Artificial neural network states for nonadditive systems

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Methods inspired from machine learning have recently attracted great interest in the computational study of quantum many-particle systems. So far, however, it has proven challenging to deal with microscopic models in which the total number of particles is not conserved. To address this issue, we propose a variant of neural network states, which we term neural coherent states. Taking the Fröhlich impurity model as a case study, we show that neural coherent states can learn the ground state of nonadditive systems very well. In particular, we recover exact diagonalization in all regimes tested and observe substantial improvement over the standard coherent state estimates in the most challenging intermediate-coupling regime. Our approach is generic and does not assume specific details of the system, suggesting wide applications.

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I. INTRODUCTION

Integration of ideas originating from machine learning into the study of quantum physics has recently attracted great interest, owing to the new possibilities it offers to tackle challenging problems in quantum physics [1–3]. As pioneered by Carleo and Troyer [4], a particularly appealing approach is to represent the quantum many-body wave function by an artificial neural network. This was first demonstrated for quantum spin systems in one and two dimensions and subsequently generalized to bosonic [5,6] and fermionic [7–9] systems. Moreover, beyond pure quantum states, artificial neural networks can also accurately represent mixed quantum states in open systems [10–13] and quantum systems at finite temperature [14].

However, all these examples involve additive many-body systems, for which by definition the total number of particles is conserved. On the other hand, there is an important class of physical systems which does not satisfy particle number conservation. Besides elementary examples including the hole theory in relativistic quantum theory and solid state physics, as well as the approximate descriptions of superfluidity and superconductivity, this comprises the important class of inherently nonadditive quantum impurity systems. Such systems include the paradigmatic Holstein [15], Fröhlich [16], and Su-Schrieffer-Heeger (SSH) [17,18] models for an electron (spin) interacting with phonons, the Dicke model [19,20] in quantum optics, and the Anderson impurity model [21] for magnetic impurities in metals. Owing to their simplicity, these models play a crucial role in the understanding of quantum many-body effects. Nevertheless, analytic solutions are often available only in limiting cases and to address the full complexity of the problem numerical methods are desired.

Neural network quantum states are, in principle, a prospective candidate for efficient representation of such complex quantum many-body states. For example, the restricted Boltzmann machine (RBM), one of the simplest and most widely used architectures [22], exhibits volume law entanglement and can represent even models with long-range interactions [23]. Analogous to variational Monte Carlo (VMC) approaches to the Holstein and SSH model [24–26], recently the electron-phonon correlation factor was represented using an RBM, while keeping a Jastrow correlation factor for the electron subsystem. Lattice polarons have also been tackled with Gaussian process regression capable of extrapolating across their phase transitions [27]. In addition, the Anderson impurity model has been addressed with machine learning methods to find the Green’s function [28] and to derive its low-energy effective model [29]. However, so far no neural network states exist which directly provide an unbiased estimate of the full many-body wave function of nonadditive systems.

In this paper we show that efficient neural network states for nonadditive systems can be constructed as a feedforward neural network with outputs inspired from the coherent states well known from quantum optics [30]. To investigate the efficiency of this architecture, we consider the Fröhlich model featuring long-range interactions between the phonon degrees of freedom and benchmark it against exact diagonalization. In all cases studied, we find that this approach outperforms the standard mean-field coherent state solution, in particular when impurity-induced phonon-phonon correlations are strong.

II. NEURAL NETWORK ARCHITECTURE

We use a basis corresponding to bosonic occupations of the system with \( n \) denoting a single bosonic configuration of the whole system,

\[
|n\rangle = |n_1, n_2, \ldots, n_i, \ldots, n_N\rangle ,
\]

where \( N \) is the number of discrete phonon modes considered. In an RBM architecture, \( N \) is equal to the number of visible neurons. However, direct application of an RBM to
nonadditive systems is not efficient. This can easily been seen by writing the neural network quantum state as $|\psi(\mathbf{n})\rangle = \psi(\hat{\mathbf{n}})|\mathbf{n}\rangle$; we have $[\psi(\hat{\mathbf{n}}), \hat{\mathbf{N}}] = 0$, $\hat{\mathbf{N}} = \sum_i \hat{n}_i$ for a function $\psi(\mathbf{n}) \sim \exp[E(\mathbf{n})]$, $E$ being linear in $\mathbf{n}$. Hence, by construction, an RBM operates in a sector of a given total number of particles [31].

