Title: A variational wave-function based method for simulating quantum field theories

Date: May 25, 2010 02:00 PM

URL: http://pirsa.org/10050065

Abstract: TBA

Variational wavefunctions for quantum field theories

Frank Verstraete, *University of Vienna*
Ignacio Cirac, *Max Planck Institute for Quantum Optics*
Tobias Osborne, Jens Eisert, *Wissenshaftskolleg Berlin*
Jutho Haegeman, Henri Verschelde, *University of Ghent*

Variational methods for strongly interacting quantum spin systems (I)

- Starting point: Wilson's numerical renormalization group for simulating Kondo impurity ('75)
  - Crucial ingredient: exponentially decreasing energy scales
  - Central problem: does not work for translational invariant systems
- Breakthrough: White's density matrix renormalization group ('92)
  - Crucial ingredient: information about all long-range correlations of the wavefunction are stored in a local density matrix
  - yields extremely precise results for simulating ground states of spin and fermionic systems in 1+1 dimension

Variational methods for strongly interacting quantum spin systems (II)

- Recent conceptual advances:
  - NRG and DMRG work so well because they are variational methods within the class of matrix product states
    (Romer, Ostlund,Nishino,Verstraete and Cirac,)
  - Matrix product states capture the physics for representing any ground state of a local Hamiltonian faithfully: area laws
    (Verstraete and Cirac, Hastings)
- Rephrasing DMRG in language of MPS allowed to extend the formalism to
  - higher dimensions: Projected Entangled Pair States
    (Verstraete and Cirac, precursors by Martin-Delgado, Sierra, Nishino)
  - real-time evolution of low-energy states (Vidal et al.)

What about using MPS-methods for simulating quantum field theories?

- Obvious approach: discretize theory and put it on a lattice
  - Example: discretization of Lieb-Liniger model leads to Bose-Hubbard model:

$$\mathcal{H} = \int_{-\infty}^{+\infty} dx \left[\frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right]$$

$$\hat{H} = -J \sum_j (\hat{a}_j^\dagger \hat{a}_{j+1} + h.a.) + \frac{U}{2} \sum_j \hat{a}_j^{\dagger 2} \hat{a}_j^2$$

- Problems:
  - For MPS, the 2-point correlation functions are decaying exponentially in the number of sites between them; so it seems impossible to construct scale-invariant solutions that yield the same correlation functions independent of the lattice parameter
  - For finite filling factor, the probability of having a particle is proportional to the lattice constant; this implies that all matrices in MPS have to become singular
  - In case of bosonic systems, we have to allow for large local occupation numbers; this increases numerical cost badly
  - Discretization of relativistic bosonic field theories: what mass to chose?
  - Fermion doubling problem

Is it possible to construct variational wavefunctions in the continuum?

- It would be very interesting to develop wave-function based formalism to describe quantum field theory
  - Divergencies may disappear automatically if the wavefunctions have some build-in cut-off
  - Would open the door for describing non-equilibrium behaviour in Minkowski space
  - Might lead to a better understanding of topological quantum order
  - Would describe current experiments in optical lattices, atom chips, etc.

- Feynman's last talk: "Difficulties in Applying the Variational Principle to Quantum Field Theories"

Proc. Int. Workshop on Variational Calculus in Quantum Field Theory, Wangerooge, West Germany, Sept. 1-4, 1987.

  - "… I didn't get anywhere. So I want to take, for the sake of arguments, a very strong view – which is stronger than I really believe – and argue that it is no damn good at all! "
  - 3 Major Objections:
    - Sensitivity to high frequencies
    - Only exponential trial states
    - We still have to do a functional integral in 1 dimension lower
  - One visionary insight: local parametetization of the global wavefunction

Feynman Objection I: Sensitivity to High Frequencies

- Energy contributions to the total energy of the high frequency modes are much more important than the low-energy ones (cfr. Zero-point energy)

- Therefore any variational method will try to get the high-frequencies right, even at the cost of getting low-energy behaviour wrong

  – "... what happens when I allow it to adjust its parameter (to lower the total energy), is it improves the imperfect function I was using at the high frequencies..."

