Title: Advances in the description of out-of-equilibrium quantum systems: from the time-dependent Variational Monte Carlo to the Neural-network Quantum States.

Date: Jun 21, 2016 03:30 PM

URL: http://pirsa.org/16060106

Abstract: <p>Strongly interacting quantum systems driven out of equilibrium represent a fascinating field where several questions of fundamental importance remains to be addressed [1].</p>

<p>These range from the dynamics of high-dimensional interacting models to the thermalization properties of quantum gases in continuous space.</p>

<p>In this Seminar I will review our recent contributions to some of the dynamical quantum problems which have been traditionally inaccessible to accurate many-body techniques.</p>

<p> </p>

<p>I will first focus on the main methodological developments we devised in the past years.</p>

<p>In particular, I will describe the time-dependent Variational Monte Carlo method [2,3] and two notable classes of variational quantum states : the time-dependent Jastrow-Feenberg expansion, and the most recently introduced Neural-network Quantum States [4]. These states can achieve high (and controllable) accuracy both in one and higher dimensions.</p>

<p>Then, I will discuss specific applications to the problem of information spreading in both short- and long-ranged interacting quantum systems [3,5]. Finally, I will also discuss recent applications to thermalization properties of Lieb-Liniger quantum gases [6].</p>

Quantum Systems Out Of Equilibrium

From Time-Dependent Variational Monte Carlo to Neural-Network Quantum States

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June 21, 2016

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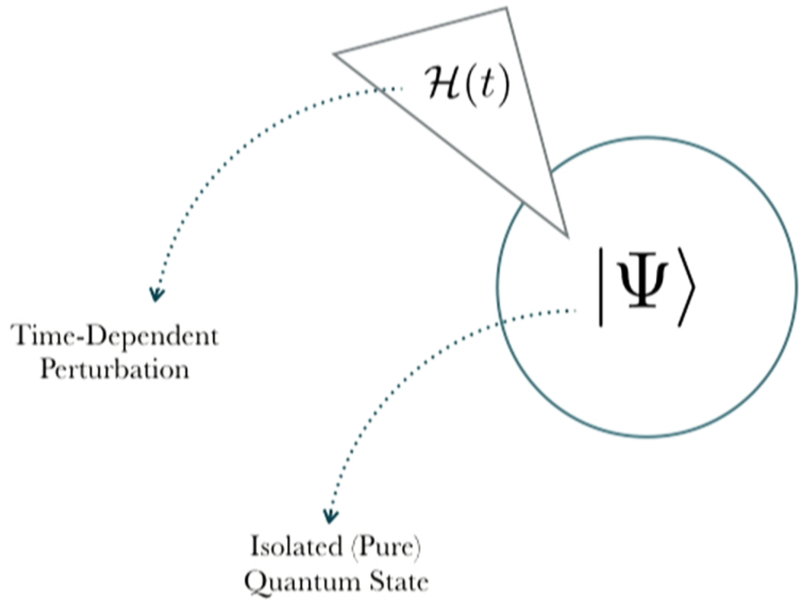
Methods
For
Which
Problems?

General Problem



Assumptions

The perturbation is **not** necessarily small
(beyond linear response)

Purely **unitary** time-evolution
(no bath, stochastic dissipation etc)

Out-Of-Equilibrium Dynamics

Quantum Quenches

$$e^{-i\mathcal{H}t}|\Psi\rangle$$

Unitary dynamics of
a pure state

Driving Hamiltonian

$$\mathcal{T}e^{-i\int_0^t dt'\mathcal{H}(t')}|\Psi\rangle$$

Unitary dynamics with
a time-varying Hamiltonian

Fundamental Questions

How to reconcile Schrödinger
with Boltzmann?

$$\mathrm{Tr}\, e^{-\frac{\mathcal{H}}{k_b T}}$$

Which Temperature?

How fast equilibrium is reached?

Defect production across
a phase Transition

Consequences for
Adiabatic Computing?

