Phase diagram reconstruction of the Bose-Hubbard model with a Restricted Boltzmann Machine wavefunction

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Recently, the use of neural quantum states for describing the ground state of many- and few-body problems has been gaining popularity because of their high expressivity and ability to handle intractably large Hilbert spaces. In particular, methods based on variational Monte Carlo have proven to be successful in describing the physics of bosonic systems such as the Bose-Hubbard model. However, this technique has not been systematically tested on the parameter space of the Bose-Hubbard model, particularly at the boundary between the Mott insulator and superfluid phases. In this work, we evaluate the capabilities of variational Monte Carlo with a trial wavefunction given by a Restricted Boltzmann Machine to reproduce the quantum ground state of the Bose-Hubbard model on several points of its parameter space. To benchmark the technique, we compare its results to the ground state found through exact diagonalization for small one-dimensional chains. In general, we find that the learned ground state correctly estimates many observables, reproducing to a high degree the phase diagram for the first Mott lobe and part of the second one. However, we find that the technique is challenged whenever the system transitions between excitation manifolds, as the ground state is not learned correctly at these boundaries. Nonetheless, we propose a method to discard noisy probabilities learned in the ground state, which improves the quality of the results produced by the method.

I. INTRODUCTION

The dimension of a Hilbert space that describes the possible states of a many-body system scales exponentially with the number of one-body states and with the number of particles. In most cases, this feature comes as an important practical difficulty for physicists to study many-body problems, because approximate techniques have to be implemented in order to perform simulations (e.g., dynamical mean-field theory, density matrix renormalization group (DMRG)). One of the most studied quantum objects is the ground state of a many-body system for a number of reasons: particles tend to occupy the lowest energy states first, as dictated by the aufbau principle; also excited states inherit the ground state structure; and most prominently, it is an object that encodes changes in observables that exhibit quantum phase transitions. Recently, the proposal of variational wavefunctions with neural networks and machine learning-inspired wavefunctions for the ground state and its optimization through variational Monte Carlo (VMC) has proven to be successful in approximating with high fidelity the ground state of several condensed matter many- and few-body systems. Some examples are atomic and molecular systems, the transverse-field Ising model with quenching, the Heisenberg model and its anti-ferromagnetic version, the quantum harmonic oscillator in electric field, the Hubbard model, the $J_1-J_2$ Heisenberg model and its antiferromagnetic version, the XXZ model, and the dipolar Bose-Hubbard system.

The success in approximating the ground state comes from two sources. The first one is technical, where the high expressivity and capabilities of neural networks to approximate arbitrary functions are exploited, as well as the thoroughly studied optimization methods in machine learning. The second one is physical: despite the Hilbert space being exponentially large with respect to one-body states and number of particles, only a small set of those states are needed to describe the ground state. Here the definition of small can vary, as it will be seen in this work.

Even though reported results indicate that the quantum ground state can be represented through neural network wavefunctions, most of these studies focus on the convergence of the energy, and few of them use the technique to characterize quantum correlations near a quantum phase transition to study the phase space of a Hamiltonian comprehensively. Indeed, the convergence of the energy comes quicker than the convergence of the state, as any first-order error in the variational state leads to only a second-order error in its corresponding energy. Therefore, focusing on energy convergence might be misleading when asserting the power of VMC with neural network trial wavefunctions. In contrast to previous works, we intensively and systematically test the capabilities of VMC to reconstruct, through a Restricted Boltzmann Machine (RBM) wavefunction, the quantum ground state of a one-dimensional Bose-Hubbard system throughout the superfluid (SF) and Mott insulator (MI).
phases. We chose the Bose-Hubbard model because of the known numerical difficulties near the MI-SF boundary, and also because the problem involves bosons, whose Hilbert space is larger than fermions, thus increasing the computational difficulty in the study. Consequently, we contrast exact diagonalization solutions with the ones provided by the VMC-RBM method in systems of 5 and 8 sites for a fine mesh in the Bose-Hubbard parameter space that exhibit the first and part of the second Mott lobes. It is only due to the sweeping of the Bose-Hubbard parameter space that we are able to see that points near the MI-SF boundary are challenging for the VMC-RBM method. However, we also find that some of the differences between the learned ground state and the ground state found through exact diagonalization are due to noise that can be cleaned. Therefore, in this work, we also contribute with a state cleaning technique that removes noise that we identify comes from over-fitting.