To bypass this problem, we propose a neural network inspired from coherent states, which may be termed neural coherent states (NCS) and is illustrated in Fig. 1. Analogous to a standard coherent state, which for a given $n$ returns an output proportional to $\lambda^n/\sqrt{n!}$, with $\lambda$ being the parameter representing the coherent state, we construct a (multilayer) feedforward neural network taking $\mathbf{n}$ as the input. For each configuration, $N$ output numbers $\lambda_i$ are generated, which are subsequently transformed according to $\lambda_i \rightarrow \lambda_i^n/\sqrt{n!}$. Then these numbers are multiplied to form the wave function. With this ansatz, we optimize the variational energy

$$
E = \frac{\langle \psi| \hat{H} |\psi \rangle}{\langle \psi| \psi \rangle} = \frac{\sum_{\mathbf{n}} \langle \psi| \mathbf{n} \rangle \langle \mathbf{n}| \hat{H} |\psi \rangle}{\sum_{\mathbf{n}} \langle \psi| \mathbf{n} \rangle \langle \mathbf{n}| \psi \rangle} = \frac{\sum_{\mathbf{n}} \psi^*(\mathbf{n}) \hat{H}_{\mathbf{n} \mathbf{n}} \psi(\mathbf{n})}{\sum_{\mathbf{n}} |\psi(\mathbf{n})|^2}.
$$

We choose Adam [33] over other commonly used methods such as stochastic reconfiguration [34] for the gradient descent algorithm in our variational Monte Carlo optimization. At each step of the descent, we sample the probability distribution given by $|\psi(\mathbf{n})|^2$. To reduce noise resulting from this stochastic estimation, we run several Monte Carlo chains in parallel and perform and update only if they are consistent [31].

### III. Hamiltonian Representation of Impurity Problems

To test the efficiency of the NCS for nonadditive systems, we focus on the Fröhlich Hamiltonian as given by

$$
\hat{H} = \frac{p^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_0 \hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} + \sum_{\mathbf{k}} \left( V_\mathbf{k} \hat{a}_\mathbf{k} e^{-ikr} + V_\mathbf{k}^* \hat{a}^\dagger_\mathbf{k} e^{ikr} \right),
$$

where $\mathbf{r}$ and $\mathbf{p}$ denote the position and momentum, respectively, of an impurity characterized by mass $m$. The three terms stand for the impurity kinetic energy, bosonic bath energy, and the impurity-bath interaction, respectively. The summation extends over all possible wave vectors $\mathbf{k}$. Here, we decided to focus on one-dimensional systems. There is, however, no fundamental limitation on the application of NCS to higher dimensions, since analogously to the original RBM the correlations induced by the hidden units are intrinsically nonlocal in space [4].

Solution of the Fröhlich model is more convenient in the impurity frame, which is achieved by the Lee-Low-Pines
transformation [35]. The Hamiltonian becomes

\[ \hat{\mathcal{H}} = \left( \sum_{k} \frac{\hbar k \hat{a}_k^\dagger \hat{a}_k}{P} \right)^2 + \sum_{k} \hbar \omega \hat{a}_k^\dagger \hat{a}_k + \sum_{k} (V_k \hat{a}_k + V_k^* \hat{a}_k^\dagger). \] (7)

The Lee-Low-Pines transformation removes the impurity degrees of freedom from the Hamiltonian. This maps the problem to a pure problem of interactions between the bosonic modes, at the price of introducing effective interactions between the phonon modes, described by the first term of the transformed Hamiltonian. The transformed impurity Hamiltonian problem is closer to the lattice boson problems such as the Bose-Hubbard problem, studied earlier with different neural quantum state (NQS) architectures [5,9]. However, the problem mentioned earlier, that the total number of bosons is not conserved, persists. Furthermore, we can set \( P = 0 \) to zero. The real number \( P \) represents the total momentum of the entire system, i.e., the impurity and the bosonic modes. Hence, setting \( P = 0 \) is without any loss of generality,

\[ \hat{\mathcal{H}} = \left( \sum_{k} \frac{\hbar k \hat{a}_k^\dagger \hat{a}_k}{2m} \right)^2 + \sum_{k} \hbar \omega \hat{a}_k^\dagger \hat{a}_k + \sum_{k} (V_k \hat{a}_k + V_k^* \hat{a}_k^\dagger). \] (8)