A Methodological Challenge in Physics

Exact Approaches

Exact Diagonalization/Lanczos

Limited to small systems

Path-Integral Monte Carlo

Severe Phase Problem

Ill-conditioned inversion of Laplace transform

Tensor Network Methods

DMRG / Matrix Product States / PEPS

Mostly limited to 1D/ short time scales

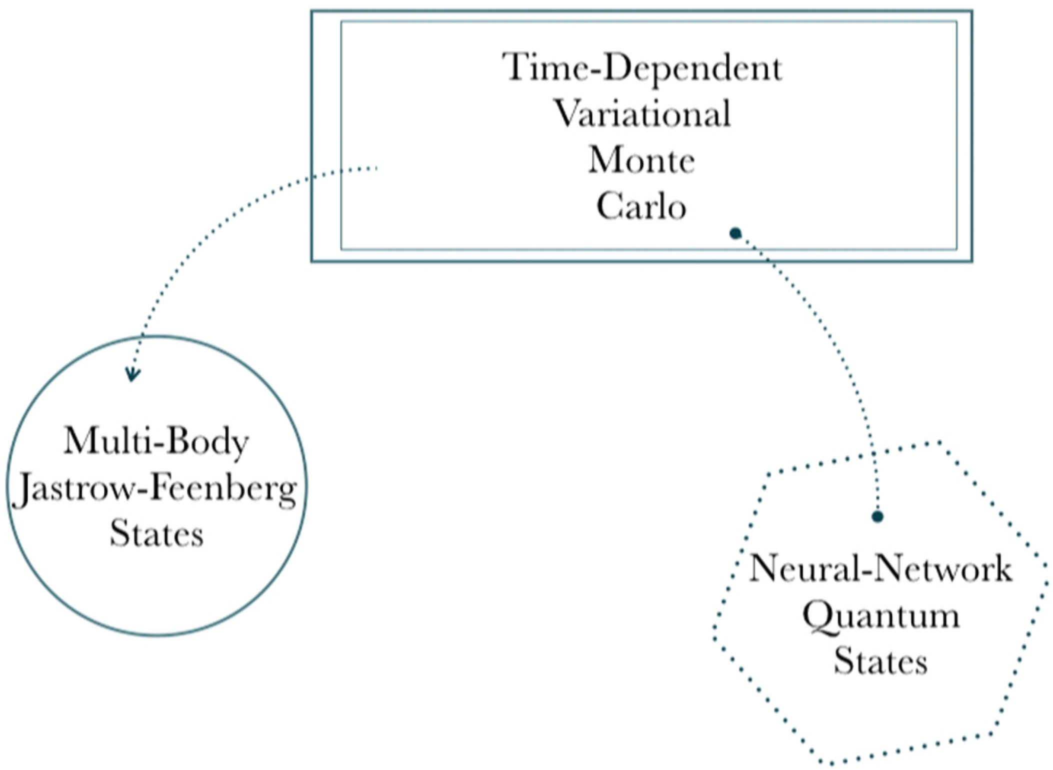
Mostly lattice systems

Mean-Field Dynamics

No limitations on geometry/timescales

Poor qualitative and quantitative accuracy

In This Talk



Time-Dependent
Variational
Monte
Carlo
Multi-Body
Jastrow-Feenberg
States
Neural-Network
Quantum
States

General Method

Time-Dependent Variational Monte Carlo

Static Variational Principle

Quantum Hamiltonian

$$\mathcal{H}$$

Variational State

$$\langle \mathbf{X} | \Psi(\alpha) \rangle$$

Variational Energy

$$E_{\text{var}}(\alpha) = \frac{\langle \Psi(\alpha) | \mathcal{H} | \Psi(\alpha) \rangle}{\langle \Psi(\alpha) | \Psi(\alpha) \rangle}$$

Functional of Variational Parameters

Optimal Variational Ground State

Minimize energy with respect to α

$$E_{\text{var}}(\alpha) = \frac{\sum_k c_k^2 E_k}{\sum_k c_k^2} \geq E_0$$

Time-Dependent Variational Principle

Dirac and Frenkel (1930's)

Exact Generator of the Dynamics

$$\frac{d}{dt}\left|\Psi_{\rm ex}(t)\right\rangle = -i\mathcal{H}(t)\left|\Psi(t)\right\rangle$$

← Time-dependent Schrödinger

Variational Generator

$$\frac{d}{dt}\left|\Psi_{\rm var}(t)\right\rangle = \sum_k \dot{\alpha}_k(t)\mathcal{O}_k\left|\Psi(t)\right\rangle$$

$$\mathcal{O}_k(X) = \frac{1}{\langle X|\Psi\rangle}\frac{\partial\langle X|\Psi\rangle}{\partial\alpha_k}$$

