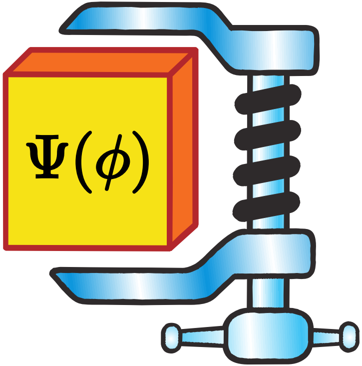
Prospects of the variational method for quantum field theory



Antoine Tilloy

April 25th, 2022

Séminaire

Quantum field theory: a bit of strategy

Two ways to attack *real world* quantum field theories non-perturbatively

1. Start **simpler** so that it becomes **simpler** [*e.g.* ϕ_2^4]
2. Start **more complex** so that it becomes **simpler** [*e.g.* $\mathcal{N} = 4$ *SYM*]

ϕ_2^4 - pile of dirt

QCD - Everest

$\mathcal{N} = 4$ *SYM* - Chrysler building

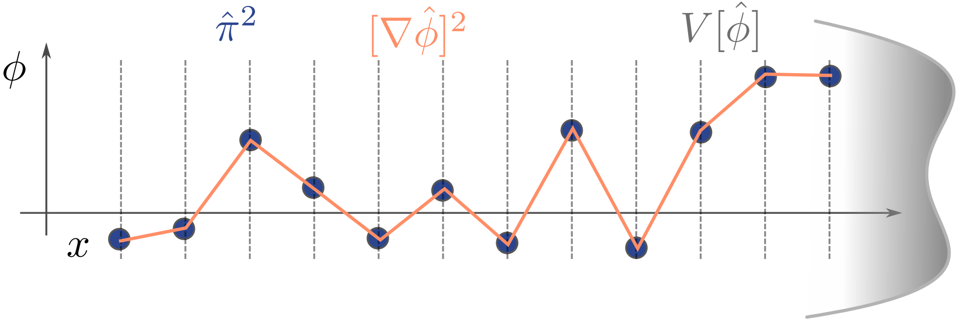
Outline

1. Scalar field theory for beginners
2. The variational method
3. Understanding on the lattice
4. Back to the continuum
5. Numerical application to ϕ^4_2 and Sinh-Gordon theories

Scalar field theory for beginners

and condensed matter theorists

Intuitive definition: canonical quantization



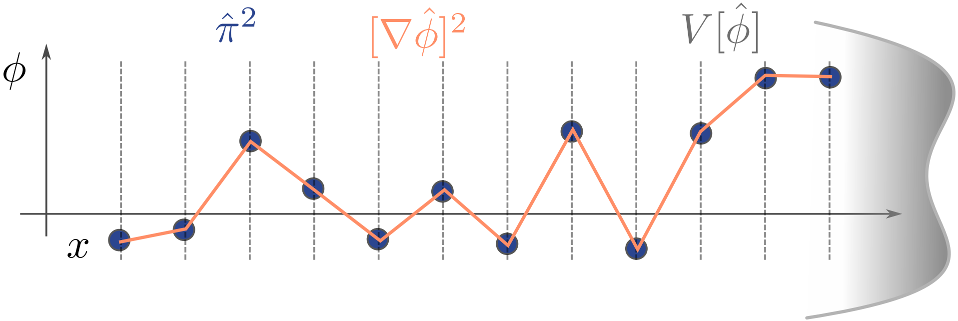
Hamiltonian

A continuum of nearest neighbor coupled anharmonic oscillators

$$\hat{H} = \int_{\mathbb{R}^d} \mathrm{d}^d x \quad \underbrace{\frac{\hat{\pi}(x)^2}{2}}_{\text{on-site inertia}} + \underbrace{\frac{[\nabla\hat{\phi}(x)]^2}{2}}_{\text{spatial stiffness}} + \underbrace{V(\hat{\phi}(x))}_{\text{on-site potential}}$$

with canonical commutation relations $[\hat{\phi}(x), \hat{\pi}(y)] = i\delta^d(x-y)\mathbb{1}$ (*i.e.* bosons)

Intuitive definition



Hilbert space

Fock space $\mathscr{H}_{\mathrm{QFT}} = \mathscr{F}[L^2(\mathbb{R}^d)]$ – just like $x, p \to (a, a^\dagger)$ do $\hat{\pi}, \hat{\phi} \to \hat{\psi}, \hat{\psi}^\dagger$

$$|\Psi\rangle = \sum_{n=0}^{+\infty} \int \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n \underbrace{\varphi_n(x_1, x_2, \cdots, x_n)}_{\text{wave function}} \underbrace{\hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\cdots\hat{\psi}^\dagger(x_n)}_{\text{local oscillator creation}} |\mathrm{vac}\rangle$$

