison, the analytical results are also shown in the solid lines. Both the inverse Hamiltonian method and the orthonormal one reproduce results accurately.

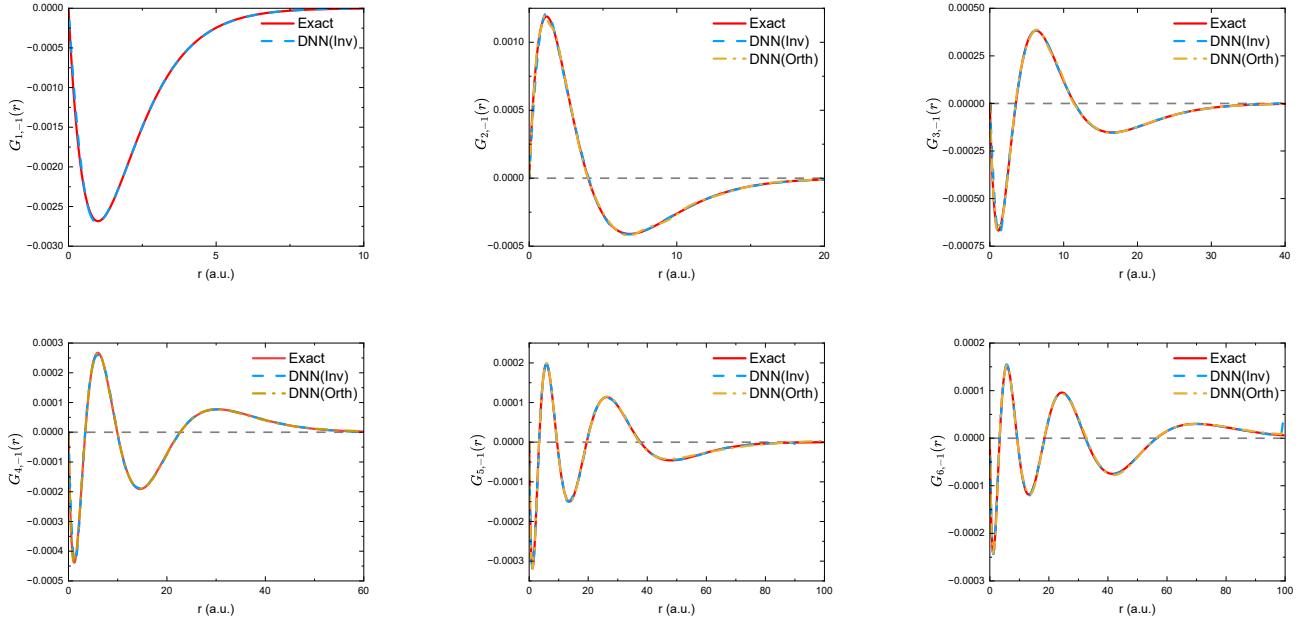


FIG. 4. Same as Fig. 3, but for the G -component.

