Title: Wick's theorem for Matrix Product states

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Abstract: Matrix product states and their continuous analogues are variational classes of states that capture quantum many-body systems or quantum fields with low entanglement; they are at the basis of the density-matrix renormalization group method and continuous variants thereof. In this talk we show that, generically, N-point functions of arbitrary operators in discrete and continuous translation invariant matrix product states are completely characterized by the corresponding two- and three-point functions. Aside from having important consequences for the structure of correlations in quantum states with low entanglement, this result provides a new way of reconstructing unknown states from correlation measurements e.g. for one-dimensional continuous systems of cold atoms. We argue that such a relation of correlation functions may help in devising perturbative approaches to interacting theories.

Joint work with Andrea Mari and Jens Eisert.
arXiv:1207.6537

Wick's theorem for matrix product states

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Waterloo, March 2013

Overview.

Main statement

Generically, in thermodynamic limit, translation-invariant (c)MPS allow for a Wick theorem.
(but based on three-point-functions)

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Why should you care?

- Wick's theorem well known for Gaussians
  - Statistics: *All the moments of a Gaussian probability distribution can be expressed as functions of the second moments alone.*
  - Physics: *Two-point-function* $\langle \phi(x)\phi(y) \rangle$ *determines properties of Gaussian states (e.g. vacuum of free theory).*
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  - important in field theory: Feynman diagrams
- MPS are totally unlike Gaussians
  - but close to important ground states (area law)
  - roughly speaking, they describe all states in 1D when entanglement saturates for large chunks
  - think of ground states of locally *interacting*, gapped Hamiltonians in 1D

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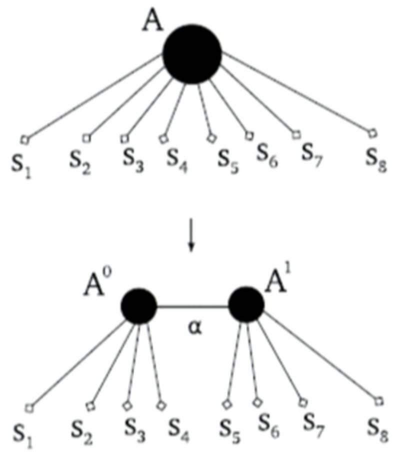
  - think of ground states of locally *interacting*, gapped Hamiltonians in 1D
- implications for
  - diagrammatic methods
  - reconstruction of field states
  - open quantum systems
  - statistics (hidden Markov models)

Background

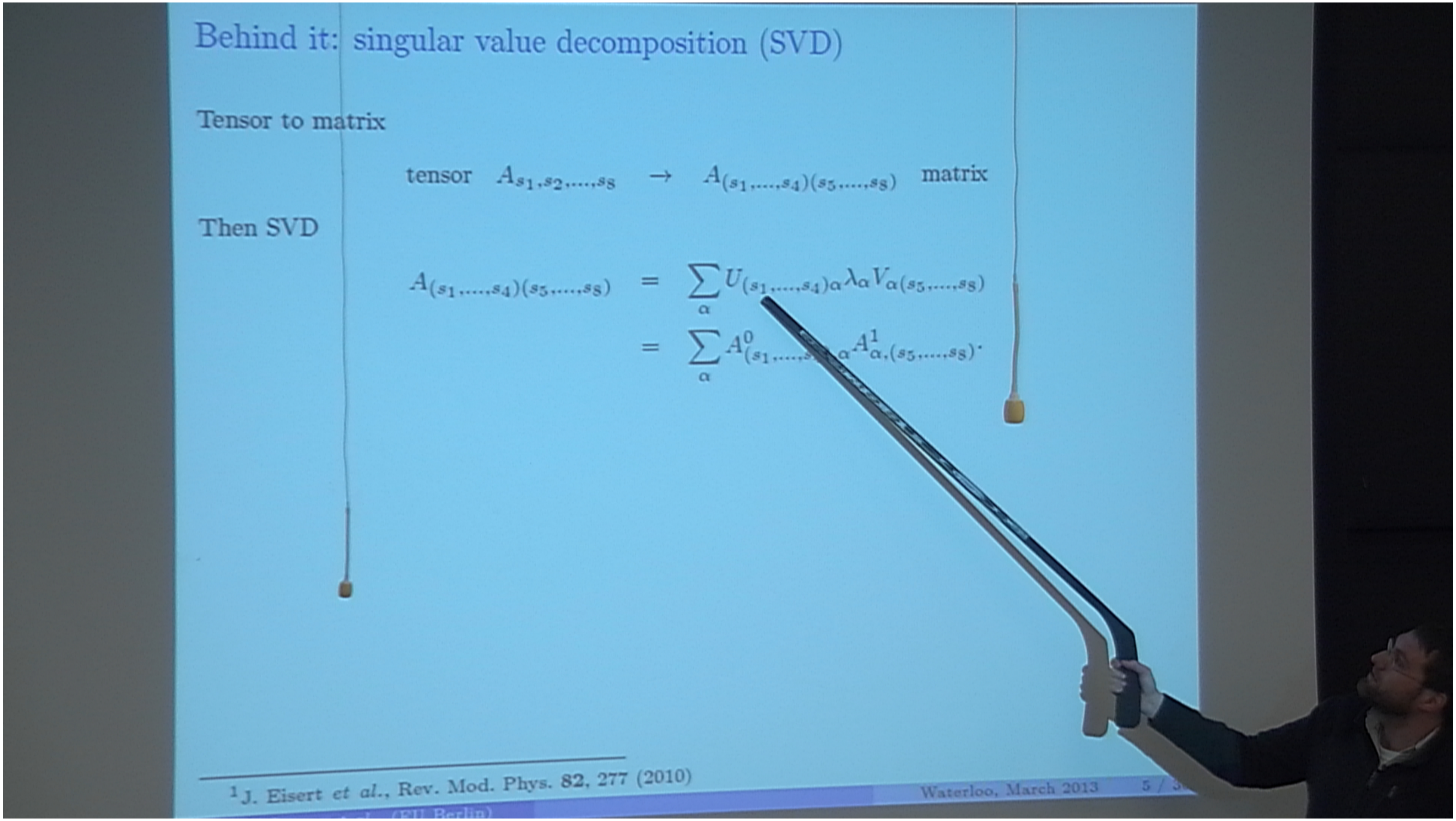
—matrix product states—

tensor splitting

$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_8} A_{s_1,s_2,\ldots,s_8} |s_1, s_2, \ldots, s_8\rangle$$



$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_8} \left(\sum_{\alpha} A^0_{s_1,\ldots,s_4,\alpha} A^1_{\alpha,s_5,\ldots,s_8} \right) |s_1, s_2, \ldots, s_8\rangle$$


Behind it: singular value decomposition (SVD)
Tensor to matrix
tensor $A_{s_1,s_2,\ldots,s_8}$ $\rightarrow$ $A_{(s_1,\ldots,s_4)(s_5,\ldots,s_8)}$ matrix
Then SVD
$A_{(s_1,\ldots,s_4)(s_5,\ldots,s_8)} = \sum_\alpha U_{(s_1,\ldots,s_4)\alpha}\lambda_\alpha V_{\alpha(s_5,\ldots,s_8)}$
$= \sum_\alpha A^0_{(s_1,\ldots} \ldots A^1_{\alpha,(s_5,\ldots,s_8)}.$
[1] J. Eisert et al., Rev. Mod. Phys. 82, 277 (2010)
Waterloo, March 2013

