Here, we propose a novel method for representation of general spin systems using Restricted Boltzmann Machine with Softmax Regression (SRBM) that follows the probability distribution of the training data. SRBM training is performed using stochastic reconfiguration method to find approximate representation of many body wave functions. We have shown that proposed SRBM technique performs very well and achieves the trial wave function, in a numerically more efficient way, which is in good agreement with the theoretical prediction. We demonstrated that the prediction of the trial wave function through SRBM becomes more accurate as one increases the number of hidden units. We evaluated the accuracy of our method by studying the spin-1/2 quantum systems with softmax RBM which shows good accordance with the Exact Diagonalization (ED). We have also compared the energies of spin chains of a few spin multiplicities (1, 3/2 and 2) with ED and DMRG results.

I. INTRODUCTION

Computationally probing the properties of quantum many-body systems have always been a challenging task in the field of condensed matter physics. In quantum systems, where correlation between the quasiparticles play a major role in defining their properties, the Hilbert space becomes exponentially large and hence the amount of data required to encode such information becomes unmanageable.

To deal with low energy properties in case of very large Hilbert spaces, Quantum Monte Carlo (QMC), Density Matrix Renormalization Group (DMRG) [1] and Dynamical Mean field theory [2] have been developed. These either rely on sampling of important configurations or compressed representation of renormalized wave functions. But there are either problems with dimensionality constraint or difficulty in finding accurate trial wave functions.

Artificial intelligence and deep learning have enabled unique achievements to address important questions in the domain of physical sciences including condensed matter physics [3–9]. A restricted Boltzmann machine (RBM) is a basic model in deep learning which was initially proposed by Smolensky [10] in 1986. RBM is two layered artificial neural network that learn the probability distribution from the input dataset [11, 12]. It is an energy-based model which comprises of one layer of visible units and one layer of hidden units, with each visible units connected to each hidden units and having no intra-layer connections. Recently, unsupervised machine learning techniques such as RBM have been implemented to find approximate representation of many body wave functions [13] that have proven to be useful in determining the low energy properties of spin-1/2 systems in one and two dimensions.

Neural network Quantum States (NQS) have gained popularity in the condensed matter physics community in recent years for their accurate representation of many body wave trial wave functions. Suitable for stochastic quantum simulations like Variational and Diffusion Monte Carlo, the NQS take into account all particle correlations whereas popular correlation factors such as Jastrow [14] are limited up to two. Nomura et al. predicted the ground state energy of Hubbard model using RBM and pair product states [15]. They observed that...
for certain cases their computation achieved better accuracy than the known many-variable variational Monte Carlo approach. Also, the entanglement properties of the RBM states were studied [7], and using deep learning techniques to explore the representational power [29, 39]. Several explicit RBM models are developed for different systems like Ising model, Heisenberg model [12], graph states [9], toric code [8], stabilizer code [15, 17], and topologically ordered states [5, 18, 19]. Furthermore, the deep Boltzmann machine (DBM), a generative model and similar to the RBM but with two or more hidden layers where the internal hidden layers capture increasingly complex higher-order correlations. Recently, the DBM states were studied in various works [9, 20, 21] and have proved to be efficient in representing quantum states.

Here we propose a unique technique based on restricted Boltzmann machine (RBM) and softmax regression for representation of a system of general spin $S$. This method performs quite well to predict the trial wavefunction and is numerically more efficient for larger system sizes, having an excellent agreement with the theoretical prediction.

II. RBM WITH SOFTMAX VISIBLE UNITS (SRBM)

The Softmax Model is introduced to model sparse count data, such as word count vectors in a document [22]. This model is a variant of Restricted Boltzmann Machine in which the visible units that are usually binary in RBM, have been changed by multinomial one of a number of different states (Fig 1). The figure shows the visible layer has $V_1$ to $V_n$ visible softmax units, and each visible softmax unit $V$ consists of $2S+1$ different binary inputs corresponding to the $z$-components of spin. The hidden layer has binary units and the network is trained by unsupervised learning. The visible softmax variables of the input data at the $i$th node are $V = (V_{i,1}(\sigma), V_{i,2}(\sigma), \ldots, V_{i,2S+1}(\sigma))$ where $\sigma$ is the $z$-component of the spin. The visible softmax inputs form a $(2S+1) \times N$ matrix, $N$ being the number of visible nodes. The ‘energy function’ of the network can be defined as

$$F_{srbm} = \sum_{\{h_i\}} \exp \left[ -\left( \sum_{i=1}^M \sum_{j=1}^F \sum_{k=1}^{2S+1} W_{ijk} V_{ik}(\sigma) h_j + \sum_{i=1}^M \sum_{k=1}^K a_{ik} V_{ik}(\sigma) + \sum_{i=1}^M b_i h_j \right) \right]$$

(1)

where $\{W_{ijk}\}$ are the symmetric weights between visible unit $i$ that takes on value $k$ and hidden unit $j$. Here, $\{a_{ik}\}$ is the bias of visible unit $i$ that takes on value $k$ and $b_i$ is the bias of hidden unit $j$. The conditional probability for the visible and hidden layers is given by:

$$\mathcal{P}(h_j = 1|V) = \text{logistic} \left( \sum_{ik} W_{ijk} V_{ik} + b_j \right)$$

