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Transition from ergodic to many-body localization regimes in open quantum systems in terms of the neural-network ansatz

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Abstract. The *purpose* of our work is to investigate asymptotic stationary states of an open disordered many-body quantum model which is characterized by an ergodic — many-body localization (MBL) phase transition. To find these states, we use the neural-network ansatz, a new *method* of modeling complex many-body quantum states discussed in the recent literature. Our main *result* is that that the ergodic phase — MBL transition is detectable in the performance of the neural network that is trained to reproduce the asymptotic states of the model. While the network is able to reproduce, with a relatively high accuracy, ergodic states, it fails to do so when the model system enter the MBL phase. We *conclude* that MBL features of the model translate into the cost function landscape which becomes corrugated and acquires many local minima.

Keywords: many-body localization, open quantum systems, neural networks.

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Переход от эргодических режимов к режимам многочастичной локализации в открытых квантовых системах с точки зрения нейросетевого представления

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Аннотация. *Целью* нашей работы является исследование асимптотических стационарных состояний открытой неупорядоченной многочастичной квантовой модели, которая характеризуется переходом эргодическая фаза — многочастичная локализация (МЧЛ). Чтобы найти эти состояния, мы используем нейросетевой анзац, новый *метод* моделирования сложных квантовых состояний многих тел, предложенный и обсуждаемый в недавних публикациях. Наш главный *результат* состоит в том, что переход эргодическая фаза – многочастичная локализация обнаруживается в работе нейронной сети, которая обучена воспроизводить асимптотические состояния модели. Хотя сеть способна воспроизводить с относительно высокой точностью эргодические состояния, она не может этого сделать, когда модельная система входит в МЧЛ-фазу. Мы *заключаем*, что особенности МЧЛ-режима трансформируются в ландшафт функции стоимости, который становится сильно неравномерным и приобретает множество локальных минимумов.

Ключевые слова: многочастичная локализация, открытые квантовые системы, нейронные сети.

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Introduction

The computational many-body quantum physics is one of the research fields that is severely subjected to the “Curse of Dimensionality” [1]. The complexity of the description of a state of a many-body system grows exponentially with the number N of system’s components, e.g., spin or qubits, so that the corresponding model becomes intractable already for relatively small values of N. The development of the computational many-body physics is the story of a constant search for new methods to compactify the description of quantum states at the price of restricting them to a subset which is constrained by some conditions [2], f.e., by area laws [3, 4].

The rise of machine learning (ML) techniques has inspired physicists to design new methods of modeling complex quantum states. One of the recent breakthroughs is the idea to use neural networks to encode many-body states, in order to benefit from the ability of the networks to compactify descriptions of complex objects and sets; see, e.g., Refs. [5, 6]. In particular, the so-called Neural Network States (NNS) [5], based on the restricted Boltzmann machines (RBMs) [7], turned out to be able to reproduce the ground states of large quantum many-body Hamiltonians [5, 8], even in the case when these ground states are characterized by long-range entanglement [9].

Open many-body open quantum systems are especially challenging to deal with computationally. Due to the growth of the number of parameters (needed to describe the state of an open system) as the square of the corresponding Hilbert space dimension, description of open quantum states by density matrices requires substantially more computational resource as compared to the states of Hamiltonian systems [2].

Numerical solution of the Lindblad master equation [10], commonly used to model evolution of open quantum systems, becomes a challenge already for $N = 10$ spins/qubits. Equally, the exact diagonalization of the Lindblad equation in order to find its stationary state — and thus to compute the asymptotic state of the corresponding model — becomes a problem starting $N = 8$ spins (if no further constraints are imposed so that the dimension of the Hilbert space can be reduced) [2]. It therefore would be beneficial to implement the machine learning techniques to model open quantum many-body states.

A progress in this direction has been made very recently [11, 12]. In particular, the fact that any mixed quantum states can be purified by using ancillary degrees of freedom, was used in the recent work by Vicentini et al. [11]. By performing the purification, mixed states can be expressed as an NNS in the extended Hilbert space [13]. The asymptotic states of the model Lindbladian can then be found by performing variational minimization of a cost function associated to the master equation. It was demonstrated that by using Markov chain Monte Carlo sampling of the gradient, it is possible to approximate the asymptotic state of the dissipative quantum transverse Ising model with high accuracy [11].

