

Variational neural network parametrisation of the micromotion operator of periodically driven quantum systems

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Periodic driving to manipulate the state and properties of a large class of physical systems, solid-state and atomic systems. The description of periodically driven many-body quantum systems cannot be captured with simple perturbative expansion, and accurate calculation of the time-evolution is required for experimental realisation of dynamical engineering regimes or robust multiqubit gates. Variational parametrisation of manybody wave function encode in neural network architectures has been recently introduced successfully for compressed representation of states with many degrees of freedom. Here we focus on the parametrisation of the Floquet operator of driven two-level system using a Restricted Boltzmann Machine. We explore the range of strong blue off-resonant driving with strength varying from weak to strong. The required complexity of the RBM with the number of Floquet manifold and we adapt the to obtain a the Floquet spectrum converges from an approximated solution the Rotating Wave Approximation. The training of the RBM presents all well-known challenges of neural network parametrisation: vanishing gradient.... These results demonstrate explicitly the capabilities and challenges of RBM in describing harmonically driven systems.

Keywords: Periodic driving, Floquet theory, Restricted Boltzmann Machine

I. INTRODUCTION

quantify the expressive power of NN there is a gap in the understanding. Well understood data sets may offer insight, such as statistical physics, manybody physics, tensor networks and renormalisation.

Training the machine may reveal correlation in the data with physical meaning. these learning task.

RBM can parametrize complex functions of visible units.

Wave functions of many-body systems and away from equilibrium

RBM representations of topological states

These developments raise questions about the expressive power of NN for physical problems. can rbm efficiently describe periodically driven systems. direct relation with exact diagonalisation techniques.

rbm can provide compact representation for a highly entangled quantum states that does not satisfy the entanglement area., with a number of parameters scaling polynomially with the system size.

conclusion: general connection between rbm and tns in arxiv 1701.04831 constitutes a bridge in using techniques for harmonically driven systems.

In the last decade Periodically driven systems are almost present in quantum mechanics. both theoretical and experimentally relevant. drastic modification of physical systems, including spectral signals [], out-of-equilibrium states driven by harmonic forces, transformation of states in . Dynamical decoupling with periodic drivings (several harmonics as in the quantum computing talk I saw), or multiqubit gates by multiple harmonic forces, to Floquet topological insulators and frequency/time-domain quantum simulations.

The time-evolution operator is key, either to define the time-evolution or for definition of effective Hamiltonians. both of them can be written in terms of the Floquet states. Floquet states perturbative theory, RWA,

Bloch-Siegert, ... expansion.... All this approximation and general solution are important to understand, for example.

ML representation of quantum states has been recently very active, showing ... and compatibility with on-line learning and experimental realisation, in particular for the control of quantum states in quantum computing architectures control with Floquet.... The reduction of the parameters required, reflection on the ... of the physically accessible states of the Hilbert space, corresponding to very restricted subsets, which can be described effectively in none such as MPS, tensor Networks.. Such a relation between ML and ... is currently an active area of research ..

Harmonically driven systems can be in the frequency space has the as a Hubbard model [?], and such that time-dependent problem can be evaluated using tools of static systems [], which has not been explored sufficiently. Here I study the parametrisation of the Floquet operator using a RBM for the archetypical case of a driven qubit. The RBM is overkill in this case, with other straight numerical diagonalisation of the Floquet Hamiltonian, however it allows to explore the capabilities of, which can be then applied to other more complex systems where exact diagonalisation or cannot be implemented so directly.

The document is as follows. In Section ?? I present the representation of the time-evolution operator in terms of Floquet states. In section ??, presents the Restricted Boltzmann Machine representation of the states and the loss functions to evaluate the Floquet spectrum. Section ?? shows the representation of Floquet states using the RBM. The central result is presented in section ??, where I discuss the evaluation of the Floquet spectrum (eigenvectors and eigenvalues) evaluated using an RBM parametrisation. Discussion of the applications are presented and conclusion are in section...