What are the problems - Hilbert space approach

The Hamiltonian is ill defined on all states in the Hilbert space because of infinite zero point energy *i.e.* terms $\propto \widehat{\psi}(x)\widehat{\psi}^\dagger(x)$

$$\langle \Psi_1 | \widehat{H} | \Psi_2 \rangle = \pm\infty \quad \text{and even} \quad \langle \text{vac} | \widehat{H} | \text{vac} \rangle \propto \delta^d(0) = +\infty$$

If the divergent vacuum terms are removed, the Hamiltonian is not bounded from below

$$\forall \ |\Psi\rangle \in \mathscr{H}, \ \langle \Psi | \widehat{H}_{\text{finite}} | \Psi \rangle = \text{finite but} \ \ \exists \ \Psi_n \ \text{s.t.} \ \lim_{n \to +\infty} \langle \Psi_n | H_{\text{finite}} | \Psi_n \rangle = -\infty$$

How are they are solved in the free case - Hamiltonian

Bogoliubov transform

Go from $\hat{\psi}(x), \hat{\psi}^\dagger(x)$ to $a(p), a^\dagger(p)$ with

$$a(p) = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_p}\,\hat{\phi}(p) + \frac{\hat{\pi}(p)}{\sqrt{\omega_p}}\right) \quad \text{with} \quad \omega_p = \sqrt{p^2 + m^2}$$

which yields

$$H_0 = \int \mathrm{d}p\, \omega_p \, \frac{1}{2}\left(a_p^\dagger a_p + a_p a_p^\dagger\right)$$

Solution

- Take $H_{\mathrm{QFT}} \equiv \, : H :_a$
- $|\text{free ground state}\rangle = |\text{vacuum}\rangle_a$
- $\mathscr{H}$ built from $a_{p_1}^\dagger \cdots a_{p_n}^\dagger |\text{vacuum}\rangle_a$

This solves the problematic free part exactly, and allows to define a finite interaction (in $1+1$)

Rigorous operator definition of ϕ_2^4

Renormalized ϕ_2^4 theory

$$H = \int \mathrm{d}x \, \frac{:\pi^2:_a}{2} + \frac{:(\nabla\phi)^2:_a}{2} + \frac{m^2}{2} :\phi^2:_a + g:\phi^4:_a$$

(note that $:\diamondsuit:_a$ depends on m)

1. Rigorously defined relativistic QFT without cutoff (Wightman QFT)
2. Vacuum energy ε_0 density finite
3. Very difficult to solve unless $g \ll m^2$ (perturbation theory)
4. Phase transition around $f_c = \frac{g}{4m^2} = 11$ i.e. $g \simeq 2.7$ in mass units

Other well defined potentials $\rightarrow$ $:\cos(\beta\phi):$ or $:\cosh(\beta\phi):$

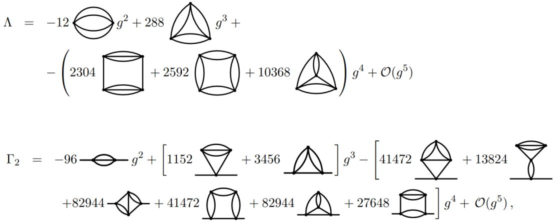
The variational method

Solving the non-exactly solvable by compressing

Two (main) games in town

Perturbation theory

+ resummation

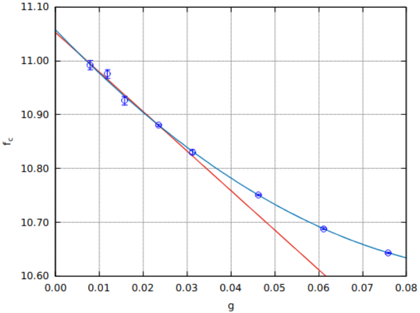


state of the art is $O(g^8)$

arXiv:1805.05882

Serone, Spada, Villadoro

Lattice Monte-Carlo



arXiv:1807.03381

Bronzin, De Palma, Guagnelli

The direct compression approach

Variational method for ground state search

1. Guess a manifold $\mathcal{M} \subset \mathscr{H}$ with few parameters ν *i.e.* $\dim \mathcal{M} \ll \dim \mathscr{H}$
2. Tune ν to minimize energy $\nu = \text{argmin}_{\nu \in \mathcal{M}} \frac{\langle \nu | H | \nu \rangle}{\langle \nu | \nu \rangle}$ and get $|\text{ground state}\rangle \simeq |\nu\rangle$

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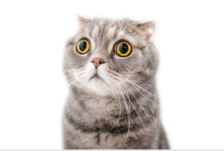
Reason for compression (classical)



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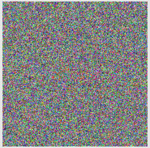

"typical" image

atypical $\Longrightarrow$ compressible

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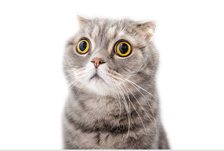

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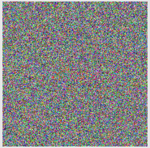

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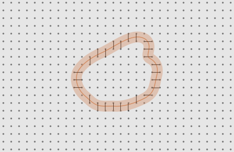
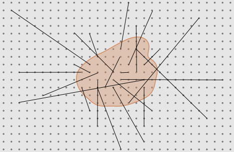
Reason for compression (quantum)



low energy state



random state

area law $=$ atypical $\Longrightarrow$ compressible

Feynman's criticism

Difficulties in Applying the Variational Principle to Quantum Field Theories[1]

so I tried to do something along these lines with quantum chromodynamics. So I'm talking on the subject of the application of the variational principle to field theoretic problems, but in particular to quantum chromodynamics.