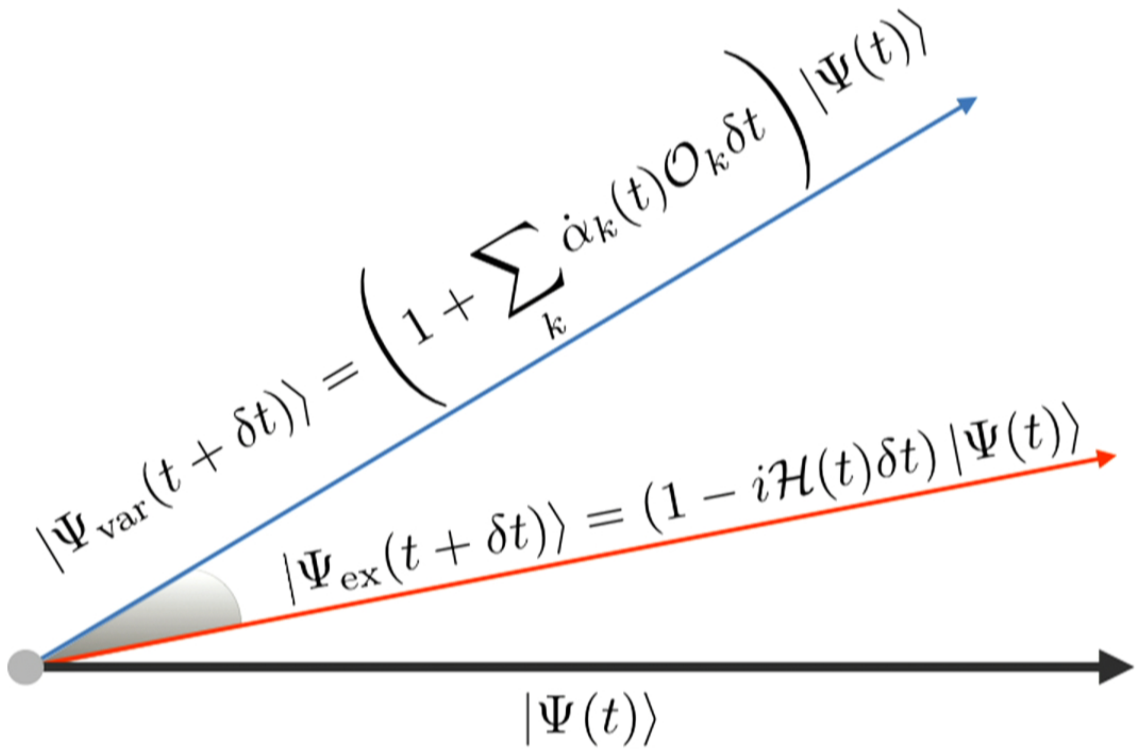
Optimal Variational Dynamics

↕

Minimize the distance between the two generators

$$\left|\frac{d}{dt}\left|\Psi_{\rm ex}(t)\right\rangle - \left|\Psi_{\rm var}(t)\right\rangle\right|^2 \geq 0$$

Geometrical Interpretation



Optimal Equations of Motion

Carleo et al. , Scientific Reports 2, 243 (2012)

$$\sum_{k'} \langle \mathcal{O}_k^\star \mathcal{O}_{k'} \rangle_t^{\mathrm{c}} \, \dot{\alpha}_{k'}(t) = -i \, \langle \mathcal{O}_k^\star \mathcal{H}(t) \rangle_t^{\mathrm{c}}$$

Connected averages

$$\langle \mathcal{AB} \rangle_t^{\mathrm{c}} = \langle \mathcal{AB} \rangle_t - \langle \mathcal{A} \rangle_t \langle \mathcal{B} \rangle_t$$

$$\langle \ldots \rangle_t = \frac{\langle \Psi(t) | \ldots | \Psi(t) \rangle}{\langle \Psi(t) | \Psi(t) \rangle}$$

Features

- Symplectic equations
- Total energy exactly conserved (time-ind. hamiltonians)
- Satisfy Ehrenfest theorem for entangling operators
- Can be derived also from principle of least action

Time-Dependent Variational Monte Carlo

Carleo et al. , Scientific Reports 2, 243 (2012)

Sample $|\langle \mathbf{X}|\ \Psi(\alpha)\rangle|^2$ with Metropolis-Hastings algorithm

Measure expectation values entering equation of motion

Solve for time-derivatives of variational parameters $\dot{\alpha}(t)$

Obtain state at next time with standard ODE scheme

Variational States

Jastrow-Feenberg States

Time-Dependent Jastrow-Feenberg Expansions

(2012-Today)

Spin/Bosons Lattice Systems

$$\langle \sigma^z | \Psi(t) \rangle = \exp\left[\sum_i J_i^{(1)}(t)\sigma_i^z + \frac{1}{2!}\sum_{i\neq j} J_{i,j}^{(2)}(t)\sigma_i^z\sigma_j^z + +\frac{1}{3!}\sum_{i\neq j\neq k} J_{i,j,k}^{(3)}(t)\sigma_i^z\sigma_j^z\sigma_k^z + \dots \right]$$

Multi-Body effective interactions

Continuos-Space Systems

$$\langle \mathbf{X} | \Psi(t) \rangle = \exp\left[\sum_{i=1} J^{(1)}(x_i, t) + \frac{1}{2!}\sum_{i\neq j} J^{(2)}(x_{ij}, t) + \frac{1}{3!}\sum_{i\neq j\neq k} J^{(3)}(x_{ijk}, t) + \dots \right]$$

Multi-Body Variational Fields

Correlated Slater-Projected Wave-Functions

Ido et al. , Phys. Rev. B 92, 245106 (2015)

Lattice Fermions

$$|\Psi\rangle = \mathcal{J} \times \mathcal{L}^K \times \mathcal{L}^S |D\rangle$$

Jastrow Factor

Momentum Projection

Spin Projection

$$|D\rangle = \left(\sum_{i,j} f_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} \right)^{N/2} |0\rangle$$

Slater Determinant

Overview
of
Some
Applications

(I)
Thermalization in Ultra-Cold Atoms

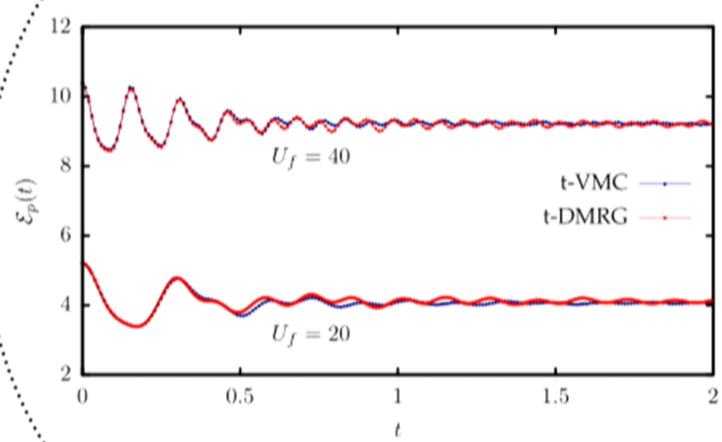
Lattice Bosons

Carleo et al., Sci. Rep. 2,243 (2012)
Carleo et al. , Phys. Rev. A 89, 031602 (Rapid) (2014)