FIG. 1. (a) Schematic energy level structure of a generic quantum system. The basis of states consist of a discrete set of energy states, which define several bands according to the level energy spacing. Inter and intra band coupling is induced by electromagnetic radiation tuned at the corresponding frequencies, as indicated by the coupling terms. The wide variety of physical systems described by this model includes (b) trapped ions [?], (c) superconducting qubits [?] and (d) diamond NV-centres [?].

II. FLOQUET FORMALISM

Periodically driven quantum systems are described by a Hamiltonian of the form:

$$H(t) = \sum_{i,j}^D E_{i,j} |i\rangle \langle j| + \sum_{i,j}^D \sum_{n \in \mathbb{Z}} V_{i,j}^n e^{in\omega t} |i\rangle \langle j| + \text{h.c.} \quad (1)$$

where D is the dimension of the Hilbert space, $E_{i,j}$ defines the static component of the Hamiltonian, $V_{i,j}^{\ell,n}$ is the coupling between the states i and j oscillating at frequency $n\omega$ (i.e. the n -th harmonic of the fundamental frequency ω).

Solutions to the corresponding Schrödinger can be build after finding a privileged frame of reference where the transformed Hamiltonian is time-independent and diagonal []. Thus, we are looking for a time-dependent unitary transformation, $U_F(t)$, that satisfies:

$$U_F^\dagger(t) H(t) U_F(t) - i\hbar U_F^\dagger(t) \partial_t U_F(t) = \sum_i \bar{E}_i |\bar{i}\rangle \langle \bar{i}| \quad (2)$$

where \bar{E}_i with $\bar{i} \in [1, D]$ is the set of eigenstates in the frame of reference where the Hamiltonian is static. In this frame of reference, the time-evolution operator is diagonal and the inverse of $U_F(t)$ can be applied to obtain the time-evolution operator in the original basis.

Considering the time-dependence of the coupling terms in the Hamiltonian, we parametrise $U_F(t)$ as a Fourier series of the form [?]:

$$U_F(t) = \sum_{n \in \mathbb{Z}} u_{i,\bar{i}}^n e^{-in\omega t} |\bar{i}\rangle \langle \bar{i}| \quad (3)$$

Using this expansion in the transformation rule Eq. (2) and taking into account the orthonormality of the Fourier basis, we obtain the eigenvalue problem:

$$\begin{aligned} \bar{E}_i U_{i,\bar{i}}^n &= \sum_{j=1}^D \sum_{n \in \mathbb{Z}} (E_{i,j} - \delta_{i,j} n \hbar \omega) U_{j,\bar{i}}^n \\ &+ \sum_{j=1}^D \sum_{m \in \mathbb{Z}} \left[V_{i,j}^m U_{j,\bar{i}}^{n+m} + V_{ji}^{m*} U_{j,\bar{i}}^{m-n} \right] \end{aligned} \quad (4)$$

which lead us to a finite matrix representation after truncating the sums in eq. (3).

For concreteness, in this paper we consider a harmonically driven qubit with the Hamiltonian:

$$H = \frac{\hbar\omega_0}{2} \sigma_z + \frac{\hbar\Omega}{2} \sigma_x \cos(\omega t + \phi) \quad (5)$$

with the Pauli matrices σ_i with $i \in [x, y, z]$ [].

In this case, the Fourier components of the unitary transformation $U_F(t)$ are the eigenvectors of the matrix:

$$\mathcal{H} = \hbar\omega_0 \begin{pmatrix} \frac{1}{2}\sigma_z + 3\bar{\omega}I & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x & 0 & 0 & 0 & 0 & 0 \\ e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z + 2\bar{\omega}I & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x & 0 & 0 & 0 & 0 \\ 0 & e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z + \bar{\omega}I & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x & 0 & 0 & 0 \\ 0 & 0 & e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x & 0 & 0 \\ 0 & 0 & 0 & e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z - \bar{\omega}I & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x & 0 \\ 0 & 0 & 0 & 0 & e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z - 2\bar{\omega}I & e^{i\phi}\frac{\bar{\Omega}}{4}\sigma_x \\ 0 & 0 & 0 & 0 & 0 & e^{-i\phi}\frac{\bar{\Omega}}{4}\sigma_x & \frac{1}{2}\sigma_z - 3\bar{\omega}I \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (6)$$

The unitary transformation is of the form.