Nonetheless, we point out that there have been previous efforts to examine the learning capability of different neural network wavefunctions for the ground state of the Bose-Hubbard Hamiltonian. However, as mentioned before, these studies do not extensively test this recent VMC framework in the Bose-Hubbard phase space. For instance, a permutation symmetric RBM implemented in NetKet has been studied to examine the energy and particle density convergence of two points in the SF and MI phases, finding a difficulty in the convergence to the numerically exact particle density in the SF phase. However, a qualitatively good localization of the boundary between the SF and MI phases for the region enclosing the first two Mott lobes was achieved using the particle density as a discriminator. RBMs have also been used to show how for a fixed number of bosons in the system, the learned ground state is able to replicate the numerically exact order parameter of the quantum phase transition. However, fixing the number of bosons greatly reduces the size of the Hilbert space that is to be sampled with VMC, implying that a more complete sampling of the basis states is possible, making the technique more exact. Also, the Bose-Hubbard model has been considered as a toy model for trying full-forward neural networks (FFNNs) and convolutional neural networks (CNNs) wavefunctions. For instance, the ground state of one and two-dimensional finite lattices with parabolic confinement potential for a fixed number of bosons was approximated through an FFNN ansatz. In the case of no confinement and periodic boundary conditions (which introduce displacement symmetry), both FFNNs and RBMs were used in large 1D lattices of up to 40 sites. CNNs have also been introduced and compared with FFNN wavefunctions to approximate this ground state. A CNN is also proposed as a means to introduce the ground state at finite temperature in a 1D lattice for larger on-site boson interaction than hopping interaction. Despite the important results derived from these works, they do not focus on the ability of the neural network ansatz to reproduce the ground state near the quantum phase transition boundary. Nevertheless, unsupervised learning has been previously used to classify states as belonging to the Mott insulator or SF phases in the Bose-Hubbard model with previously obtained states or physical quantities, for several values of the order parameters.

We believe that the ability of VMC technique to reproduce the ground state near the quantum phase transition has to be extensively tested, which is why we pay close attention to the description of the variational ground state near the SF-MI phase for a small number of sites to compare it with the numerically exact ground state. This paper is organized as follows. Section II exposes the main features of the Bose-Hubbard Hamiltonian and describes the SF-MI transition in the system. In this section, an overview of the VMC technique is given, discussing the difficulties that must be faced and overcome in order to learn the ground state of the Bose-Hubbard model. In section III, the main results are given, including energy convergence, the overlap of the approximated and exact ground states, the reproduction of the phase diagram via two different order parameters, as well as tomographies indicating relevant Fock states for the ground state. Finally, in section IV conclusions of this work are given.

II. MODEL AND VARIATIONAL MONTE CARLO

A. Bose-Hubbard Hamiltonian

The Bose-Hubbard Hamiltonian describes the interactions between bosons that can occupy sites in a d-dimensional lattice. These interactions are characterized by hopping energy $t$, an on-site interaction $U$ and a chemical potential $\mu$, so that the grand-canonical Hamiltonian reads ($\hbar = 1$)

$$\hat{H} = -t \sum_{\langle ij \rangle} (\hat{a}_i \hat{a}_j^\dagger + \text{H.c.}) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i,$$

(1)

where $\hat{a}_i$ is the annihilation operator at site $i$, and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the number operator. The notation $\langle ij \rangle$ indicates that the sum runs over pairs of neighbor sites in the lattice. The Bose-Hubbard model is able to reproduce experimental results in Josephson-junction networks and in lattices of ultra-cold atoms. The latter offers precise control of the lattice parameters. Theoretically, a lot of attention has been devoted both to understand the quantum phases of the system (the ones that arise from eq. (1)) and from the disordered or extended Bose-Hubbard model with longer range interactions, as well to calculate the quantum phase transition boundaries, whose precision has improved over the years with better calculation techniques and computing power, revealing features such as the re-entrance phenomenon, where for particular values of the chemical potential, the system switches between the MI phase to
the SF phase, and back to the MI phase before definitely entering the SF phase after an increase of $t/U$.