I'm going to give away what I want to say, which is that I didn't get anywhere! I got very discouraged and I think I can see why the variational principle is not very useful. So I want to take, for the sake of argument, a very strong view – which is stronger than I really believe – and argue that it is no damn good at all!

Feynman's requirement in a nutshell

1. **Extensive parameterization**
   Number of parameters $\propto L^{\alpha}$ at most for system size L (not $\propto \mathrm{e}^{L}$)
2. **Computable expectation values**
   ψ known $\implies \langle \mathcal{O}(x)\mathcal{O}(y)\rangle_{\psi}$ computable
3. **Not oversensitive to the UV**
   no runaway minimization where higher and higher momenta get fitted

Elegantly swallowing the bullet

Example: naive Hamiltonian truncation

With an IR cutoff L, momenta are discrete. Take as submanifold $\mathscr{M}$ the **vector space** spanned by:

$$|k_1, k_2, \cdots, k_r\rangle = a^\dagger_{k_1} a^\dagger_{k_2} \cdots a^\dagger_{k_r} |0\rangle_a$$

such that $\langle k_1 k_2 \cdots k_r | H | k_1 k_2 \cdots k_r \rangle \leqslant E_{\text{trunc}}$ $\rightarrow$ finite dimensional

Breaks **extensiveness**

- number of parameters $\propto \mathrm{e}^{L \times E_{\text{trunc}}}$
- error $\propto E_{\text{trunc}}^{-3}$ (with renormalization refinements)

still good results, see Rychkov & Vitale `arXiv:1412.3460`

Relativistic continuous matrix product states

RCMPS: *A variational ansatz to solve $1+1d$ relativitic QFT without discretization or cutoff and to arbitrary precision*

Definition

(Verstraete & Cirac 2010 for non-relativistic $\longrightarrow$ AT 2021 for relativistic)

A RCMPS is a manifold of states parameterized by 2 $(D \times D)$ matrices Q, R

$$|Q, R\rangle = \text{tr}\left\{\mathcal{P}\exp\left[\int \mathrm{d}x\, Q \otimes \mathbb{1} + R \otimes a^\dagger(x)\right]\right\}|0\rangle_a$$

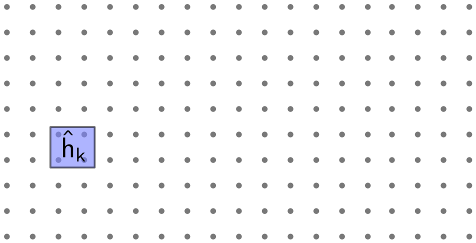
with

- $a(x) = \frac{1}{2\pi}\int \mathrm{d}k\, \mathrm{e}^{ikx} a_k$ where $a_k = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_p}\,\hat{\phi}(p) + i\frac{\hat{\pi}(p)}{\sqrt{\omega_p}}\right)$
- trace taken over $\mathbb{C}^D$
- $\mathcal{P}$ path-ordering exponential

On the lattice

the variational method with tensor networks in a simpler context

Quantum many-body problem on the lattice



Typical many-body problem

N spins on a lattice

$\mathscr{H} = \bigotimes_{j=1}^{n} \mathscr{H}_j$ with $\mathscr{H}_j = \mathbb{C}^2$

$|\psi\rangle = \sum c_{i_1, i_2, \cdots, i_n} |i_1, i_2, \cdots i_N\rangle$

Problem:

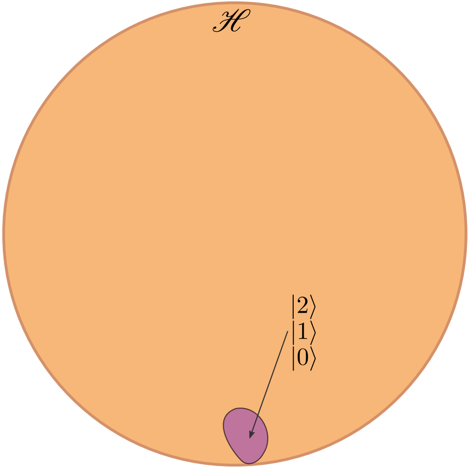
Finding the low energy states of

$$H = \sum_{k=1}^{N} h_k$$

is **hard** because $\dim \mathscr{H} = 2^N$ for spins

Fugaku – 2 EFLOPS – 150 PB
cannot do $4 \times 4 \times 4$ spins

Variational optimization



Generic (spin $d/2$) state $\in \mathscr{H}$:

$$|\psi\rangle = \sum_{i_1, i_2, \cdots, i_n} c_{i_1, i_2, \cdots, i_N} |i_1, \cdots, i_N\rangle$$