- This is obviously not what we want!
  – We are interested in long-range low-energy physics, this is the point of a quantum field theory

Feynman Objection II: Only exponential trial states

- For atoms, very good variational wavefunctions are of the form

$$\psi(x) \approx \left(1 - \beta x^4\right)\exp\left(-\alpha x^2\right)$$

- This is not possible in the case of QFT, as the dimensions do not fit in formulae like

$$\psi(x) \approx \left(1 - \beta \int \phi(x)^4 dx\right)\exp\left(-\int\int \phi(x) K(x,y) \varphi(y) dx dy\right)$$

as the wavefunction has to be "size extensive"

- What we want instead is corrections of the form $\exp\left(-\beta \int \phi(x)^4 dx\right)$ but then we have to evaluate non-Gaussian functional integrals which is extremely hard to do with good enough precision

Feynman Objection III: We still have to do a functional integral

- Very much related to objection II: we wanted to avoid taking functional integrals in the first place, and the only thing the variational treatment helps if a good wavefunction has been found is that the functional integral has now to be taken in 3 dimensions instead of 4; this is still a very hard problem

Feynman visionary suggestion as a way out:

"It's really quite insane actually: we are trying to find the energy by taking the expectation of an operator which is located here and we present ourselves with a functional which is dependent on everything all over the map. That's something wrong. Maybe there is some way to surround the object, or the region where we want to calculate things, by a surface and describe what things are coming in across the surface. It tells us everything that's going on outside. I'm talking about a new kind of idea but that's the kind of stuff we shouldn't talk about at a talk, that's the kind of stuff you should actually do!"

Continuous Matrix Product States

- Provides an ansatz for low-energy quantum states of quantum field theories for which none of the objections of Feynman apply, and which actually implement his idea as a way out
  - cMPS have an automatic high-energy cut-off built in
  - cMPS are of the exponential form but not Gaussian
  - Expectation values can be calculated exactly and with minimal effort
  - All information about long-range correlations is stored in the "density matrix"
- Furthermore:
  - Allow for large local occupation number without an increase in the total number of variational parameters
  - Scale invariant by construction
  - Seem to capture the physics for describing low-energy behaviour of any local quantum field theory (just as MPS to for quantum spin systems)

Definition of cMPS:

$$|\chi\rangle = \mathrm{Tr}_{aux}\left[\mathcal{P}e^{\int_0^L dx\left[Q(x)\otimes\mathbb{1}+R(x)\otimes\hat{\psi}^\dagger(x)\right]}\right]|\Omega\rangle$$

$$[\hat{\psi}(x),\hat{\psi}(y)^\dagger]=\delta(x-y)$$

Q(x), R(x) are DxD matrices acting on an auxiliary Hilbert space. The wavefunction is automatically normalized and the total number of parameters is exactly D^2 if we use the gauge condition

$$Q=-\frac{1}{2}R^\dagger R-iH$$

Verstraete, Cirac, PRL 2010

cMPS in second quantization

$$|\chi\rangle = \sum_{n=0}^{\infty} \int_{0<x_1<\ldots<x_n<L} dx_1 \ldots dx_n \phi_n \hat{\psi}^\dagger(x_1) \ldots \hat{\psi}^\dagger(x_n)|\Omega\rangle$$

$$\phi_n = \mathrm{Tr}_{aux}\left[u_Q(x_1, 0) R u_Q(x_2, x_1) R \ldots R u_Q(L, x_n)\right]$$

$$u_Q(y, x) \;=\; \mathcal{P}\exp\left[\int_x^y Q(x) dx\right]$$

How to calculate expectation values?

$$\langle \hat{\psi}(x)^\dagger \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{TL}(R \otimes \bar{R})\right],$$

$$\langle \hat{\psi}(x)^\dagger \hat{\psi}(0)^\dagger \hat{\psi}(0) \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{T(L-x)}(R \otimes \bar{R}) e^{Tx}(R \otimes \bar{R})\right]$$

$$\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2}\right] \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{TL}([Q,R] \otimes [\bar{Q},\bar{R}])\right], \qquad ($$

$$T = Q \otimes \mathbb{1} + \mathbb{1} \otimes \bar{Q} + R \otimes \bar{R}$$

Using the abovementioned gauge condition, the real parts of the eigenvalues of T are guaranteed to be non-positive, and there is 1 eigenvalue equal to 0

