Title: Solving Non-relativistic Quantum Field Theories with continuous Matrix Product States

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Abstract: Since its proposal in the breakthrough paper [F. Verstraete, J.I. Cirac, Phys. Rev. Lett. 104, 190405(2010)], continuous Matrix Product States (cMPS) have emerged as a powerful tool for obtaining non-perturbative ground state and excited state properties of interacting quantum field theories (QFTs) in (1+1)d. At the heart of the cMPS lies an efficient parametrization of manybody wavefunctionals directly in the continuum, that enables one to obtain ground states of QFTs via imaginary time evolution. In the first part of my talk I will give a general introduction to the cMPS formalism. In the second part, I will then discuss a new method for cMPS optimization, based on energy gradient instead of the usual imaginary time evolution. This new method overcomes several problems associated with imaginary time evolution, and allows to perform calculations at much lower cost / higher accuracy than previously possible.

Solving Non-Relativistic Quantum Field Theories with Continuous Matrix Product States

Martin Ganahl, Julian Rincon, Guifre Vidal

Many Electron
Simons Collaboration

PERIMETER INSTITUTE

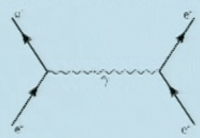
Tensor Networks Initiative
Perimeter Institute

Integrable: e.g.
Bethe Ansatz

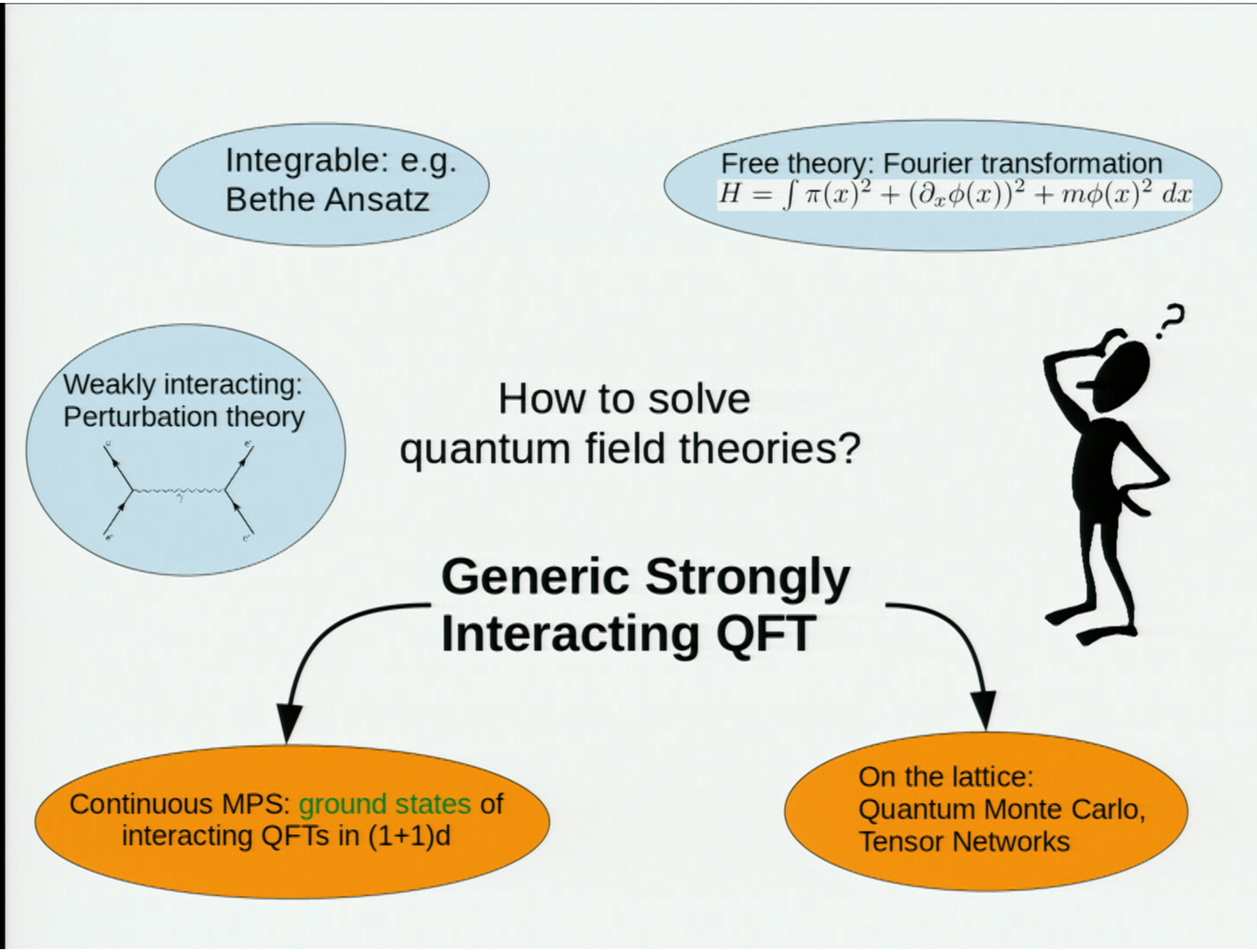
Free theory: Fourier transformation

$$H = \int \pi(x)^2 + (\partial_x \phi(x))^2 + m\phi(x)^2 \, dx$$

Weakly interacting:
Perturbation theory



How to solve
quantum field theories?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How to solve
quantum field theories?
Generic Strongly
Interacting QFT
Continuous MPS: ground states of
interacting QFTs in (1+1)d
On the lattice:
Quantum Monte Carlo,
Tensor Networks

Short summary

Continuous MPS: ground states of interacting QFTs in (1+1)d

Example: Lieb Liniger bosons (can also be solved by Bethe Ansatz)

$$H = \int_{-\infty}^{\infty} dx \left(\frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x) + g(\psi^\dagger(x))^2(\psi(x))^2 + \mu\psi^\dagger(x)\psi(x) \right)$$

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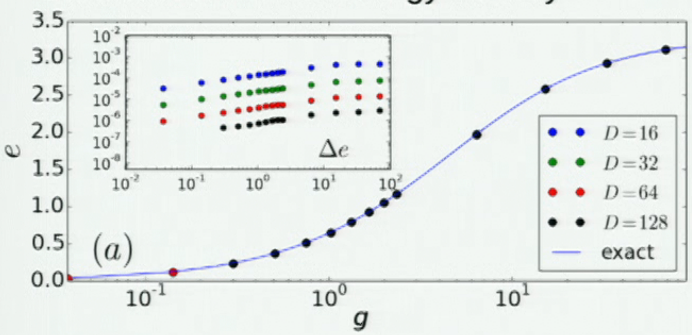
Local observables: energy density



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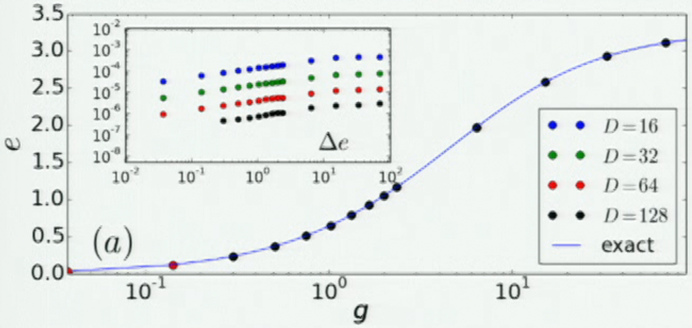
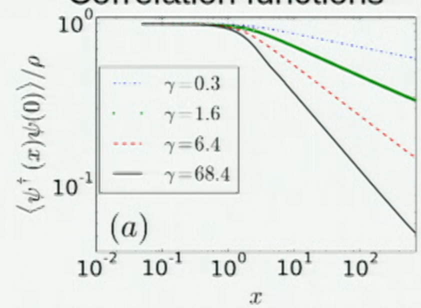
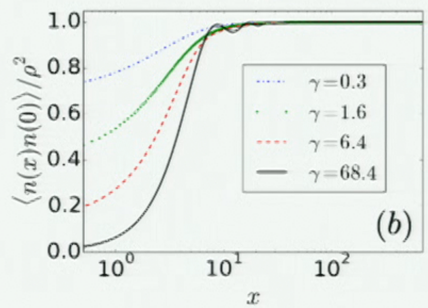


c=1 CFT with varying compactification radius

Correlation functions





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Non Relativistic:

$$\frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x)$$

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Which QFTs?