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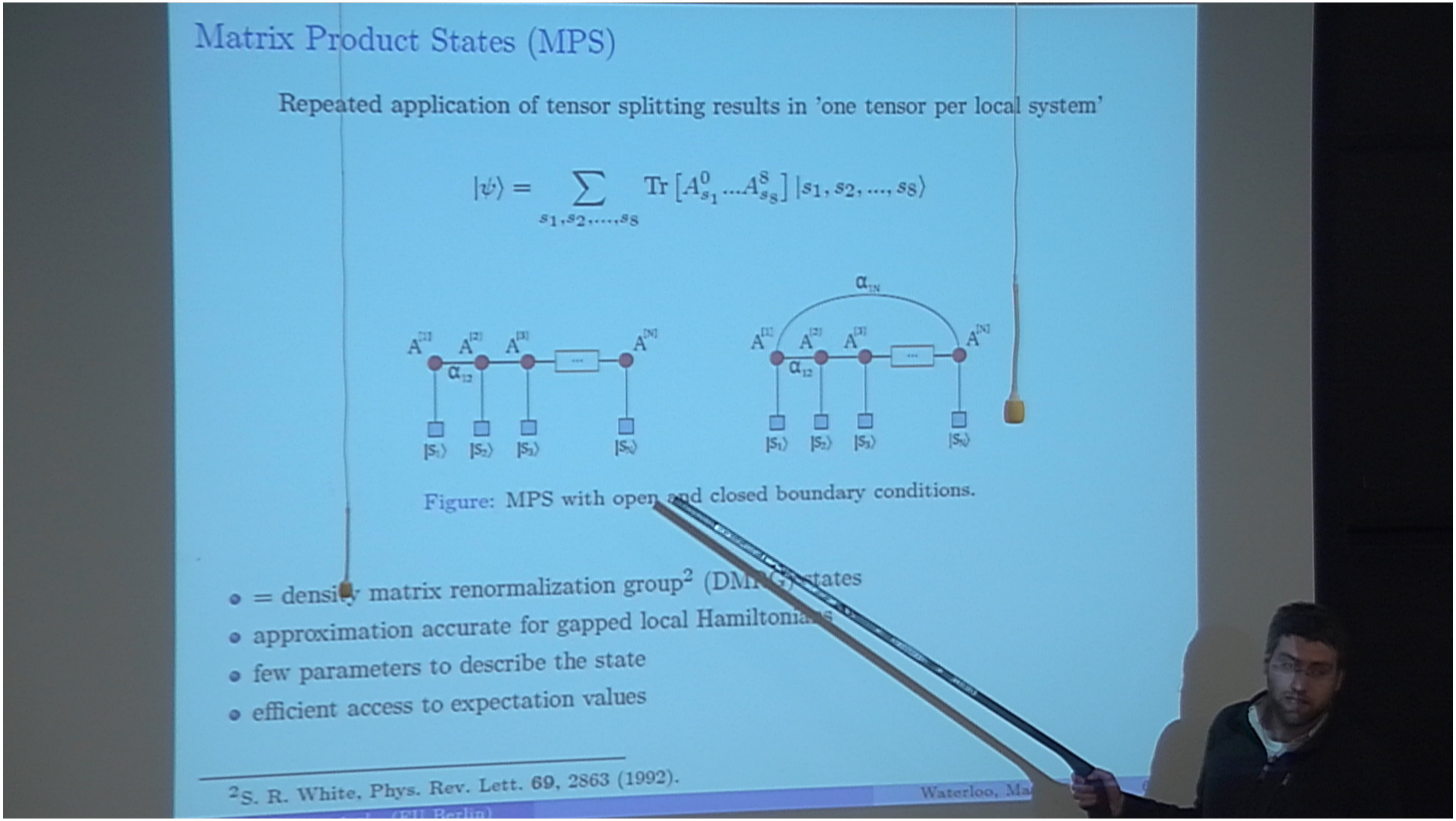
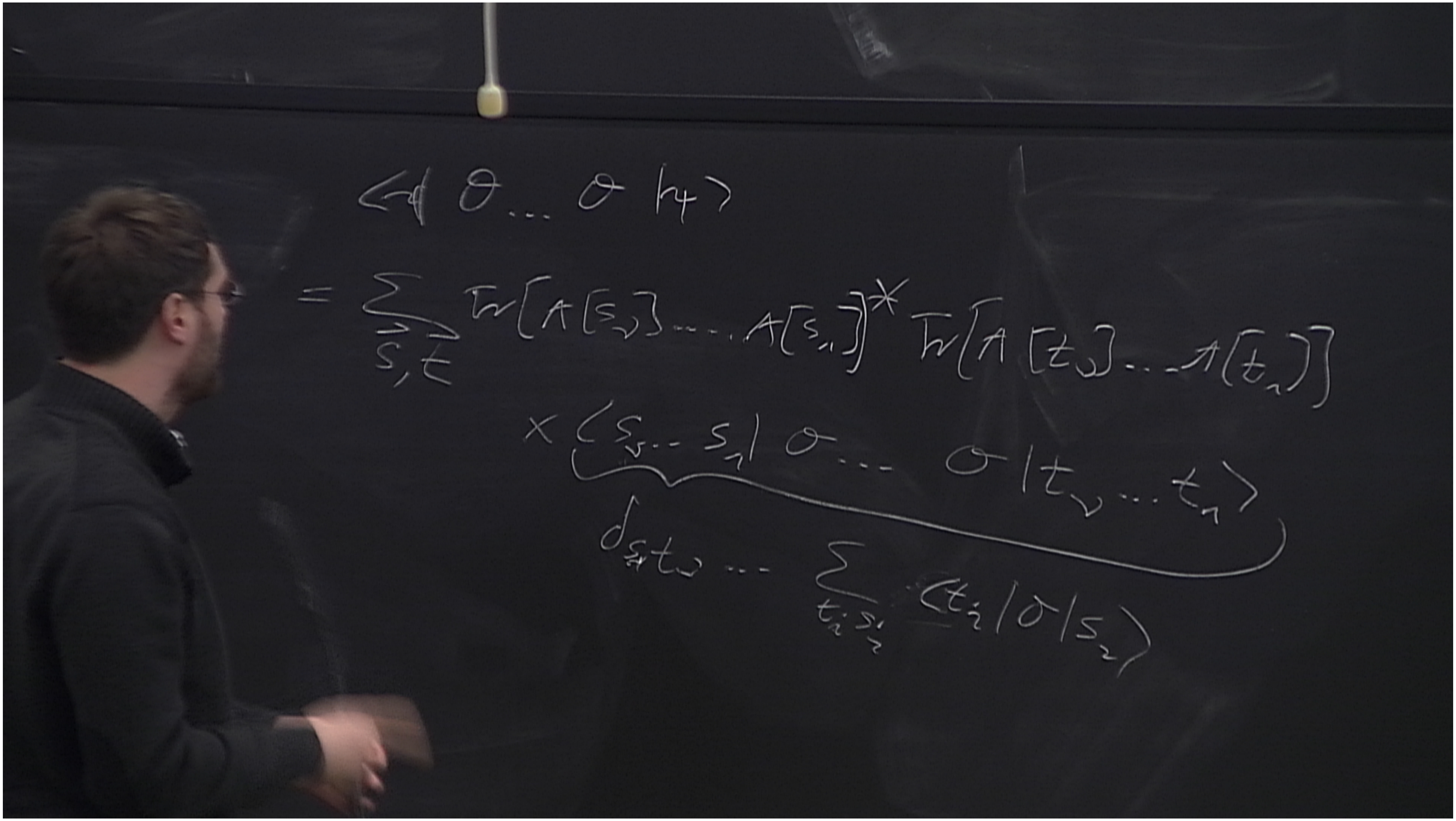
- $\{\lambda_\alpha\}$ very interesting: contains all important info about bipartite entanglement between both parties
- set $\{\lambda_\alpha\}$, ordered by magnitude, usually decays very quickly for physical states in 1D: area law[1]
- λ_α with small magnitude can be discarded, while resulting approximation remains norm-close
- ability to transform states with local operations into each other dictated by $\{\lambda_\alpha\}$
- it is a relaxation of *mean-field*

[1] J. Eisert *et al.*, Rev. Mod. Phys. **82**, 277 (2010)


Matrix Product States (MPS)
Repeated application of tensor splitting results in 'one tensor per local system'
$|\psi\rangle = \sum_{s_1, s_2, ..., s_8} \mathrm{Tr}\left[A^0_{s_1} ... A^8_{s_8}\right] |s_1, s_2, ..., s_8\rangle$
α12
α1N
Figure: MPS with open and closed boundary conditions.
• = densi y matrix renormalization group[2] (DM states
• approximation accurate for gapped local Hamilton
• few parameters to describe the state
• efficient access to expectation values
[2] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
Waterloo, Ma