(2)

$$\mathcal{P}(V_{ik} = 1|h) = \frac{\exp \left( \sum_{j} W_{ijk} h_j + a_{ik} \right)}{\sum_{k} \exp \left( \sum_{j} W_{ijk} h_j + a_{ik} \right)}$$

(3)

III. SPIN INFORMATION ENCODED IN SOFTMAX UNITS AS DISCRETE PROBABILITIES

For a general spin $S$ there are $2S+1$ possibilities for the $z$-component, i.e. $S^2 \in \{-S, -S+1, \ldots, S-1, S\}$. The spin information at each site is encoded by $2S+1$ binary values for discrete ‘probabilities’; the way the information of spin at each site, is encoded, is as follows: Each visible softmax unit will have $2S+1$ entries. For example, if there is a spin $-S$ sitting at the $i$th site, the probability $V(\sigma = -S)_{ik} = 1$ and for all other $2S$ entries, it is $V(\sigma)_{i,k 
eq k} = 0$. Thus, for a site having spin-3/2 we have the following entries at the $i$th visible node:

| Entries | $S^2$ value ($\sigma_k$) |
|---------|-------------------------|
| $V(\sigma)_{ik}$ | $\frac{3}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{1}{2}$ |
| $\sigma_i = \frac{3}{2}$ | 1 | -1 | -1 | -1 |
| $\sigma_i = \frac{1}{2}$ | -1 | 1 | -1 | -1 |
| $\sigma_i = \frac{-1}{2}$ | -1 | -1 | 1 | -1 |
| $\sigma_i = \frac{-3}{2}$ | -1 | -1 | -1 | 1 |

constraint on the SRBM for encoding spin information is: Always one of the $V(\sigma)_{ik}$ should be 1 and others should be 1 and others will be -1.

IV. TRAINING SRBM WITH STOCHASTIC RECONFIGURATION METHOD

A. Gibbs Sampling with Categorical Distribution

The forward pass (visible to hidden) is similar to the normal RBM in which the choice of the hidden node is decided between $-1$ and 1, according to the logistic function (Eq 2). But for the backward pass, there are $2S+1$ choices for one of the values at each node to be 1. Thus, we need to sample from the categorical distribution of $V_{ik}(\sigma)$ at the $i$th node. So we compare the Cumulative Distribution Function (CDF) (evaluated for all the possibilities of spin at each node) by comparing it with a uniformly distribution. Thus the sampling algorithm may be described by the following steps:
1. Generate a uniform random number $r_1 \in [0,1]$ for each hidden node $j$. Set $b_j = 1$ if $P(h_j = 1|\mathbf{V})$ (Eq.2) exceeds $r_1$, otherwise $b_j = -1$.

2. Calculate the $k$ probabilities $P(V_{ik} = 1|h)$ at the $i^{th}$ visible node.

3. Evaluate the CDF $\mathcal{F}(V_{ik}(\sigma)) = \sum_{x_k \leq P(\sigma)_k} P(x_k)$ (eq.3).

4. Generate a uniform random number $r_2 \in [0,1]$. Set the value of $V_{ik}(\sigma)$ if it just exceeds the value of $r_2$. Set all other $\{V_{ik}(\sigma) = -1\}$

B. Variational Monte Carlo and Optimization of Parameters with Stochastic Reconfiguration Method

Generally, the optimum values for the weights and the biases are obtained through training of the SRBM, and it’s achieved by minimizing the KL-divergence or contrastive divergence. But here instead, we minimize the average energy calculated using Variational Monte Carlo. The initial trial wave function is taken to be $\psi_{\text{trial}}(x) = \sqrt{P_{\text{srbm}}}$ with as the initial trial wave function the antiferromagnetic Heisenberg Hamiltonian for a general spin-$S$ given by

$$
\mathcal{H} = \sum_{\langle ij \rangle} S_i^+ S_j^- + \frac{1}{2} \left( S_i^+ S_j^+ + S_i^- S_j^- \right)
$$ (4)

The energy expectation value $\langle \mathcal{H} \rangle$ can be expressed as the average of the local energies, i.e. $E = \langle \mathcal{H} \rangle = \langle E_{\text{loc}} \rangle$ where

$$
E_{\text{loc}}(x) = \sum_{x'} \frac{\psi_{\text{trial}}(x')}{\psi_{\text{trial}}(x)}
$$ (5)

$E_{\text{loc}}(x)$ being the local energy for the configuration $x$. The change in the variational parameters, or, in this case the weights $\{W_{ijk}\}$ and the biases $\{a_{ik}\}$ and $\{b_j\}$ of the SRBM are obtained by the Stochastic Reconfiguration(SR) method proposed by Sorella et al. This method equates the change in $\psi_{\text{trial}}(x)$ w.r.t to the parameters with the power method obtained by repeatedly operating the Hamiltonian, which eventually reaches the ground state.