From another perspective, asymptotic states of disordered open many body-system models can be continuously tuned from the ergodic phase, characterized by long-range entanglement (and therefore similar to the state addressed in Ref. [11, 14]) to MBL states, characterized short-ranged entanglement [15]. It is interesting to study the validity of the variational neural-network ansatz for the two types of states as well as to explore the transition between these types through the prism of neural network training. This is the main motivation of our work.

1. Model

We use an open disordered many-body model proposed in Ref. [15]. It was shown that, by tuning the strength of the disorder, it is possible to change the asymptotic states of the model from ergodic to the ones bearing the footprints of MBL. Below he briefly outline the model.

We consider an open-ended chain of N (an even number) sites occupied by $N/2$ spinless fermions. The fermions interact only when occupying neighboring sites and are additionally subjected to random on-site potentials h_l, $l = 1, \ldots, L$. The model Hamiltonian is

$$H = -J \sum_{l=1}^{L} \left(c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l \right) + U \sum_{l=1}^{L} n_l n_{l+1} + \sum_{l=1}^{L} h_l n_l, \tag{1}$$

where $c_l^\dagger$ (c_l) creates (annihilates) a fermion at site l, and $n_l = c_l^\dagger c_l$ is the local particle number operator. Values h_l are drawn from an uncorrelated uniform distribution on the interval $[-h, h]$. For $J = U = 1$ (our choice here) this system undergoes a many-body localization transition when $h > h_{\mathrm{MBL}} \backsimeq 3.6$ [16]. By using the Jordan–Wigner transformation, the system can be mapped onto a model of L spins confined to the manifold $S^z = \sum_{l=1}^{L} s_l^z = 0$. This relation allows us to implement the time-evolving block decimation (TEBD) scheme generalized to matrix product operators [4] and propagate the model system to its steady state. As the initial state we use $\varrho(0) = |\psi_0\rangle\langle\psi_0|$, $|\psi_0\rangle = |1010...10\rangle$.

The dissipation is captured with the Lindblad master equation,

$$\dot{\varrho}(t) = \mathcal{L}\varrho(t) = -i\,[H, \varrho(t)] + \sum_{s=1}^{L} \gamma_s \left[A_s \varrho(t) A_s^\dagger - \frac{1}{2}\{A_s^\dagger A_s, \varrho(t)\} \right],$$

where $\varrho(t)$ is the system density operator, and A_s is the jump operator mimicking the s-th dissipative channel of the environment, with rate γ_s. The non-local dissipative operators act on a pair of neighboring sites,

$$A_l = (c_l^\dagger + c_{l+1}^\dagger)(c_l - c_{l+1}), \qquad \forall \gamma_l = \gamma. \tag{2}$$

In Ref. [15] it was demonstrated that, by increasing disorder strength h, we can detect ergodic – MBL transition at $h \approx 7$. This transition can be detected by using several quantifiers, including the spectral statistics and structure of the density matrices describing to the asymptotic states. We will use this type of quantifiers here.

2. Neural-network ansatz

Here we briefly outline the idea of the ansatz presented in Ref. [11].

By using some basis in the system's Hilbert space, $\{|\boldsymbol{\sigma}\rangle = |\sigma_1, \sigma_2, ..., \sigma_N\rangle\}$ (which is the Fock basis in the case of our model), the density operator can be represented as matrix $\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'})$,

$$\hat{\rho}(\boldsymbol{v}) = \sum_{\boldsymbol{\sigma},\boldsymbol{\sigma'}} \rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) \, |\boldsymbol{\sigma}\rangle \, \langle \boldsymbol{\sigma'}| \, . \tag{3}$$

In order to use the NNS representation, this density matrix has to represented at as a partial trace over a pure state living in a higher dimensional Hilbert space, $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_A$ where $\mathcal{H}_{S,A}$ are the system and ancillary Hilbert spaces, respectively. The extended space is spanned by basis $\{|\boldsymbol{\sigma}, \boldsymbol{a}\rangle\}$ where $\boldsymbol{a} = (a_1, a_2, ..., a_{N_a})$ labels the ancillary degrees of freedom. The density matrix of the original system S is obtained by tracing out the ancillary degrees freedom [13],

$$\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) = \sum_{\boldsymbol{a}} \psi_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{a}) \psi^{\star}_{\boldsymbol{v}}(\boldsymbol{\sigma'}, \boldsymbol{a}). \tag{4}$$