However, due to the symmetry of the, we can select any set of and. It is natural to select the central columns and repeat, we have to parametrise only a reduced set of the elements of the matrix.

In the regime of off-resonant + weak-to-strong driving. More precisely, our numerical results are obtained for the parameters $\omega = 1.7\omega_0$ and the Rabi frequency $\Omega \in [0, 10] \times \omega_0$. Figure presents the energy gap between the dressed states as a function of the Rabi frequency Ω and the eigen states of selected parameters.

The wavefunction has the symmetry, $n \rightarrow n + m$,

$$U_{i,\bar{i}}^n = U_{i,\bar{i}}^{m+n} \quad (7)$$

which is used to reduce the number of parameter below. The

III. PARAMETRISATION OF THE MICROMOTION OPERATOR

The dressed states defined by U_F are time-dependent superposition of the elements of the basis:

$$|\bar{i}\rangle = \sum_{j,n} u_{j,\bar{i}}^n e^{in\omega t} |j\rangle \quad (8)$$

with the coefficients of U_F .

Following the Troyer Calero ... and tohre, we parametrise theses elements with a pair of Restricted Boltzman Machines (RBM) that define their amplitude and phase. Simple generalisation of the RBM for spin systems. In this case, the state of each cell of the visible layer is given by a set of integers that identify the element. $\sigma = j, \tilde{i}, n$, the projection of angular momentum of the bare and dressed states, and $n \in Z$ the Floquet manifold index. The state of the hidden layer is $\mathbf{h} = (h_1, h_2, h_3, \dots, h_M)$ with the binary variables $h_i \in -1, 1$ for $i = 1, \dots, M$.

The micromotion fourier components can be parametrized by:

$$u_{j,\tilde{i}}^n = \sqrt{\frac{P_\lambda(\sigma)}{Z}} \exp(\phi_\mu(\sigma)) \quad (9)$$

with the marginal probabilities:

$$P_\kappa(\sigma) = \sum_{\{\mathbf{h}\}} p_\kappa(\sigma, \mathbf{h}) \quad (10)$$

obtained from the ... probability.

$$p_\kappa(\sigma, \mathbf{h}) = \exp(\mathbf{b}_\sigma \cdot \sigma + \mathbf{c}_\mathbf{h} \cdot \mathbf{h} + \mathbf{h}^T \cdot \mathbf{W}_{\mathbf{h},\sigma} \cdot \sigma) \quad (11)$$

for $\kappa = \lambda$ and μ .

In this case, the symbol σ is an array of numbers that labels the element of the Floquet matrix. For the driven two level system, we choose $\sigma = i, \tilde{i}, 1/n$, with $i, \tilde{i} \in -1/2, 1/2$ the projection of angular momentum of the bare and dressed states, and $n \in Z$ the Floquet manifold index.

The single layer RBM allows us to obtain an analytical expression for the marginal probabilities:

$$P_\kappa(\sigma) = \exp(\mathbf{b}_\sigma \cdot \sigma) \prod_{j=1}^h \cosh(\mathbf{c}_j + \mathbf{W}_j \cdot \sigma) \quad (12)$$

The ... function can be build from our objective of diagonalizing the matrix. We define the distance of matrix from a diagonal form ...

$$\text{norm}(\mathcal{H}) = \sum_i \sum_j \quad (13)$$

IV. RBM PARAMETRISATION OF FLOQUET STATES

The numerically exact Floquet states (the fourier coefficients of expansion...) straigh forward by diagonalisin eq [? ?].

teh Kull-lll loss function:

$$k = \sum_i p_i \log \frac{p_i}{p_i} \quad (14)$$

The training starts of wit a random distribution of all parameters with choosen as ..to train both RBm

parametrisation of the amplitude and the phase, I loop swapping one, starting of a random initialiaization of the RBM parameters. The parameers of the amplitude are choosen as randon, while

Typical training problems and parameters. Accuracy.