For simplicity, we will restrict our analyses to the $d = 1$ case, where only two quantum phases are possible. When the on-site interaction energy is much larger than the hopping energy, the latter becomes negligible, and the Hamiltonian is written as the sum of independent Hamiltonians for each site $\sum_{i} \tilde{H}_i$, which can be immediately diagonalized by the number basis. The corresponding eigenenergies are $\sum_{i} \frac{\mu}{2} n_i - \mu n_i$, which reach minimum values for fixed $\mu$ and $U$ at $n_i = \max\{0, |\mu|/U\}$ (note that all sites are equivalent). Moreover, in this regime, the expected variance of the local number operator is 0, i.e. $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2 = 0$. This regime characterizes the MI phase. On the other hand, when the hopping energy is much larger than the on-site interaction energy, the latter becomes negligible. Thus, the Hamiltonian can also be written as the sum of independent Hamiltonians, but in momentum space, where $\hat{a}_k = N^{-1/2} \sum_{j=1}^{N} \hat{a}_j e^{-ix_jp_k/\hbar}$ is the annihilation boson operator in momentum representation. Here, $x_j = c \times j$, where $c$ is the lattice constant, and $p_k = 2\pi k h/[N \times c]$. Each independent Hamiltonian in momentum space ($\sum_{k} (-2t \cos(2\pi k/N) - \mu) \hat{a}_k^\dagger \hat{a}_k$) has eigenenergies $-2t \cos(2\pi k/N) - \mu$, which reach their minimum when all bosons condense with 0 momenta. Note that the energies are independent of the states’ occupation, meaning that the ground state is degenerate for any number of particles. This regime is known as the SF phase, characterized by a delocalized wave function (formally described by algebraic decaying spatial correlations[44-45], which is why the SF phase in 1D is not a true Bose-Einstein condensate) which has a non-zero expected variance of the local number operator. In fact, the probability distribution for the local occupation is Poissonian, meaning that $\langle n_i^2 \rangle - \langle n_i \rangle^2 = \langle n_i \rangle$. For a fixed chemical potential and an infinite number of sites, there exists a continuous phase transition from the MI phase to the SF phase as $U$ decreases with respect to $t$, apart from a range in $\mu$ in the first Mott lobe, where re-entrance exists.

### B. Variational Monte Carlo with Restricted Boltzmann Machine Wave Function

In this section, a review of the method introduced by Carollo and Troyer[46] is given, where a VMC setup is used to find the ground state, formally written as a trial wavefunction given by an RBM. In the Fock space basis, the ground wave function of the Bose-Hubbard system can be written as[47]

$$|\Psi\rangle = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \Psi(n_1, n_2, \ldots) |n_1, n_2, \ldots\rangle,$$

where $n_i$ is the occupation number of the $i$-th site, and $|\Psi(n_1, n_2, \ldots)\rangle^2$ are the probability amplitudes corresponding to the Fock states $|n_1, n_2, \ldots\rangle$. In order to map the wave function to a computer, both the number of sites and the number of possible particles in each site have to be truncated. We will refer to the number of sites as $N$ and to the maximum number of particles in each site as $M - 1$. The coefficients $\Psi(n_1, n_2, \ldots, n_N)$ are approximated by an RBM. RBMs are generative neural networks, formally described by a bipartite undirected graph such as the one shown in fig. 1, where there is a layer of visible neurons denoted by $\mathbf{v}$ that are used to input real data, and a layer of hidden neurons denoted by $\mathbf{h}$ that are used as latent variables of the model[48]. In particular, the wavefunction coefficients take the form

$$\Psi(n_1, n_2, \ldots, n_N) = \psi_\theta(n_1, \ldots, n_N) = \sum_{\mathbf{h}} e^{-E_{\text{RBM}}(\mathbf{v}(n), \mathbf{h})},$$