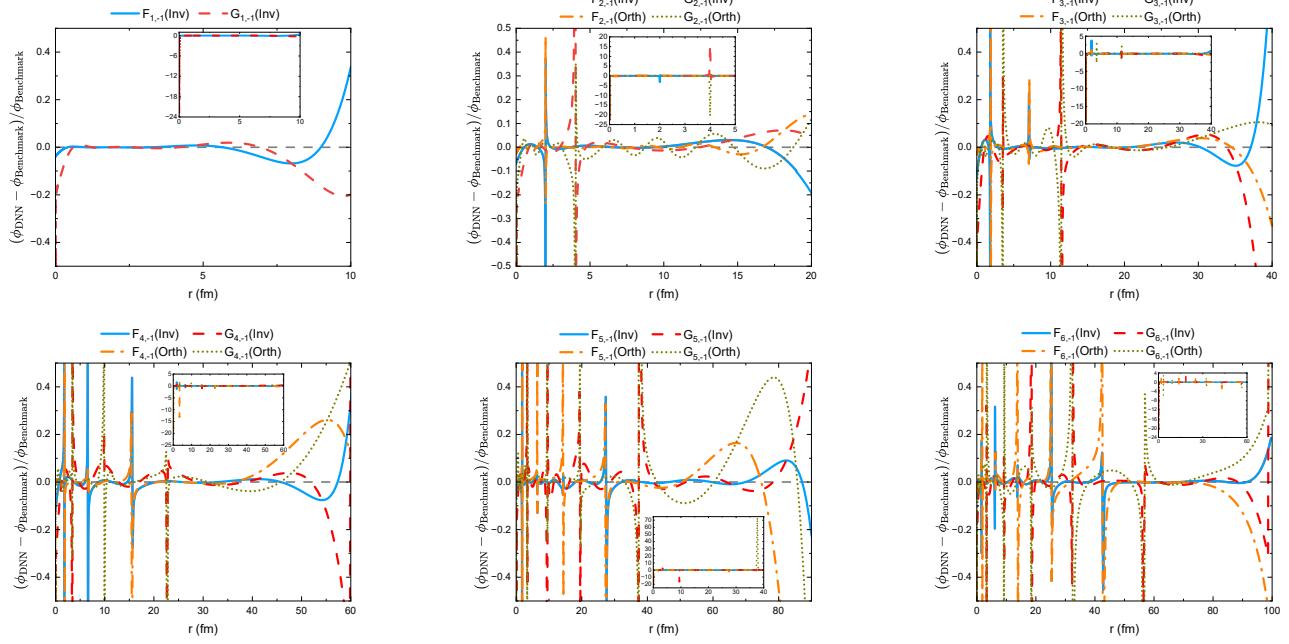


FIG. 5. Relative errors of DNN wave functions to the exact benchmark results for a hydrogen atom. The positions of peaks correspond to the node of wave functions.

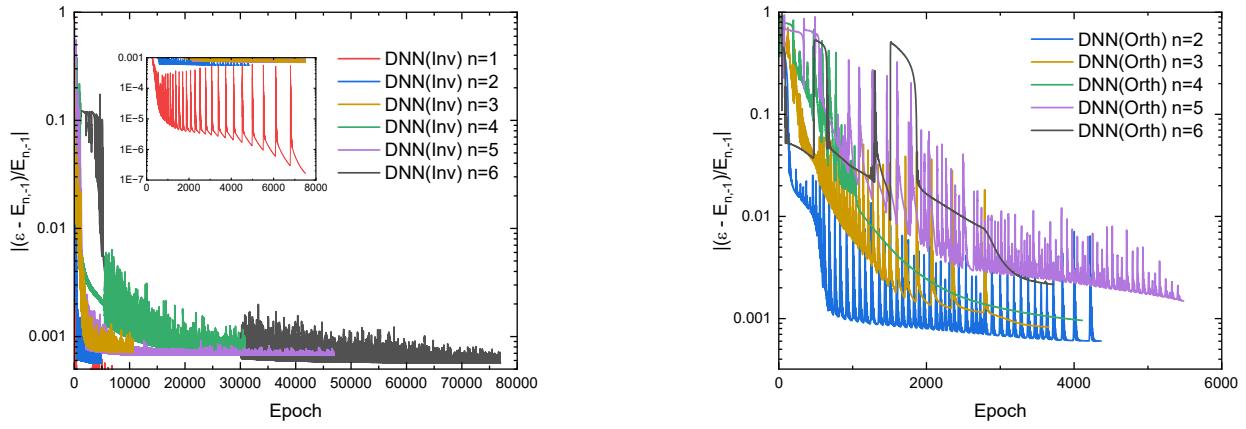


FIG. 6. Relative errors of energy of different states of $\kappa = -1$ as functions of epochs for a hydrogen atom. Because of the randomness in the optimization process, the number of epochs fluctuates in each run. The left panel is for the inverse Hamiltonian method, and the right panel is for the orthonormal method.

TABLE I. Energies with $\kappa = -1$ of the hydrogen atom from $n = 1$ to 6. The ε_{Inv} and $\varepsilon_{\text{Orth}}$ denote the energy obtained by the inverse Hamiltonian method and the orthonormal one, respectively. Rows with “—” in the column denote this state cannot be calculated by the orthonormal method. Except for the $n = 5$ and $n = 6$ states with the orthonormal method achieving the 1×10^{-3} level of precision, the rest calculations reach at least 1×10^{-4} level of precision.