IV. NUMERICAL RESULTS

To make the Hamiltonian more convenient for numerical computation, we measure energy in units of \( \hbar \omega_0 \). This allows us to show the results as functions of \( 1/m \) and \( V_k \), for which analytical results exist in the limiting cases \( 1/m \to 0 \) and \( V_k \to 0 \). Moreover, we discretize the \( k \) grid to include \( N \) points \( k_i \) ranging from \(-k_0 \) to \( k_0 \) with step \( \Delta k \). This finally puts the Hamiltonian into the following form in one dimension:

\[ \hat{\mathcal{H}} = \left( \sum_{k} \frac{\hbar k \hat{a}_k^\dagger \hat{a}_k}{2m} \right)^2 + \sum_{k} \hbar \omega \hat{a}_k^\dagger \hat{a}_k + \sum_{k} (V_k \hat{a}_k + V_k^* \hat{a}_k^\dagger). \] (9)

To benchmark our results, we compare them with two approaches—exact diagonalization (ED), and the mean-field approach [36], where the ground state \( |\psi_{\text{MF}}\rangle \) is a direct product of coherent states, resulting in energy \( E_{\text{MF}} \):

\[ |\psi_{\text{MF}}\rangle = \bigotimes_i \left| \frac{-V_k}{1 + \hbar^2 k^2 / 2m} \right\rangle, \quad E_{\text{MF}} = -\sum_k \frac{|V_k|^2}{1 + \hbar^2 k^2 / 2m}. \] (10)

By such a choice of benchmarks, we are able to quantify the correlations expressed with our ansatz. To facilitate the comparison with ED, we restrict the maximum number of bosons at each mode at a value \( n_{\text{max}} \), ranging between three and eight, depending on the parameter regime, which we determine until convergence is obtained. This improves the stability of training by reducing the risk of the Monte Carlo sampler exploring irrelevant local maxima of \( |\psi(n)|^2 \). We attribute this risk reduction to the reduction of the size of the Hilbert space. This leads to simplification of the \( |\psi(n)|^2 \) landscape explored by the sampler.

As the first test, we take a small system with \( N = 2 \) \( k \) points \(-k_0 \) and \( k_0 \). We fix the impurity-bath potential at \( V = 0.9 \). Correspondingly, we use a high cap of the number of bosons, \( n_{\text{max}} = 10 \). Moreover, using the convenient unit \( n_{\text{0}} = \hbar k_0^2 / (2\omega_0) \) for the mass, such that \( \hbar^2 k_0^2 / (2m_0) = \hbar \omega_0 \), we fix the inverse mass at \( m = 0.6 (1/m_0) \). We vary the number of nodes in the single hidden layer, thus changing the number of variational parameters and, consequently, the representational power of the network. For each number of nodes, we perform stochastic optimization of the energy and compare the obtained energy with the ED. Only for the final determination of the energy do we employ the full summation to reduce the stochastic error. The results are shown in Fig. 2.

We observe that increasing the number of hidden nodes systematically reduces the energy until convergence with ED is found, with a relative difference below \( 10^{-6} \) which indicates that the NCS can represent the state accurately. The remaining discrepancy is attributed to the stochastic error arising during the variational optimization.

To further evaluate the ability of NCS to express correlations between different bosonic modes, we study the performance of our approach for more visible nodes and in different regimes of impurity mass \( m \) and impurity-bath coupling \( V \). Low mass is associated with a high correlation level, while high mass brings the Hamiltonian closer to the infinite mass regime, where an analytic solution in the form of a coherent state exists. We consider three values of \( V \) to demonstrate mass dependence: \( V = 0.2, V = 0.4, \) and \( V = 0.6 \). The results are shown in Fig. 3(a), where we plot the ground state energy difference as compared to the mean field both for the NCS approach and for exact diagonalization.

To reduce computational efforts, the energy is now evaluated by stochastic estimation as well. This consistently yields a stochastic error of \( 10^{-3} \) for all data points considered below, which is sufficient to investigate the improvement as compared to the mean field and consistency with ED. We found that a further reduction of the stochastic error is challenging, probably due to the different signs in the wave function for odd and even \( n \) at negative \( \lambda \). Similar challenges with
stochastic optimization have been observed for nonstoquastic yet additive systems [37–40].