where $E_{\text{RBM}}(\mathbf{v}(n), \mathbf{h})$ is the energy of the RBM[49] and $\theta$ are the variational parameters of the RBM. As a short-hand notation, an occupation configuration is denoted as $\mathbf{n}$, and it is inputted to the visible layer of the RBM. However, the configuration first needs to be one-hot encoded as follows: each occupation $n_i$ is encoded into an $M$-component vector whose $j$-th component is $\delta_{j,n_i}$, $j = 0, 1, \ldots, M - 1$; then, the vectors for every occupation are concatenated into $\mathbf{v}(n)$. Moreover, if the $N_H$ hidden neurons are restricted to binary values 1 or −1, the approximated wave function coefficients can be written as

$$\psi_\theta(\mathbf{n}) = e^{\sum_{j} a_j v_j(\mathbf{n})} \prod_{\ell=1}^{N_H} 2 \cosh \left( b_\ell + \sum_{j} W_{\ell j} v_j(\mathbf{n}) \right),$$

where $a_j$, $b_\ell$ and $W_{\ell j}$ are the complex-valued visible bias, hidden bias and connection matrix of the RBM, respectively, which are to be learned to approximate the ground state.

![FIG. 1. Illustration of the used RBM, where each site occupation is one-hot encoded into $M$ visible neurons, depicted with different colors for different sites in the top layer. There are $N_H$ hidden neurons in the bottom layer connected with the visible neurons through weights $W_{\ell j}$ that connect the $\ell$-th hidden neuron with the $j$-th visible neuron.](image)

Thus, the approximation of the wave function coefficients is done through the adjustment of the parameters $\theta : \{a_j, b_\ell, W_{\ell j}\}$ that minimize the energy $\langle \psi_\theta | H | \psi_\theta \rangle$. At each step of the minimization, a set $\mathcal{M}$ of configurations $\mathbf{n}$ is sampled from $|\psi_\theta(\mathbf{n})|^2$ using the Metropolis-Hastings algorithm, so that the energy can be efficiently
More explicitly, the following steps are carried out to generate the sample \( \mathcal{M} \). At the first iteration, a state \( n_0 \) is randomly proposed. Then, at the \( i \)-th iteration:

1. Under some updating rule, propose a new state \( n_i' \) from \( n_i \).
2. With probability \( \min\{1, |\psi_\theta(n_i')/\psi_\theta(n_i)|^2\} \) accept the state \( n_i' \), i.e. \( n_{i+1} \leftarrow n_i' \). If it is not accepted, then \( n_{i+1} \leftarrow n_i \).

To build the sample \( \mathcal{M} \) a total of 1000 iterations are performed. Then, through either stochastic gradient descent or stochastic reconfiguration \( \theta \), as explained by Carleo and Troyer \( ^2 \). Both the sampling and minimization of the energy with respect to the RBM parameters are repeated iteratively until the RBM parameters converge, resembling an Expectation Maximization algorithm \( ^2 \). A schematic representation of the variational Monte Carlo technique is shown in fig. 2.

![Diagram](image)

**FIG. 2.** Representation of the variational Monte Carlo technique. With randomly initialized parameters \( \theta \), a set of states from the Hilbert space \( \mathcal{H} \) is sampled. By minimizing the energy defined in eq. (4), the parameters \( \theta \) are updated. These two steps are repeated \( n \) times with the objective of sampling the states (in the occupation basis) that are relevant for the ground state, depicted by a red dot, with the correct probability distribution.

Once the RBM has been trained, the state can be reconstructed by sampling states from \( |\psi_\theta(n)|^2 \). An important issue that immediately arises is that for an unknown target probability distribution \( |\Psi(n)|^2 \), the sampling can be too small or too large. If it is small, important information about the ground state might not be taken into account, whereas if it is large, noisy probability from other states can be taken into account. However, the small or large nature of the sampling is relative to the number of states that contribute significantly to the ground state. Critically, if the number of states that contribute significantly to the ground state is minimal, then the sampling might never be able to visit those states in the Hilbert space (especially for intractably large Hilbert spaces). This is the case of the Mott insulator phase, where the ground state corresponds to \( |n_1 = m, n_2 = m, \ldots \rangle \) for the \( m \)-th Mott lobe.