n	1	2	3	4	5	6
Exact (Hartree)	-0.50000666	-0.125002	-0.055556	-0.0312503	-0.020000	-0.013889
ε_{Inv} (Hartree)	-0.50000657	-0.124931	-0.055516	-0.0312271	-0.019987	-0.013881
Relative Error of ε_{Inv}	1.79×10^{-7}	5.68×10^{-4}	7.20×10^{-4}	7.42×10^{-4}	6.50×10^{-4}	5.76×10^{-4}
Time per Epoch of ε_{Inv} (s)	0.0553	0.0562	0.0575	0.0567	0.0557	0.0570
ε'_{n-1} (Hartree)	-0.51	-0.13	-0.06	-0.04	-0.021	-0.015
$\varepsilon_{\text{Orth}}$ (Hartree)	—	-0.124927	-0.055510	-0.0312204	-0.019970	-0.013859
Relative Error of $\varepsilon_{\text{Orth}}$	—	6.00×10^{-4}	8.28×10^{-4}	9.57×10^{-4}	1.50×10^{-3}	2.16×10^{-3}
Time per Epoch of $\varepsilon_{\text{Orth}}$ (s)	—	0.111	0.120	0.125	0.126	0.136

V. RESULTS FOR WOODS-SAXON POTENTIALS

A. The Woods-Saxon potentials

In this section, we apply the DNN model to a neutron in the Woods-Saxon potentials of ^{16}O and ^{208}Pb nuclei. In this section, we use $\hbar = c = 1$.

The scalar potential $S(r)$ and vector one $V(r)$ of Woods-Saxon potentials for neutrons, respectively, read

$$U(r) = V(r) + S(r) = \frac{V_N^0}{1 + \exp((r - R_0)/a)}, \quad (31\text{a})$$

$$W(r) = V(r) - S(r) = \frac{-\lambda_n V_N^0}{1 + \exp((r - R_0^{\text{ls}})/a^{\text{ls}})}, \quad (31\text{b})$$

$$V_N^0 = V' \left(1 - \kappa' \frac{N - Z}{N + Z} \right), \quad (31\text{c})$$

$$R_0 = r_0 A^{\frac{1}{3}}, \quad (31\text{d})$$

$$R_0^{\text{ls}} = r_0^{\text{ls}} A^{\frac{1}{3}}, \quad (31\text{e})$$

with $\lambda_n = 11.12$, $V' = -71.28 \text{ fm}$, $\kappa' = 0.462$, $r_0 = 1.233 \text{ fm}$, $a = 0.615 \text{ fm}$, $r_0^{\text{ls}} = 1.144 \text{ fm}$ and $a^{\text{ls}} = 0.648 \text{ fm}$ [38], where A , N , and Z denote the number of nucleons, neutrons and protons, respectively.

B. Discrete representations with uniform mesh

The uniform mesh is adopted to calculate for the Woods-Saxon potential, where r is uniformly distributed with mesh size Δr . The derivative matrix of the first-order differential operator $\frac{\partial}{\partial r}$ reads

$$\frac{\partial}{\partial r} \simeq \frac{1}{2\Delta r} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 0 \end{pmatrix}. \quad (32)$$

C. DNN results

In this section, we use a 20 fm box with $M = 2000$ meshes for the DNN calculation. The general pseudospectral method [39, 40] is adopted to calculate benchmark wave functions and energies with the mapping parameter $L = 10$ and the number of mesh points 600.

Table II lists the energies of three states below the Fermi energy for ^{16}O ($Z = N = 8$) by the inverse Hamiltonian method, i.e., the $1s_{1/2}$, $1p_{3/2}$, and $1p_{1/2}$ states. All the states are “ground state” for the given l and j (i.e., κ). The precision reaches at least 1×10^{-4} . Figure 7

TABLE II. Energies of ^{16}O below the Fermi energy calculated by the Woods-Saxon potential. The benchmark is obtained by the general pseudospectral method.

κ	-1	-2	1
Benchmark (MeV)	-43.16880	-24.6354	-18.9746
ε_{Inv} (MeV)	-43.16859	-24.6353	-18.9772
$\varepsilon'_{1\kappa}$ (MeV)	-45.0	-28.0	-20.0
Relative Error of ε_{Inv}	4.86×10^{-6}	4.06×10^{-6}	1.37×10^{-4}

TABLE III. Same as Table II but for ^{208}Pb . Only $\kappa = -1$ states are shown.

n	1	2	3
Benchmark (MeV)	-58.0026	-41.0773	-18.7560
ε_{Inv} (MeV)	-58.0028	-41.0791	-18.7626
ε'_{n-1} (MeV)	-60.0	-45.0	-20.0
Relative Error of ε_{Inv}	3.45×10^{-6}	4.38×10^{-5}	3.52×10^{-4}
$\varepsilon_{\text{Orth}}$ (MeV)	—	-41.0789	-18.7597
Relative Error of $\varepsilon_{\text{Orth}}$	—	3.90×10^{-5}	1.97×10^{-4}

shows the corresponding wave functions. The DNN wave functions show good agreements with the benchmark.

