Time-Dependent Variational Monte Carlo
In Collaboration With

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A Method For Which Problems?
General Problem

$|\Psi\rangle$

$\mathcal{H}(t)$

Time-Dependent Perturbation

Isolated (Pure) Quantum State

Assumptions

The perturbation is \textbf{not} necessarily small (beyond linear response)

Purely \textit{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?

$$\text{Tr} e^{-\frac{\mathcal{H}}{k_B T}} \quad \text{Which Temperature?}$$

How fast equilibrium is reached?

Defect production across a phase transition

Consequences for Adiabatic Computing?
A Challenge in Computational 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
- Quench Dynamics
- Adiabatic Quantum Computing
Method and Variational States
Static Variational Principle

Quantum Hamiltonian

\[ \mathcal{H} \]

Variational State

\[ \langle X | \Psi(\alpha) \rangle \]

Variational Energy

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

Optimal Variational Ground State

Minimize energy with respect to \( \alpha \)

\[ E_{\text{var}}(\alpha) = \frac{\sum_k c_k^2 E_k}{\sum_k c_k^2} \geq E_0 \]
Time-Dependent Variational Principle
Dirac and Frenkel (1930’s)

**Exact Generator of the Dynamics**

\[
\frac{d}{dt} |\Psi_{\text{ex}}(t)\rangle = -i\mathcal{H}(t) |\Psi(t)\rangle
\]

\[\longleftrightarrow\text{ Time-dependent Schrödinger}\]

**Variational Generator**

\[
\frac{d}{dt} |\Psi_{\text{var}}(t)\rangle = \sum_k \dot{\alpha}_k(t) \mathcal{O}_k |\Psi(t)\rangle
\]

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

**Optimal Variational Dynamics**

Minimize the distance between the two generators

\[
\left| \frac{d}{dt} |\Psi_{\text{ex}}(t)\rangle - |\Psi_{\text{var}}(t)\rangle \right|^2 \geq 0
\]
Geometrical Interpretation

\[ |\Psi_{\text{var}}(t + \delta t)\rangle = \left(1 + \sum_k \dot{\alpha}_k(t) O_k \delta t\right) |\Psi(t)\rangle \]

\[ |\Psi_{\text{ex}}(t + \delta t)\rangle = (1 - i\mathcal{H}(t) \delta t) |\Psi(t)\rangle \]
Optimal Equations of Motion

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

\[
\sum_{k'} \langle \mathcal{O}^*_k \mathcal{O}_{k'} \rangle^c_t \dot{\alpha}_{k'}(t) = -i \langle \mathcal{O}^*_k \mathcal{H}(t) \rangle^c_t
\]

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

Connected averages

\[
\langle AB \rangle^c_t = \langle AB \rangle_t - \langle A \rangle_t \langle B \rangle_t
\]

\[
\langle \ldots \rangle_t = \frac{\langle \Psi(t)| \ldots |\Psi(t) \rangle}{\langle \Psi(t)|\Psi(t) \rangle}
\]
Obtain state at next time with standard ODE scheme

Measure expectation values entering equation of motion

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

Sample $|\langle X | \Psi(\alpha) \rangle|^2$ with Metropolis-Hastings algorithm
Time-Dependent Jastrow-Feenberg Expansions

(2012-Today)

Spin/Bosons Lattice Systems

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

Multi-Body effective interactions

Continuos-Space Systems

\[ \langle X \mid \Psi(t) \rangle = \exp \left[ \sum_{i=1} J_i^{(1)}(x_i, t) + \frac{1}{2!} \sum_{i \neq j} J_{i,j}^{(2)}(x_{ij}, t) + \frac{1}{3!} \sum_{i \neq j \neq k} J_{i,j,k}^{(3)}(x_{ijk}, t) + \ldots \right] \]

Multi-Body Variational Fields
**Correlated Slater-Projected Wave-Functions**


\[ |\Psi\rangle = J \times L^K \times L^S |D\rangle \]

- **Jastrow Factor**
- **Momentum Projection**
- **Spin Projection**
- **Slater Determinant**

\[ |D\rangle = \left( \sum_{i,j} f_{i,j} c_{i,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} \right)^{N/2} |0\rangle \]
Overview of Some Applications

(I) Thermalization in Ultra-Cold Atoms
Lattice Bosons

Quantum Quench in the Bose-Hubbard Model

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

Quench from a superfluid phase

\[ \frac{\partial}{\partial t} \Psi = \mathcal{H} \Psi \]

\[ \xi(t) = e^{\langle \phi^2 \rangle(t) - \langle \phi^2 \rangle(t_0) / 2} \]

Comparison with t-DMRG in one dimension

Non-Thermal Behavior In Two Dimensions

The above results have been obtained for out-of-equilibrium one-dimensional results for the time-dependent expectation value of the on-site potential energy as a function of the time. As we see from Fig. 5, in the region of very large anticipated dynamical effects that drive the dynamics in this regime.