### III. RESULTS

We swept several values of chemical potential and hopping energy corresponding to the first and part of the second Mott lobe in the \( t/U-\mu/U \) space, with \( U = 1 \), performing 12000 sampling and optimization steps with NetKet \( ^2 \), where 1000 Metropolis-Hastings steps were done for each sampling step. This was done for three different scenarios: for 5 sites, we used 8 and 20 hidden neurons, and for 8 sites, we used 11 hidden neurons. In all cases, the maximum number of bosons allowed per site was 4.

#### A. Energy convergence

Since the VMC minimizes the energy, we check that the energy computed with eq. (4) converges by measuring its variance for the last 500 sampling-optimization steps, as well as by measuring the absolute error of the energy when compared to the exact ground state energy found through Lanczos diagonalization. For the aforementioned three scenarios, the variance for the last 500 sampling-optimization steps is shown in fig. 3(a)-(c), and the corresponding absolute errors with respect to the exact ground state energy are shown in fig. 3(d)-(f). It is seen that in the Hamiltonian parameter space, the majority of the energies have low-variance, showing convergence towards a value that is in excellent agreement with the exact ground-state energies.

Since the Hilbert spaces are small enough to compute all the probability amplitude coefficients for every state in the Fock basis, we can also compute any observable \( \hat{O} \) as

\[
\langle \psi_\theta | \hat{O} | \psi_\theta \rangle = \frac{\sum_{n \in \mathcal{H}} |\psi_\theta(n)|^2 \langle n | \hat{O} | n \rangle}{\sum_{n \in \mathcal{H}} |\psi_\theta(n)|^2}.
\]  

(5)

In particular, the absolute error of the energy computed through eq. (5) is shown in fig. 3. It is clear that in the case of 5 sites and 20 neurons, a very large region both in the SF and MI phases show a strong disagreement between the energy calculated through eqs. (4) and (5), showing that even though the energy converged, the state did not. Another recurrent pattern in the energies calculated through eqs. (4) and (5) is an arc of high absolute

Estimated as \( ^2 \)

\[
\langle \psi_\theta | \hat{H} | \psi_\theta \rangle \approx \frac{1}{|\mathcal{M}|} \sum_{n \in \mathcal{M}} \sum_{n'} \langle n | \hat{H} | n' \rangle \frac{\psi_\theta(n')}{\psi_\theta(n)}.
\]

(4)
FIG. 3. Energy variance and absolute error of the last 500 sampling-optimization steps. Dashed lines show the phase boundaries computed for 128 sites with DMRG by Ejima et al.23 In (a), the two first Mott lobes and the SF region are labeled explicitly. (a)-(c) show the variance for the last 500 sampling-optimization steps for the cases of 5 sites and 8 hidden neurons, 8 sites and 11 hidden neurons, and 5 sites and 20 hidden neurons, respectively. (d)-(f) show the corresponding absolute errors between the average energy value for the last 500 sampling-optimization steps and the exact ground state energy.

B. Overlap

The RBM state non-convergence for the case of 5 sites and 20 hidden neurons is further confirmed when we measure the overlap between the exact ground state \(|\psi_{\text{exact}}\rangle\) and the RBM ground state \(|\psi_\theta\rangle\), shown in fig. 5(c). It is now clear why the expected energy with respect to the complete RBM state shown in fig. 4(c) presents large errors when compared to the expected energy with respect to the exact ground state: it appears that the RBM has not learned the ground state in the bottom-right region of the plot, which is a region that covers part of the Mott lobe, as well as part of the SF phase region. In fact, since the minimization is carried out with eq. (4), the RBM only learns relative probability amplitudes between the sampled states, and due to a large number of hidden neurons, the RBM overfits. Moreover, in the case of 5 sites and 8 hidden neurons, and the case of 8 sites and 11 hidden neurons, the RBM finds difficulty in learning the ground state in the limit between the MI and the SF phase as shown in fig. 5(a) and (b). The difficulty in learning those states, and, in general, in treating the ground state near the MI-SF boundary comes from the Kosterlitz-Thouless-like quantum phase transition in 1D systems,86 where an exponentially small Mott gap exists. We see once again that there are arcs of low overlap points formed in the left-most side of the Mott lobes. Within the SF phase, there are also lines of low overlap, which appear because of the finite size effects of the sites chain. Note that there are as many of these fictitious boundaries as there are sites in the periodic chain under study. Nevertheless, when comparing the 5 sites cases, it is seen that for values of \(\mu/U > 1\) the states at the MI-SF phases boundary are better learned when 20 hidden neurons are used in the RBM (as in cf. fig. 5(c)) than when only 8 hidden neurons are used (see fig. 5(a)).