Likewise, we consider three different inverse mass values to study the performance at different impurity-bath couplings $V$: $1/m = 0.6 (1/m_0)$, $1/m = 1.2 (1/m_0)$, and $1/m = 2.0 (1/m_0)$. The results for the $V$ dependence are shown in Fig. 3(b). In all regimes of $V$ and $m$, we observe very stable performance—-the NCS is able to match ED within the stochastic error and, as such, outperform the mean-field approach across the range of (inverse) mass tested, in particular in the most challenging regime where $m \sim 1$ (note that at large $m$ the system is close to the uncorrelated vacuum state). This holds in a regime for which the number of parameters $N_W$ in the network is much smaller than the size of the Hilbert space $N_H$: $N_W/N_H \approx 4 \times 10^{-3}$.

The observed efficiency of the network suggests access to system sizes beyond ED. To provide further evidence for this, we gradually increase the number of $k$ points and benchmark the ability of the NCS approach to express the correlations between a larger number of bosonic modes. To this end we take $k$ being an equidistant grid between $-k_0$ and $k_0$ with a varying number of points. The constant impurity-bath interaction potential is $V_c \equiv 0.3$, which corresponds to contact interactions in real space, which is reasonable for one-dimensional systems. We fix the mass at $1/m = 2 (1/m_0)$ and the ratio between the number of hidden to visible nodes to 10. In Fig. 4 we show the results of a benchmark against the mean-field approach and, where feasible, exact diagonalization. We observe that the difference between the energy reached using our NCS state and the mean-field solution increases with increasing the number of phonon modes, which is consistent with the fact that the amount of modes that are coupled to each other increases as well. Moreover, within the range where ED is feasible, we observe that the NCS results match ED, while the mean-field energy is systematically higher. These results confirm the efficiency of the NCS, where for 11 visible nodes $N_W/N_H \approx 7 \times 10^{-7}$. Thus, our results suggest a great potential to exploit this approach beyond the regime accessible with exact diagonalization.

V. CONCLUSIONS

In summary, we introduced an approach to solve nonadditive systems with artificial neural networks. By benchmarking against exact diagonalization, we obtained accurate results for small systems and all parameter regimes studied. In particular, we were able to capture the challenging intermediate-coupling regime at the same accuracy as weak-coupling results, illustrating that this method provides an unbiased approach to strong correlations in nonadditive systems, which moreover is accessible with only a moderate number of network parameters.

Natural next steps include benchmarks against other methods for impurity systems. This is particularly interesting for applications in two or three dimensions, where numerically exact solutions are available [41,42] and a quantitative comparison for a large number of phonon modes can be made. Similarly, generalizations to other impurity models, such as the Holstein and SSH models, are very interesting to further assess the quality of the NCS approach. It would also be beneficial to include studies of other observables derived from the obtained variational wave function. This could for example include a correlation function between different phonon modes, bosonic occupations in different modes, or the polaron effective mass, and beyond such additional benchmarks, generalizations to other neural network architectures and more complex impurity models, such as the angulon quasiparticle [43–45] which is the rotational counterpart of the polaron. The main complication is the noncommutative SO(3) algebra describing quantum rotations, which is inherently involved in the angulon problem. Some work in a similar direction has already been done for spin models [46], where irreducible representations of SU(2) were considered as inputs for the network. An appealing feature of variational neural network algorithms is their direct extension to unitary quantum dynamics of the system [4,47–50]. This requires generalizing

FIG. 3. The energy difference in the mean-field solution as a function of (a) inverse mass in units $1/(m_0 m) = \hbar \omega_0^2/(2m_0)$ for three different values of $V$ and (b) impurity-bath coupling $V/\hbar \omega_0$ for three different values of $1/m$.

FIG. 4. The energy difference as compared to the mean-field solution calculated with the NCS approach (orange points) as a function of the number of $k$ points on an equidistant grid between $k = -k_0$ and $k = k_0$. Black crosses indicate the corresponding values obtained with exact diagonalization, where accessible.

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the current approach to complex valued network parameters, yielding the possibility of an extension of the presented work to the case of impurity dynamics, the understanding of which is a subject of intensive ongoing research [51–56].

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