Quantum Quench in the Bose-Hubbard Model

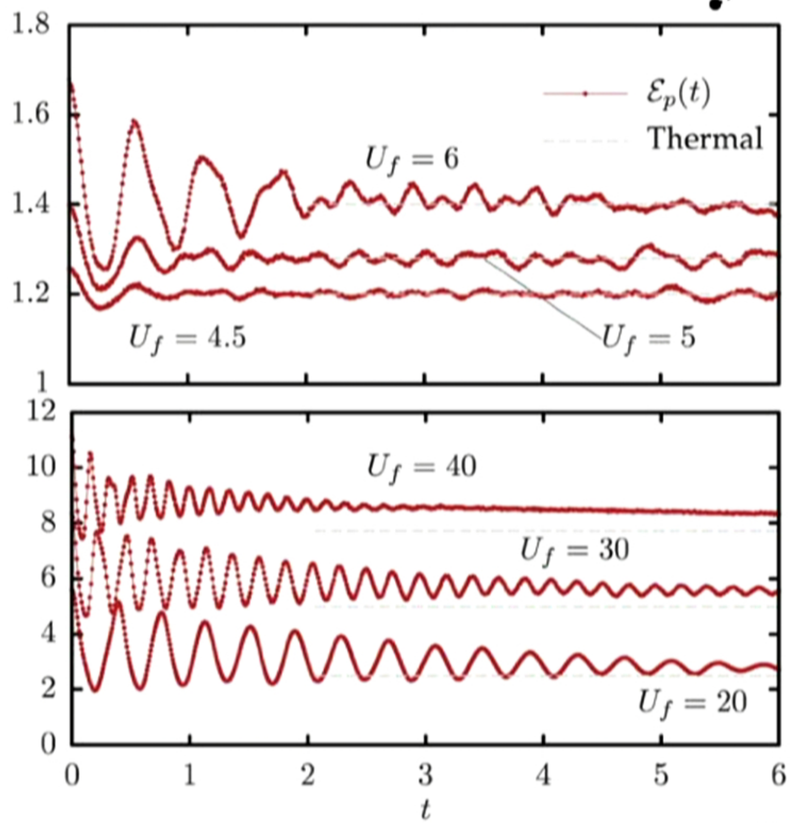
$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + \frac{U}{2} \sum_i n_i \left(n_i - 1 \right)$$

Quench from a superfluid phase



Comparison with t-DMRG in one dimension

Non-Thermal Behavior In Two Dimensions



Thermal Behavior quenching to small interactions

Non-Thermal Behavior quenching to strong interactions

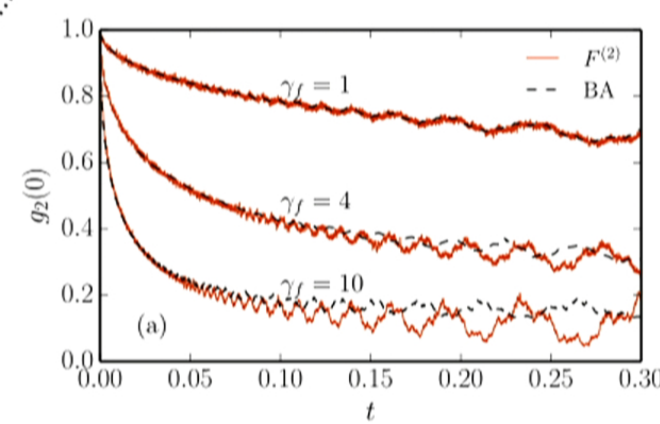
One-Dimensional Quantum Gases

Carleo, Cevolani, Sanchez-Palencia, and Holzmann
In preparation (2016)

Quantum Quench in the Lieb-Liniger Model

$$\mathcal{H} = \int dX \left[\frac{\hbar^2}{2m} \nabla\psi^\dagger \nabla\psi + \frac{g}{2}\psi^\dagger\psi^\dagger\psi\psi \right]$$

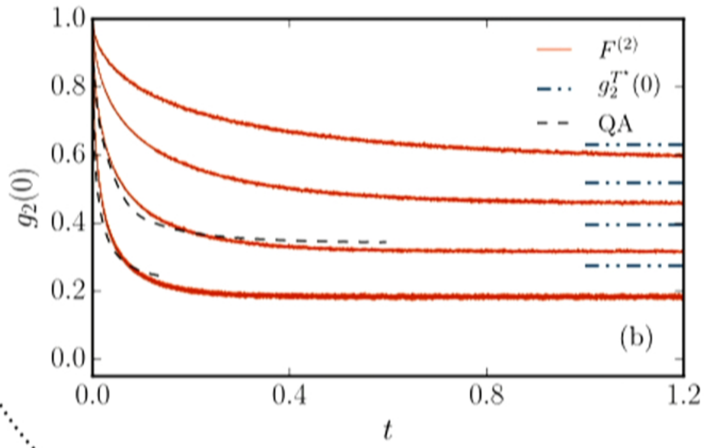
Quenches in the interaction strength

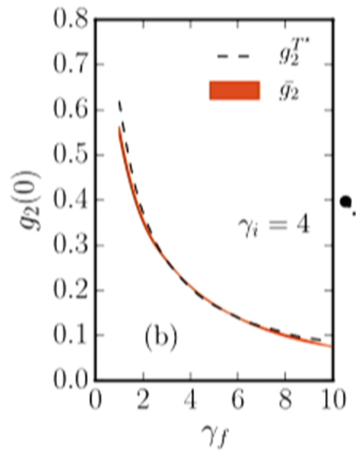


Comparison with Bethe Ansatz for Small Systems

Integrability in Quantum Gases

Carleo, Cevolani, Sanchez-Palencia, and Holzmann
In preparation (2016)