FIG. 4. Absolute error between the RBM state expected energy computed through eq. (5) and the exact ground state energy for (a) 5 sites and 8 hidden neurons, (b) 8 sites and 11 neurons, and (c) 5 sites and 20 neurons. Dashed lines are the MI-SF boundaries as in fig. 3.

FIG. 5. Overlap \(|\langle \psi_{\text{exact}} | \psi_\theta \rangle|^2\) between the exact and RBM ground states for (a) 5 sites and 8 hidden neurons, (b) 8 sites and 11 neurons, and (c) 5 sites and 20 neurons. Dashed lines are the MI-SF boundaries as in fig. 3.

Since the advantage of VMC over exact diagonalization comes for intractably large Hilbert spaces, it is not always possible to compute the probability amplitudes for all of the Fock states basis. In such a case, the RBM state can be built as

\[
|\psi_\theta\rangle = \frac{\sum_{n \in \mathcal{M}'} \psi_\theta(n) |n\rangle}{\sqrt{\sum_{n \in \mathcal{M}'} |\psi_\theta(n)|^2}},
\]

where \(\mathcal{M}'\) is a sample of Fock states sampled with the Metropolis-Hastings algorithm, with an acceptance probability of \(\min\{1, p_{\text{GC}}(n_{i+1})/p_{\text{GC}}(n_i)\}\), where \(p_{\text{GC}}(n) = Z^{-1} \exp \left(-\langle n | \hat{H} | n \rangle\right)\) is the probability associated with the grand canonical ensemble (note that the term \(\mu \langle \hat{N} \rangle\) has already been introduced in the Hamiltonian). This strategy was used to generate a sample \(\mathcal{M}'\) of up to 2048 Fock states yielding a state \(|\psi_\theta\rangle\) for every point in the phase diagram. The overlap between the exact ground state \(|\psi_{\text{exact}}\rangle\) and the sampled RBM ground state \(|\psi_\theta\rangle\) is shown in fig. 5 for the three studied scenarios. Comparing fig. 5 with fig. 3, it is seen that the retrieved sampled state “cleans” the RBM state by removing Fock states for which the probability amplitudes were badly learned, and leaves the Fock states that are relevant to the actual ground state. Despite this cleaning, the larger the
FIG. 6. Overlap $|\langle \psi_{\text{exact}} | \tilde{\psi}_\theta \rangle|^2$ between the exact and sampled RBM ground states for (a) 5 sites and 8 hidden neurons, (b) 8 sites and 11 hidden neurons, and (c) 5 sites and 20 hidden neurons, for a maximum of 2048 states sampled from the Hilbert space. Dashed lines are the MI-SF boundaries as in fig. 5.