The correlation functions are decaying exponentially fast, and the correlation length is proportional to the inverse gap of the Lindbladian

cMPS in second quantization

$$|\chi\rangle = \sum_{n=0}^{\infty} \int_{0<x_1<\ldots<x_n<L} dx_1 \ldots dx_n \phi_n \hat{\psi}^\dagger(x_1) \ldots \hat{\psi}^\dagger(x_n)|\Omega\rangle$$

$$\phi_n = \mathrm{Tr}_{aux}\left[u_Q(x_1, 0) R u_Q(x_2, x_1) R \ldots R u_Q(L, x_n)\right]$$

$$u_Q(y, x) \; = \; \mathcal{P}\exp\left[\int_x^y Q(x)dx\right]$$

How to calculate expectation values?

$$
\begin{aligned}
\langle \hat{\psi}(x)^\dagger \hat{\psi}(x) \rangle &= \mathrm{Tr}\left[e^{TL}(R \otimes \bar{R})\right], \\
\langle \hat{\psi}(x)^\dagger \hat{\psi}(0)^\dagger \hat{\psi}(0) \hat{\psi}(x) \rangle &= \mathrm{Tr}\left[e^{T(L-x)}(R \otimes \bar{R}) e^{Tx}(R \otimes \bar{R})\right] \\
\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2}\right] \hat{\psi}(x) \rangle &= \mathrm{Tr}\left[e^{TL}([Q,R] \otimes [\bar{Q},\bar{R}])\right], \quad (
\end{aligned}
$$

$$T = Q \otimes \mathbb{1} + \mathbb{1} \otimes \bar{Q} + R \otimes \bar{R}$$

Using the abovementioned gauge condition, the real parts of the eigenvalues of T are guaranteed to be non-positive, and there is 1 eigenvalue equal to 0

The correlation functions are decaying exponentially fast, and the correlation length is proportional to the inverse gap of the Lindbladian

cMPS as limit of MPS

$$|\chi_\epsilon\rangle = \sum_{i_1\cdots i_N} \mathrm{Tr}\left[A^{i_1}\cdots A^{i_N}\right]\left(\hat{\psi}_1^\dagger\right)^{i_1}\cdots\left(\hat{\psi}_N^\dagger\right)^{i_N}|\Omega\rangle$$

$$\begin{aligned} A^0 &= \mathbb{1} + \epsilon Q \\ A^1 &= \epsilon R \\ A^n &= \epsilon^n R^n / n! \\ \hat{\psi}_i &= \frac{\hat{a}_i}{\sqrt{\epsilon}} \end{aligned}$$

$$_{kin} = L\langle\chi|\left(\frac{\hat{\psi}_{i+1}^\dagger - \hat{\psi}_i^\dagger}{\epsilon}\right)\left(\frac{\hat{\psi}_{i+1} - \hat{\psi}_i}{\epsilon}\right)|\chi\rangle.$$

Divergencies 1/eps and 1/eps^2 automatically cancel in the case of bosons; in case of fermions, we require R^2=0 for the (non-relativistic) kinetic energy to be finite

Illustration: the Lieb-Liniger model (I)

$$\mathcal{H} = \int_{-\infty}^{+\infty} dx \left[\frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right]$$

