Quantum quenches in 2D via arrays of coupled chains

Andrew James
University College London

Robert Konik
Brookhaven National Laboratory
Quantum quenches in 2D via arrays of coupled chains

• **Introduction**
  - many body states with MPS
  - entanglement and dimension

• **MPS for arrays of coupled chains**

• **Time evolution for arrays of coupled chains**
  - Perturbative limit
  - ‘Dynamical phase transitions’
Representing Many-Body Quantum States

General many-body state

\[
|\psi\rangle = \sum_{\{\sigma\}} c_{\sigma_1 \cdots \sigma_N} |\sigma_1 \cdots \sigma_N\rangle
\]

Need exponentially many \(c\) numbers to completely specify state

\[d_{\sigma}^N = \dim(\sigma)^N\]

But typical states we deal with need far fewer

In particular for a simple product state only need 1

\[
|\psi\rangle = |\sigma_1 \cdots \sigma_N\rangle
\]
What is an efficient representation between these extremes?
How do we choose which contributions are ‘small’ and can be neglected?

$$c_{\sigma_1, (\sigma_2 \cdots \sigma_N)}$$

- $d_{\sigma}^{N-1}$
- $d_{\sigma}^{N-1}$

General

Product state
A bipartite system

\[ |\psi\rangle = \sum_{ab} c_{ab} |a\rangle |b\rangle, \quad c_{ab} \Rightarrow d_a \times d_b \]

Change basis for A and B using Schmidt (singular value) decomposition of state

\[ |\psi\rangle = \sum_{i} s_i |i\rangle_A |i\rangle_B, \quad s_i \Rightarrow \min(d_a, d_b) \]

Less redundancy and ranks importance of contributions
A bipartite system

\[ |\psi\rangle = \sum_i s_i |i\rangle_A |i\rangle_B \]

Distribution of singular values gives a measure of entanglement

\[ \sum_i s_i^2 = 1, \quad S_E = -\sum_i s_i^2 \log s_i^2 \]

Zero for product state, maximum log(N) for N states
Carry out iterative SVD on a 1D system with N sites.

\[ |\psi\rangle = \sum_{\sigma} A_{a_1 a_1 a_2}^{\sigma_1} A_{a_{N-1}, 1}^{\sigma_N} |\sigma_1 \cdots \sigma_N\rangle \]
Matrix Product States

\[ |\psi\rangle = \sum_{\sigma} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1 a_2} \cdots A^{\sigma_N}_{a_{N-1}, 1} |\sigma_1 \cdots \sigma_N\rangle \]

- Restrict to largest $D$ singular values at each bond
- Max independent coefficients for matrix dimension $D$?

\[ (d_\sigma - 1) N D^2 \quad \text{vs.} \quad d^N_\sigma \]

- Max entanglement entropy at a bond is given by flat distribution of singular values

\[ \log D \]
Density matrix renormalisation group

- Iterative construction and optimisation of MPS with energy minimisation for 1D problems
- High accuracy, controlled by bond dimension D, (even near critical points, e.g. Pollmann et al. PRL 2009)
Density matrix renormalisation group

Density Matrix Formulation for Quantum Renormalization Groups

Steven R. White

Department of Physics, University of California, Irvine, California 92717
(Received 22 May 1992)

SVD
Why does it work?

Success of MPS methods in 1D relies on, at worst, log growth of entanglement

\[ S_A = \frac{c}{6} \log L_{eff} + \cdots \]

\[ L_{eff} = \begin{cases} \frac{L}{\pi} \sin \frac{\pi x}{L} & \text{critical} \\ \frac{\xi}{a} & \text{gapped} \end{cases} \]

Holzhey, Larsen & Wilczek 1994, Calabrese & Cardy 2004

Bipartite 1D system
How do we extend MPS to higher dimensions?
How does entanglement entropy behave for $D>1$?