Figure 8 shows the energy spectrum of ^{208}Pb ($Z = 82$, $N = 126$) below the Fermi energy. The left-hand side is the benchmark and the right-hand side is the DNN results with the inverse Hamiltonian method. All the energies obtained by the DNN are identical (within 0.002 %) to the benchmark calculation. The first three states of $\kappa = -1$ as an example are listed in Table III with both the inverse Hamiltonian and the orthonormal method, which give almost the same accuracy.

The F - and G - components for $\kappa = -1$ of ^{208}Pb are shown in Figs. 9 and 10, respectively. Both methods show good agreements with the benchmark for the F -component. According to Eq. (17), the accuracy of the orthonormal method depends on the accuracy of lower-state wave functions, which means it also depends on the the inverse Hamiltonian method which provides the lowest state data.

VI. SUMMARY

In this paper, we extended the deep neural network method proposed in Ref. [28] to the Dirac equation, where the existence of the Dirac sea leads to the variational collapse for the usual variational method. To avoid such a problem, we applied the inverse Hamiltonian method, which reverses the order of the energy spectrum so that the target state is at the bottom, thus making the method applicable to both the ground and excited states. Besides the inverse Hamiltonian method, we also extended the orthonormal method [28] to calculate excited states. By applying the orthonormal condition, a state that is orthonormal to all the lower states is obtained to calculate the loss function so that components

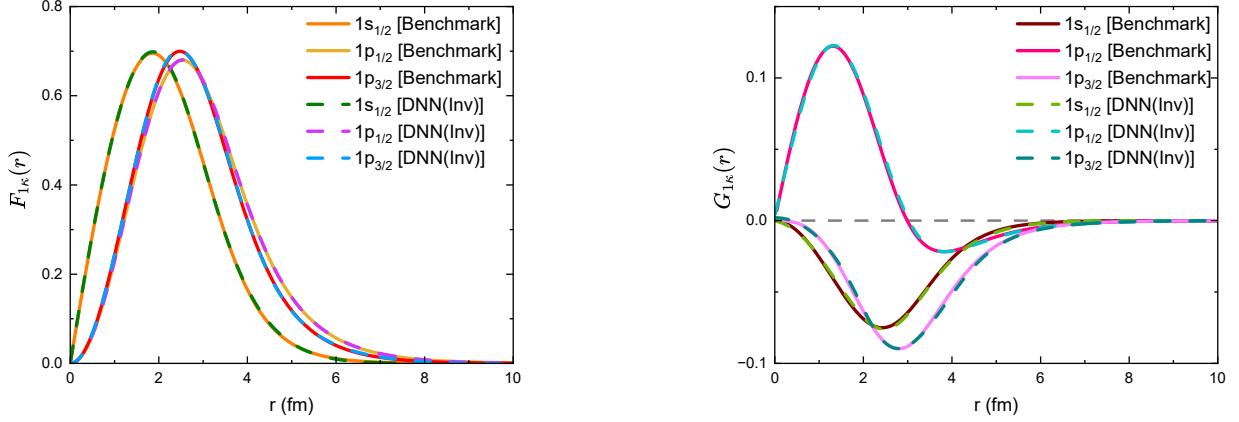


FIG. 7. Same as Figs 3 and 4 but for the Woods-Saxon potential for ^{16}O below the Fermi energy.