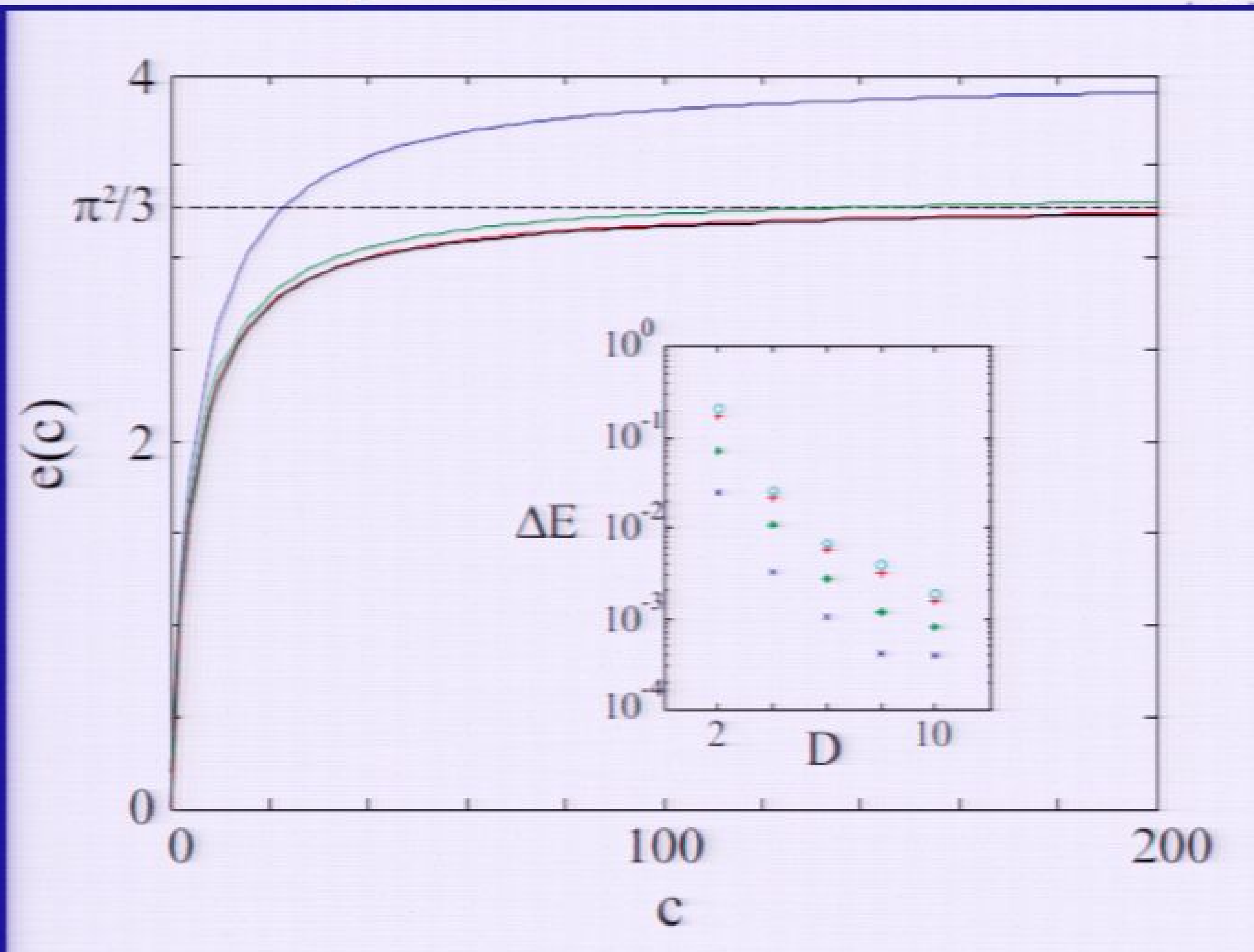
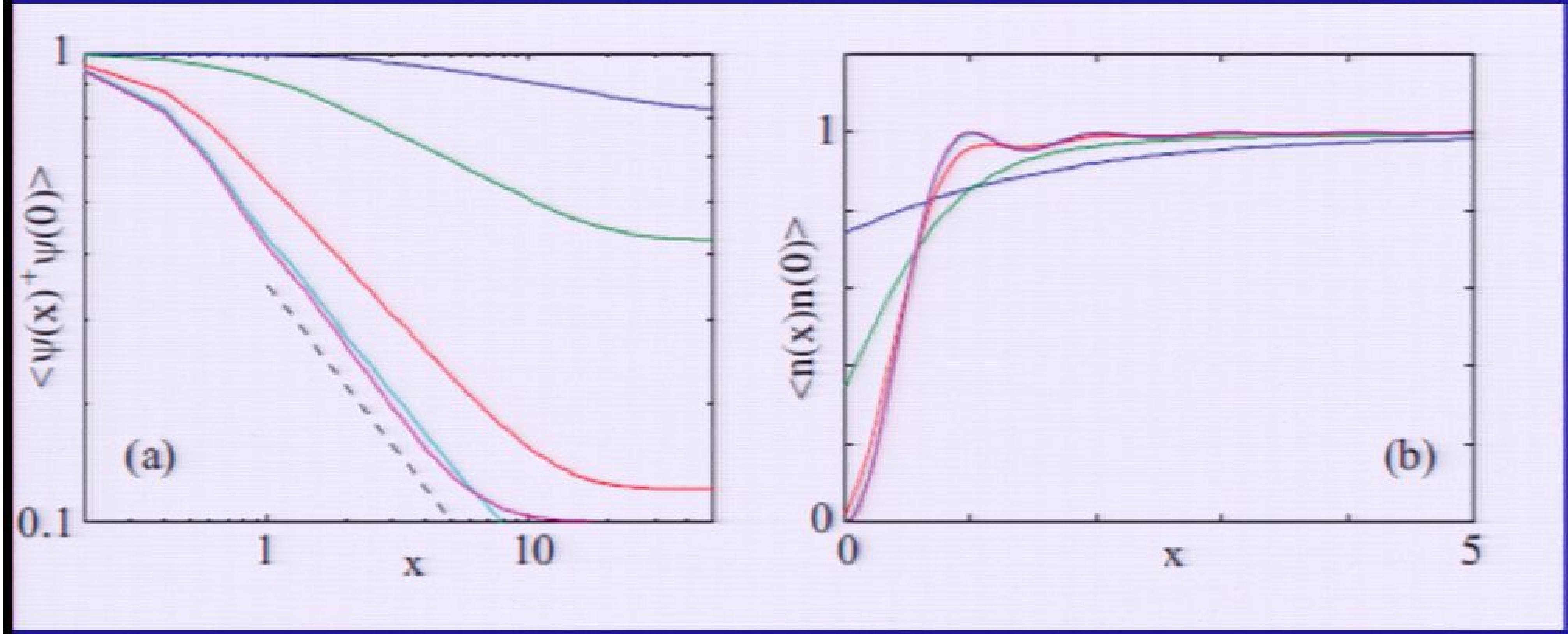