Non Relativistic:

$$\frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x)$$

Relativistic: *need UV regularization*

$$\pi(x)^2 + (\partial_x \phi(x))^2$$

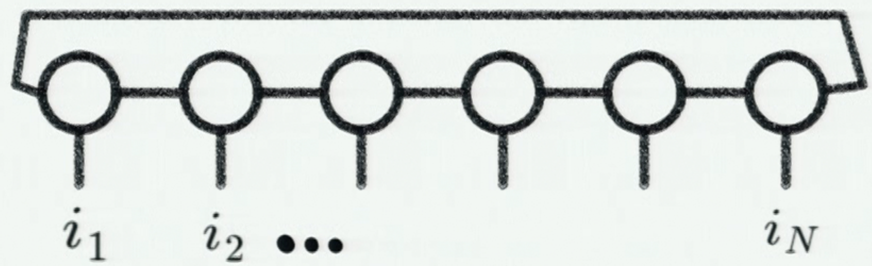
$$\psi(x) = (\phi(x) + i\pi(x))/\sqrt{2}$$

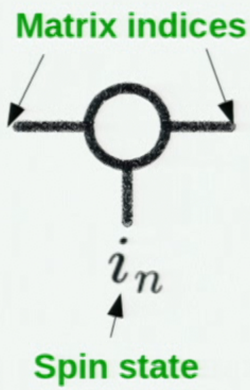
Part 1
An Introduction to cMPS

Basic notation

Matrix Product State wave functions (e.g. spins)

$$|\psi\rangle = \sum_{\{i_1 \ldots i_N\}} tr\left[A^{i_1} A^{i_2} \ldots A^{i_N}\right] |i_1 \ldots i_N\rangle$$





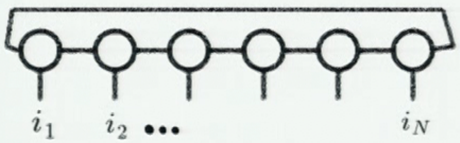
$$= A^{i_n} = \begin{pmatrix} A^0 \\ A^1 \\ \vdots \end{pmatrix}$$

Short outline

Continuous Tensor networks for quantum fields

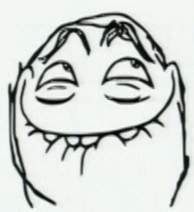
Previous talks: Put field theory on a lattice
by discretization:

Matrix Product States



 $= A[n]$

Powerful lattice MPS toolbox:
DMRG, TEBD, TDVP, ...



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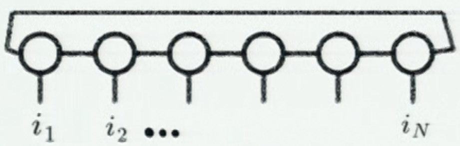

 $= A[n]$ → Tensor density $A[x]$

Powerful lattice MPS toolbox:
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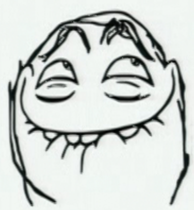
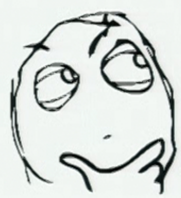
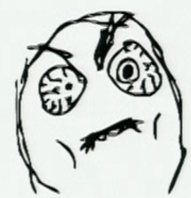


This talk: how to take the continuous limit of an MPS? (Verstraete and Cirac, 2010)

?

 → 

The continuum limit of a lattice MPS

Constructive approach:
Fine graining of a bosonic lattice MPS

$$|\psi\rangle = \sum_{\{i_n\}} tr(A^{i_1} \dots A^{i_N})[b_1^\dagger]^{i_1} \dots [b_N^\dagger]^{i_N} |0_1 \dots 0_N\rangle$$

$$A^0 \sim |0\rangle \qquad\qquad A^0 A^0 A^0 A^0 A^0 \sim |00000\rangle$$

$$A^1 \sim b^{\dagger 1} |0\rangle \qquad\qquad A^0 A^0 A^1 A^0 A^0 \sim |00100\rangle$$

$$\vdots$$

The continuum limit of a lattice MPS

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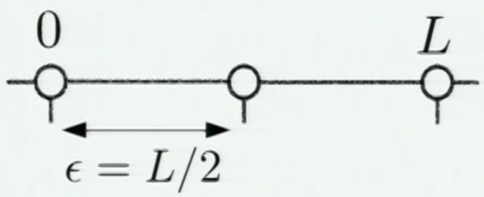

$$= \begin{pmatrix} A^0 \\ A^1 \\ A^2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbb{1} + \epsilon Q \\ \sqrt{\epsilon} R \\ \sqrt{\epsilon^2/2!} R^2 \\ \vdots \end{pmatrix}$$

$$A^0 = \mathbb{1} + \epsilon Q \sim |0\rangle$$

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(Verstraete and Cirac, 2010)

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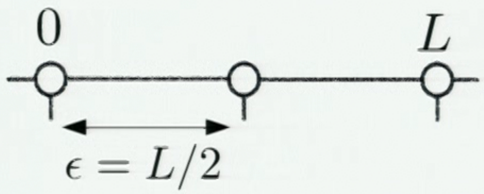

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Variational parameters: Q, R

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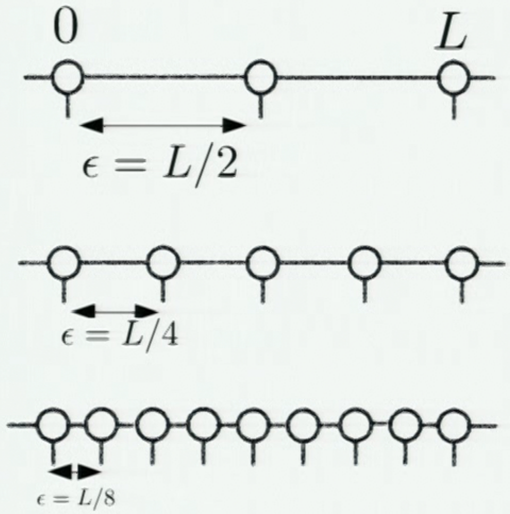

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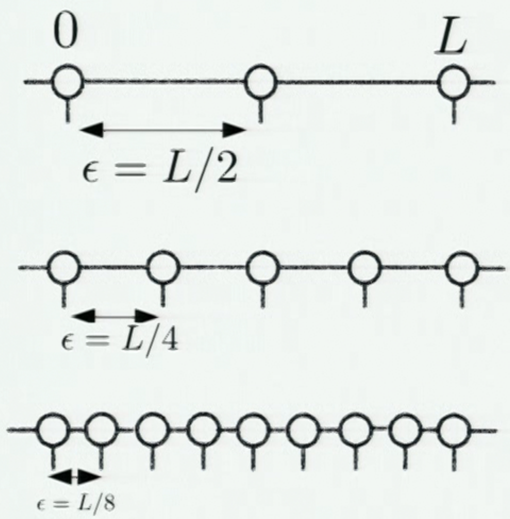

$$\lim_{\substack{\epsilon \to 0 \\ N \to \infty}} N\epsilon = L$$

$$= \begin{pmatrix} A^0 \\ A^1 \\ A^2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbb{1} + \epsilon Q \\ \sqrt{\epsilon} R \\ \sqrt{\epsilon^2/2!} R^2 \\ \vdots \end{pmatrix}$$

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Variational parameters: Q, R

$$|\Psi\rangle = tr\left[\mathcal{P} e^{\int_0^L Q \otimes \mathbb{1} + R \otimes \psi^\dagger(x) dx}\right] |0\rangle$$

(Verstraete and Cirac, 2010)

The continuum limit of a lattice MPS

Is this limit trivial??