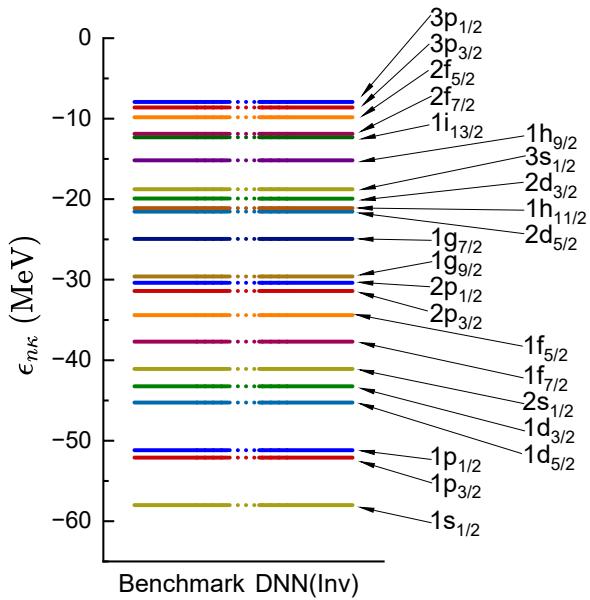


FIG. 8. Spectrum of neutrons calculated by the Woods-Saxon potential of ^{208}Pb . The benchmark is given by the general pseudospectral method and the inverse Hamiltonian method is used for the DNN.

of all the lower states are eliminated in the DNN results.

To verify the feasibility of our method, we applied our method to calculate a hydrogen atom and the Woods-Saxon potentials of ^{16}O and ^{208}Pb . We found that both methods show good agreements with the benchmark with about the same accuracy (up to 0.15 % difference) for the both systems.

We believe one promising extension of our work is to solve the relativistic many-body systems. In the case of the two-body systems, the two-body Dirac equation [41] describes two particles with interaction, where our DNN

method may help in finding the solution especially for the excited states.

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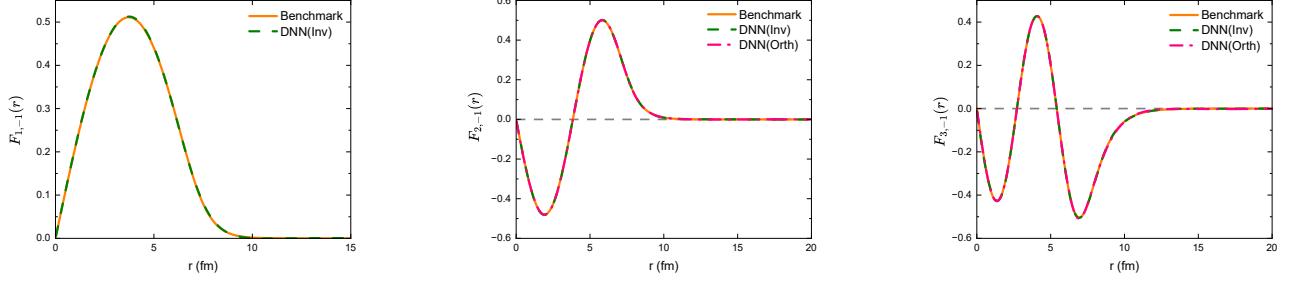


FIG. 9. Same as Fig. 3 but for the Woods-Saxon potential for ^{208}Pb . Only $\kappa = -1$ states below the Fermi energy are shown.

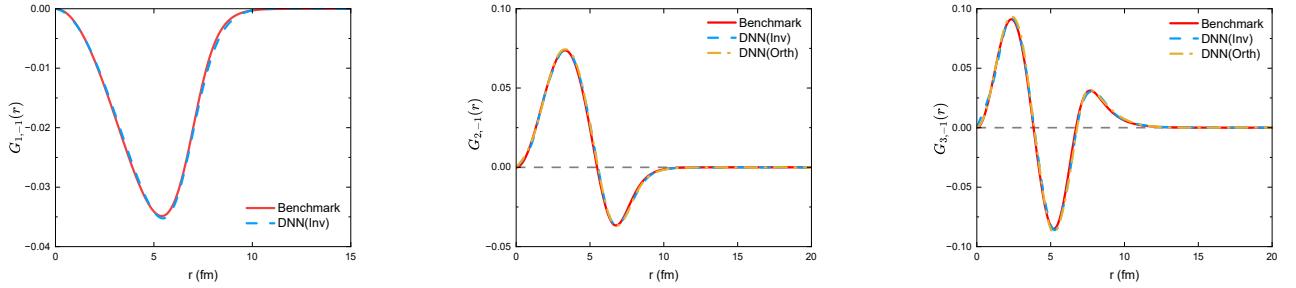


FIG. 10. Same as Fig. 9 but for the G -component.