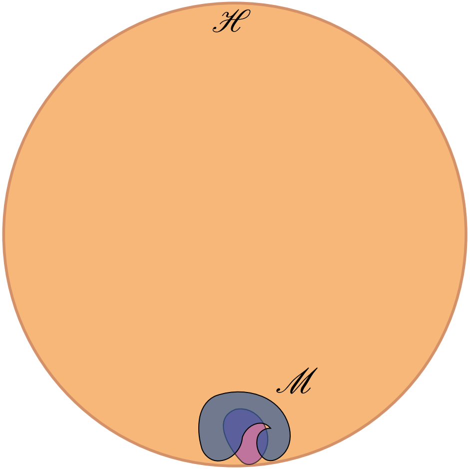
Exact variational optimization

To find the ground state:

$$|0\rangle = \min_{|\psi\rangle \in \mathscr{H}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

- $\dim \mathscr{H} = d^N$

Variational optimization



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$$|\psi\rangle = \sum_{i_1, i_2, \cdots, i_n} c_{i_1, i_2, \cdots, i_N} |i_1, \cdots, i_N\rangle$$

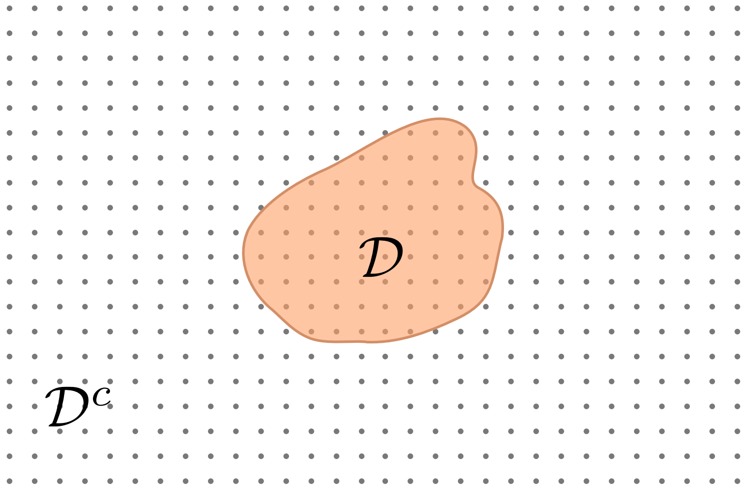
Approx. variational optimization

To find the ground state:

$$|0\rangle = \min_{|\psi\rangle \in \mathscr{M}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

- $\dim \mathscr{M} \propto \mathrm{Poly}(N)$ or fixed

Interesting states are weakly entangled



Low energy state

$|\psi\rangle = |0\rangle$ or $|1\rangle$ ...

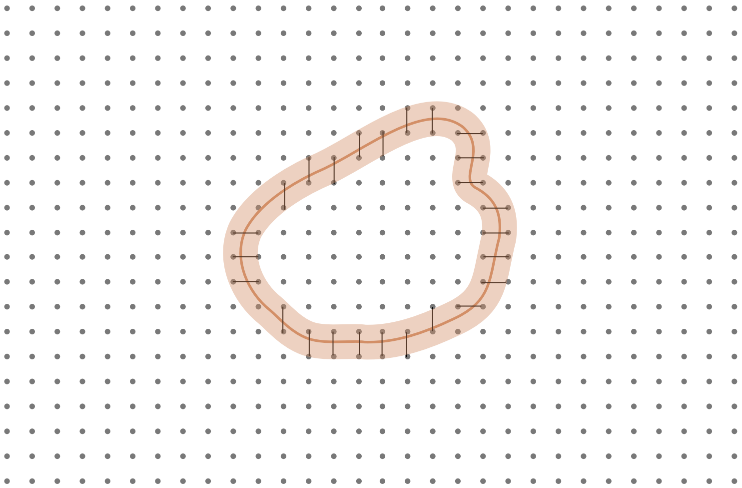
Reduced density matrix
$\rho = \mathrm{tr}_{\mathcal{D}^c}\left[|\psi\rangle\langle\psi|\right]$