$$= \begin{pmatrix} \mathbb{1} + \epsilon Q \\ \sqrt{\epsilon} R \\ \sqrt{\epsilon^2/2!} R^2 \\ \vdots \end{pmatrix} = \begin{pmatrix} A^0 \\ A^1 \\ A^2 \\ \vdots \end{pmatrix}$$

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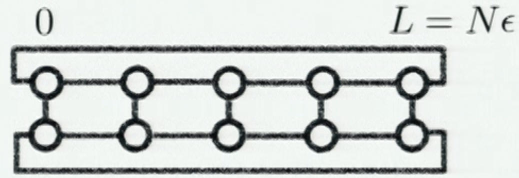
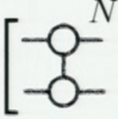
No: $\lim_{\epsilon \to 0} (1 + \epsilon x)^{\frac{1}{\epsilon}} = e^x$

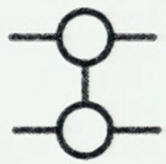
Continuous limit at finite density $\langle \psi^\dagger \psi \rangle$

Calculus of continuous Matrix Product States

the norm of a cMPS

$\langle\Psi|\Psi\rangle =$ 

$= tr\Big[$  $\Big]^N$

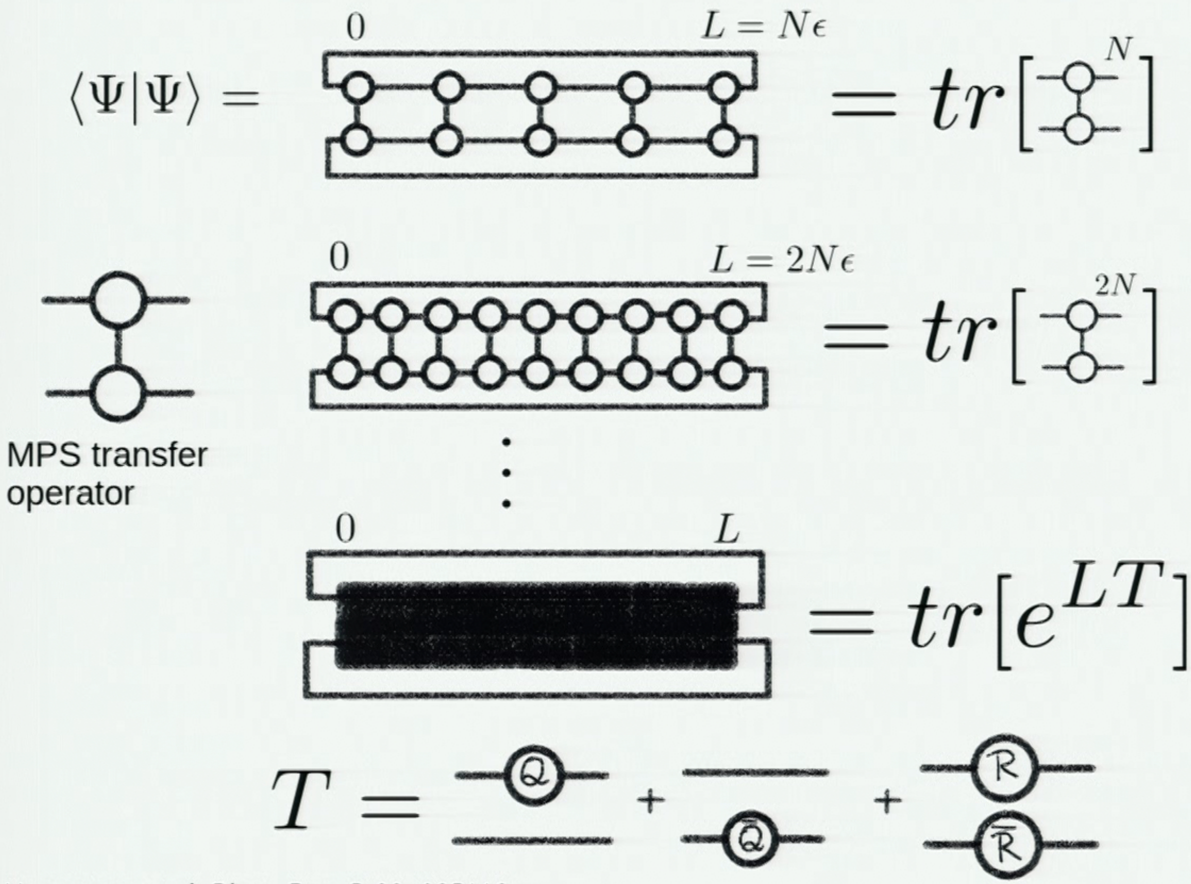


MPS transfer
operator

Haegeman et al. Phys. Rev. B 88, 085118

Calculus of continuous Matrix Product States

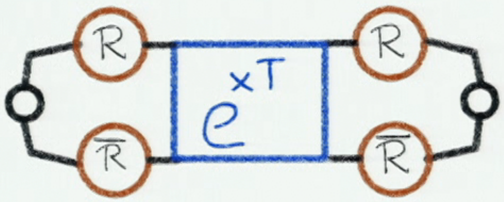
the norm of a cMPS



Haegeman et al. Phys. Rev. B 88, 085118

Observables

$\langle \psi^\dagger(0)\psi(0)\psi^\dagger(x)\psi(x)\rangle$



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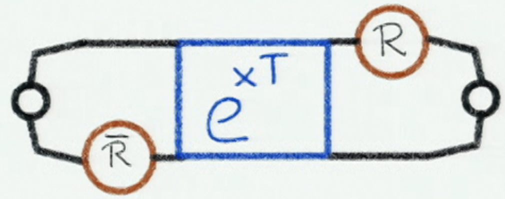
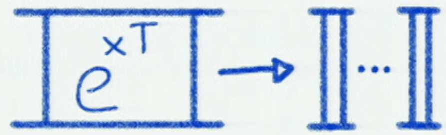


Differential equation with boundary condition



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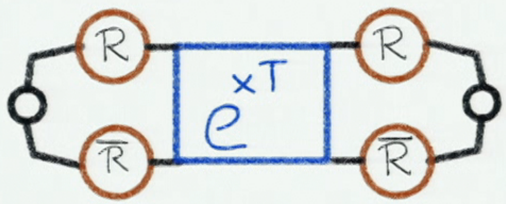

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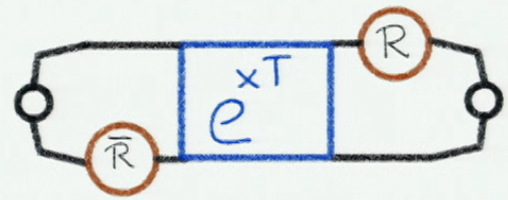

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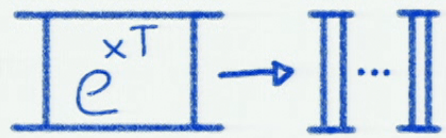

Efficient evaluation of energy densities of interacting QFTs!

$$\langle H\rangle = \int_{-\infty}^{\infty} \langle \frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x)\rangle + c\,\langle [\psi^\dagger(x)]^2[\psi(x)]^2\rangle + \mu\,\langle \psi^\dagger(x)\psi(x)\rangle$$

Basis for numerical optimization techniques

Why cMPS?

Class of variational many-body states
directly in the continuum

Why cMPS?

One alternative: lattice discretizations (for non-relativistic Hamiltonians), e.g.

$$H = \sum_{i \in \mathbb{N}} \frac{1}{2m(\Delta x)^2}(c_{i+1}^\dagger - c_i^\dagger)(c_{i+1} - c_i) + \frac{g}{\Delta x} c_i^\dagger c_i^\dagger c_i c_i + \mu_i c_i^\dagger c_i.$$

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Separation of energy scales!