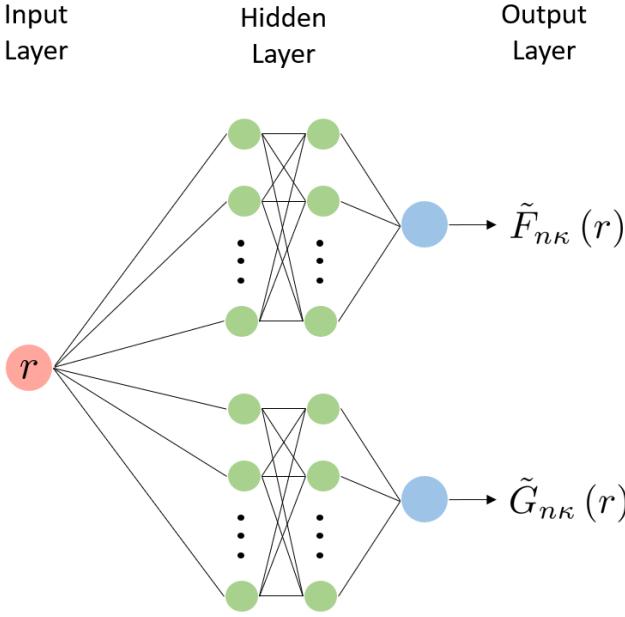


FIG. 11. The structure of the non-fully connected DNN. One output unit generates the F -component of the wave function, while the other generates the G -component. For each output, the units in the hidden layers are fully connected, while the hidden layer units of different outputs are not connected to each other.

Appendix A: Failed training set-ups

In this appendix, we discuss which DNN structure and output fail to generate the accurate G -component wave function and results of minimizing the energy without the inverse Hamiltonian.

1. Employing a non-fully connected neural network

Besides the fully-connected DNN used in the main text, we also test a non-fully connected deep neural network to generate the F - and G -components, whose structure is shown in Fig. 11, where $F_{n\kappa}$ and $G_{n\kappa}$ are generated by two output units, respectively. For each output, the units of the hidden layers are fully connected, while the hidden layer units of different outputs are not connected to each other.

As shown in Fig. 12, the G -component is largely different from the benchmark. This is because the G -component contributes to the norm [Eq. (12)] in about 0.001 %, and thus its contribution to the loss function is too small for optimization. Therefore, even if the G -component behaves strangely, the loss function can easily satisfy the convergence criteria. Although the G -component contributes to the norm in 0.39 % in the case of ^{208}Pb , it is still not large enough to be well optimized with the non-fully connected neural network as shown in Fig. 13.

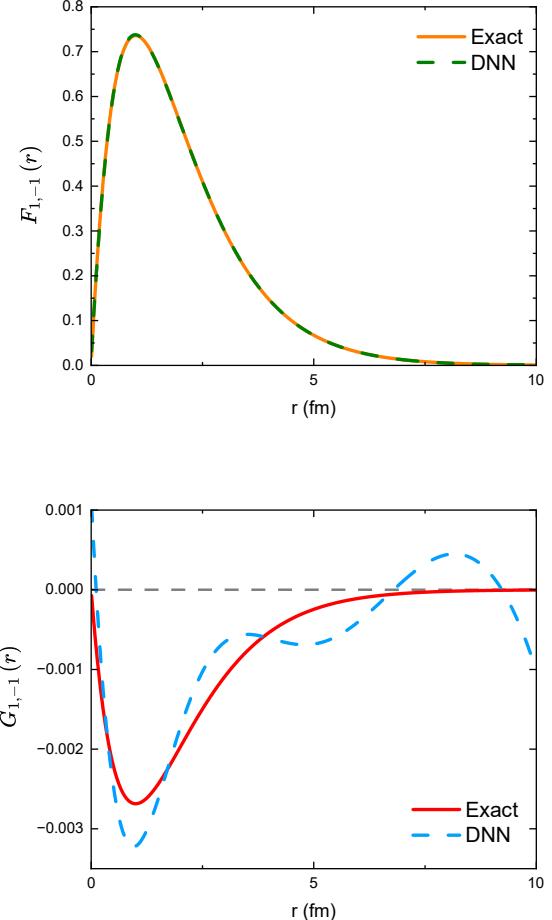


FIG. 12. The ground-state wave functions of a hydrogen atom calculated by the non-fully connected DNN. The F -component is consistent with the benchmark, while the G -component is largely different from the benchmark.

2. Usage of the trial wave function $f_{n\kappa}$

In Sec. III A, a trial wave function $f_{n\kappa}$ is used as the DNN output to calculate $F_{n\kappa}$ and $G_{n\kappa}$. The denominator r improves the accuracy of $F_{n\kappa}$ and $G_{n\kappa}$ close to the origin.