C. Order parameter

The phase diagram of the Bose-Hubbard model can be reconstructed by measuring quantities in the sampled RBM ground state that exhibit the phase transition. As mentioned before, we choose the variance of the local number operator, in particular, of the first site. In fig. 7(a) and (b), the order parameter measured with the exact ground state is shown for 5 and 8 sites, respectively. It is seen that in the Mott insulator phase, the variance of the number of bosons in the first lattice site is near to 0, but not exactly 0 because of finite size effects. On the other hand, fig. 7(d) and (e) show the order parameter for the sampled RBM ground state with 2048 Fock states for the cases of 8 and 20 hidden neurons for 5 sites, which show excellent agreement with their exact counterpart fig. 7(a). However, at the boundary between the MI and SF phases, there are absolute errors that could be as high as 0.15, which come from the difficulty of learning the ground state near the phase transition boundary. In spite of these differences at the boundaries, it is clear that the learned RBM ground state mimics the re-entrance phenomenon shown in finite 1D chains. Finally, fig. 7(c) shows the order parameter for the exact RBM ground state for 8 sites and 11 hidden neurons. Figure 7(f) also shows the order parameter for 8 sites and 11 hidden neurons but with a different sampling limit. Instead of fixing a number of Fock states to be sampled (2048 and 4096 were insufficient, data not shown), we build the sample $\mathcal{M}'$ by accepting states with the Metropolis-Hastings algorithm until there is a run of 400 consecutive state proposals that do not raise a new accepted state into $\mathcal{M}'$. In this case, the state is cleaned (note that the arc of badly learned order parameter almost completely disappears). A clear indicator of the number of Fock states to represent the ground state emerges: for very low values of $t$, within the first Mott lobe, only one sampled state $|\langle 1,1,1,1,1 \rangle\rangle$ is needed to reproduce the exact ground state; in the SF phase, up to 30000 states are sampled before hitting a 400 streak of no newly accepted states into the sample that constitutes the RBM ground state.

![Order parameter graph](image)

FIG. 7. Order parameter $\text{Var}(\tilde{n}_1)$ for the ground state obtained through exact diagonalization for 5 sites (a), and 8 sites (b); for the sampled RBM ground state with 2048 Fock states for 5 sites with 8 hidden neurons (d) and 20 hidden neurons (e); and for the exact RBM ground state for 8 sites with 11 neurons (c) and the sampled RBM ground state (f). The white line is the 0.001 contour line, and the yellow one corresponds to the 0.01 contour line in all plots. Dashed lines are the MI-SF boundaries as in fig. 5.

Other quantities can be used as an order parameter, which more explicitly relate to quantum correlations such as entanglement. For instance, a partial trace carried out over all degrees of freedom except the first site yields a reduced density matrix $\rho_1(t,\mu)$, from which the linear entropy $S(t,\mu) = 1 - \text{Tr} \{ \rho_1^2(t,\mu) \}$ can be measured (the von Neumann entanglement entropy can also be used, e.g., [50]). Figure 8 shows the absolute errors between the exact and the sampled RBM ground states for the three studied scenarios, where the errors in the MI-SF boundary become large.

D. Tomography

In all the studied scenarios, there are problems for learning the ground state at the MI-SF boundaries, as well as the mini-plateaus boundaries within the SF...
The exact ground states show very similar distributions over three rungs of the one-filling manifold: \( |1, 1, 1, 1\rangle, |0, 1, 1, 1, 2\rangle \) and \( |0, 1, 1, 2, 1\rangle \). Increasing \( \mu \) up to the first MI-SF boundary (slightly within the SF phase), we see that the probability amplitude distribution starts to differ between the exact and the RBM ground states, and the RBM struggles to identify if the ground state is now in an excitation manifold above the one-filling manifold, represented by the rungs \( |1, 1, 1, 1\rangle \), or in the MI phase which is represented by the rung \( |1, 1, 1, 1\rangle \). Increasing again \( \mu \) in order to be at the middle of the first plateau within the SF phase shows that both the RBM and the exact ground states have similar probability amplitude distributions, even though the RBM assigns a probability to other rungs (not shown in the plot because their contribution is less than 0.01). It is clear that this first plateau is mostly represented by the rung \( |1, 1, 1, 1, 2\rangle \) which is in the 6-th excitation manifold. If we continue to increase \( \mu \), we see that near the boundaries between the MI-SF phases and between the plateaus within the SF phase, the RBM and the exact ground states exhibit differences in the probability amplitude distributions. On the contrary, in the middle of those plateaus, the probability amplitude distributions from both RBM and exact ground states are very similar (which is also seen in fig. (a)). Moreover, each time the tomography moves onto a new plateau (with a higher value of \( \mu \)), the excitation manifold increases by one, up to the 10-th excitation manifold, which corresponds to the two-filling manifold at the second Mott lobe, characterized by the rung \( |2, 2, 2, 2\rangle \) as well as the rungs \( |1, 2, 2, 2, 3\rangle \) and \( |1, 2, 3, 1, 3\rangle \).