Generally an ‘area law’ is expected

$$S_E \sim \mathcal{A}/a^{D-1}$$

An exception: massless free fermions in $D$ dimensional cube (Gioev and Klich 2006)

$$S_E \sim L^{D-1} \log L$$
DMRG in 2D

MPS methods less efficient in 2D than in 1D due to area law growth of entanglement

Effective long range interactions
General problem for tensor methods
Truncated Spectrum Approach DMRG
Chain, length $R$, periodic b.c.s, with continuum Hamiltonian that is either conformal or integrable

- Continuum limit: finite size corrections exponential, keep $R$ small $\sim e^{-\Delta R}$
- Integrable or conformal: exact spectrum and matrix elements known
- Use chains as sites in normal 1D DMRG?

$$H = \sum_i H_{i}^{1D} + J_{\perp} \sum_{\langle ij \rangle} O_i O_j$$
Bending the area law

\[ H = \sum_i H_{i}^{1D} + J_\perp \sum_{\langle ij \rangle} \mathcal{O}_i \mathcal{O}_j \]
The spectrum of each chain is infinite…

However for finite $R$ it is discrete, so we can order by energy and truncate

When can we expect/hope to get away with this?
Inspiration from TCSA

Truncated Conformal Space Approach

\[ H = H_{CFT} + \lambda_0 \int d^2 x \phi_0(x) \]

Relevant perturbing operator, most important effect is mixing of low energy states
Critical Ising chain in magnetic field well described (error \( \sim 1\%\)) by keeping only 39 states
Truncated spectrum approach to DMRG

- Control area law with small R
- Requires re-truncation in energy after each DMRG step to keep consistent cutoff
- In general don’t need to keep too many reduced density matrix eigenvalues, ~30 in gapped phase to 100’s nearer criticality for $10^{-5}$ truncation error
Example: Quantum Ising chain

- Continuum limit of lattice Ising chain in transverse field
- Can study negative mass, $\Delta$, (disordered) or positive $\Delta$ (ordered) chains

\[ H_{\text{lattice}}^{1D} = -J \sum_m \left( \sigma_m^z \sigma_{m+1}^z + (1 + g) \sigma_m^x \right) \]

\[ H^{1D} = \int dx \left[ \frac{v}{2} \left( \bar{\Psi} \frac{\partial \bar{\Psi}}{\partial x} - \Psi \frac{\partial \Psi}{\partial x} \right) + \Delta \bar{\Psi} \Psi \right] \]

\[ \Delta = -2gJ, \quad v = 2Ja \]
Example: Quantum Ising chain

• Chain eigenstates organised into two ‘sectors’ Ramond and Neveu-Schwarz with integer and half-integer momenta

\[ \text{NS: } |p_1, p_2, \cdots, p_{N_f}\rangle = \alpha^\dagger_{p_1} \alpha^\dagger_{p_2} \cdots \alpha^\dagger_{p_{N_f}} |0\rangle_{NS}, \quad p_i \in (\mathbb{Z} + 1/2) \frac{2\pi}{R} \]

\[ \text{R: } |k_1, k_2, \cdots, k_{N_f}\rangle = \alpha^\dagger_{k_1} \alpha^\dagger_{k_2} \cdots \alpha^\dagger_{k_{N_f}} |0\rangle_{R}, \quad k_i \in \mathbb{Z} \frac{2\pi}{R} \]

• Permissible states depend on sign of mass

\[ \Delta > 0, \quad \text{NS states when } N_f \text{ even, R states when } N_f \text{ even.} \]

\[ \Delta < 0, \quad \text{NS states when } N_f \text{ even, R states when } N_f \text{ odd.} \]

• Fermion energies

\[ E_{k_i} = \sqrt{\Delta^2 + k_i^2} \]
2D Quantum Ising model (2+1)

- Should be an order/disorder transition (disordered chains will order with enough coupling)

- Start with disordered (negative mass) chains and sweep chain coupling, study the energy gap
- Test that the correct many-body behaviour is captured
2D Quantum Ising model (2+1)

\[ \Delta_{2DQI} \sim |J_c - J_\perp|^\nu \]

\[ N = 60, \; R\Delta = 10, \; E_c = 7.8\Delta \]

R. M. Konik and Y. Adamov, PRL 102, 097203 (2009)

In 3D classical Ising universality class, \[ \nu = 0.630 \]
2D Quantum Ising model (2+1)

Finite size scaling \( \nu = 0.630 \)

- \( R=6, N=60 \)
- \( R=7.6, N=76 \)
- \( R=8, N=80 \)
- \( R=9.2, N=92 \)