State $\psi_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{a})$ can be encoded via a neural network ansatz [13],

$$\psi_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{a}) = \sqrt{\mathcal{P}_{\boldsymbol{v}_A}(\boldsymbol{\sigma}, \boldsymbol{a})} \exp[-1/2 \log(\mathcal{P}_{\boldsymbol{v}_\theta}(\boldsymbol{\sigma}, \boldsymbol{a}))]. \tag{5}$$

Amplitude $\mathcal{P}_{\boldsymbol{v}_A}(\boldsymbol{\sigma}, \boldsymbol{a})$ and phase function $\mathcal{P}_{\boldsymbol{v}_\theta}(\boldsymbol{\sigma}, \boldsymbol{a})$ are given by $\mathcal{P}_\nu(\boldsymbol{\sigma}, \boldsymbol{a}) = \sum_{\boldsymbol{h}} \exp[-E_\nu(\boldsymbol{\sigma}, \boldsymbol{a}, \boldsymbol{h})]$ (with $\nu \in \{\boldsymbol{v}_A, \boldsymbol{v}_\theta\}$), where the energy functional is defined as

$$E_\nu(\boldsymbol{\sigma}, \boldsymbol{a}, \boldsymbol{h}) = \boldsymbol{\sigma} \cdot \mathbf{b}_\nu^{(\sigma)} + \boldsymbol{a} \cdot \boldsymbol{b}_\nu^{(a)} + \boldsymbol{h} \cdot \boldsymbol{b}_\nu^{(h)} + \boldsymbol{\sigma}^T \boldsymbol{W}_\nu \boldsymbol{h} + \boldsymbol{\sigma}^T \boldsymbol{U}_\nu \boldsymbol{a}. \tag{6}$$

The ansatz parameters are $\boldsymbol{v} = (\boldsymbol{v}_A, \boldsymbol{v}_\theta)$ where $\boldsymbol{v}_\nu = (\mathbf{b}_\nu^{(\sigma)}, \boldsymbol{b}_\nu^{(a)}, \boldsymbol{b}_\nu^{(h)}, \boldsymbol{W}_\nu, \boldsymbol{U}_\nu)$. The rectangular matrix $\boldsymbol{W}_\nu$ weighs the connections between the system variables (visible layer) to the auxiliary variables (hidden layer), while the weight matrix $\boldsymbol{U}_\nu$ quantifies the connection between the system variables and the ancillary ones (ancillary layer). Such neural-network ansatz is represented by a tri-partite Restricted Boltzmann Machine depicted in Fig. 1. In other words, there are two independent artificial neural networks, one for the amplitude ($\nu = A$) and one for the phase ($\nu = \theta$).

By substituting above expressions into Eq. (4) and performing tracing over the ancillary degrees of freedom, we obtain the expressions for the elements of the density matrix*:

$$\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) = \exp\left[\Gamma^{-}_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) + \Gamma^{+}_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'}) + \Pi_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma'})\right]. \tag{7}$$

The descriptive power of the neural-network ansatz can be improved by increasing the density of the hidden ($\alpha = N_h/N$) and ancillary ($\beta = N_a/N$) layers.

The search for the asymptotic state can be recast into a minimization problem for a cost function,

$$\mathcal{C}(\boldsymbol{v}) = \frac{\|d\hat{\rho}_{\boldsymbol{v}}/dt\|_2^2}{\|\hat{\rho}_{\boldsymbol{v}}\|_2^2} = \frac{\mathrm{Tr}\left[\hat{\rho}^{\dagger}_{\boldsymbol{v}} \mathcal{L}^{\dagger} \mathcal{L} \hat{\rho}_{\boldsymbol{v}}\right]}{\mathrm{Tr}\left[\hat{\rho}^{\dagger}_{\boldsymbol{v}} \hat{\rho}_{\boldsymbol{v}}\right]}, \tag{8}$$

*The expression of $\Gamma^{+/-}$ and Π can be found in the Supplemental Material of [11].