Non-Thermal
Behavior
quenching
from ideal BEC

Thermal
Behavior
quenching
from finite
interactions

Lieb-Robinson Bounds

Short-range Hamiltonians

$$\langle \mathcal{A}(R,t)\mathcal{B}(0,t)\rangle - \langle \mathcal{A}(R,0)\mathcal{B}(0,0)\rangle \leq \text{const} \times \exp\left[-(|R| - v|t|)\right]$$

Correlations suppressed outside the "light-cone" region $t < R/v$

E. H. Lieb and D. W. Robinson (1972)

Long-Range Hamiltonians

$$\mathcal{H}_{\text{nl}} \simeq \frac{1}{R^{\alpha}}$$

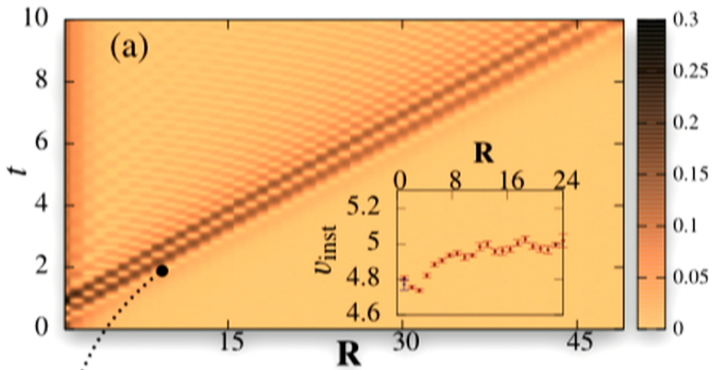
Unbounded correlations for $\alpha < D$ — *M. B. Hastings (2010)*

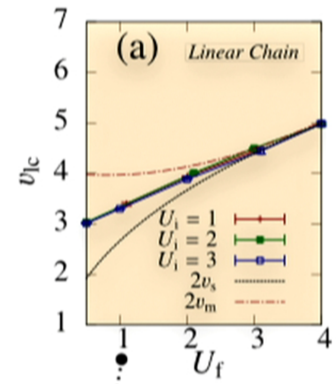
Superballistic bound for $\alpha > D$ — *M. Foss-Feig et al. (2015)*

Information Spreading in Superfluids

Carleo et al., Phys. Rev. A 89, 031602 (Rapid) (2014)

$$G(R,t) = \langle n_i n_{i+R} \rangle_t$$



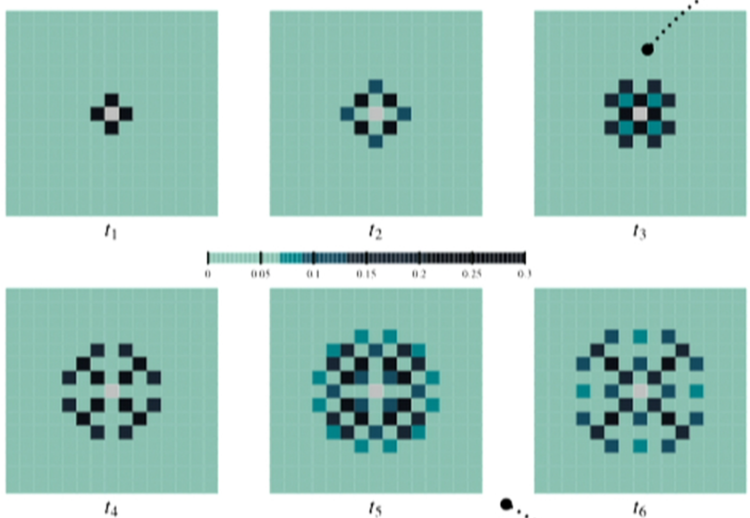


- Light-Cone Effect

  Ballistic regime only for sufficiently long times

  Universality of Light-Cone velocity

"Light-Cone" Effect in Two Dimensions

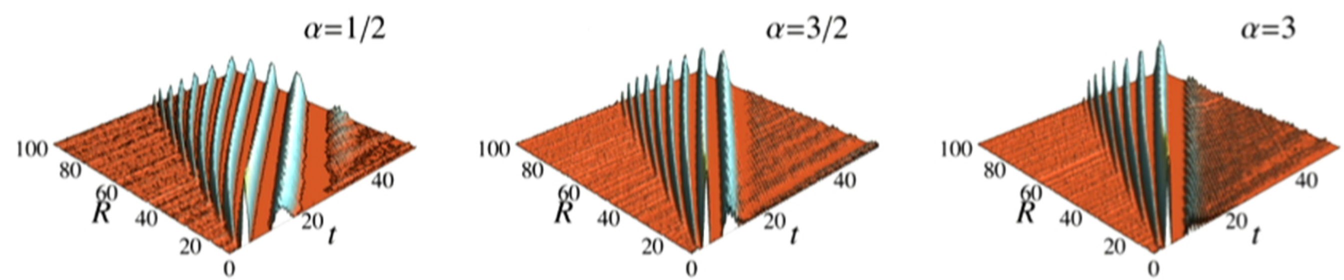


Local
Spreading of
Information
Lieb-Robinson
Bounds

Anisotropic
Spreading
Due to Lattice
Effects.
Observable in
Experiments

What About Long-Range Bosons?