Illustration: The Lieb-Liniger model (II)

- Not just energies are well reproduced, also the correlation functions!



What about high frequencies?

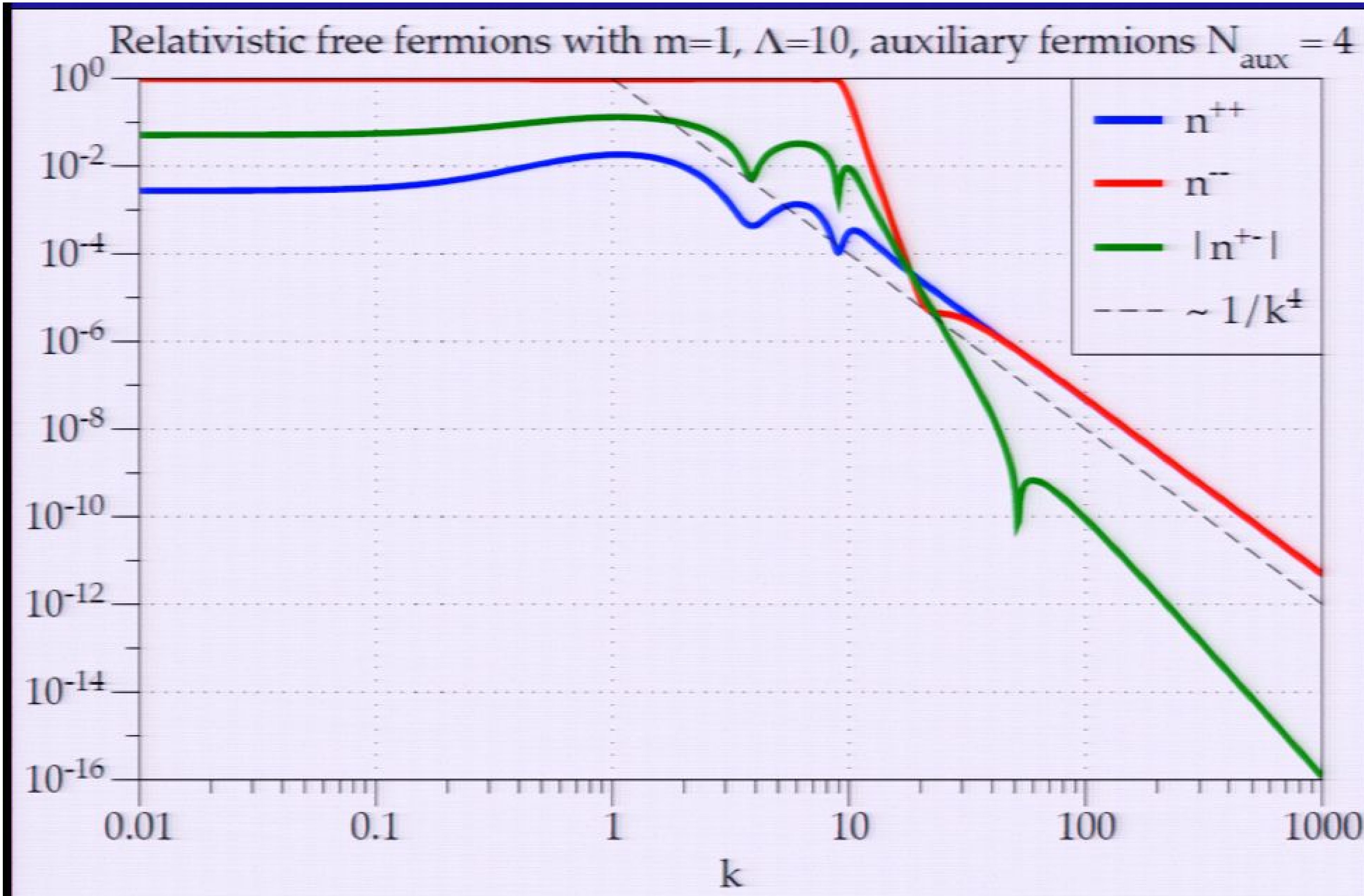
- Expectation value of the non-relativistic kinetic energy:

$$\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2} \right] \hat{\psi}(x) \rangle \;=\; \mathrm{Tr}\left[e^{TL} ([Q,R] \otimes [\bar{Q},\bar{R}]) \right]$$

  - This is automatically bounded if all matrices involved are bounded in norm
  - If a cMPS wavefunction is such that its second order derivative is continuous, then the expectation value of its high-frequency components scales like

$$n(k) \approx \frac{1}{k^4}$$

    - This imposes an effective high-energy cut-off as all expectation values become finite; hence we can go and look at relativistic theories!



ulation of free Dirac fermions by introducing an effective cut-off; plotted is n(k) obtained as Fourier transform of the 1-particle density matrix $\langle\chi|\hat{\psi}^\dagger_\alpha(x)\hat{\psi}_\beta(x')|\chi\rangle = C_{\alpha,\beta}(x-x')$

Scale invariance of cMPS

Recall:

$$\langle \hat{\psi}(x)^\dagger \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{TL}(R \otimes \bar{R})\right],$$

$$\langle \hat{\psi}(x)^\dagger \hat{\psi}(0)^\dagger \hat{\psi}(0) \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{T(L-x)}(R \otimes \bar{R}) e^{Tx}(R \otimes \bar{R})\right]$$

$$\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2}\right] \hat{\psi}(x) \rangle = \mathrm{Tr}\left[e^{TL}([Q,R] \otimes [\bar{Q},\bar{R}])\right], \quad ($$

$$T = Q \otimes \mathbb{1} + \mathbb{1} \otimes \bar{Q} + R \otimes \bar{R}$$

Those formulae yield right scaling transformation by changing

$$Q \to cQ \quad ; \quad R \to \sqrt{c}R \quad ; \quad \mathrm{L} \to \frac{\mathrm{L}}{\mathrm{c}}$$

cMPS are therefore invariant under coarse-graining: there are exact fixed points of coarse-graining transformations on the state.

- This situation is much simpler than in case of MPS in quantum spin systems: cMPS have nicer and more natural properties (Verstraete, Wolf, Rico, Latorre, Cirac '05)
- Note that cMPS do not violate an area law!
- Is it possible to formulate field-theoretic version of MERA ?