⟨ψ| O ... O |ψ⟩
= Σ_{s,t} Tr[A[s_N] ... A[s_1]]* Tr[A[t_N] ... A[t_1]]
× ⟨s_N ... s_1| O ... O |t_N ... t_1⟩
δ_{s_N t_N} ... Σ_{t_i s_i} ⟨t_i|O|s_i⟩

$$\langle\psi| O \dots O |\psi\rangle$$

$$= \sum_{\vec{s},\vec{t}} \mathrm{Tr}[A[s_1]\cdots A[s_n]]^* \, \mathrm{Tr}[A[t_1]\cdots A(t_n)]$$

$$\times \underbrace{\langle s_1 \dots s_n | O \dots O | t_1 \dots t_n \rangle}$$

$$\delta_{s_1 t_1} \dots \sum_{t_2 s_2} \langle t_2 | O | s_2 \rangle$$

$$\mathrm{Tr}[A]\,\mathrm{Tr}[B] = \mathrm{Tr}[A \otimes B]$$

$$\mathrm{Tr}[(AB)\otimes(CD)] = \mathrm{Tr}[(A\otimes C)(B\otimes D)]$$

Definition of the term "generic"

Observation: gauge freedom

- remember

$$\langle O^{(i_N)} O^{(i_{N-1})} \dots O^{(i_1)} \rangle = \mathrm{Tr}\,[M E^{n_{N-1}} M \dots M E^{\infty}] =: C^{(N)}(\mathbf{n}),$$

- possible simultaneous conjugation of all matrices

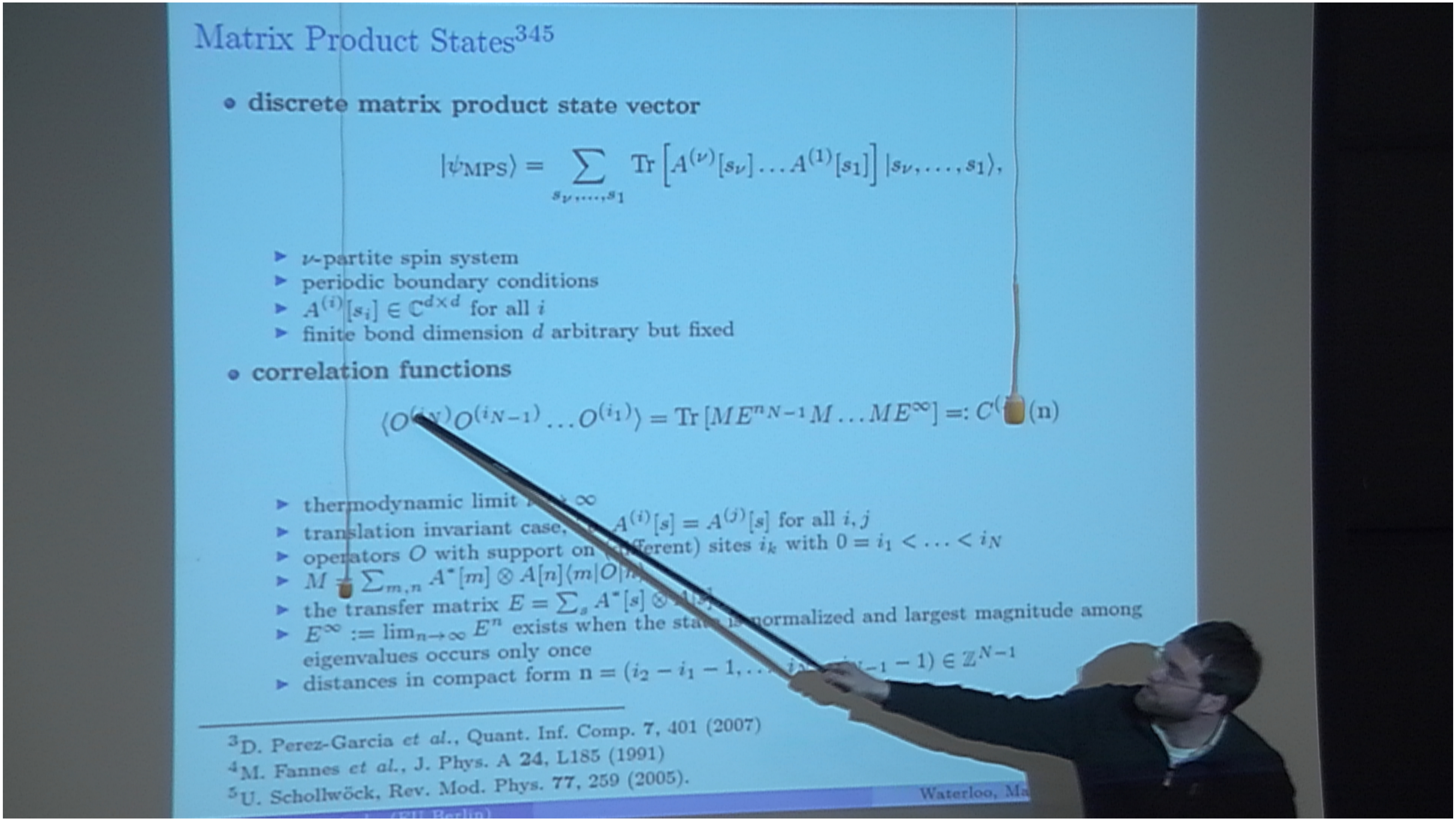
$$E \to X E X^{-1}, \quad M \to X M X^{-1}$$

- e.g. Jordan transformation of $E \to J(E)$

Definition

We say the MPS is *generic* if

- $J(E)$ is non-degenerate
- largest magnitude among eigenvalues occurs only once


Matrix Product States3 4 5
discrete matrix product state vector
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ν-partite spin system
periodic boundary conditions
$A^{(i)}[s_i] \in \mathbb{C}^{d\times d}$ for all i
finite bond dimension d arbitrary but fixed
correlation functions
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Main result

Situation

- In general, to characterize the full state of a quantum system one needs to specify all the correlation functions.
- One may ask the following question: *"Is it possible to completely characterize a (continuous) matrix product state from low order correlation functions?"*

Main statement of this talk

With the only initial assumption of a bond dimension d (= limited entanglement) we can

1. Certify that the given (c)MPS is generic.
2. Reconstruct the full state of a (c)MPS from low order correlation functions once (1) has been verified.

Data structure and transformations

Consider discrete MPS

- correlation functions

$$\langle O^{(i_N)} O^{(i_{N-1})} \dots O^{(i_1)} \rangle = \mathrm{Tr}\,[M E^{n_{N-1}} M \dots M E^{\infty}] =: C^{(N)}(\mathbf{n}),$$

- Z-transform

$$\mathcal{Z}^{(N)}(\mathrm{s}) := \sum_{n_1,\dots,n_{N-1}} s_1^{n_1} \dots s_N^{n_{N-1}} C^{(N)}(\mathbf{n}), \quad s_1,\dots,s_{N-1} \in \mathbb{C}$$

- key observation: when $J(E)$ is non-degenerate

$$C^{(N)}(\mathbf{n}) = \sum_{k_{N-1},\dots,k_1=1}^{d^2} c^{(N)}(k_{N-1},\dots,k_1) \times (\mu_{k_{N-1}})^{n_{N-1}} \dots (\mu_{k_1})^{n_1},$$

  with μ_i, the eigenvalues of E
- application of Z-trafo to correlators

$$\mathcal{Z}^{(N)}(\mathrm{s}) = \sum_{k_1,\dots,k_{N-1}}^{d^2} \frac{c^{(N)}(k_{N-1},\dots,k_1)}{(1-\mu_{k_{N-1}} s_{N-1}) \cdots (1-\mu_{k_1} s_1)}$$

- meromorphic function. has characteristic poles and residues

$$c^{(N)}(k_{N-1},\dots,k_1) = \langle 1|M|k_{N-1}\rangle\langle k_{N-1}|M \dots |k_1\rangle\langle k_1|M|1\rangle$$

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Example

Consider the following case.

- Given a generic MPS with finite d, let the operators O and the state be such that the corresponding matrices XMX^{-1} have only *non-zero* elements.
- Under this condition, all two-point function transforms show all the poles
- Computationally, all residues of all the poles of all N-point functions with $N \leq 3$ can be obtained.