Entanglement entropy
$S = -\mathrm{tr}\left[\rho \log \rho\right]$

Area law

$$S \propto |\partial\mathcal{D}|$$

Interesting states are weakly entangled



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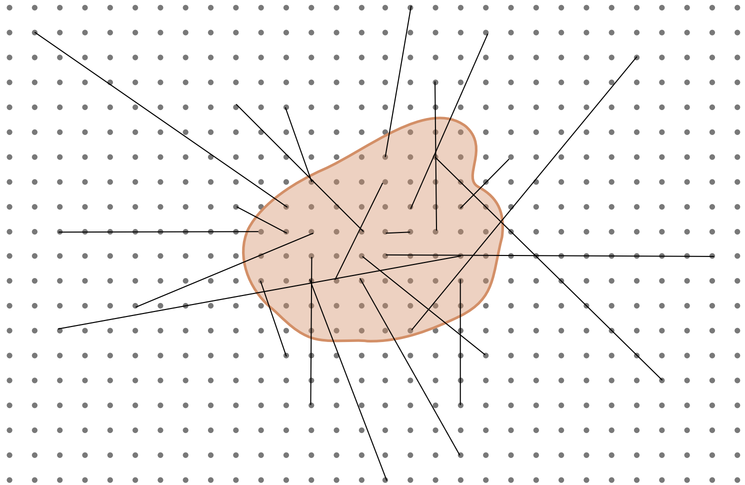
Typical states are strongly entangled



Random state

$|\psi\rangle = U_{\text{Haar}}|\text{trivial}\rangle$

Reduced density matrix
$\rho = \text{tr}_{\mathcal{D}^c}\left[|\psi\rangle\langle\psi|\right]$

Entanglement entropy
$S = -\text{tr}\left[\rho \log \rho\right]$

Volume law

$S \propto |\mathcal{D}|$

The solution in 1 +1: Matrix Product States (MPS)

Definition

A MPS for a translation invariant chain of N qudits ($\mathbb{C}^d$) with periodic boundary conditions is a state

$$|\psi(A)\rangle := \sum_{i_1,i_2,\ldots,i_N} \mathrm{tr}\left[A_{i_1} A_{i_2} \cdots A_{i_N}\right] |i_1, i_2, \ldots, i_N\rangle$$

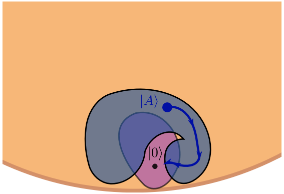
where A_i are d matrices $\in \mathcal{M}_D(\mathbb{C})$.

- The matrices A_i for $i = 1 \ldots d$ are the free parameters
- The size D of the matrices is the **bond dimension** (quantifies freedom)
- Correlation functions (and $\langle H \rangle$) efficiently computable
- Entanglement entropy verifies Area Law

Optimization

To find lowest energy state, with generic TNS, still need to optimize the $\text{poly}(D)$ parameters

- Naive gradient descent inefficient (works only for $D \leqslant 10$)
- Riemanian gradient descent highly efficient ($=$ TDVP)



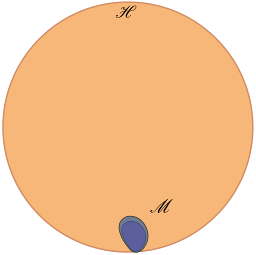
Metric on tensor network state manifold

1. $|\psi(A)\rangle \in \mathscr{M}$ a state in the tensor network manifold
2. $|\psi(A), W\rangle = W \cdot \nabla_A |\psi(A)\rangle$ the tangent vector in A along direction W
3. $g_A(V, W) := \text{Re}\,\langle \psi(A), V | \psi(A), W \rangle$ induced Hilbert metric

Note: best is to do Riemanian quasi-Newton, like Riemanian conjugate gradient or Riemanian LBFGS $\rightarrow$ `OptimKit.jl` by Haegeman et al.

Some facts

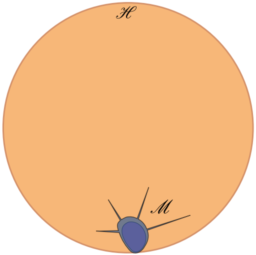
1 spatial dimension



Theorems (colloquially)

1. For gapped H, tensor network states $|A\rangle$ approximate well $|0\rangle$ as D increases
2. **All** $|A\rangle$ are ground states of local gapped H

$\geqslant 2$ spatial dimension



Folklore

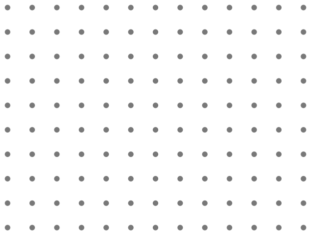
1. For gapped H, tensor network states $|A\rangle$ approximate well $|0\rangle$ as D increases
2. **Most** $|A\rangle$ are ground states of local gapped H

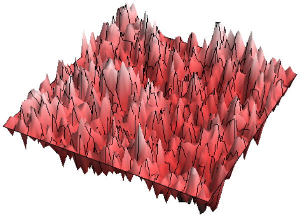
Relativistic matrix product states

taking MPS to the limit

The quantum many-body problem in the continuum

From the lattice to the continuum and Quantum Field Theory (QFT)





$$|\Psi\rangle = \sum_{i_1, i_2, \cdots, i_N} c_{i_1 i_2 \cdots i_N} |i_1 i_2 \cdots i_N\rangle \quad \longrightarrow \quad |\Psi\rangle = \int \mathcal{D}\phi \, \psi(\phi) \, |\phi\rangle$$

New problem: 2^N $\mathbb{C}$-parameters $\rightarrow \dim \mathscr{H} = \infty^\infty$ even at finite size!