The density matrix (I)

- There is a simple way of calculating expectation values of CMPS in terms of a Lindblad equation if working in the natural gauge:

$$\frac{d}{dx}\rho(x) = -i[\tilde{H}, \rho(x)] + R\rho(x)R^\dagger - \frac{1}{2}\left[R^\dagger R, \rho(x)\right]_+$$

$$\begin{aligned}
\langle \hat{\psi}(x)^\dagger \hat{\psi}(x) \rangle &= \mathrm{Tr}\left[R^\dagger R \rho_{ss}\right], \\
\langle \hat{\psi}(0)^\dagger \hat{\psi}(x)^\dagger \hat{\psi}(x) \hat{\psi}(0) \rangle &= \mathrm{Tr}\left[(R e^{\tilde{T}x}(R\rho_{ss}R^\dagger)R^\dagger\right] \\
\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2}\right] \hat{\psi}(x) \rangle &= \mathrm{Tr}\left[([Q,R])^\dagger [Q,R]\rho_{ss}\right],
\end{aligned}$$

- The density matrix of the auxiliary field is exactly the density matrix arising in DMRG, and it parameterizes all the correlations present in the state.

The density matrix (II)

- The dynamics of this density matrix is governed by a local Markovian Lindblad equation (cfr. CP-map in case of MPS)

$$\frac{d}{dx}\rho(x) = -i[\tilde{H},\rho(x)] + R\rho(x)R^{\dagger} - \frac{1}{2}\left[R^{\dagger}R,\rho(x)\right]_{+}$$

- The eigenvalues of this density matrix are the Schmidt coefficients of the half-chain

    - Note 1: entanglement entropy for cMPS is always bounded by the dimension of underlying matrices Q,R; to get a divergence, those matrices have to become infinite dimensional (cfr. Cirac, Sierra '10)

    - Note 2: relativistic theories always exhibit infinite entanglement entropy, but the divergence is due to the high-frequency modes, and those are not present if a cut-off is imposed.

Holographic quantum states

Osborne, Eisert, Verstraete '10

- This connection to the evolution of the auxiliary system exactly does what Feynman envisaged: if yields a local parameterization of global properties !

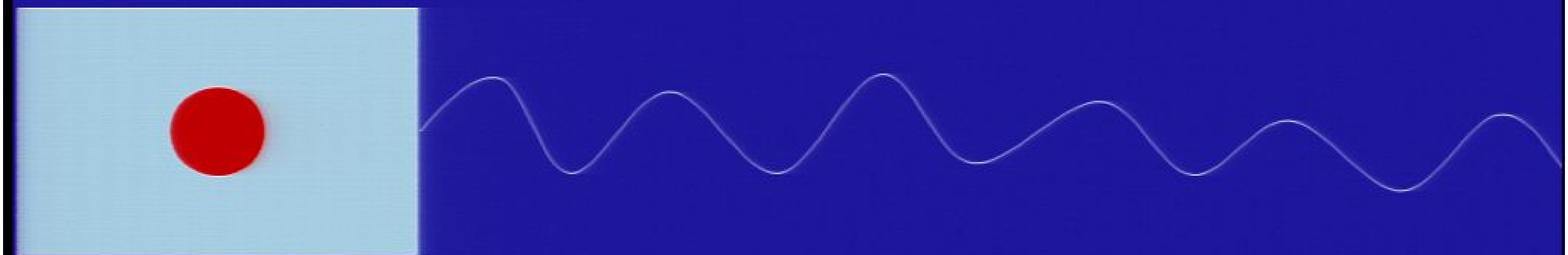
- It also leads to an equivalent way of parameterizing cMPS:

  – the physical system of interest can be interpreted as the purification of the dissipative evolution of the auxiliary system!

  – This is continuum version of the sequential generation scheme of MPS using a quantum circuit

Schon, Wolf, Verstraete, Solano, Cirac '05

Cavity QED



- D-level atom in the cavity
- Coupled to the cavity modes by a Hamiltonian H
- Photons leak out of the cavity
- Evolution of atom described by a Lindblad equation; the Lindblad terms correspond to quantum jumps and generate photons leaking out of the cavity
- Global quantum State of all photons leaking out of cavity is precisely described by a cMPS!