Cevolani et al., Phys. Rev. A 92, 041603 (Rapid) (2015)



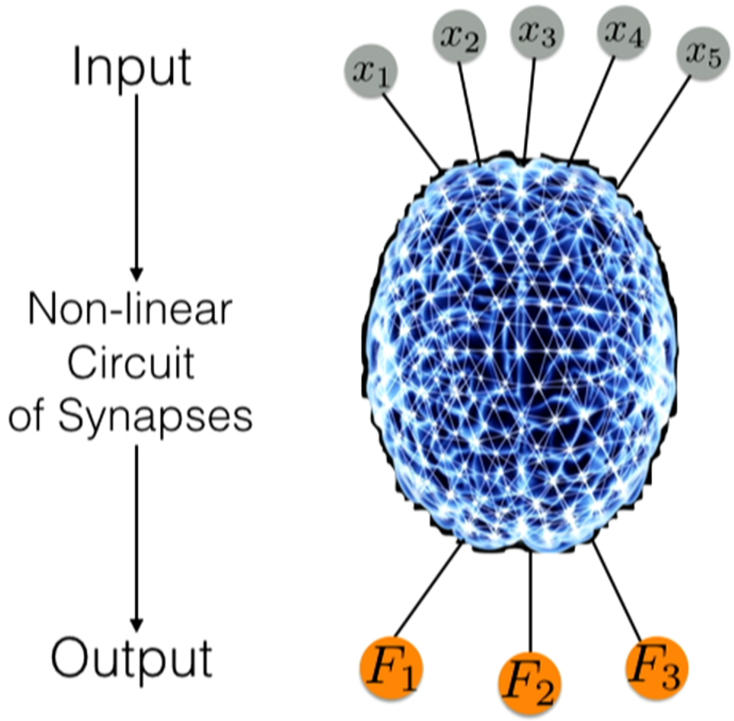
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_{i<j} \frac{n_i n_j}{R_{i,j}^\alpha}$$

- Strong Light-Cone Effect
- Locality Preserved even at Small Alpha
- Non-Local Modes Have Small Weights

New-Born Variational States

Neural-Network Quantum States

Neural Networks in Brief

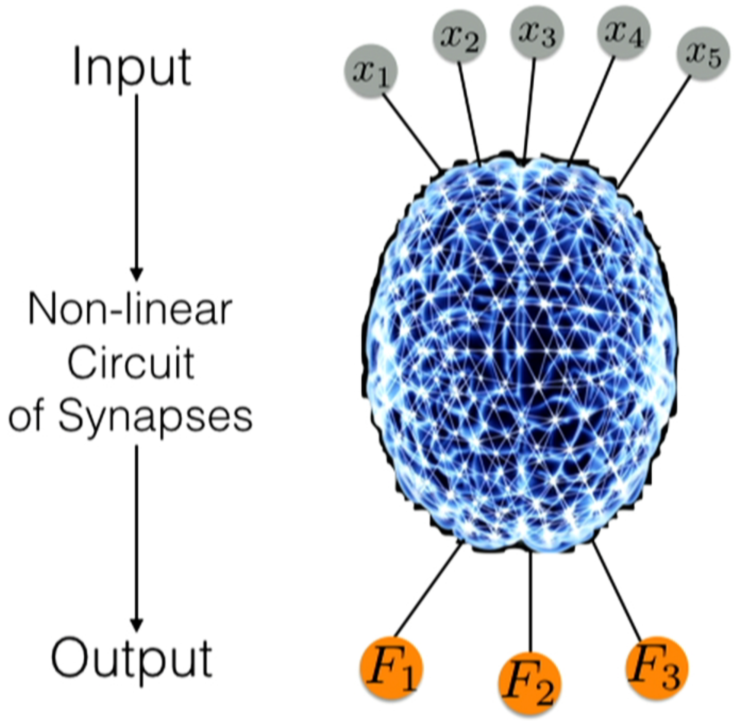


A brain can be seen as a function of high-dimensional input

$$\mathbf{F}(\mathbf{x};\mathbf{W})$$

network weights (to be learned from experience)

Neural Networks in Brief



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$$\mathbf{F}(\mathbf{x}; \mathbf{W})$$

network weights (to be learned from experience)