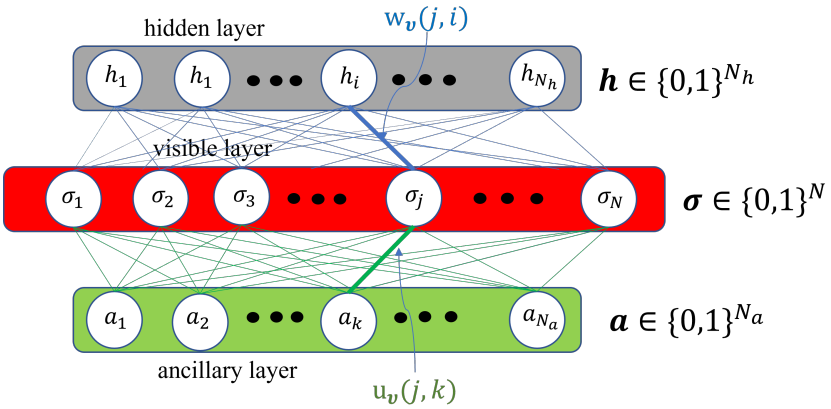

Fig. 1. The neural network used for the ansatz. The vector $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, ..., \sigma_N)$ contains the variables of the system (visible layer, in red on the plot). The vector $\boldsymbol{a} = (a_1, a_2, ..., \sigma_{N_a})$ contains the ancillary degrees of freedom of the extended Hilbert space (ancilla layer, green). The vector $\boldsymbol{h} = (h_1, h_2, ..., h_{N_h})$ contains variables of auxiliary nodes (hidden layer, grey). The network is specified wit the set of parameters $\boldsymbol{v}_\nu = (\mathbf{b}_\nu^{(\sigma)}, \boldsymbol{b}_\nu^{(a)}, \boldsymbol{b}_\nu^{(h)}, \boldsymbol{W}_\nu, \boldsymbol{U}_\nu)$. Local biases, $\boldsymbol{b}_\nu^{(h)}, \boldsymbol{W}_\nu, \boldsymbol{U}_\nu$, acts on the neurons of the hidden, visible, and auxiliary layers, respectively. Another network, with the same structure is used to represent the phase ($\nu = \boldsymbol{v}_0$), Eq. (5) (color online)

It is known that, because the absence of the normalization in density matrices obtained using the purification technique [13], it is not possible to base the optimization procedure on the elements of the density matrices encoded in the network. It was propose to use Markov Chain Monte Carlo [17] with Metropolis update rules, and, at every sampling step, a new configuration $(\boldsymbol{\sigma}, \tilde{\boldsymbol{\sigma}}) \to (\boldsymbol{\sigma}', \tilde{\boldsymbol{\sigma}}')$ is created by switching a random number of spins and it is accepted with probability $\min(\exp\left[p_{\boldsymbol{v}}(\boldsymbol{\sigma}, \tilde{\boldsymbol{\sigma}})/p_{\boldsymbol{v}}(\boldsymbol{\sigma}', \tilde{\boldsymbol{\sigma}}')\right], 1)$.

Finally, on every step of the optimization procedure, physical observables of interest are sampled through another Markov chain,

$$\langle\hat{\Theta}\rangle = \frac{\mathrm{Tr}\left[\hat{\rho}\ \hat{\Theta}\right]}{\mathrm{Tr}[\hat{\rho}]} = \sum_{\boldsymbol{\sigma}} p_{\boldsymbol{v}}^{\mathrm{obs}}(\boldsymbol{\sigma}) \sum_{\tilde{\boldsymbol{\sigma}}} \frac{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \tilde{\boldsymbol{\sigma}})\Theta(\tilde{\boldsymbol{\sigma}}, \boldsymbol{\sigma})}{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma})}, \tag{9}$$

where $p_{\boldsymbol{v}}^{\mathrm{obs}}(\boldsymbol{\sigma}) = \rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma})/\,\mathrm{Tr}[\hat{\rho}]$.