- More formally:

$$H_{tot} = H \otimes I + i\left(R \otimes \psi^* - R^* \otimes \psi\right)$$

$$\Rightarrow \exp(-i\varepsilon H_{tot})|\chi\rangle|\Omega\rangle \approx \left(-i\varepsilon H \otimes I + \varepsilon R \otimes \psi^* - \frac{\varepsilon^2}{2} R^* R \otimes \psi\psi^*\right)|\chi\rangle|\Omega\rangle$$

$$\approx \exp\left(\varepsilon\left(Q \otimes I + R \otimes \psi^*\right)\right)|\chi\rangle|\Omega\rangle$$

  - H specifies the internal dynamics of the atom
  - R specifies how the atom couples to the cavity field

- Those are precisely the type of systems that have been studied in cavity QED since the '80s

  - Time-time-time-… correlation functions of photons are equivalent to all correlations functions of cMPS: P. Zoller et al. effectively wrote down formulae for cMPS back in the '80s!
  - Provides connection between quantum measurement theory and quantum field theory!
  - This opens up possibility of simulating quantum field theories like Lieb-Liniger with cavity QED

Holographic quantum states

Osborne, Eisert, Verstraete '10

- This connection to the evolution of the auxiliary system exactly does what Feynman envisaged: if yields a local parameterization of global properties !

- It also leads to an equivalent way of parameterizing cMPS:

  - the physical system of interest can be interpreted as the purification of the dissipative evolution of the auxiliary system!

  - This is continuum version of the sequential generation scheme of MPS using a quantum circuit

    Schon, Wolf, Verstraete, Solano, Cirac '05

- More formally:

$$H_{tot} = H \otimes I + i\left(R \otimes \psi^* - R^* \otimes \psi\right)$$

$$\Rightarrow \exp\left(-i\varepsilon H_{tot}\right)|\chi\rangle|\Omega\rangle \approx \left(1 - i\varepsilon H \otimes I + \varepsilon R \otimes \psi^* - \frac{\varepsilon^2}{2} R^* R \otimes \psi\psi^*\right)|\chi\rangle|\Omega\rangle$$

$$\approx \exp\left(\varepsilon\left(Q \otimes I + R \otimes \psi^*\right)\right)|\chi\rangle|\Omega\rangle$$

  - H specifies the internal dynamics of the atom
  - R specifies how the atom couples to the cavity field

- Those are precisely the type of systems that have been studied in cavity QED since the ‘80s

  - Time-time-time-… correlation functions of photons are equivalent to all correlations functions of cMPS: P. Zoller et al. effectively wrote down formulae for cMPS back in the ’80s!
  - Provides connection between quantum measurement theory and quantum field theory!
  - This opens up possibility of simulating quantum field theories like Lieb-Liniger with cavity QED

non-equilibrium dynamics of a zero-dimensional vs static properties of a 1-dimensional system

- Interestingly, this way of looking at the problem indicates that static properties of quantum field theories have a counterpart into time-time correlation functions of non-equilibrium systems in a dimension lower: HOLOGRAPHIC principle
  - Cfr. Classical stochastic processes in 1-D that exhibit phase transitions (traffic!) very much like 2-D classical partition functions
  - Same holds of course for MPS: instead of continuous evolution, we have evolution using CP-maps. This picture provides intuitive explanation for the emergence of the density matrix
- Dissipative systems actually exhibit very rich structure
  - Other manifestations: universal quantum computation using dissipative dynamics (Verstraete, Wolf, Cirac Nat. Phys. '09), quantum Metropolis sampling (K. Temme. K. Vollbrecht, T. Osborne, D. Poulin, F. Verstraete '09), mixiing times in random walk algorithms (K. Temme. M. Kastoryano, M. Ruskai, M. Wolf, F. Verstraete '10)

Conclusions

- We have a dream that we can develop quantum field theory with wavefunctions instead of functional integrals
- Feynman's obstacles can in principle be overcome
- Continuous Matrix Product States seem to capture the low-energy physics of 1+1 dimensional quantum field theories (both relativistic and non-relativistic)
- Intriguing connections between quantum field theory, quantum measurement theory, dissipative non-equilibrium phenomena and the holographic principle