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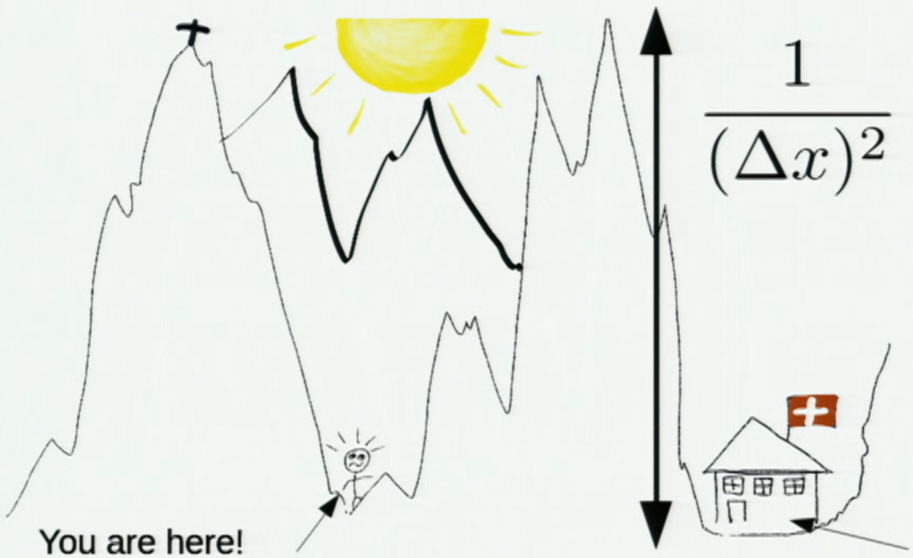


$\Delta x \to 0$ not possible
Usually "finite Δx scaling"

Why cMPS?

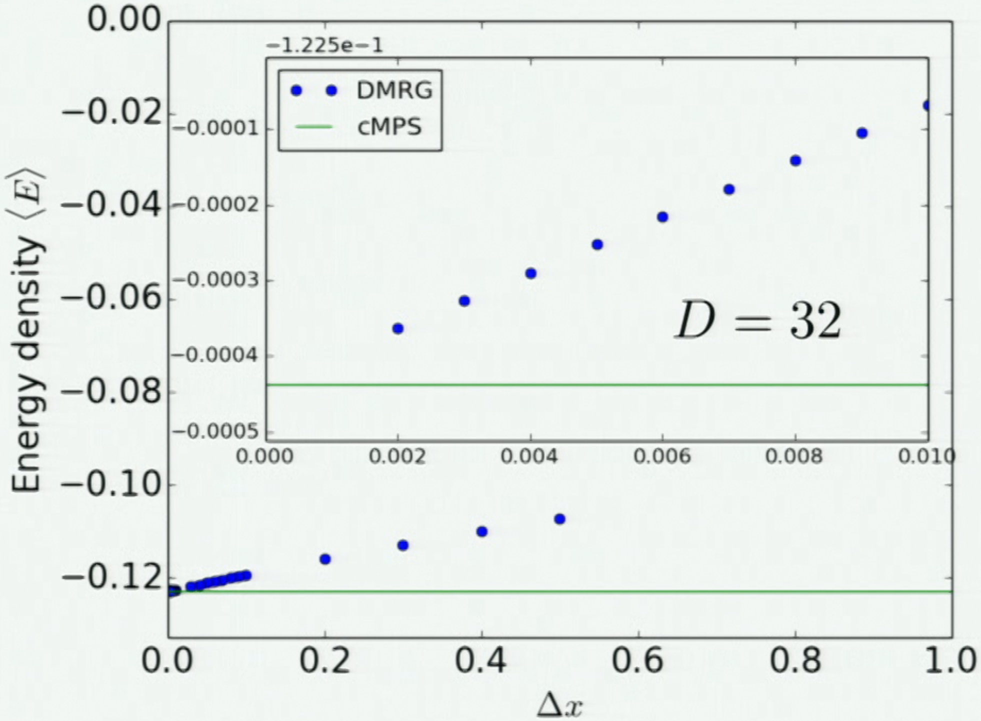
Variational parameters are “small”!!

$$= \begin{pmatrix} A^0 \\ A^1 \\ A^2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbb{1} + \epsilon Q \\ \sqrt{\epsilon} R \\ \sqrt{\epsilon^2/2!} R^2 \\ \vdots \end{pmatrix}$$

DMRG — cMPS

Keep ϵ explicit, and don't
waste your time on $\mathbb{1}$!!

DMRG vs cMPS



Blue dots: "interpolating DMRG" with iterative refinement of discretization → many simulations

Green line: cMPS results
Single shot calculation

Part 2

Variational optimization for cMPS

arXiv:1611.03779

cMPS ground states for QFTs

Imaginary time evolution

$$\lim_{\tau \to \infty} \frac{e^{-H\tau} |\Psi\rangle}{|e^{-H\tau} |\Psi\rangle|}$$

Time dependent
variational principle (TDVP)
(Haegeman et al.
Phys. Rev. Lett. 107, 070601)

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Gradient optimization

$$\min_{Q,R} E(Q,R) \equiv \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

MG, J. Rincon, G. Vidal arXiv:1611.03779

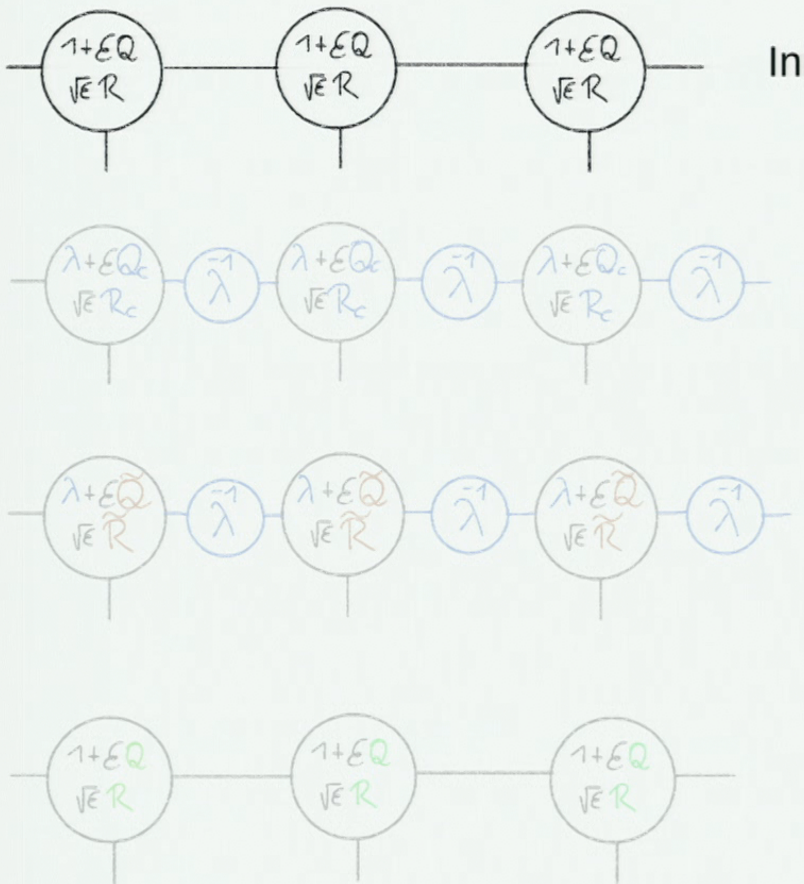
use $\frac{\partial E}{\partial(Q^*,R^*)}$ to lower energy:

$$\begin{pmatrix} Q \\ R \end{pmatrix} \to \begin{pmatrix} \tilde{Q} \\ \tilde{R} \end{pmatrix} = \begin{pmatrix} Q \\ R \end{pmatrix} - \alpha \begin{pmatrix} \partial E/\partial Q^* \\ \partial E/\partial R^* \end{pmatrix}$$