Matrix Product States[3,4,5]

- **discrete matrix product state vector**

$$|\psi_{\mathrm{MPS}}\rangle = \sum_{s_\nu,\ldots,s_1} \mathrm{Tr}\left[A^{(\nu)}[s_\nu]\ldots A^{(1)}[s_1]\right]|s_\nu,\ldots,s_1\rangle,$$

  - ν-partite spin system
  - periodic boundary conditions
  - $A^{(i)}[s_i] \in \mathbb{C}^{d\times d}$ for all i
  - finite bond dimension d arbitrary but fixed

- **correlation functions**

$$\langle O^{(i_N)}O^{(i_{N-1})}\ldots O^{(i_1)}\rangle = \mathrm{Tr}\left[ME^{n_{N-1}}M\ldots ME^{\infty}\right] =: C^{(\text{[illegible]}}(\mathrm{n})$$

  - thermodynamic limit $\nu \to \infty$
  - translation invariant case, i.e. $A^{(i)}[s] = A^{(j)}[s]$ for all i, j
  - operators O with support on (different) sites i_k with $0 = i_1 < \ldots < i_N$
  - $M = \sum_{m,n} A^*[m] \otimes A[n]\langle m|O|n\rangle$
  - the transfer matrix $E = \sum_s A^*[s] \otimes A[s]$
  - $E^\infty := \lim_{n\to\infty} E^n$ exists when the state is normalized and largest magnitude among eigenvalues occurs only once
  - distances in compact form $\mathrm{n} = (i_2 - i_1 - 1, \ldots, i_N - i_{N-1} - 1) \in \mathbb{Z}^{N-1}$

[3] D. Perez-Garcia *et al.*, Quant. Inf. Comp. **7**, 401 (2007)

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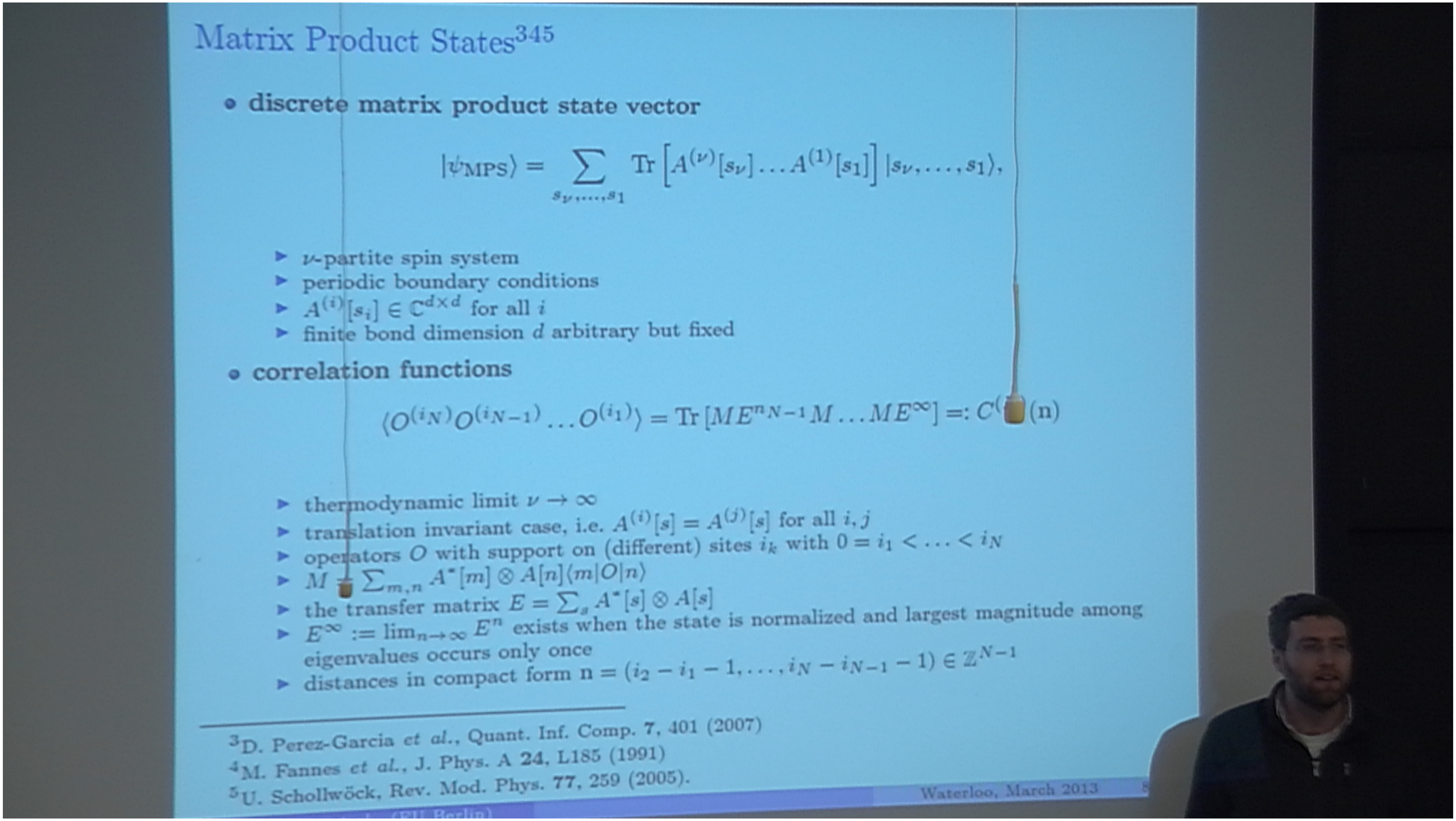
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Example

Consider the following case.

- Given a generic MPS with finite d, let the operators O and the state be such that the corresponding matrices XMX^{-1} have only *non-zero* elements.
- Under this condition, all two-point function transforms show all the poles
- Computationally, all residues of all the poles of all N-point functions with $N \leq 3$ can be obtained.

Now we can, using the construction above, give explicit formulas that express all N-point functions in terms of the 2- and 3-point functions.

- We have

$$\mathbb{C} \ni 1 = 1^{(k)} := \frac{M_{1,k} M_{k,1}}{c^{(2)}(k)}.$$

- The residues are, e.g.,

$$\begin{aligned}
c^{(4)}(k_3, k_2, k_1) &= M_{1,k_3} M_{k_3,k_2} M_{k_2,k_1} M_{k_1,1} \\
&= M_{1,k_3} 1^{(k_3)} M_{k_3,k_2} 1^{(k_2)} M_{k_2,k_1} 1^{(k_1)} M_{k_1,1} \\
&= \frac{(M_{1,k_3} M_{k_3,1})(M_{1,k_3} M_{k_3,k_2} M_{k_2,1})(M_{1,k_2} M_{k_2,k_1} M_{k_1,1})(M_{1,k_1} M_{k_1,1})}{c^{(2)}(k_3) c^{(2)}(k_2) c^{(2)}(k_1)} \\
&= \frac{c^{(3)}(k_3, k_2) c^{(3)}(k_2, k_1)}{c^{(2)}(k_2)}
\end{aligned}$$

Wick's theorem—interaction picture—"Feynman approach"

- interaction picture in field theory
  - starting point is vacuum of free theory, i.e. Gaussian states
  - perturbation is interaction term V, polynomials in field-operators
  - formal S-matrix

$$S = \sum_{n=0}^{\infty} \frac{i^n}{n!} \mathcal{T} \prod_{j=1}^{n} dx_j^4 V(\mathbf{x}_j)$$

  - Wick's theorem: Gaussians? We can express everyting with two-point-functions!

$$\langle \mathcal{T} \prod_{j=1}^{n} V(\mathbf{x}_j) \rangle_0 = \sum_{\text{all contractions}} (\pm) \mathcal{N} \overline{\phi(x_{\sigma_1}) \phi(x_{\sigma_2})}\, \overline{\phi(x_{\sigma_3}) \phi(x_{\sigma_4})} \ldots$$