\( J_c = 0.185 \)
\( \nu = 0.630 \)
Other things to look at

- Entanglement (James, Konik PRB 87, 2013)
- Generalise to other chain Hamiltonians
  - Coupled XXZ
  - Coupled Hubbard chains
- Infinite DMRG for thermodynamic limit
- Take advantage of other MPS/MPO algorithms
  - Time evolution and iTEBD
  - Finite temperature
Time evolution and out-of-equilibrium
Quantum quenches

- Take an eigenstate of some ‘initial’ Hamiltonian and time evolve it with respect to a new Hamiltonian

\[ |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \]

- How do we approach stationary state and thermalise?
- What is the return probability (Loschmidt echo)

\[ \mathcal{L}(t) = |\langle \psi(0) | e^{iH_0t} e^{-iHt} |\psi(0)\rangle|^2 \]

- In 1D, can use MPS based time evolution and analytic methods
Quantum quenches in cold atoms

\[ |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \]

Quantum Quench in an Atomic One-Dimensional Ising Chain


1Institut für Experimentalphysik und Zentrum für Quantenphysik, Universität Innsbruck, 6020 Innsbruck, Austria
2Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA

(Received 9 April 2013; published 31 July 2013)

We study nonequilibrium dynamics for an ensemble of tilted one-dimensional atomic Bose-Hubbard chains after a sudden quench to the vicinity of the transition point of the Ising paramagnetic to antiferromagnetic quantum phase transition. The quench results in coherent oscillations for the orientation of effective Ising spins, detected via oscillations in the number of doubly occupied lattice sites. We characterize the quench by varying the system parameters. We report significant modification of the tunneling rate induced by interactions and show clear evidence for collective effects in the oscillatory response.
Time evolving block decimation

- Trotter decomposition of time steps into odd and even bond operations

\[
|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle = \prod_{n}e^{-iH_{tn}}|\psi(0)\rangle, \quad \sum_{n}t_n = t
\]

\[
e^{-iH_{tn}} \approx e^{-iH_{\text{odd}t_n}}e^{-iH_{\text{even}t_n}}
\]

\[
e^{-iH_{\text{odd}t_n}} = e^{-iH_{1,2t_n}}e^{-iH_{3,4t_n}}\ldots e^{-iH_{N-1,Nt_n}}
\]
Time evolving block decimation

- Trotter decomposition of time steps into odd and even bond operations
- Compress MPS after time step
- Time step error can be controlled with smaller steps or higher order decompositions
- Error due to truncation is more problematic
Time evolving block decimation

- Trotter decomposition of time steps into odd and even bond operations
- Compress MPS after time step
- Time step error can be controlled with smaller steps or higher order decompositions
- Error due to truncation is more problematic

Entanglement grows (at worst) linearly with time (Lieb Robinson bounds), P. Calabrese and J. Cardy (2006)
MPS dimensions grow (at worst) exponentially

\[ S_E(t) \leq S_E(0) + ct \]
\[ D \lesssim \#^S \Rightarrow D \lesssim \#^t \]
Infinite MPS in 1D: iTEBD

Infinite time evolving block decimation

- Impose translational invariance
- Work with two site fragment
- Fast compared to finite chains (only 2 matrices instead of N)
- Better numerical stability than for large finite N
For a finite system we can do the full contraction over MPS indices

\[ \langle \tilde{\psi} | \psi \rangle \]

For the infinite case we must work with the transfer operator

\[ T(\tilde{a}_l a_l), (\tilde{a}_{l+2} a_{l+2}) \]

\[ = \left\{ \tilde{A}^{\sigma_l+1 \ast}_{\tilde{a}_{l+2}, \tilde{a}_{l+1}} \tilde{A}^{\sigma_l \ast}_{\tilde{a}_{l+1}, \tilde{a}_l} \right\} \left\{ A^{\sigma_l}_{a_l, a_{l+1}} A^{\sigma_{l+1}}_{a_{l+1}, a_{l+2}} \right\} \]

Overlap/site is given by (square root of) the dominant eigenvalue
Quantum quenches for coupled chains
Global quench setup

- Start with product state (interchain coupling zero), for disordered (negative mass) chains
- Know ground state exactly, $D=1$, $S_E=0$, MPS is easy to form