$\frac{\partial E}{\partial(Q^*,R^*)}$ is a **local** gradient

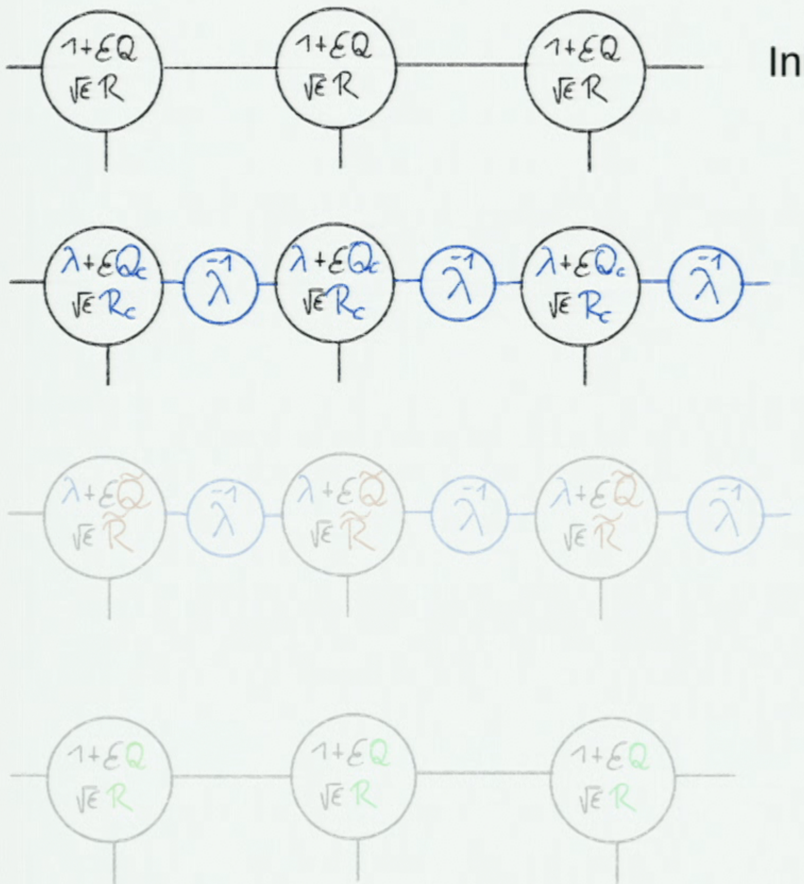
$\left\| \begin{pmatrix} \partial E/\partial Q^* \\ \partial E/\partial R^* \end{pmatrix} \right\|$ measures convergence

Gradient optimization details



Initial state

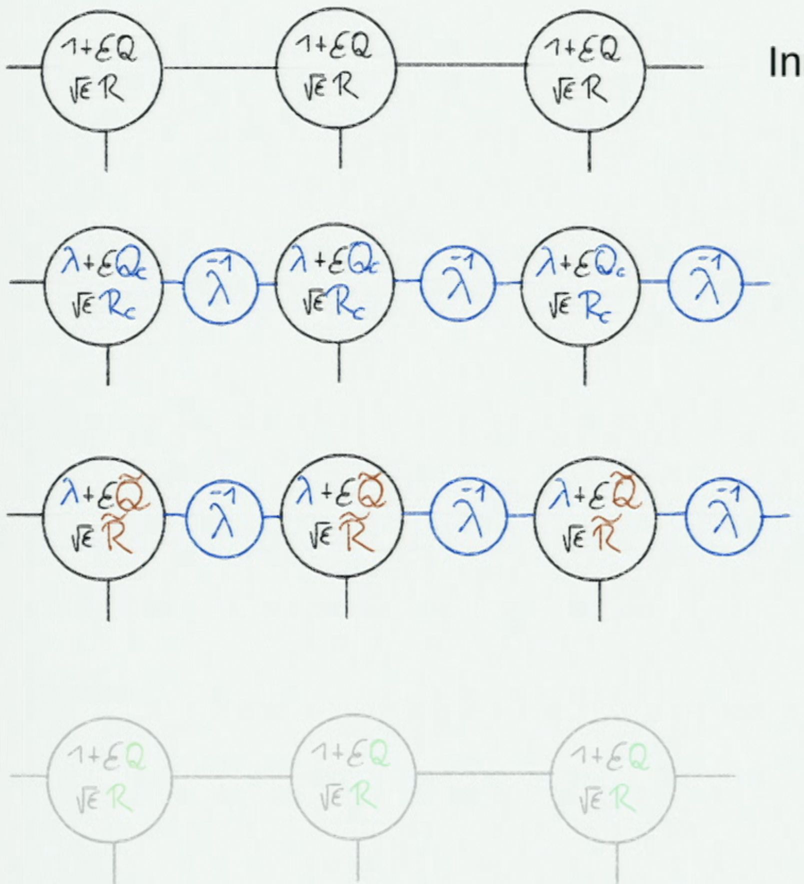
Gradient optimization details



Initial state

Regauge to
central canonical form

Gradient optimization details



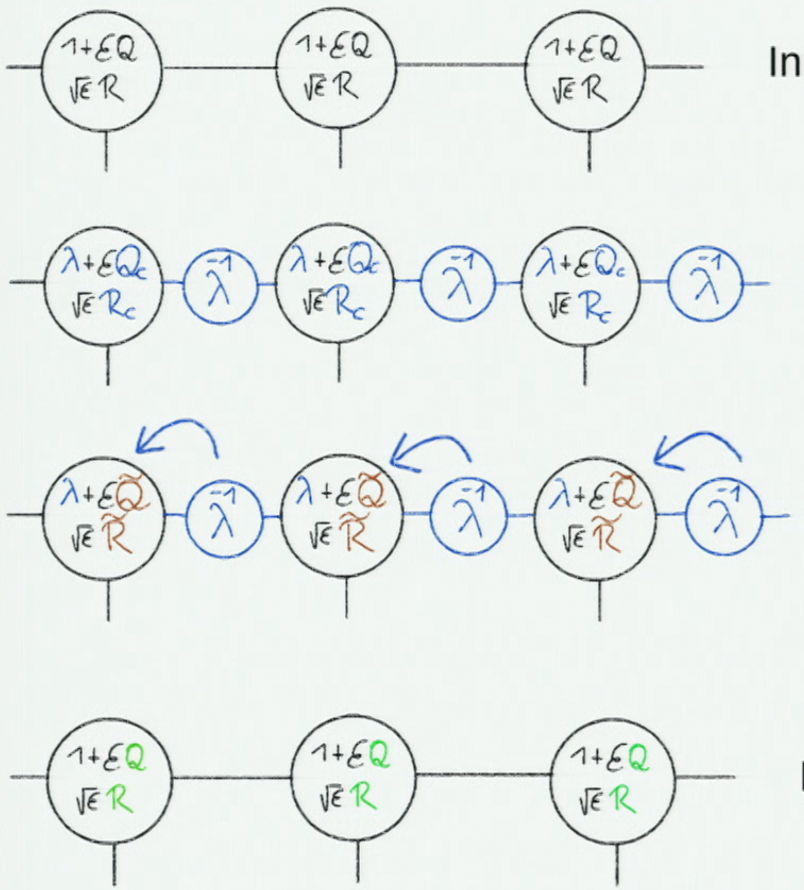
Initial state

Regauge to
central canonical form

Update

$$\begin{pmatrix} \tilde{Q} \\ \tilde{R} \end{pmatrix} = \begin{pmatrix} Q_c \\ R_c \end{pmatrix} - \alpha \begin{pmatrix} \partial E / \partial Q_c^* \\ \partial E / \partial R_c^* \end{pmatrix}$$

Gradient optimization details



Initial state

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central canonical form

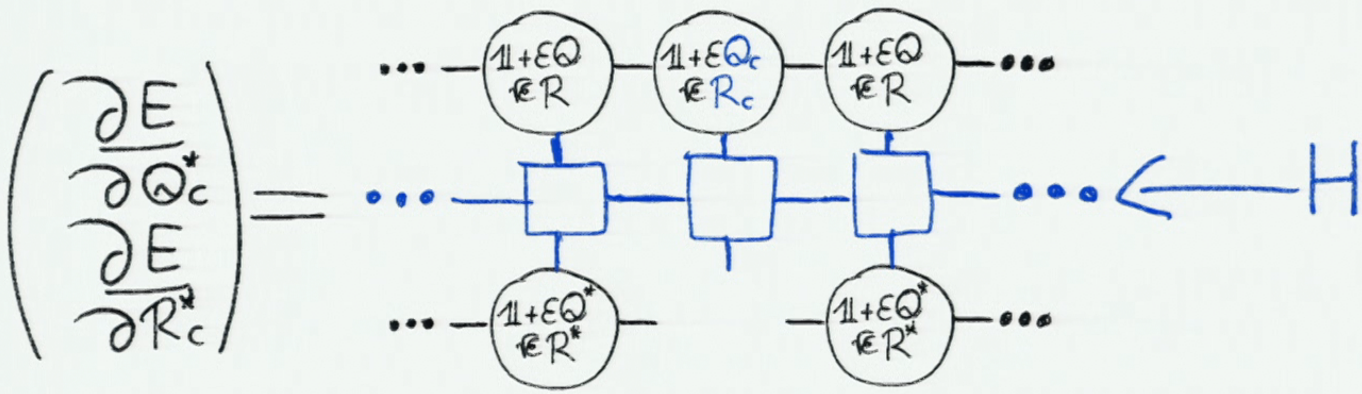
Update

$$\begin{pmatrix} \tilde{Q} \\ \tilde{R} \end{pmatrix} = \begin{pmatrix} Q_c \\ R_c \end{pmatrix} - \alpha \begin{pmatrix} \partial E / \partial Q_c^* \\ \partial E / \partial R_c^* \end{pmatrix}$$