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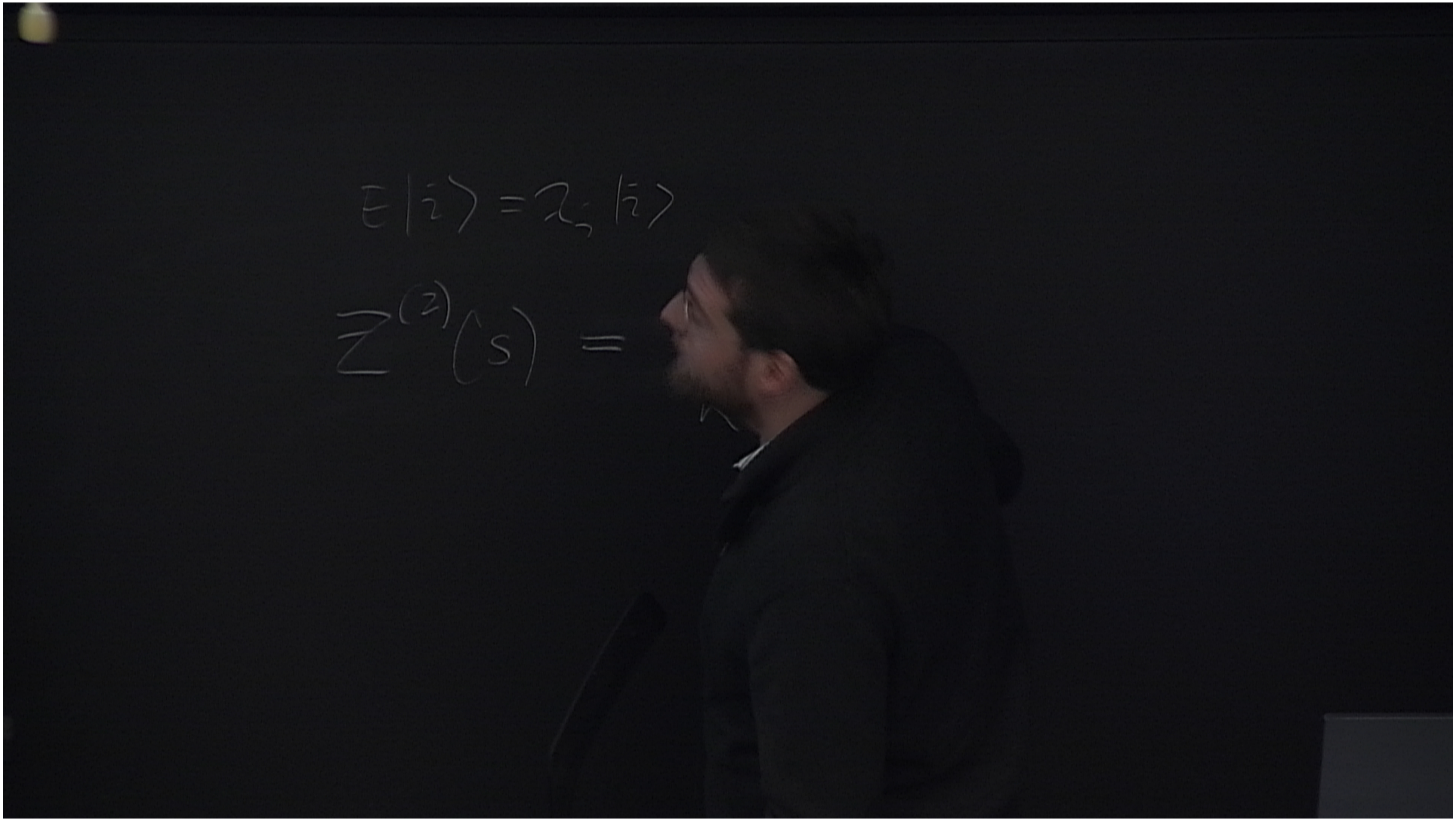
- Essentially the same applies to the associated *field* states, continuous MPS!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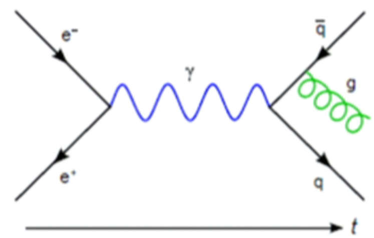
- $\overline{\phi(x_{\sigma_1})\phi(x_{\sigma_2})}$ are propagators, i.e. two-point-functions in quasi-free vacuum states of non-interacting theories
- mental image is



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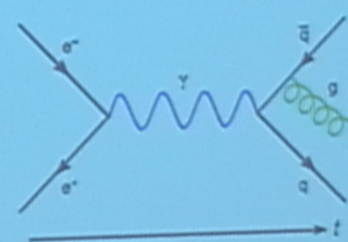
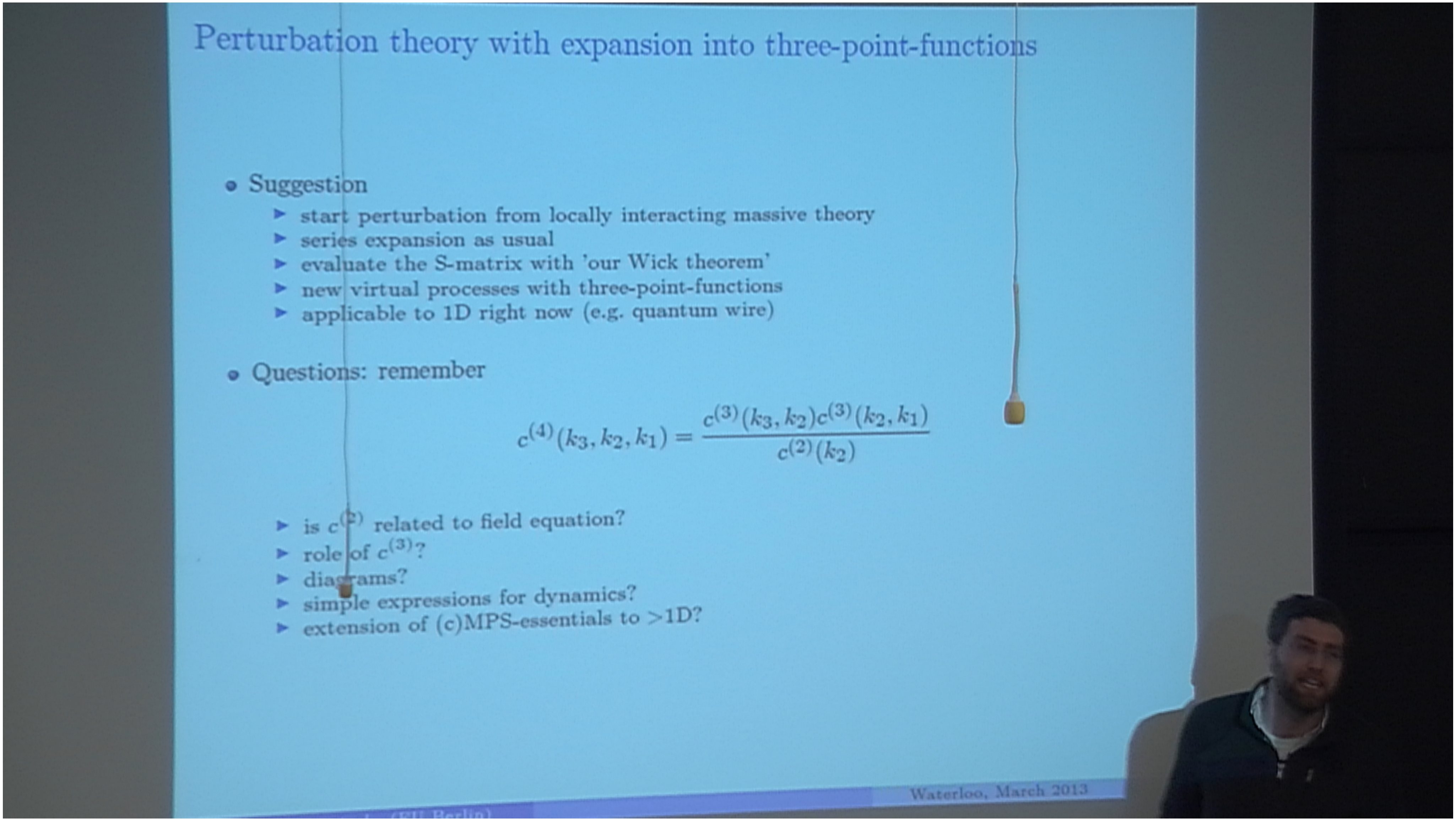
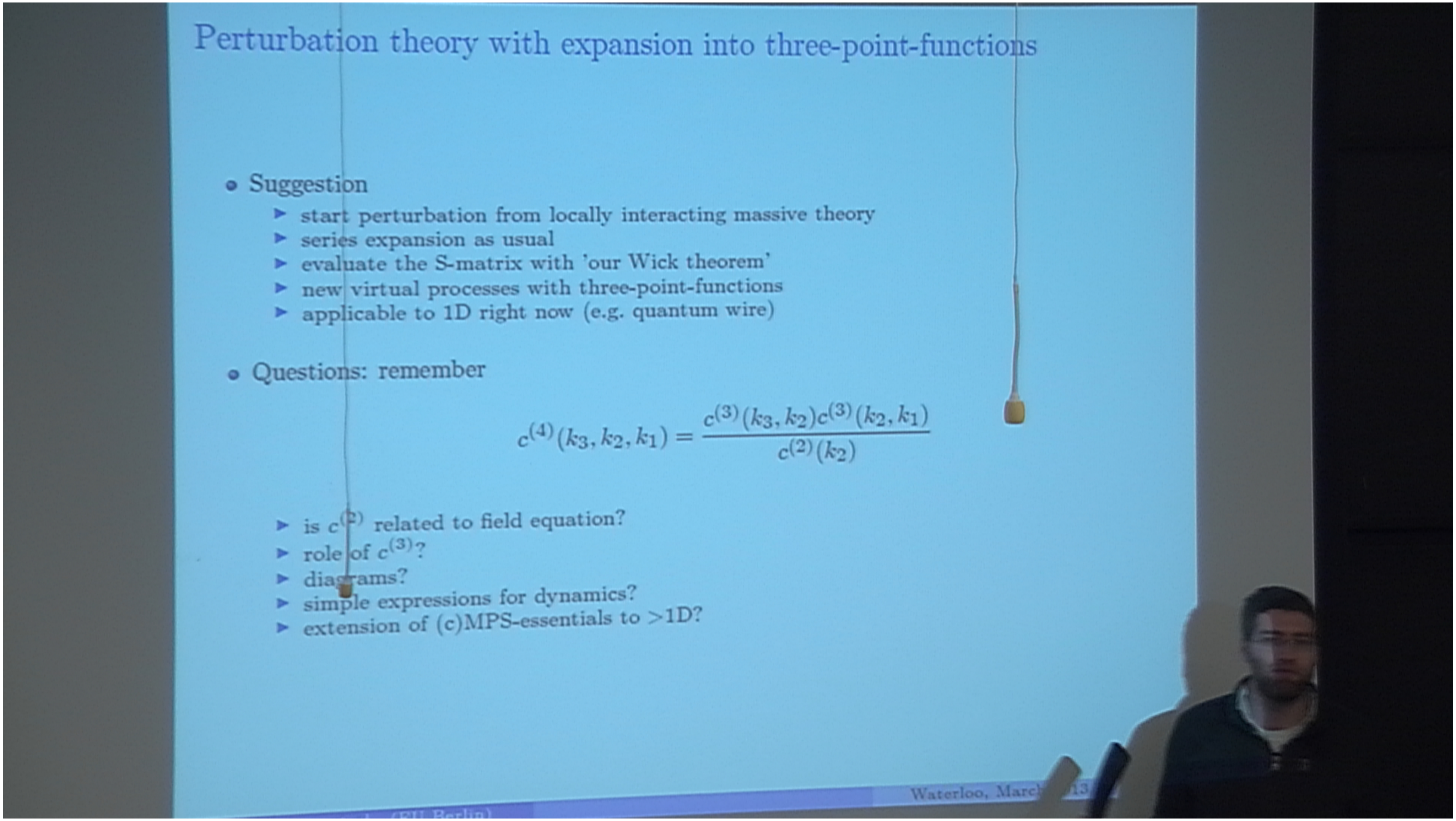