If $F_{n\kappa}$ is used as the DNN output, $G_{n\kappa}$ of a hydrogen atom diverges at the origin as shown in Fig. 14. The ground state wave functions of ^{208}Pb are shown in Fig. 15. The divergence at the origin is smaller compared to the Coulomb results but still exists. This may be because the gradient of $F_{n\kappa}$ of ^{208}Pb at the origin is smaller compared with the hydrogen atom, which is easier for the DNN to optimize. So that the $G_{n\kappa}$ calculated by the $F_{n\kappa}$ from Eq. (11) is more accurate for ^{208}Pb than the hydrogen atom.

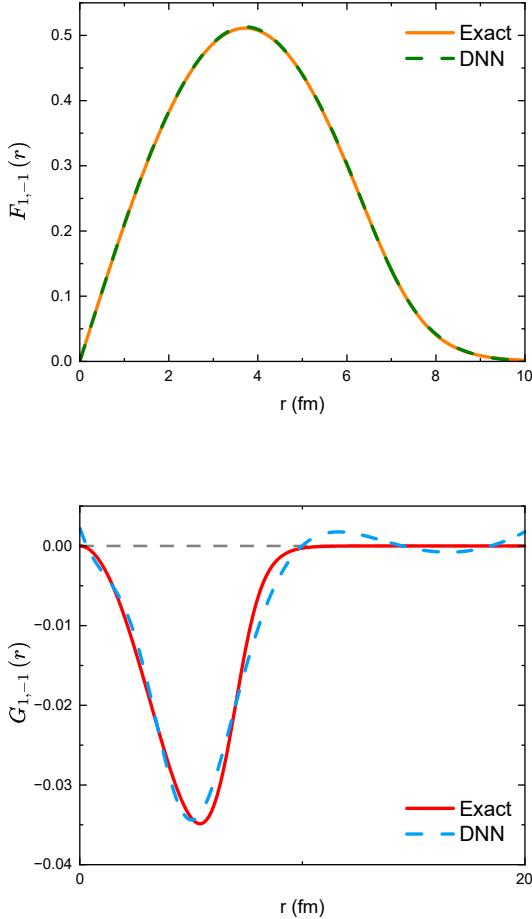


FIG. 13. Same as Fig. 12 but for the Woods-Saxon potential for ^{208}Pb .

3. Minimizing without the inverse Hamiltonian

Because of the existence of the Dirac sea, the ground state is no longer the lowest energy of the Dirac Hamiltonian H'_{Dr} . We employ the fully connected DNN in the main text and the non-fully connected DNN in Appendix A 1 to minimize the energy expectation value of H'_{Dr}

$$\varepsilon_D = \min \frac{\langle \phi | H'_{Dr} | \phi \rangle}{\langle \phi | \phi \rangle} \quad (\text{A1})$$

as the loss function, where the potential is the Coulomb potential as an example.

As shown in Fig. 16(a) for the non-fully connected DNN, it is observed that ε_D falls into the Dirac sea, which is the so-called variational collapse. For the fully connected DNN, as shown in Fig. 16(b) we discover that ε_D can converge at the ground state energy. This may because the local minimum of the ground state is too deep for the fully connected DNN so that the loss function is