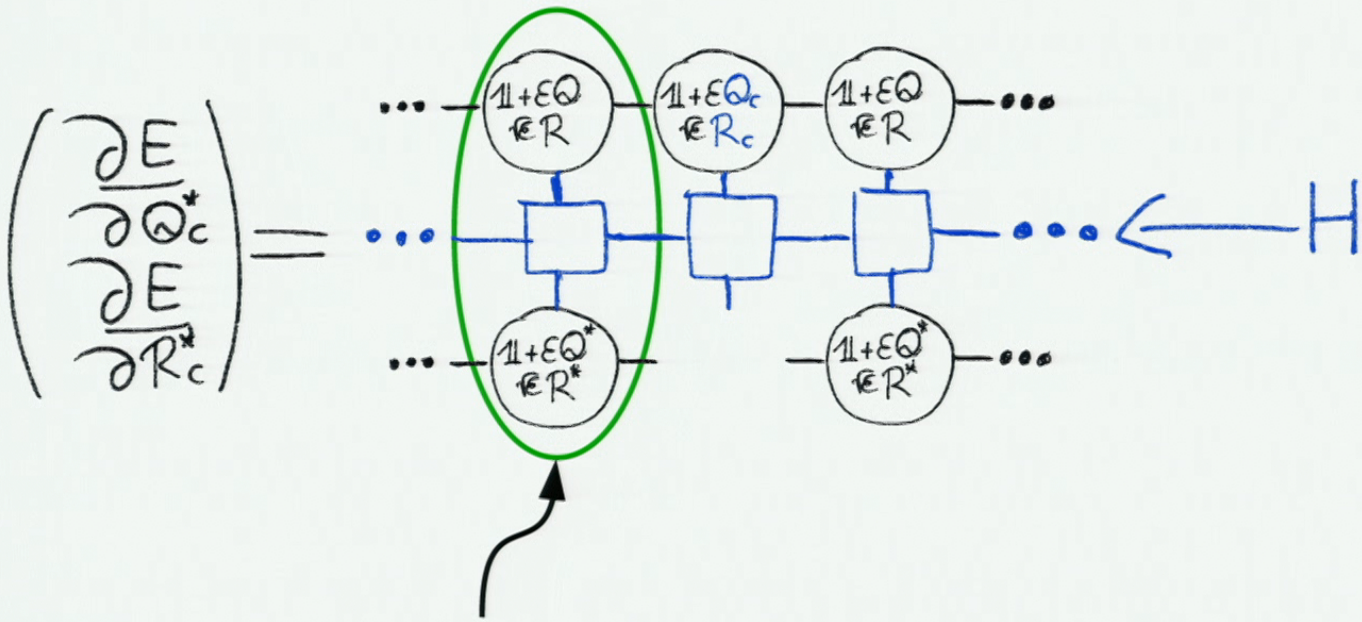
Absorb λ^{-1}

Final state

Here is the gradient



Here is the gradient



Infinitesimal layer

Benchmark: Lieb Liniger Model

Bosons with $\delta(r)$ interaction:

$$H = \int_{-\infty}^{\infty} \frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x) + g(\psi^\dagger(x))^2(\psi(x))^2 + \mu\psi^\dagger(x)\psi(x)$$

Bethe ansatz: $$g(z) - \frac{1}{2\pi}\int_{-1}^{1} dy \frac{2cg(y)}{c^2 + (y-z)^2} = \frac{1}{2\pi}$$

particle density $\rho \equiv \langle n \rangle = \int_{-1}^{1} dz g(z)$

energy density $e = \frac{1}{\langle n \rangle^3}\int_{-1}^{1} k^2 g(k)$

Why cMPS?

Variational parameters are “small”!!

$$= \begin{pmatrix} A^0 \\ A^1 \\ A^2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbb{1} + \epsilon Q \\ \sqrt{\epsilon} R \\ \sqrt{\epsilon^2/2!} R^2 \\ \vdots \end{pmatrix}$$

DMRG cMPS

Keep ϵ explicit, and don't waste your time on $\mathbb{1}$!!

Gradient optmization vs. imaginary time evolution: a comparison

Imaginary time evolution:
(Haegeman et al. 2012)

$$\lim_{\tau \to \infty} \frac{e^{-H\tau}\,|\Psi\rangle}{|e^{-H\tau}\,|\Psi\rangle\,|}$$

Largest bond dimensions $D = 64$

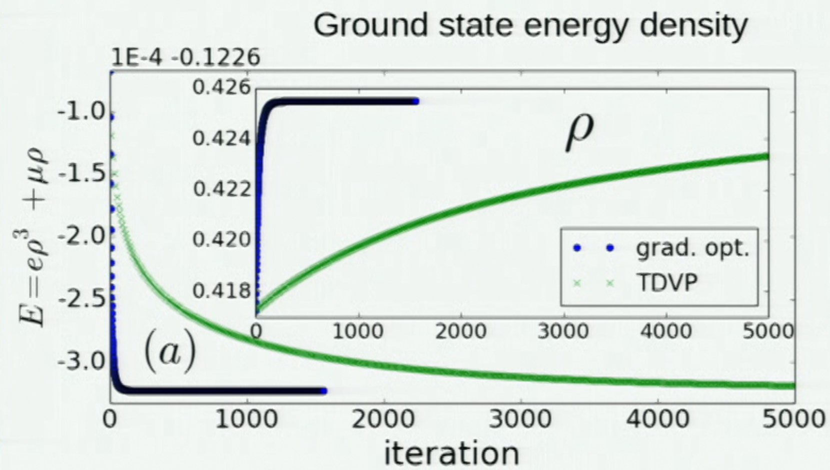
Slow convergence

Gradient optimization:

Fast convergence

Large bond dimensions $D = 256$

Non-linear conjugate gradient extension



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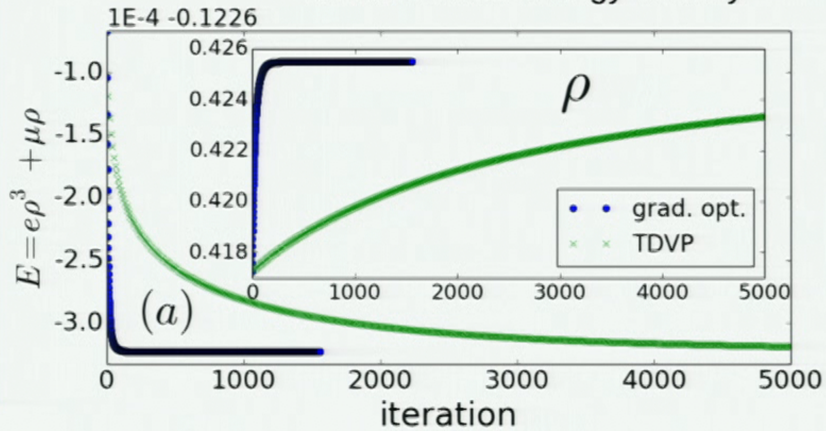
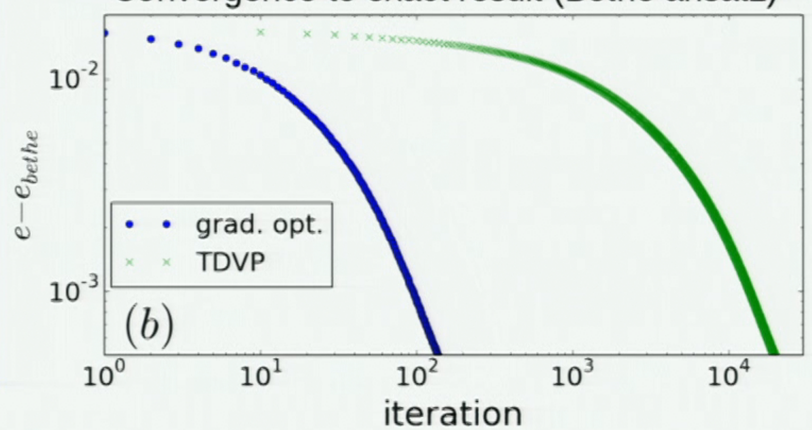
Ground state energy density