- problem: the quasi-free theory is *very different* from the interacting theory
- problem: representations and questions about what kind of mathematical object is constructed this way


Perturbation theory with expansion into three-point-functions
Suggestion
start perturbation from locally interacting massive theory
series expansion as usual
evaluate the S-matrix with 'our Wick theorem'
new virtual processes with three-point-functions
applicable to 1D right now (e.g. quantum wire)
Questions: remember
$$c^{(4)}(k_3, k_2, k_1) = \frac{c^{(3)}(k_3, k_2)c^{(3)}(k_2, k_1)}{c^{(2)}(k_2)}$$
is $c^{(2)}$ related to field equation?
role of $c^{(3)}$?
diagrams?
simple expressions for dynamics?
extension of (c)MPS-essentials to >1D?
(FU Berlin)
Waterloo, March 2013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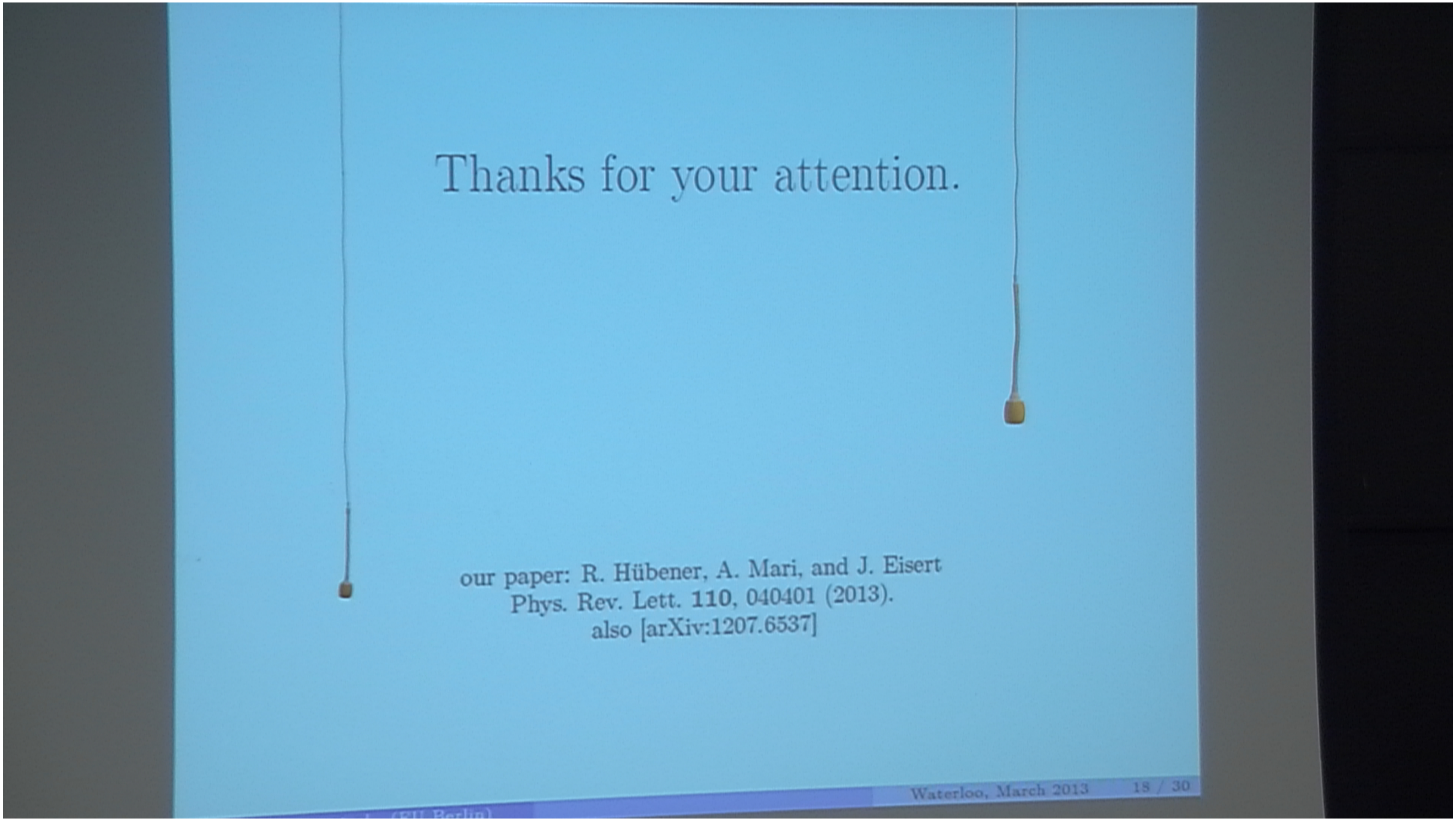
Thanks for your attention.
our paper: R. Hübener, A. Mari, and J. Eisert
Phys. Rev. Lett. 110, 040401 (2013).
also [arXiv:1207.6537]
Waterloo, March 2013
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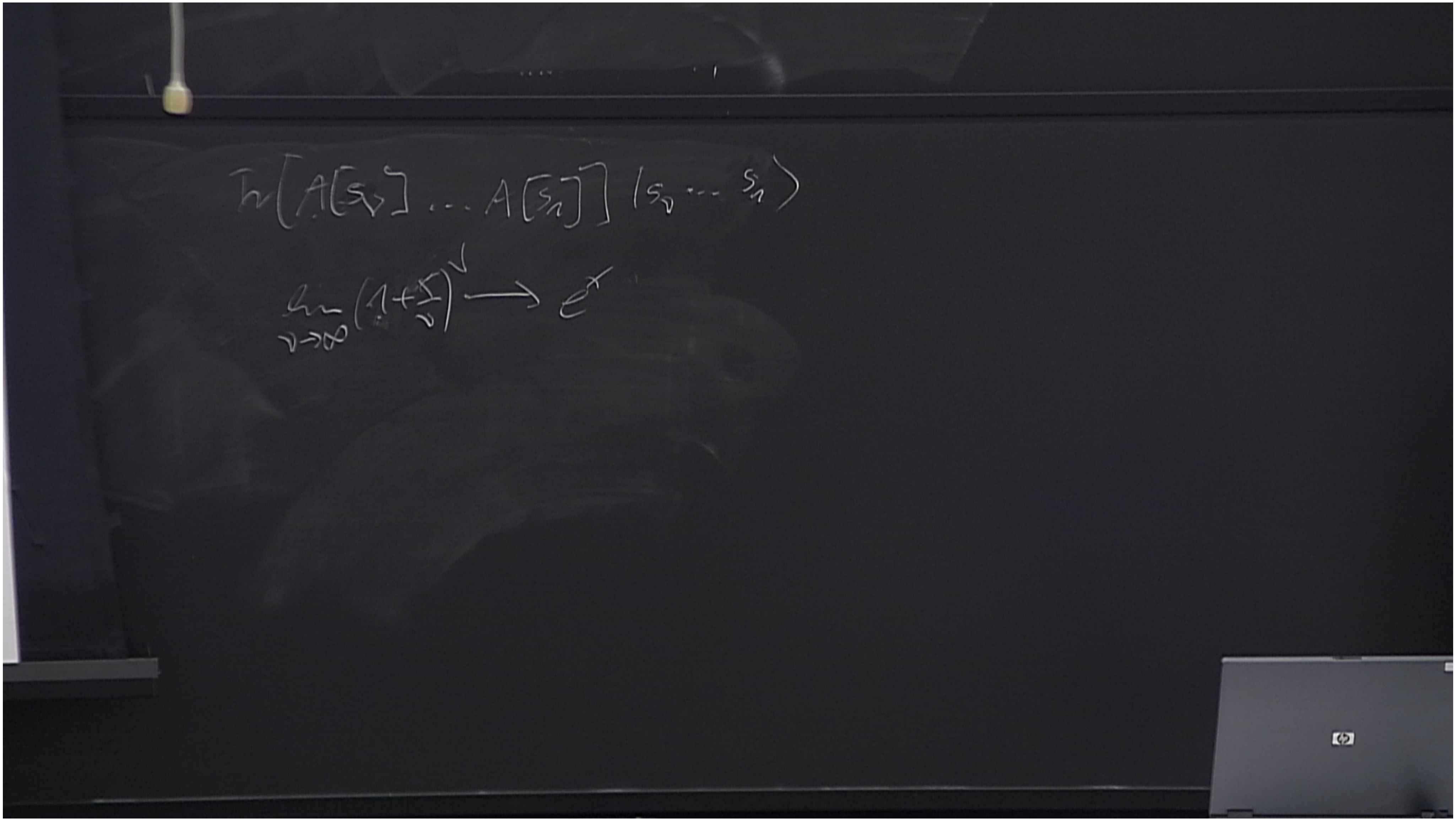
continuous MPS[6,7]