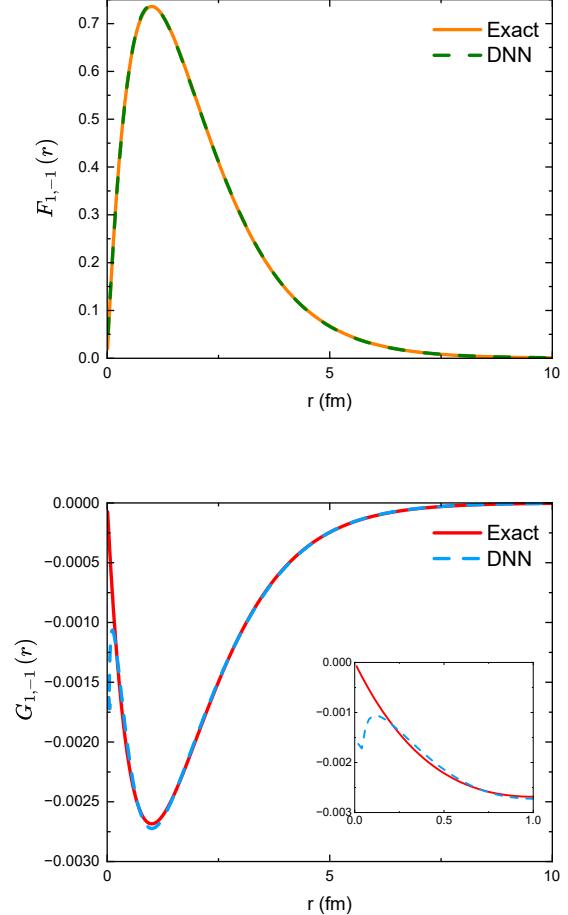


FIG. 14. The F - and G -components of the ground-state wave functions of a hydrogen atom with using $F_{n\kappa}$ as the DNN output.

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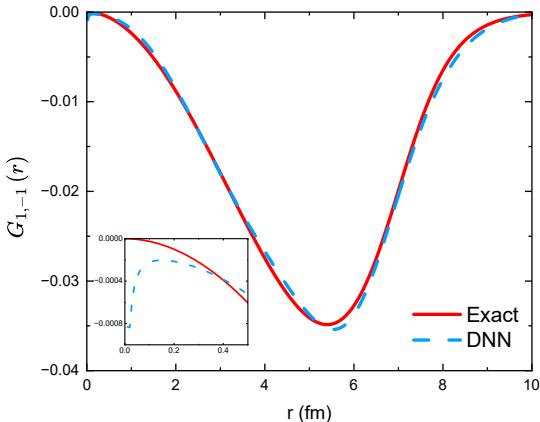
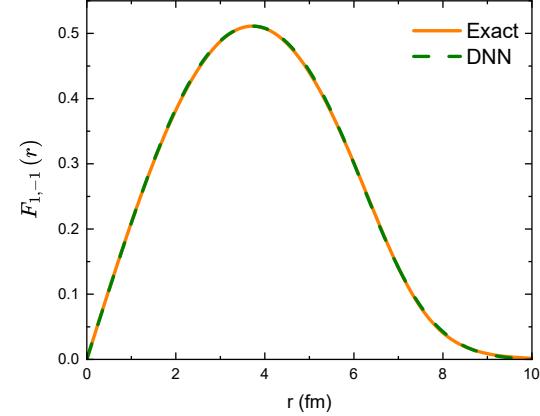
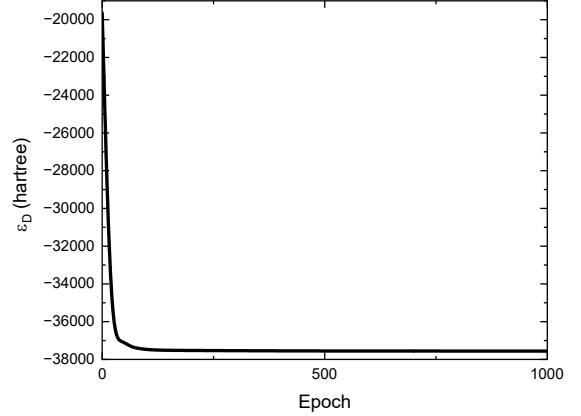
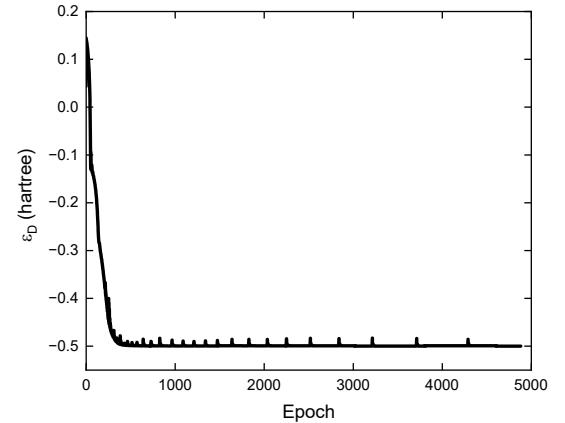


FIG. 15. Same as Fig. 14 but for the Woods-Saxon potential for ^{208}Pb .

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(a) Non-fully connected DNN



(b) Fully connected DNN

FIG. 16. The energy of the Dirac Hamiltonian H'_{Dr} for a hydrogen atom with minimizing ε_D directly as a function of epochs. In the case of the non-fully connected DNN, the program doesn't converge and falls into the Dirac sea. In the case of the fully connected DNN, the loss function converges at the ground state energy.

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