Figure 5

The initial state is the ground state of the Bose-Hubbard Hamiltonian with values of the on-site potential energy. It is natural to identify the considered system size as a function of the time. As occurs even in two dimensions. In Fig. 6, we show the results of the time-dependent variational scheme, verifying that a similar behavior is observed even in higher dimensions, provided that the inter-atomic interactions induce sufficiently strong dynamical constraints. In this regard, we have studied the two-dimensional case by means of our action-induced quenching to strong interactions. Moreover, we have shown that the time evolution of the many-body system is almost independent on the dimensionality and the symmetry breaking.

However, the anomalously long-time relaxation of the density auto-correlation points towards a kind of glassy behavior that should be further investigated. This fast time quenching to small interactions is recognized to play a role in the density relaxation processes of purely homogeneous systems through a dynamical arrest visible in the long-lived inhomogeneous pattern, resembles closely a kind of glass transition.

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One-Dimensional Quantum Gases

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

Quantum Quench in the Lieb-Liniger Model

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

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)

![Graphs showing non-thermal and thermal behavior](image)

- **Non-Thermal Behavior**
  - Quenching from ideal BEC

- **Thermal Behavior**
  - Quenching from finite interactions
Overview of Some Applications

(II)
Locality and Information Spreading
Short-range Hamiltonians

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

Correlations suppressed outside the "light-cone" region \( t < R/v \)

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

Long-Range Hamiltonians

\[ H_{nl} \approx \frac{1}{R^\alpha} \]

Unbounded correlations for \( \alpha < D \)

M. B. Hastings (2010)

Superballistic bound for \( \alpha > D \)

M. Foss-Feig et al. (2015)
Information Spreading in Superfluids


\[ G(R, t) = \langle n_in_{i+R} \rangle_t \]

(a) Density-density correlations

(b) Time dependence of correlations

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?


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

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

(III)

Lattice Fermions
Interaction Ramps in the Fermi-Hubbard

\[ \mathcal{H}(t) = -J \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U(t) \sum_i n_{i\uparrow} n_{i\downarrow} \]

Linear Ramp in the Interaction

\[ \Delta \rho(t) = \frac{1}{4} \left( n_{i\uparrow} + n_{i\downarrow} - n_{\uparrow}^\dagger n_{\downarrow}^\dagger - n_{\downarrow} n_{\uparrow} \right) \]

One Dimension

Two Dimensions
Overview of Some Applications

(IV) Adiabatic Quantum Computing
Adiabatic Quantum Computing

Slow Adiabatic Driving

Slow unitary evolution

\[ \mathcal{H}(t) = \left( 1 - \frac{t}{T} \right) \sum_i \sigma_i^x + \frac{t}{T} \sum_{i<j} V_{i,j} \sigma_i^z \sigma_j^z \]

Open Questions

Is Adiabatic Optimization Better than Classical One?

How to Describe a Large Number of Qubits?

How to Validate Future Generations of Quantum Computers? (à la D-Wave)
Accuracy For Spin Glass Problem

Carleo, Bauer, and Troyer
In preparation (2016)

Comparison with Matrix Product States
Quantum Speed-Up

Carleo, Bauer, and Troyer
In preparation (2016)

Performance Comparison with Classical Simulated Annealing

Median Time To Solution Exhibits Quantum Speedup
A Call for Quantum Monte Carlo People in The Audience
Spectral and Dynamical Properties

**Imaginary-Time Correlations**

- Severely ill-posed problem
- Just Another Reformulation of the Sign Problem
- Bayesian Voodoo
- Hard to Obtain Systematic Errors
- Limited to Linear Response
- Many Interesting Experiments are non-linear

**Time-Dependent Variational Monte Carlo**

- Inherits From Static Variational Monte Carlo
- Can be implemented in a day of work
- Accurate For Both Linear Response and Violent Non-Linear Response
- Polynomial Increase in the Wave-Functions can lead to exponentially better accuracy
- More Controlled Approximation
- You’d better Improve your wave-function, than try to exponentially reduce your error bars