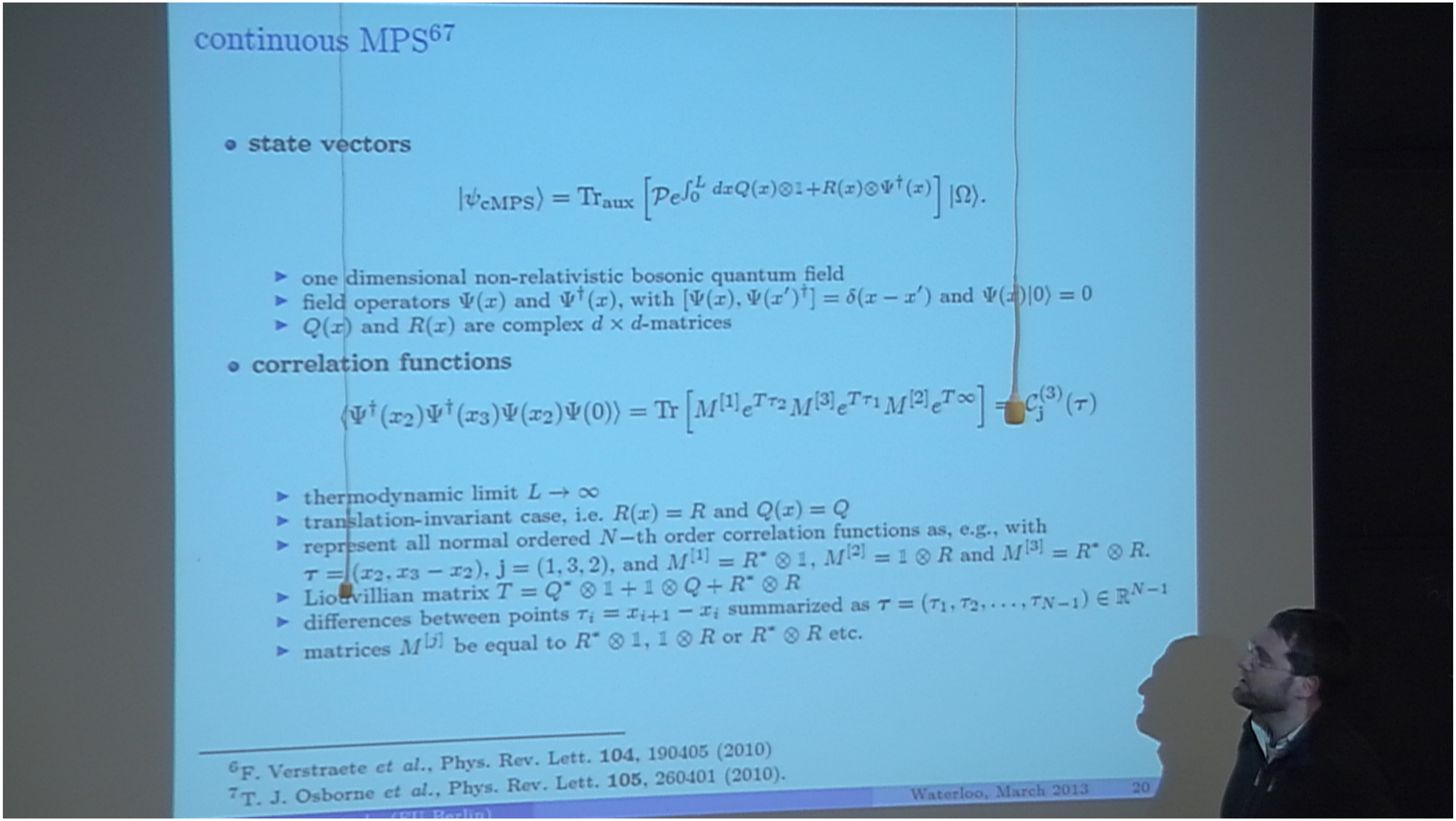
- **state vectors**

$$|\psi_{\text{cMPS}}\rangle = \text{Tr}_{\text{aux}}\left[\mathcal{P}e^{\int_0^L dx Q(x)\otimes\mathbb{1}+R(x)\otimes\Psi^\dagger(x)}\right]|\Omega\rangle.$$

  - one dimensional non-relativistic bosonic quantum field
  - field operators $\Psi(x)$ and $\Psi^\dagger(x)$, with $[\Psi(x),\Psi(x')^\dagger]=\delta(x-x')$ and $\Psi(x)|0\rangle=0$
  - $Q(x)$ and $R(x)$ are complex $d\times d$-matrices

[6] F. Verstraete *et al.*, Phys. Rev. Lett. **104**, 190405 (2010)
[7] T. J. Osborne *et al.*, Phys. Rev. Lett. **105**, 260401 (2010).