![Diagram showing product state with interchain coupling zero]

- Turn on small interchain coupling

![Diagram showing product state with small interchain coupling]

- Evolve in time
Perturbative treatment of a quench

- As a check, consider very shallow quenches that can be treated perturbatively \textit{(in particular, do not cross critical coupling)}

\[ H = H_0 + gH_1, \quad g \ll 1 \]

- Need unitary perturbation theory to avoid terms that grow in time without bound

\[ |\phi(t)\rangle = e^{-iHt}|\phi(0)\rangle = e^{-S}e^{-iH_{\text{diag}}t}e^S|\phi(0)\rangle \]

Moeckel and Kehrein, PRL 100, 175702 (2008)
Kollar, Wolf and Eckstein, PRB 84, 054304 (2011)
Perturbative treatment for coupled Ising chains

- Expectation of an operator on chain $i$ at time $t$

$$\langle O_i \rangle_t = \langle O_i \rangle_0 + 8J_\perp^2 R^2 \sum_{n_i,n_{i+1}} \left( \frac{\sin^2(t[E_i + E_{i+1}]/2)}{(E_i + E_{i+1})^2} \right)$$

$$\times \delta_{k_i,-k_{i+1}} \left| \langle 0 | \sigma_i | n_i \rangle \langle 0 | \sigma_{i+1} | n_{i+1} \rangle \right|^2 \langle n_i | O_i | n_i \rangle$$

- States of system are tensor products of states on individual chains

$$|\Phi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_N\rangle$$

$$|\Phi(0)\rangle = |0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle$$

$$H_{1D,i} |\phi_i\rangle = E_{\phi_i} |\phi_i\rangle$$
Perturbative treatment for coupled Ising chains

- Expectation of an operator on chain $i$ at time $t$

$$\langle O_i \rangle_t = \langle O_i \rangle_0 + 8J_\perp^2 R^2 \sum_{n_i,n_{i+1}} \left( \frac{\sin^2(t[E_i + E_{i+1})/2)}{(E_i + E_{i+1})^2} \right)$$

$$\times \delta_{k_i, -k_{i+1}} \langle 0 | \sigma_i | n_i \rangle \langle 0 | \sigma_{i+1} | n_{i+1} \rangle^2 \langle n_i | O_i | n_i \rangle$$

Key features at 2\textsuperscript{nd} order:
- No dependence on number of chains or boundary (except trivial factor of 2 at edges if O.B.C.)
- Sum of terms periodic in $t$, overlap with initial state is trivial to this order:

$$\mathcal{O} = |0\rangle\langle 0| \Rightarrow \langle \mathcal{O} \rangle_t = 1$$
Chain momentum occupation number

Consider number operator for excitations on chain $i$ with chain momentum $k$

- Chain excitations are fermions, maximum value is 1 for each $(k,i)$ pair
- Gives a measure of how far each chain is from its (uncoupled) groundstate
Small quench $J_\perp = 0.01 \ll J_c \sim 0.18$

$R=2$

\begin{align*}
\text{for } n_{0,i} / 10^{-4} \\
\text{and } n_{0,i} / 10^{-5}
\end{align*}

- $E_c = 4$
- $E_c = 8$
- Perturbative

$1.101 \times 10^{-4}$
Small quench $J_\perp = 0.01 \ll J_c \sim 0.18$

$R=8$

![Graph of oscillating functions with labels: $E_c=4$, $E_c=8$, Perturbative. The graph shows two sets of oscillations with different amplitudes and phases.](Image)
Longer times

\[ J_\perp = 0.01 \ll J_c \approx 0.18 \]

\[ n_{0,j} / 10^{-4} \]

- \( s_{\text{min}} = 10^{-4} \)
- \( s_{\text{min}} = 10^{-5} \)
- \( s_{\text{min}} = 10^{-6} \)

\[ R=8, E_c=4.0, J_\perp=0.01 \]
Momentum modes versus $R$

Chain $k=0$ mode saturates quickly with $R$

Higher $k$ modes take longer…
Half integer chain momentum modes

\[ k = \frac{2\pi n}{R}, \quad n \in \mathbb{Z} + 1/2 \]  

NS half integer modes

\[ J_\perp = 0.01 \ll J_c \sim 0.18 \]