3. Results

In order to approximate the asymptotic states of the model (1)–(2), we use the *NetKet* [18] package developed by the authors of Ref. [11]. We have modified the original code in order to take the symmetry of the model system into account and thus to reduce the dimension of the Fock space to $N = \binom{L}{L/2}$, where L is the number of the lattice sites. Finally, we keep fixed the density of neurons in the hidden $\alpha = N_h/N$, and ancillary layer, $\beta = N_a/N$, fixed, $\alpha = \beta = 2$.

In order to measure the distance between the density matrix ϱ_{exact}, obtained with the exact diagonalization of $\mathcal{L}$, Eq. (2), and the density matrix obtained with the neural-network ansatz, ϱ_{NNA}, we use the standard fidelity measure, $d(\varrho_{\mathrm{exact}}, \varrho_{\mathrm{NNA}}) = 1 - F(\varrho_{\mathrm{exact}}, \varrho_{\mathrm{NNA}})$, where $F(\varrho, \sigma) = = \left(\mathrm{tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2$.

The results for the two extreme cases, $h = 0$ and $h = 10$, corresponding to the ergodic and deep MBL phases, respectively, are presented in Fig. 2. While in the first case the distance drops to relatively low value and then slowly tends to zero upon the increase of the number of iterations, in the second case the distance drops to a value which more or less corresponds to a distance between two randomly-chosen states and does not decrease further.

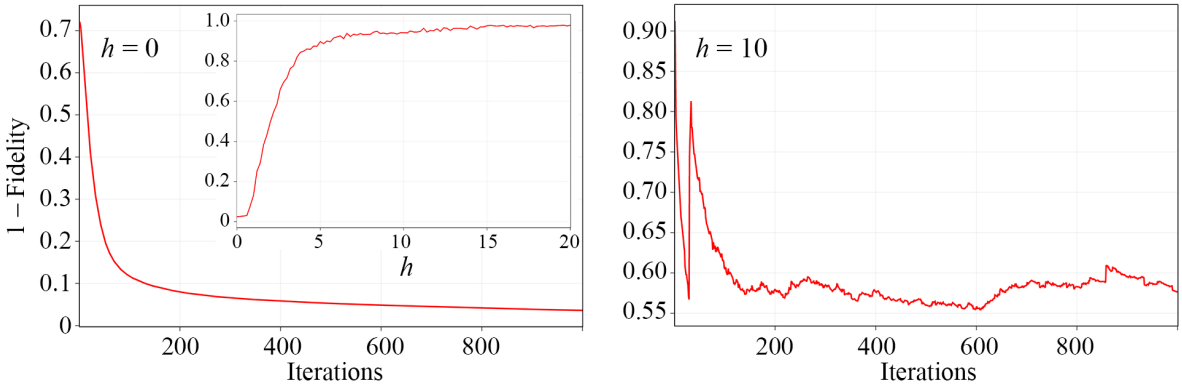

Fig. 2. Distance between the density matrices describing the asymptotic states of the model (1)–(3), $1 - F(\varrho_{\text{exact}}, \varrho_{\text{NNA}})$ as a function of the number of iterations, for $h = 0$ (left panel) and one particular realization of the disorder, $h = 10$ (right panel). ϱ_{exact} is obtained with the diagonalization of the Lindblad superoperator $\mathcal{L}$, while ϱ_{NNA} is obtained with neural-network ansatz (see text for more details). Inset: The distance between the density matrices averaged over 10^4 realizations of disorder as a function of the disorder strength. The number of iterations in all cases was 10^3. Parameters of the model are $\gamma = 0.1$, $U = J = 1$, and $L = 8$

We inspect structures of the density matrices corresponding to the asymptotic states of two particular realizations of the disorder in the ergodic phase, $h = 0$ and $h = 1$. Following the ideas of Ref. [15], we plot the absolute value of the matrix elements. We find a good agreement between the patterns produced by ϱ_{exact} and ϱ_{NNA}; see Fig. 3. Namely, both density matrices, exact and NNA ones, when expressed in the standard lexicographically ordered Fock, exhibit similar fine-structured pattern typical to ergodic states found in Ref. [15].