IV. CONCLUSIONS

In this work, we systematically tested the capabilities of VMC with a trial ground wavefunction given by an RBM on the one-dimensional Bose-Hubbard model. The motivation for the technique comes from the possibility of incorporating it into the toolbox of quantum physics to tackle theoretical problems that are difficult to study numerically due to the intractably large Hilbert spaces. Thus, it is first needed to intensively test the technique to reproduce known results, and it is also needed to theoretically explain why the technique works (this is a challenging open question which involves the question of why neural networks work well). Only if the community identifies the strengths and weaknesses of the technique is it possible to use it to explore problems of interest that involve vast Hilbert spaces. Regarding the model under study, we repeatedly found differences between the exact ground state found through the exact diagonalization of the Bose-Hubbard Hamiltonian and the learned ground state. We did so in one-dimensional chains of 5 and 8 sites. In order to better learn the ground state, the variational trial wavefunction was enriched in the case of 5 sites by increasing the number of hidden units in the RBM’s hidden layer. Although results improved near the
MI-SF boundary, other regions of the Bose-Hubbard parameter space suffered from badly learned ground states. For that reason, we proposed a sampling technique that cleans the ground state, getting rid of contributions that arise because of over-fitting. However, the VMC-RBM method to find the ground state was proven to yield good results not only in computing the energy (with low errors and clear signs of convergence in most of the parameter space) but also in computing other observables which explicitly involve quantities related to quantum correlations, such as the linear entropy of one of the chain’s sites. In particular, we reconstructed with excellent accuracy the phase diagram of the Bose-Hubbard model using the local occupation variance as an order parameter for most of the parameter space. Nevertheless, we also carried out quantum state tomographies to understand the composition of the ground states at the interfaces between the MI-SF phases and also within the excitation manifold plateaus formed for finite chains in the SF phase, which revealed significant differences between the Fock states distributions of the exact ground state and the learned ground state.

Accordingly, we must raise the attention that the VMC technique is consistently challenged near the quantum phase transition of the Bose-Hubbard model. We do not doubt that the high-expressivity of neural quantum states are capable of improving those results under more extensive sampling, or more complex variational trial wavefunctions apart from RBMs; however, we report that some questions have to be answered with precision before confidently using VMC as a method to accurately explore the physics of a many-body problem without the support of any other numerical method. In the first place, we observed that not every point of the phase diagram requires the same amount of computational work to learn the ground state. Most notably, the ground state in the MI phase is mostly explained by only one Fock state, whereas the number rapidly grows for ground states in the SF phase. Therefore, automated ways of stopping sampling within the sampling steps should be taken into consideration. In particular, when using the Metropolis-Hastings algorithm, we found that if a Markov chain of a certain length was formed with no new sampled states, we could stop sampling, yielding a high-quality ground state. Secondly, the VMC technique showed badly learned ground states along arcs formed within the Mott lobes. Why these form remains unanswered, as they are not related to the structure of the MI-SF boundaries. However, after we clean the learned ground state, these arcs almost completely disappear. Thus, it might be the case that they
are related to over-fitting, which traduces in noisy probability from Fock states that are not relevant to the ground state. Finally, concerning the first question, the number of optimization steps required to learn the ground state has to be better understood, as it is only clear when the energy converges, but not the state.\textsuperscript{[72]}

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If instead the sample is built from the distribution $|\psi_n|^2$, then the acceptance probability becomes $\min\left\{1, |\psi_\theta(n_{i+1})/\psi_\theta(n_i)|^2\right\}$ and the state build through eq. (5) inherits the RBM state problems (data not shown).

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In this regard, NetKet team has included the Gelman-Rubin statistics.

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