Not captured by the perturbative result
Dynamics of overlap

\[ G(t) = \langle \Psi_0 | e^{-iHt} | \Psi_0 \rangle \]

c.f. trivial overlap to 2\textsuperscript{nd} order in perturbative calculation

\[ l(t) = -\frac{2}{R_N} \log |G(t)| \]

\[ E_c = 4.0, \ J_\perp = 0.01 \]
Deeper quenches for coupled chains
Moving away from the perturbative limit

Departure from simple oscillatory behaviour
Moving away from the perturbative limit

\[ n_{0,i}/J_\perp^2 \]

- \( J_\perp = 0.01 \)
- \( 0.05 \)
- \( 0.1 \)
- \( 0.2 \)

\( R = 4, E_c = 8 \)
Moving away from the perturbative limit

Half integer modes become ‘large’
Dynamical Phase Transitions?

Heyl, Polkovnikov and Kehrein, PRL 110, 135704 (2013)

For TFIM, nonanalytic ‘rate’ if quench is through critical point

\[ l(t) = - \lim_{N \to \infty} \frac{1}{N} \log |G(t)|^2 \]

Karrasch and Schuricht
PRB 87, 195104 (2013)
Dynamical Phase Transitions?

Heyl, Polkovnikov and Kehrein, PRL 110, 135704 (2013)

For TFIM, nonanalytic ‘rate’ if quench is through critical point

More generally not periodic, nor uniquely associated with equilibrium critical points

Andraschko and Sirker, PRB 89 (2014)

Fagotti, arXiv:1308.0277

Karrasch and Schuricht, PRB 87, 195104 (2013)
Deep quenches for coupled chains

\[ H = \sum_i \left\{ H_{1D,i} + J_\perp \int_0^R dx \, \sigma_i(x) \sigma_{i+1}(x) \right\} \]

As a check, start with small \( R \)

Chain fermion energies diverge for all but the lowest excited state

\[ E_n \sim \sqrt{\Delta^2 + \left( \frac{2\pi n}{R} \right)^2} \]
Deep quenches for coupled chains

\[ H = \sum_i \left\{ H_{1D,i} + J_{\perp} \int_0^R \text{d}x \ \sigma_i(x)\sigma_{i+1}(x) \right\} \]

- As a check, start with small \( R \)

- Only ground state and first excited state on each chain survive, recover 1D TFIM

\[
\lim_{R \to 0} H = \sum_i \tilde{h} \sigma_i^z + \tilde{J}_{\perp} \sigma_i^x \sigma_{i+1}^x
\]

\[
\tilde{h} = \Delta + E_{RM,0} - E_{NS,0}
\]

\[
\tilde{J}_{\perp} = J_{\perp} |\langle RM, 0|\sigma|NS, 0\rangle|^2
\]
Quench of coupling in TFIM limit $J_\perp = 0$ to $J_\perp = 1.5$

$J_{\perp,\text{crit}} \approx 0.5$

Can study the infinite chains case (iTEBD)

Times for nonanalytic behaviour can be calculated exactly, $t^* = 0.4693...$
Boundary conditions and finite systems

Even for large finite systems, b.c.s make a difference

Important if looking for this behaviour in e.g. cold atoms

- iTEBD
- N=100 (PBC)
- N=50 (OBC)
- N=200 (OBC)
Both solutions are visible in the eigenvalues of the iTEBD transfer operator
Deeper quenches for coupled chains

For larger $R$, $J_{\perp,c} \approx 0.18$

\[ E_c = 8.0, \; J_{\perp} = 0.5 \]

- $R=2$
- $R=4$
- $R=6$
- $R=8$
Conclusions

• Coupling integrable chains together allows straightforward extension of 1D MPS methods to 2D systems

• Extra control parameters are chain length, R, and energy cutoff

• Can work with infinitely many chains

• Uses
  • Low lying spectrum and phase transitions
  • Investigating entanglement entropy
  • Time evolution, great for shallow quantum quenches, deeper quenches possible for short times
Future work

- Other integrable chains
- XXZ with J.S. Caux (Amsterdam)
- iDMRG for studying phase transitions
- Better understanding of energy cutoff
- Finite temperature
- Supercomputing