As much as a cow can be assumed to be spherical…

Example of Use : Classification

Input Space : Image Bits

Output Space : class to which the image belongs to

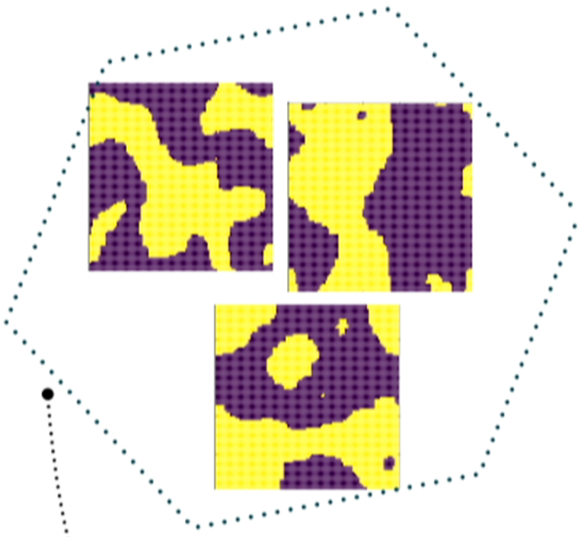
Training : fit network weights to (a few) known cases

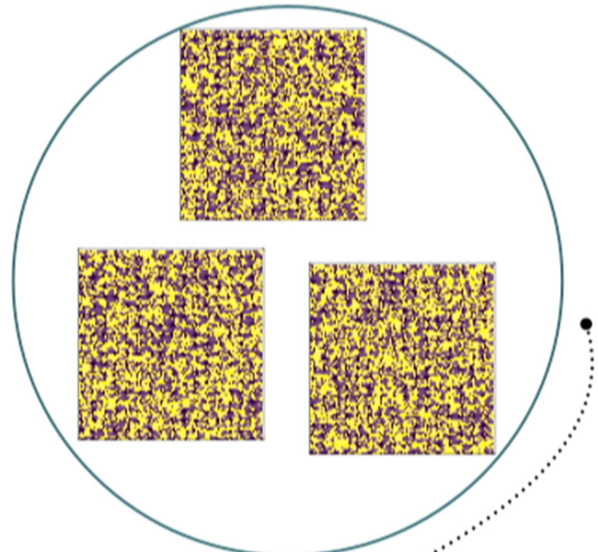
Generalization : classify never-seen images

Recent Applications to Phase Transitions

J. Carrasquilla, and R. Melko, arXiv:1605.01735 (2016)

L. Wang, arXiv:1606.00318 (2016)





- Classification of phases of matter
- Very useful when order parameter is unknown

Reinforcement Learning

(For example, the game of Go)
D. Silver et al., Nature 529, 484 (2016)

Play a game with the current game policy
(interactive learning)

Obtain the final score

Change the game policy

Game policy is a high dimensional function
Encoded with complex neural networks

Neural-Network Quantum States (I)

G. Carleo, and M. Troyer, arXiv:1606.02318 (2016)

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A Many-Body Wave-Function can be approximated by a neural network

$$\Psi(\sigma_1^z, \sigma_2^z, \ldots \sigma_N^z; \mathbf{W})$$

network weights (to be learned from quantum mechanics rules)

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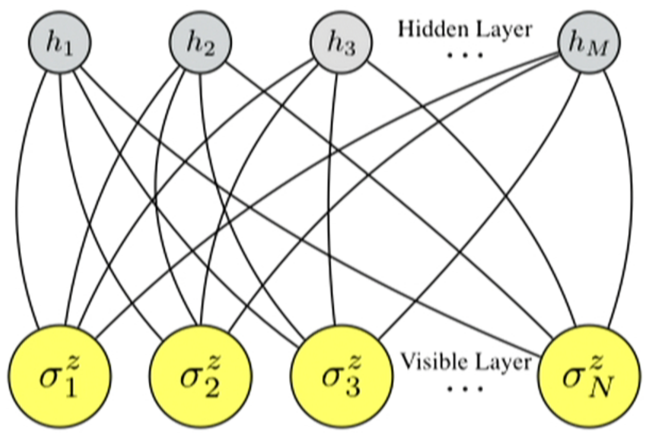

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$$\Psi(\sigma_1^z, \sigma_2^z, \ldots \sigma_N^z; \mathbf{W})$$

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Restricted Boltzmann Machine

More Hidden Neurons Make it Smarter (and more accurate)

Neural-Network Quantum States (II)

G. Carleo, and M. Troyer, arXiv:1606.02318 (2016)

$$\Psi(\sigma_1^z, \sigma_2^z, \dots \sigma_N^z; \mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Variational Parameters

Accuracy increased adjusting $\alpha = M/N$

Correlating part consists of αN^2 parameters

> Representability theorems guarantee that arbitrary accurate approximations of bounded functions exist

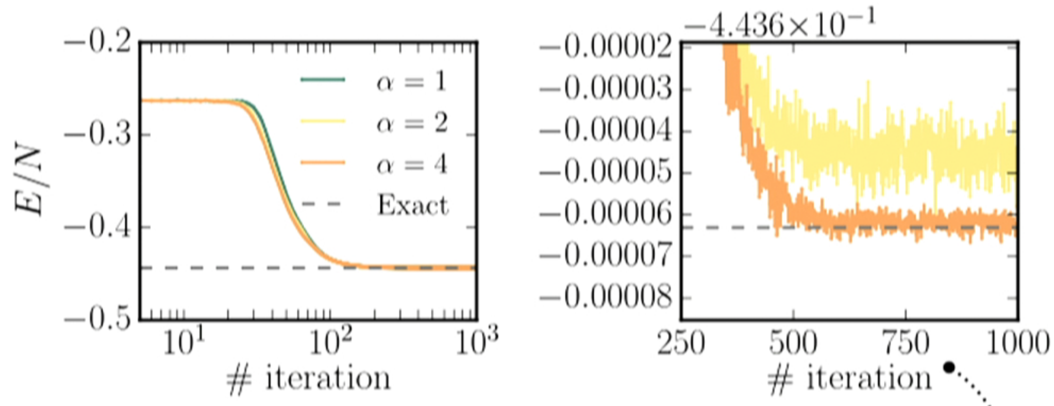
The Game of Quantum Mechanics

Sample wave-function with current set of network parameters

Obtain the average energy
(Or t-VMC quantities)