In the case of MBL regimes, the difference between the structures is distinctive. However, it is not random: While the pattern produced by ϱ_{exact} is dominantly diagonal, with several 'hot spots' along

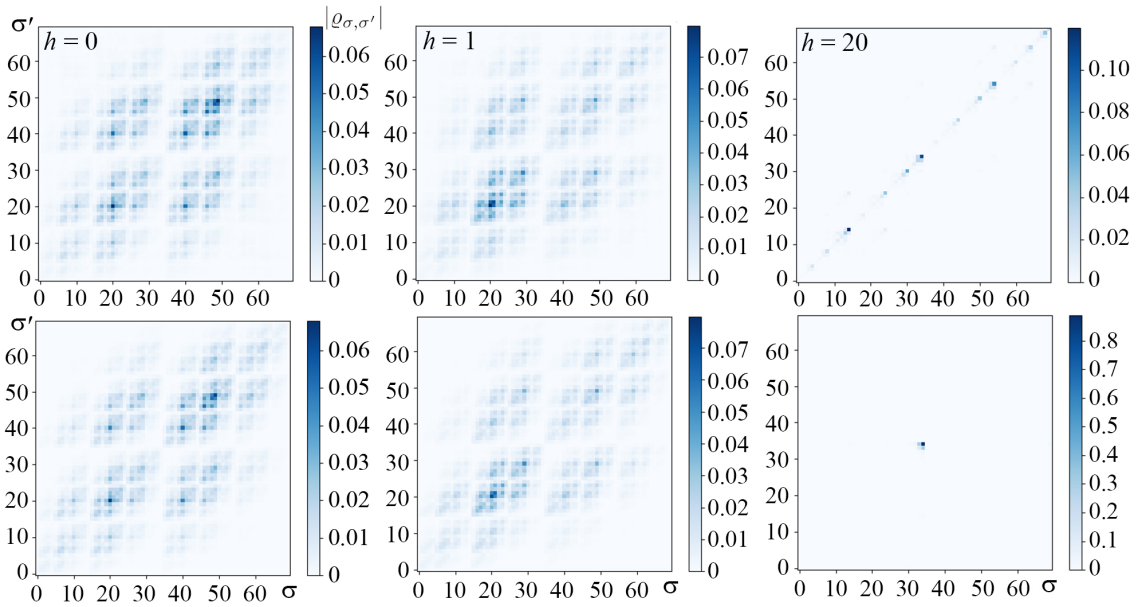

Fig. 3. Absolute values of the elements of the asymptotic density matrix for a single disorder realization and three different values of h. Upper panel: Density matrices ϱ_{exact} obtained with the diagonalization of the Lindblad superoperator $\mathcal{L}$. Lower panel: Density matrices ϱ_{NNA} obtained with the neural-network ansatz. Other parameters are the same as in Fig. 2

the main diagonal (this pattern is typical to the MBL states [15]), ϱ_{NNA} is able to reproduce only one of these spots. By launching the neural network from a randomly chosen initial configuration, we can obtain another density matrix, which reproduces another hot spot.

Conclusions

By using the variations neural-network ansatz proposed in Ref. [11], we analyzed the asymptotic states of the model exhibiting transition between the many-body ergodic and MBL phases.

We found that the performance of the neural network is very different in the two phases. Our conclusion is that many-body localization is somehow imprinted in the cost function landscape which becomes rough upon the increase of the disorder strength and acquires many local minima. Each local minimum corresponds to a single localization hot spot, that is a very localized probability distribution concentrated around single Fock state. The overall MBL density matrix can be represented as a weakly entangled combination of single-hot-spot density matrices. We guess that deep in the MBL state, the exact density matrix can be represented, as a convex combination of single-hot-spot density matrices, $\varrho_{\mathrm{exact}} \approx \sum_{s=1}^{M} p_s \varrho^s_{\mathrm{NNA}}$, where M is the number of localization spots in the Fock basis. Probabilities p_s can be estimated by performing statistical sampling and launching the network from random initial configurations. We plan to move further in this direction; in case this hypothesis is collaborated with numerical results, the link between a genuine quantum phenomena, MBL, and a famous problem of machine learning such as corrugated cot landscape with many local minima, will be established.

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