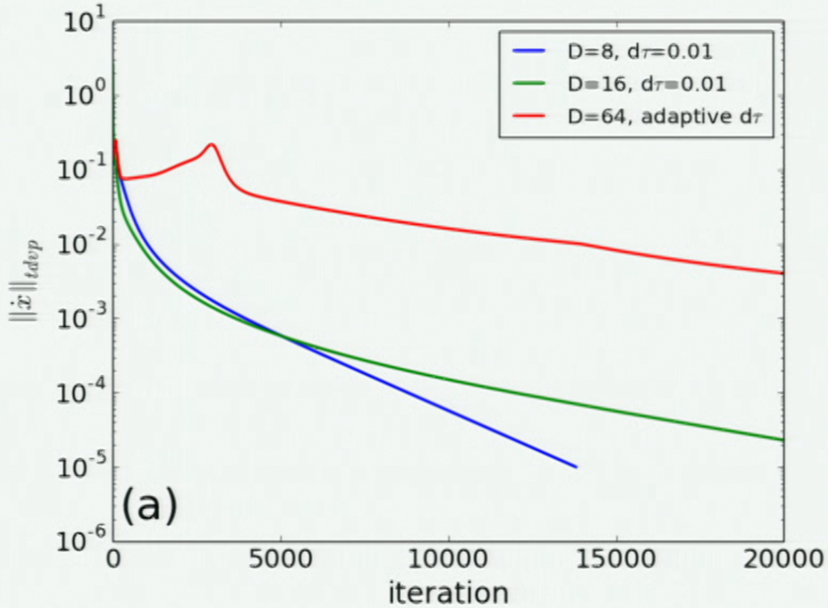


Convergence to exact result (Bethe ansatz)



The role of initialization

Imaginary time evolution can get lost



Gradient optimization can get lost, too!!

Reduce the problem with a good initial guess

DMRG preconditioning

Use **DMRG on coarse grids** Δx to get good initial states (there DMRG is very fast)

Substantial speed up due to *"DMRG preconditioning"*

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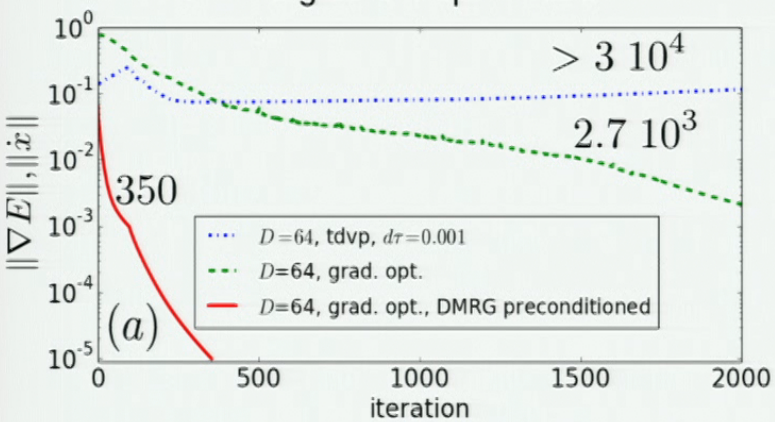
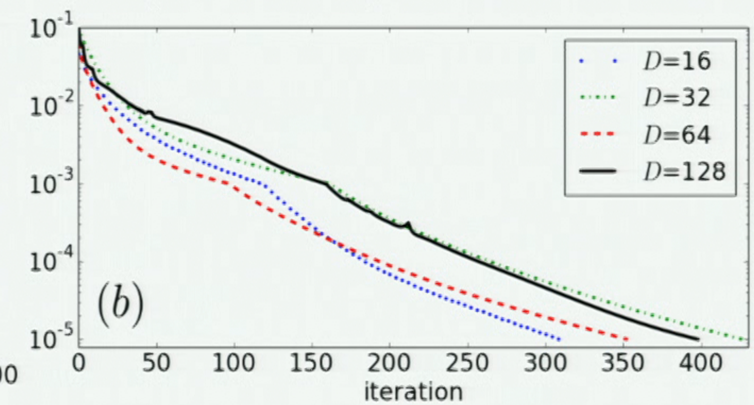
Convergence towards the ground state

TDVP vs gradient optimization



Gradient optimization with DMRG preconditioning

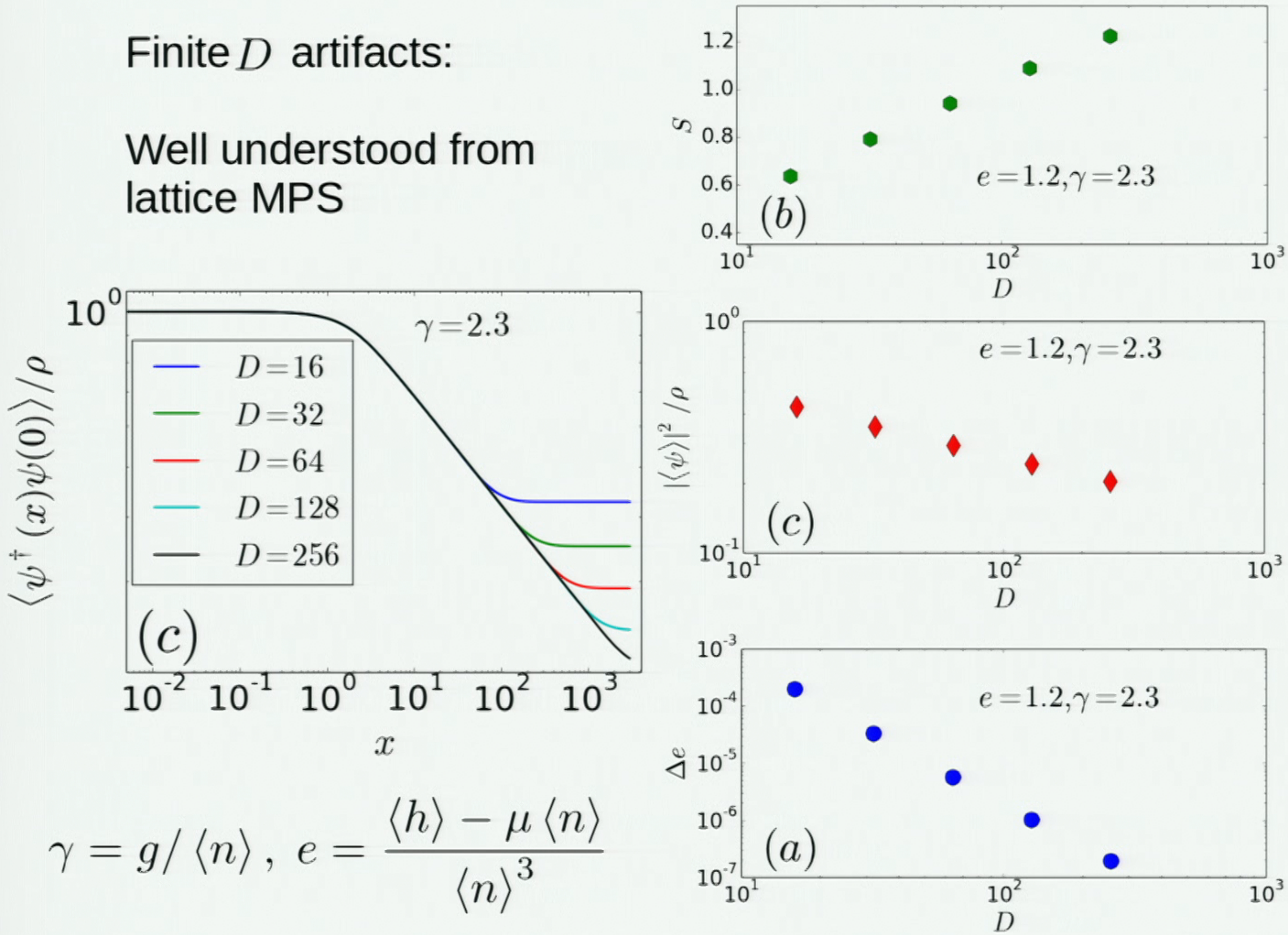


TDVP: D=64 runs for several days

D=128 in 2.5 h

Finite D artifacts:

Well understood from lattice MPS



$$\gamma = g/\langle n\rangle\,,\ e = \frac{\langle h\rangle - \mu\langle n\rangle}{\langle n\rangle^3}$$

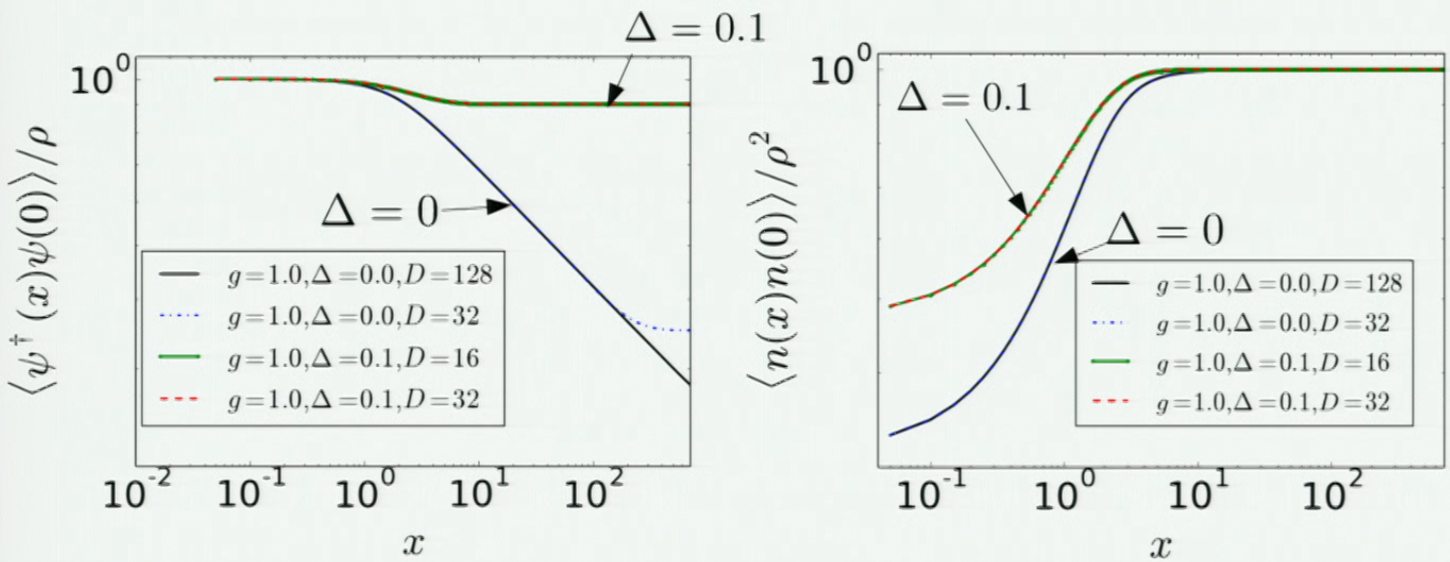
Non-integrable model

$$H = \int_{-\infty}^{\infty} \frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x) + g(\psi^\dagger(x))^2(\psi(x))^2 + \mu\psi^\dagger(x)\psi(x)$$

Lieb Liniger

$$+\Delta(\psi^\dagger(x)\psi^\dagger(x) + \psi(x)\psi(x))$$

pairing term



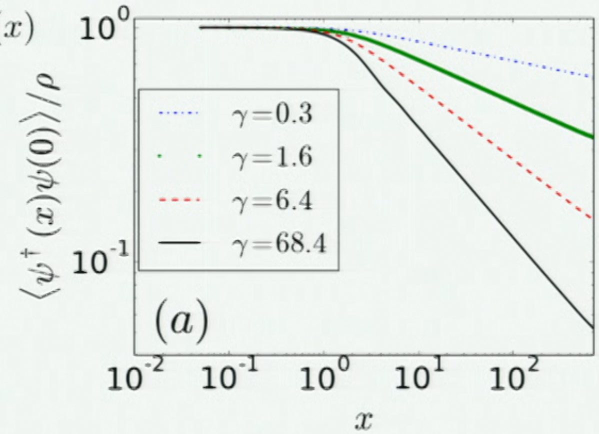
Δ opens a gap

Observables

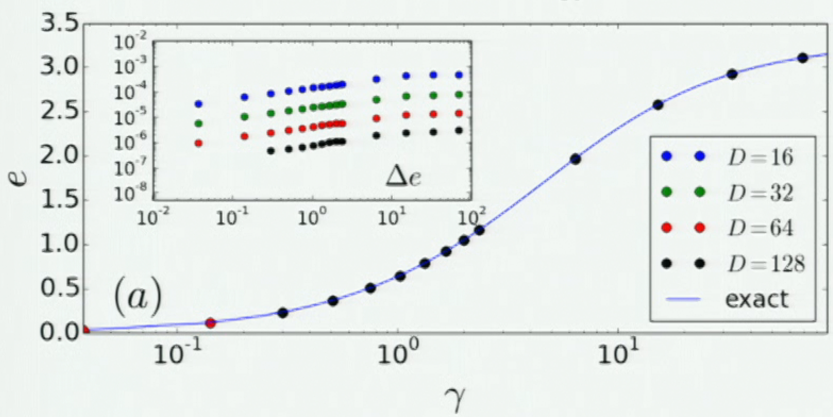
$$H = \int_{-\infty}^{\infty} \frac{d\psi^\dagger}{dx}(x)\frac{d\psi}{dx}(x) + g(\psi^\dagger(x))^2(\psi(x))^2 + \mu\psi^\dagger(x)\psi(x)$$

$$\gamma = g/\langle n\rangle\,,\ e = \frac{\langle h\rangle - \mu\langle n\rangle}{\langle n\rangle^3}$$

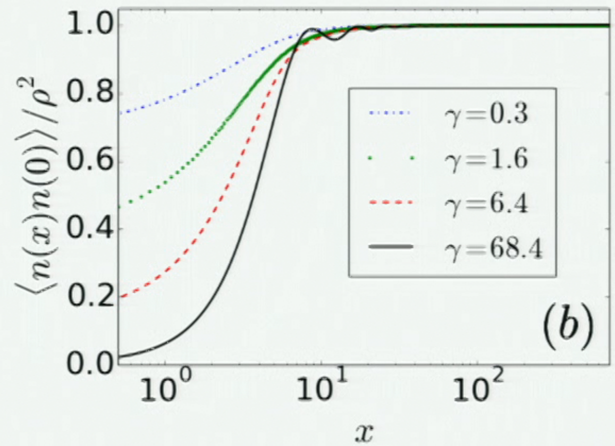
Structure factor



Ground state energy



Pairing correlation function



Conclusions

- Steepest descent gradient optimization is ~50 to 100 times faster that imaginary time evolution for cMPS
- Previously inaccessible bond dimensions can now be done with moderate resources
- Non-linear conjugate gradient can be easily implemented and gives another speedup of ~ 5 (see paper)
- DMRG is an excellent preconditioner for cMPS (factor ~5)

Outlook

- Fermions and multiple bosons
- Relativistic systems (phi-four)
- Cold atoms