Question Can one compress ∞^∞ down to a manageable number of parameters?

Relativistic continuous matrix product states

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Definition

(Verstraete & Cirac 2010 for non-relativistic $\longrightarrow$ AT 2021 for relativistic)

A RCMPS is a manifold of states parameterized by 2 $(D \times D)$ matrices Q, R

$$|Q,R\rangle = \mathrm{tr}\left\{\mathcal{P}\exp\left[\int \mathrm{d}x\, Q\otimes \mathbb{1} + R\otimes a^\dagger(x)\right]\right\}|0\rangle_a$$

with

- $a(x) = \frac{1}{2\pi}\int \mathrm{d}k\, \mathrm{e}^{ikx} a_k$ where $a_k = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_p}\,\hat{\phi}(p) + i\frac{\hat{\pi}(p)}{\sqrt{\omega_p}}\right)$
- trace taken over $\mathbb{C}^D$
- $\mathcal{P}$ path-ordering exponential

Basic properties of RCMPS

$$|Q,R\rangle = \mathrm{tr}\left\{\mathcal{P}\exp\left[\int \mathrm{d}x\, Q\otimes \mathbb{1} + R\otimes a^\dagger(x)\right]\right\}|0\rangle_a$$

Feynman's checklist:

1. **Extensive** because of $\mathcal{P}\exp\int$
2. Obervables **computable** at cost D^3 (non trivial!)
   requires $[a(x), a^\dagger(y)] = \delta(x-y)$ i.e. *quantum noise* techniques
3. **No UV problems**
   $|0,0\rangle = |0\rangle_a$ is the ground state of H_0 hence exact CFT UV fixed point
   $\langle Q,R|h_{\phi^4}|Q,R\rangle$ is finite for all Q,R (not trivial!)

The variational algorithm

Procedure:
Compute $e_0 = \langle Q, R | h_{\phi^4} | Q, R \rangle$ and $\nabla_{Q,R} e_0$
Minimize e_0 with **TDVP** aka gradient descent with a metric

Computations of e_0 and ∇e_0 in a nutshell:

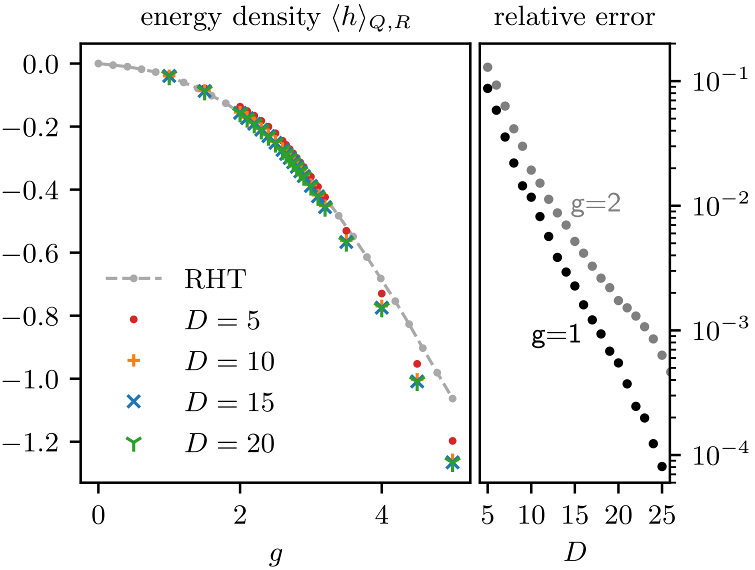
1. $V_b = \langle :e^{b\phi(x)}: \rangle_{QR}$ computable by solving an ODE with cost $\propto D^3$
2. $\langle :\phi^n: \rangle_{QR}$ computable doing $\partial_b^n V_b \Big|_{b=0} \quad \rightarrow \quad \propto D^3$
3. $e_0 = \langle h \rangle_{QR}$ computable by summing such terms at cost $D^3 \quad \rightarrow \quad \propto D^3$
4. ∇e_0 computable by solving the adjoint ODE (backpropagation) $\quad \rightarrow \quad \propto D^3$