If $\alpha = \{\alpha_1, \ldots, \alpha_N\} = \{\{a_{ik}\}, \{b_j\}, \{W_{ijk}\}\}$ be the set of all variational parameters then the change in those parameters is obtained by

$$
\Delta \alpha = \gamma (S + \epsilon \mathbf{1})^{-1} \hat{f}
$$ (6)

where the entries matrix $S_{\alpha'} = \langle \Delta \alpha \rangle - \langle \Delta \alpha \rangle/\langle \mathcal{H} \rangle$ and the elements of the vector $\hat{f}_1 = (\Delta \mathcal{H})/\langle \mathcal{H} \rangle$. The quantity $\Delta \alpha$ is given by

$$
\Delta \alpha = \frac{1}{\psi_{\text{trial}}(x)} \frac{\partial \psi_{\text{trial}}(x)}{\partial \alpha_k}
$$ (7)

The parameter $\gamma$ is the ‘learning rate’ of the SRBM. For $\psi_{\text{trial}}(x) = \sqrt{P_{\text{srbm}}}$ the above expressions turn out to be

$$
\Delta_{i\in\{a_{ik}\}} = \frac{1}{2} \sum_{\langle ij \rangle} W_{ijk} V_{ik} \quad \Delta_{b_j} = \frac{1}{2} \tanh \left( \sum_{\langle ik \rangle} W_{ijk} V_{ik} + b_j \right) \quad \Delta_{i\in\{W_{ijk}\}} = \frac{1}{2} \tanh \left( \sum_{\langle ik \rangle} W_{ijk} V_{ik} + b_j \right) V_{ik}(\sigma)
$$ (8)

The term scalar $\epsilon 1$ with $\epsilon = 10^{-4}$ (in our case) is added, in case the the matrix $S$ is not invertible.

V. RESULTS: VALIDATION AND PERFORMANCE OF THE RESTRICTED BOLTZMANN MACHINE WITH SOFTMAX VISIBLE UNITS.

A. Validation of spin-$\frac{1}{2}$ quantum system using SRBM

We validate the accuracy of our method by studying the spin-$\frac{1}{2}$ quantum systems. In this case, the SRBM has 2 inputs per visible node. Although this is computationally expensive than the normal RBM, this result can be useful to validate the SRBM algorithm. Fig.2 shows the prediction for the ground state energy of a 16-site Heisenberg chain with Periodic Boundary Conditions (PBC) using SRBM. We have considered two different cases having 16 visible units with 16 and 24 hidden units respectively.

![Fig. 2: Validation of the result of an RBM spin-1/2 Heisenberg chain of 16 sites using SRBM. The plot shows the evolution of the ground state energy per site as a function of epochs for a network with 16 and 24 hidden units. The exact value obtained by ED is -0.43198. The plot shows that the prediction have a good agreement with ED.](image-url)
It is evident from these results that the predictions for
the spin-1/2 system have a good agreement with or Exact
diagonalization (ED) calculations.

B. Performance of the Restricted Boltzmann
Machine with Softmax visible units for general spin
system

We have initially considered one dimensional chains
of length 10 for spins 1, and 2 with periodic boundary
conditions where each node in the visible layer has 3,
4 and 5 possibilities respectively. The hyperparameter
learning rate for training of the model is 0.005. In each
epoch, 400 steps of Gibbs sampling were performed to
calculate the local energies and derivatives.

The convergence plot for the ground state energy
of a 10-site Heisenberg spin chain with PBC using SRBM
is shown in Figure 3. Here the green line represents the
ground state energy obtained via ED and the blue, orange
and red curves denote the prediction obtained through
SRBM for a network with 10, 15 and 20 hidden units re-
spectively. The rolling average of the y-axis with a win-
dow of 20 is plotted to reduce the fluctuation. Also, as we
increase the number of hidden units the fluctuation in the
numerical prediction of energy per site reduces consid-
erably and approach the analytical value asymptotically,
which is evident from the red curve with hidden dimen-
sion (hdim) equal to 20.

Fig. 4 shows the plot of ground state energy per site vs
epochs for a spin-3/2 Heisenberg chain and (b) a
spin-2 Heisenberg chain with visible layer dimension 10
and for hidden layer dimension 10, 15. The exact value
obtain by ED is: (a) -2.8518 and e (b) -4.7948

VI. CONCLUSION

We have shown that the proposed restricted Boltz-
mann machine with Softmax Regression (SRBM) algo-
rithm for systems of general spin $S \left( S = \frac{1}{2}, 1, \frac{3}{2}, 2, \text{etc.} \right)$
achieves the trial wave function, in a numerically effi-
cient way considering all body correlations into account and having a good agreement with the theoretical prediction. Our results also demonstrated that the prediction of the trial wave function through SRBM becomes more accurate as one increases the number of hidden units. Furthermore, we validate the accuracy of our method by studying the spin-1/2 quantum systems with softmax RBM which also shows a good agreement with the Exact Diagonalization results.

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