Tr[A[s_ν] ... A[s_1]] |s_ν ... s_1⟩
lim_{ν→∞} (1 + x/ν)^ν ⟶ e^x


continuous MPS[6,7]
state vectors
$|\psi_{cMPS}\rangle = \mathrm{Tr}_{aux}\left[\mathcal{P}e^{\int_0^L dx Q(x)\otimes 1 + R(x)\otimes\Psi^\dagger(x)}\right]|\Omega\rangle.$
one dimensional non-relativistic bosonic quantum field
field operators $\Psi(x)$ and $\Psi^\dagger(x)$, with $[\Psi(x),\Psi(x')^\dagger] = \delta(x-x')$ and $\Psi(x)|0\rangle = 0$
$Q(x)$ and $R(x)$ are complex $d\times d$-matrices
correlation functions
$\langle\Psi^\dagger(x_2)\Psi^\dagger(x_3)\Psi(x_2)\Psi(0)\rangle = \mathrm{Tr}\left[M^{[1]}e^{T\tau_2}M^{[3]}e^{T\tau_1}M^{[2]}e^{T\infty}\right] = C_j^{(3)}(\tau)$
thermodynamic limit $L\to\infty$
translation-invariant case, i.e. $R(x) = R$ and $Q(x) = Q$
represent all normal ordered $N-$th order correlation functions as, e.g., with
$\tau = (x_2, x_3 - x_2)$, $j = (1,3,2)$, and $M^{[1]} = R^*\otimes 1$, $M^{[2]} = 1\otimes R$ and $M^{[3]} = R^*\otimes R$.
Liouvillian matrix $T = Q^*\otimes 1 + 1\otimes Q + R^*\otimes R$
differences between points $\tau_i = x_{i+1} - x_i$ summarized as $\tau = (\tau_1,\tau_2,\ldots,\tau_{N-1})\in\mathbb{R}^{N-1}$
matrices $M^{[j]}$ be equal to $R^*\otimes 1$, $1\otimes R$ or $R^*\otimes R$ etc.
[6] F. Verstraete et al., Phys. Rev. Lett. 104, 190405 (2010)
[7] T. J. Osborne et al., Phys. Rev. Lett. 105, 260401 (2010).
Waterloo, March 2013
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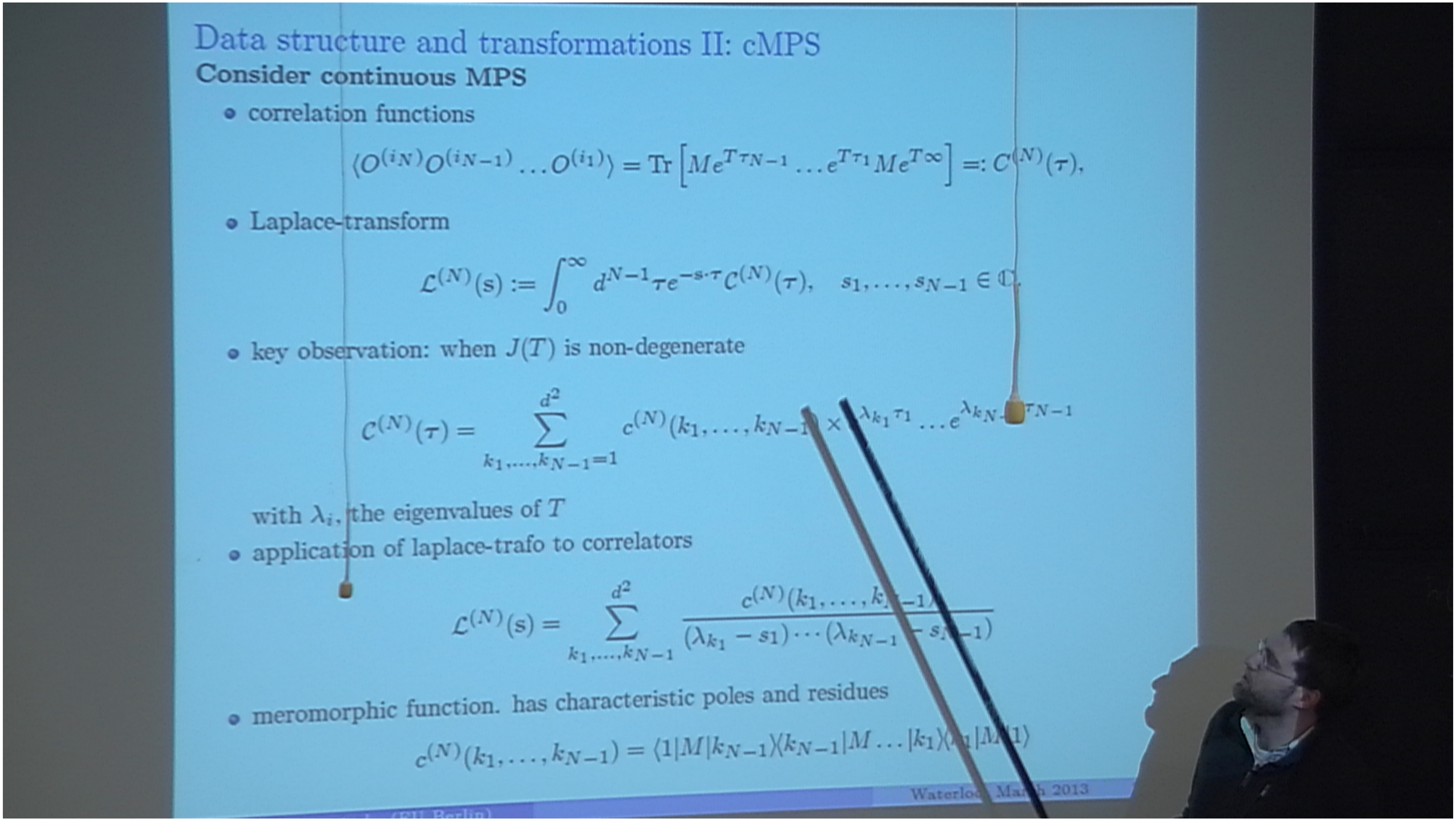
Data structure and transformations II: cMPS
Consider continuous MPS
correlation functions
$\langle O^{(i_N)} O^{(i_{N-1})} \dots O^{(i_1)} \rangle = \mathrm{Tr}\left[M e^{T\tau_{N-1}} \dots e^{T\tau_1} M e^{T\infty} \right] =: \mathcal{C}^{(N)}(\tau),$
Laplace-transform
$\mathcal{L}^{(N)}(\mathrm{s}) := \int_0^\infty d^{N-1}\tau e^{-\mathrm{s}\cdot\tau} \mathcal{C}^{(N)}(\tau), \quad s_1, \dots, s_{N-1} \in \mathbb{C}.$
key observation: when $J(T)$ is non-degenerate
$\mathcal{C}^{(N)}(\tau) = \sum_{k_1,\dots,k_{N-1}=1}^{d^2} c^{(N)}(k_1,\dots,k_{N-1}) \times e^{\lambda_{k_1}\tau_1} \dots e^{\lambda_{k_{N-1}}\tau_{N-1}}$
with λ_i, the eigenvalues of T
application of laplace-trafo to correlators
$\mathcal{L}^{(N)}(\mathrm{s}) = \sum_{k_1,\dots,k_{N-1}}^{d^2} \frac{c^{(N)}(k_1,\dots,k_{N-1})}{(\lambda_{k_1} - s_1)\cdots(\lambda_{k_{N-1}} - s_{N-1})}$
meromorphic function. has characteristic poles and residues
$c^{(N)}(k_1,\dots,k_{N-1}) = \langle 1|M|k_{N-1}\rangle\langle k_{N-1}|M \dots |k_1\rangle\langle k_1|M|1\rangle$
(FU Berlin)
Waterloo, March 2013