ϕ^4_2 theory

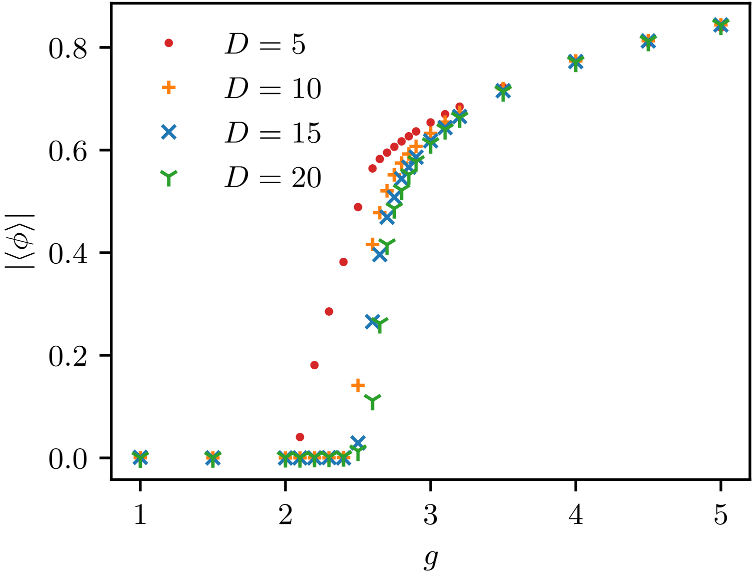
$$H = \int \mathrm{d}x \, \frac{:\pi^2:}{2} + \frac{:(\nabla\phi)^2:}{2} + \frac{m^2}{2} :\phi^2: + g :\phi^4:$$

1. Well-defined
2. Non-integrable - hard to carry accurate computations
3. Well understood qualitatively
4. phase transition for $g \simeq 2.7$

Results: ϕ_2^4 energy density



Results: ϕ_2^4 – field expectation value $\langle\phi\rangle$

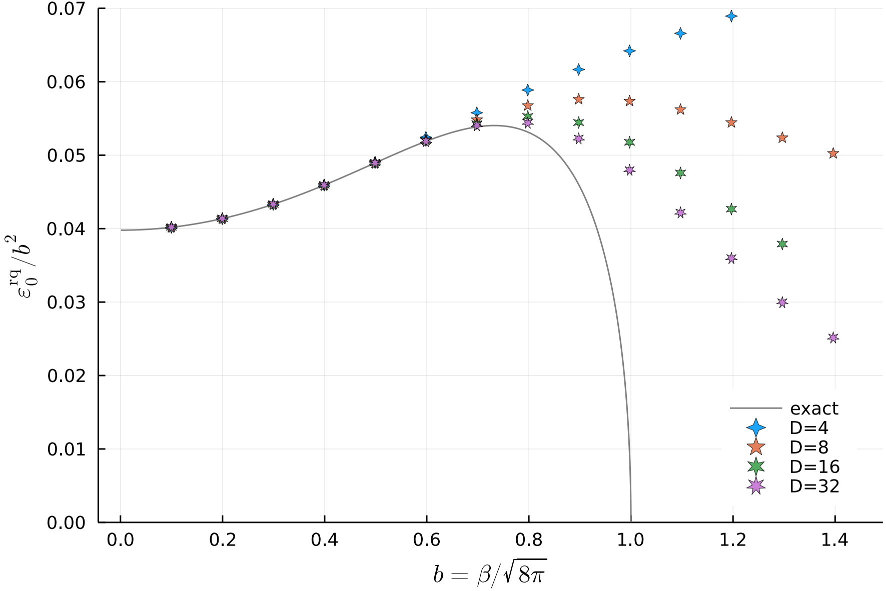


Sinh-Gordon theory

$$H = \int dx \, \frac{:\pi^2:}{2} + \frac{:(\nabla\phi)^2:}{2} + \mu :\cosh(\beta\phi):$$

1. Well-defined (at least for $\beta \leqslant \sqrt{4\pi}$ and probably $\beta \leqslant \sqrt{8\pi}$)
2. Integrable - exact results by Zamolodchikov et al.
3. Controversies about qualitative behavior
   [see Konik Lajer Mussardo arXiv:2007.00154]
4. Phase transition at $\beta = \sqrt{8\pi}$ (??)