V. EVALUATING THE FLOQUET SPECTRUM USING ARBM

Finding the full spectrum of quasienergies and the .

As an initial guess for the parameters, we train the RBM to fit the RWA, which can be evaluated in . The second is the definition of a loss fuction. IN this case we wnat a that the matrix ooperion... lead to a diagonal form .we define distance as the difference between the of the values with the correponding diagonal elelmemtn. The training of this .. shown in ...

As a second form of the loss function is a quantification of the diffeence between the lefhs vectors and the initila vectors. They should only differr in the scale, such . the candidate eigenvalue is chooslen as teh ratio between ... and Then we evaluate the difference. The traing .. suffer similar difficulties taking a long number of steps and requirieing a small loss rate.

Combination of the two loss functions during traingin in a randomly between loss functions. We observe a spped up of the traing, improve of the fidelity with the esxac, as well an improvment of the numerically exact Floquet spectrum.

VI. DISCUSSION

Loss function with slow learning. Investigation in better loss function as well as dragging tools from ML to speep up ..

The difficultly of training consittues a tool for characterising physicl system as Hre we have observed that complex wavefuntion rquire more traing effort. application for example to floque driven systems.

Applicaton for evaluating the longtime evluation. nitial guess functions to improve convegency. CONversely, the training wave functin and the distribution/correlation of the coefficients correlated with othe critier of the system..

The application of symmetries an boundary coditions to the floquet states. Also, this can be readly extended to multimode scaling of multimodedriven system (with uncommensurable frequencies).

RBM parametrisation fits any function.

Floquet states requiring more Fourier components are harder to train.

several ways to define a loss function.

Slow gradient

random selection of criteria similar to ensemble learning

the RWA approximation is a good start generically and evolves towards the solution. speeding up the convergence ML .

More interesting is the construction of the initial guess and restriction of the solutions explored, for example that the amplitude of Floquet manifolds should be small.

here we explored the RBM parametrisation to build the micromotion operator. Other parametrisation can be more efficient for optimisation. Such construction of the initial guess and constraints can be come from using Tensor Networks parametrisation, or ...

VII. CONCLUSION

In this paper we present a premier explorative study of the use of RBM for the parametrisation of Floquet operators, in an archetypical periodically driven system. We obtain that training of the can be done , which is equivalent to the experimentally demonstrated in .. with online learning of the wavefunction.

The evaluation of the Floquet spectrum is a more difficult task. the initial guess guides the minimum of the defined loss function. simple definitos vse on the properties of a diagonal matrix and present low gradients . combination of loss function sa better, reflection on the ensemble learning combination fo other simple architecture of the wave function, eg a NN can led to for more complex systems tahtn the studeid here.

In this work we present a initial exploration of using RBM for Floquet problems. the Floquet states staes can be parametrised efficiently following similar approaches, even with an alternative fitting of the complex and the

wavefunction amplitude. this task can be qualified as easy, rapid from random distributon.

Finding the Floquet sates is a harder task. using as initial guess the RWA training . the function has a slow after a fast decline. however a combination of loss functions satisfied by any dagonal matrix or the eigne vectors helps to guide the search. configuraiotn.. . Perhaps a different . The micromotion operator is the time-evolution operator, then other ML architehqure might present better. Also

This starting point for exploratioon of the use of parametrisatio for more complex ...like .. . The numerical effort for the case studied here is overkilling, however we explore typical taht might be present in other driven quantum systems.

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APPENDIX A: RESTRICTED BOLTZMAN MACHINE PARAMETRISATION OF $u_{j,i}^n$

APPENDIX B: TYPICAL AND NO SO TYPICAL TRAINING RESULTS

APPENDIX A: TYPICAL EXAMPLE OF THE MATRIX REPRESENTATION OF THE MULTIMODE HAMILTONIAN