Change network parameters

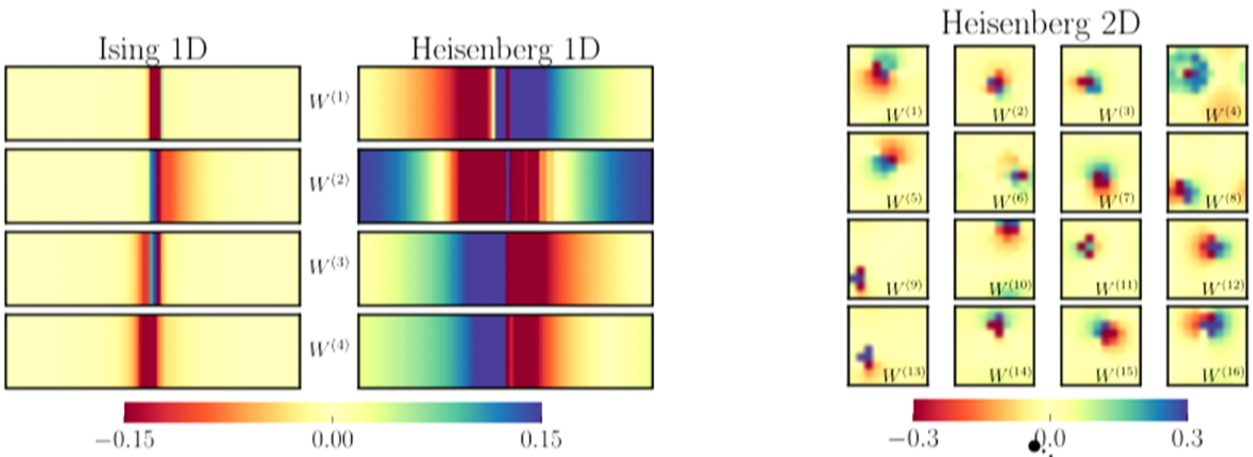
Ground-State Properties with NQS (I)



Stochastic approach to optimization (SR method)

Very High Accuracy can be systematically obtained

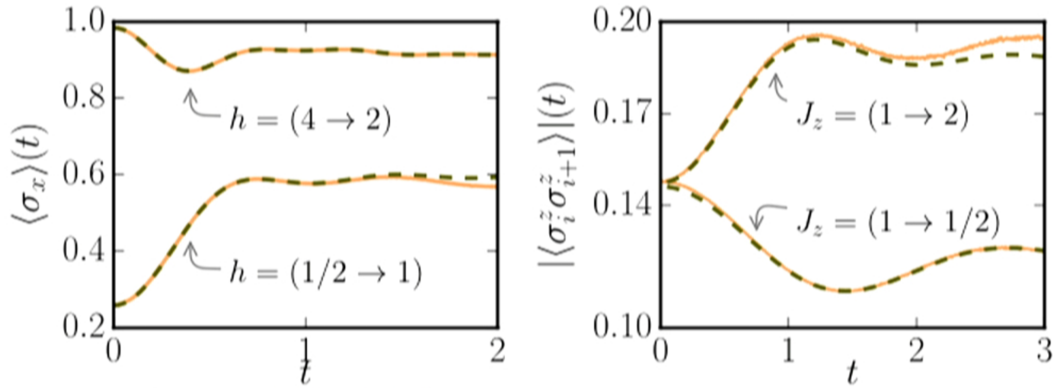
How the Ground State Looks Like



Feature filters for translation invariant systems

In 2D a larger number of filters is needed
(more symmetries to be learned)

Quantum Dynamics with NQS



1D Transverse-Field Ising

1D Heisenberg Model

Quantum Quenches in 1d Model

Shown results at alpha=4

High precision and improvable at larger alphas

Effective solution of the phase problem

Why These States Work

Nature Likes "Simple" Things

Physical States in the Hilbert space are characterized by (a few) important features

Neural Networks effectively identify and described these features

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NQS Have Long-Range Correlations

Network connections are non-local in space

Suitable to describe critical phases in any dimension

Outlook

Time-Dependent Variational Monte Carlo

Quantum Monte Carlo method can **actually** do unitary dynamics → Just elude the phase problem with accurate variational wave-functions

Accurate access to traditionally hard regimes and systems

- High-Dimensional lattice systems
- Continuos-Space models
- Adiabatic Computing For Large # of qubits

Outlook

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Neural Network Quantum States

A new powerful tool to solve ground-state and dynamics → *It learned Bethe Ansatz much faster than I ever did*

Controlled approximation → *Make your wave-function smarter increasing the number of neurons*

A new challenge for quantum information → *Is entanglement what matters for these states? Why can they be much more compact than MPS?*