Results for Sinh-Gordon – energy density



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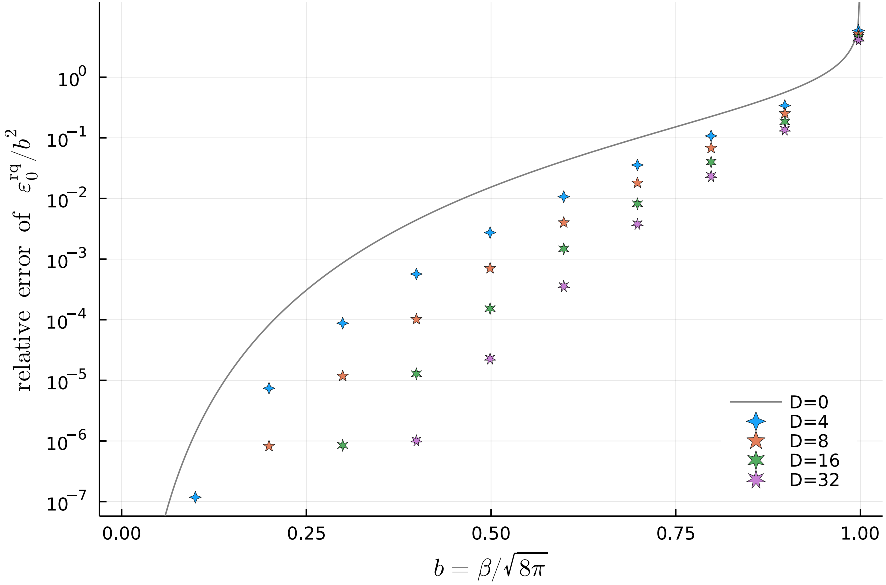
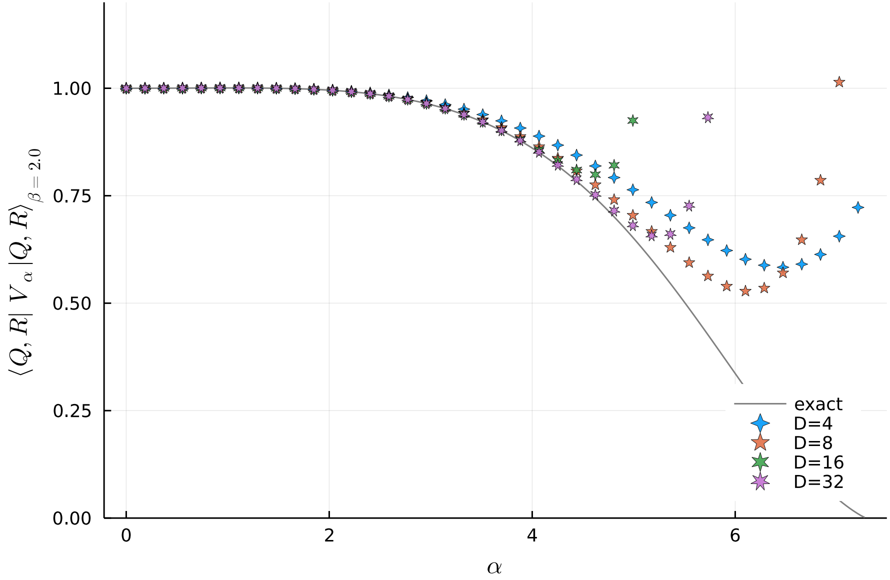
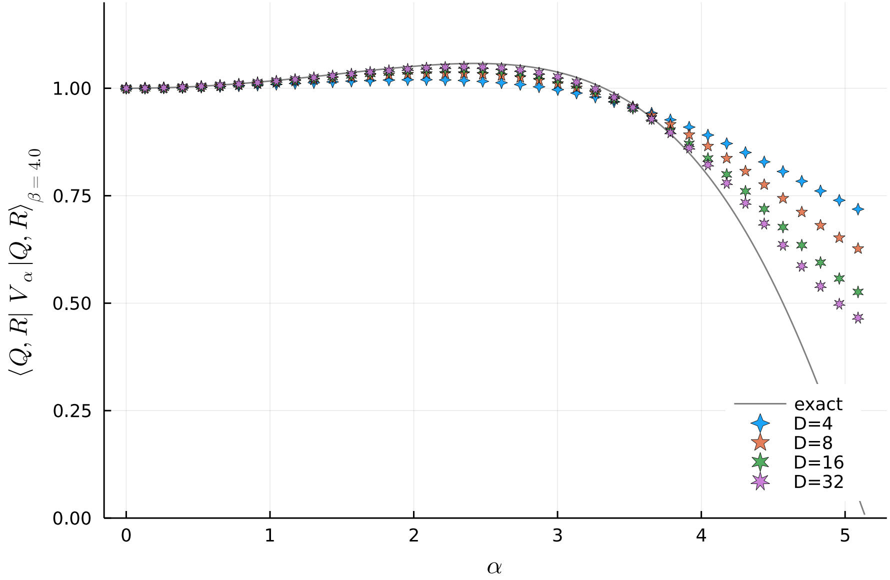


Results for Sinh-Gordon – $\langle : \exp(\alpha\phi) : \rangle$ at $\beta = 2.0$



Results for Sinh-Gordon – $\langle : \exp(\alpha\phi) : \rangle$ at $\beta = 4.0$



Discussion

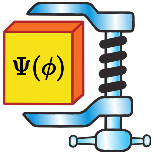
Remaining objectives do more realistic theories

	non-relativistic	relativistic	critical
$d = 1$ space	Verstraete-Cirac 2010	AT 2021	
$d \geqslant 2$ space	AT-Cirac 2019		

no idea	heuristics	clear definition	fast algorithm

Summary

$$|Q, R\rangle = \operatorname{tr}\left\{\mathcal{P}\exp\left[\int \mathrm{d}x\, Q\otimes\mathbb{1} + R\otimes a^\dagger(x)\right]\right\}|0\rangle_a$$



1. Ansatz for $1+1$ relativistic QFT
2. No cutoff, UV or IR, extensive, computable
3. UV is captured exactly even at $D=0$
4. Efficient (cost poly D, error 1/superpoly D) and now competitive
5. Rigorous (variational)