

Title: Non-Gaussian fermionic ansatzes from many-body correlation measures

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Series: Quantum Matter

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Abstract: The notorious exponential complexity of quantum problems can be avoided for systems with limited correlations. For example, states of one-dimensional systems with bounded entanglement are approximable by matrix product states. We consider fermionic systems, where correlations can be defined as deviations from Gaussian states. Heuristically, one expects a link between compact non-Gaussian ansatzes and bounded fermionic correlations. This connection, however, has not been rigorously demonstrated. Our work resolves this conceptual gap.

We focus on pure states with a fixed number of fermions. Generalizing the so-called Plücker relations, we introduce k -particle correlation measures χ_k . The vanishing of χ_k at a constant k defines a class \mathcal{H}_k of states with limited correlations. These sets \mathcal{H}_k are nested, ranging from Gaussian for $k=1$ to the full n -fermion Hilbert space \mathcal{H} for $k=n+1$. States in $\mathcal{H}_{\{k=O(1)\}}$ can be represented using a non-Gaussian ansatz of polynomial size. Classes \mathcal{H}_k have physical meaning, containing all truncated perturbation series around Gaussian states. We also identify non-perturbative examples of states in $\mathcal{H}_{\{k=O(1)\}}$, by a numerical study of excited states in the 1D Hubbard model. Finally, we discuss the information-theoretic implications of our results for the widely used coupled-cluster ansatz.

Zoom Link: TBD

Relations on modes

$$\{\psi_q^+, \psi_q\} = \delta_{q,p} \quad p, q \in [l] = \{1, 2, \dots, l\}$$

$$\{\psi_q, \psi_p\} = 0; \quad \sum_{q=1}^l \psi_q^+ \psi_q \equiv n$$



$$S = (s_1, s_2, \dots, s_n) \in [l]$$

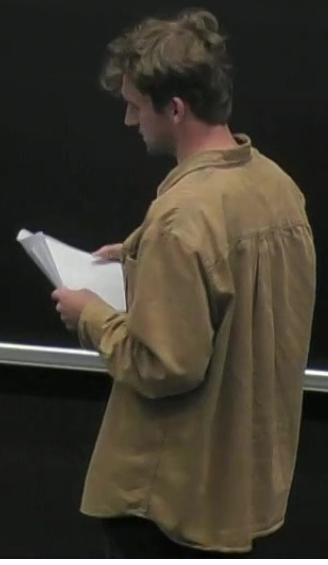
$$|S\rangle \equiv \psi_S^+ | \rangle \equiv \psi_{s_n}^+ \dots \psi_{s_1}^+ | \rangle$$

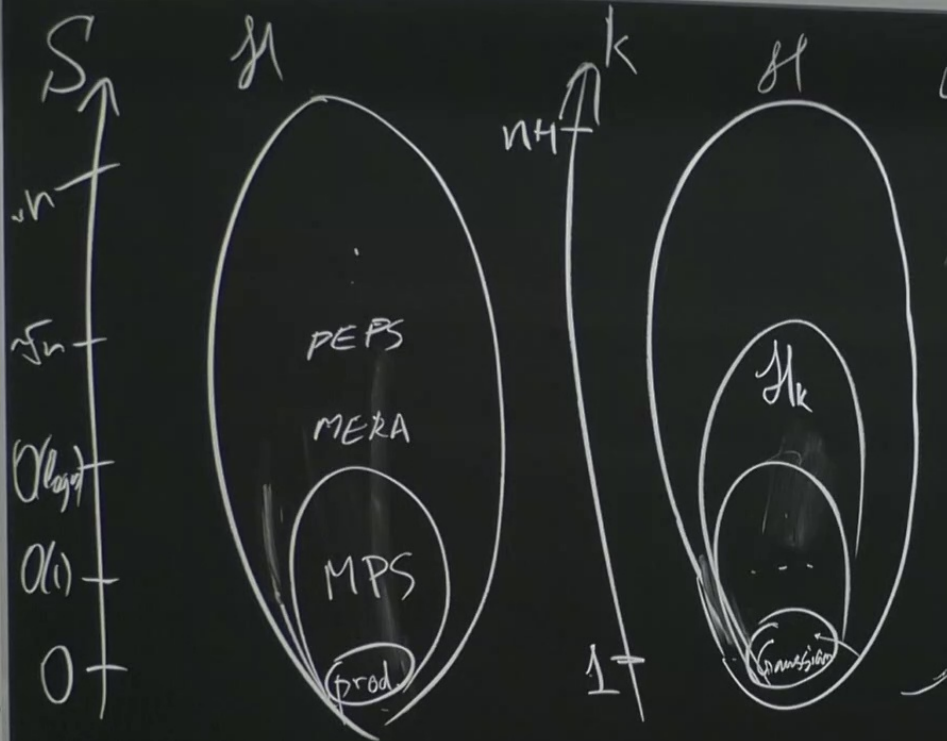
$$|v\rangle = \sum v(S) |S\rangle \in \mathcal{L} \quad \text{e.g., } |v\rangle = v(1,2)|1,2\rangle + v(1,3)|1,3\rangle + v(3,4)|3,4\rangle \quad \begin{matrix} l=4 \\ n=2 \end{matrix}$$

Gaussian states

$$|G\rangle = \exp\left(\sum_{pq} \theta_{pq} \psi_q^+ \psi_p\right) |S_0\rangle$$

Properties.





1. Relationship
2. Exponential poly-

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 Do not touch the chalkboard
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 use the eraser.

n fermions on l modes

$$\psi_q \quad \{\psi_q^\dagger \psi_q\} = \delta_{q,p} \quad p, q \in [l] = \{1, 2, \dots, l\}$$

$$\{\psi_q, \psi_p\} = 0; \quad \sum_{q=1}^l \psi_q^\dagger \psi_q \equiv n$$



$$S = (s_1, s_2, \dots, s_n) \in [l]$$

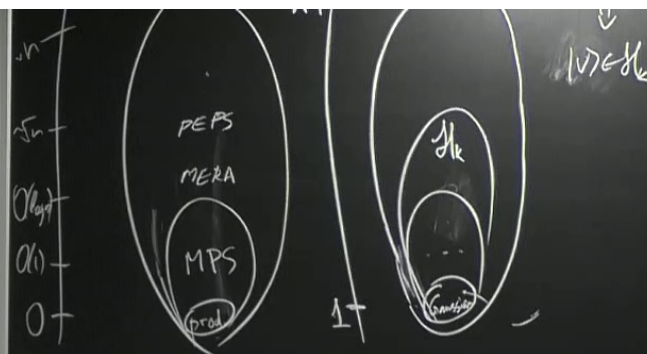
$$|S\rangle \equiv \psi_S^\dagger |0\rangle \equiv \psi_{s_n}^\dagger \dots \psi_{s_1}^\dagger |0\rangle$$

$$|\psi\rangle = \sum v(S) |S\rangle \in \mathcal{H} \quad \text{e.g., } |\psi\rangle = v(1,2)|1,2\rangle + v(1,3)|1,3\rangle + v(3,4)|3,4\rangle \quad \begin{matrix} l=4 \\ n=2 \end{matrix}$$

Gaussian states

$$|\psi\rangle = \exp\left(\sum_{pq} \theta_{pq} \psi_q^\dagger \psi_p\right) |S_0\rangle$$

Properties.



1. Relevant correlations
2. Explicit poly-sized ansatz
3. Is comput. useful

$$|V\rangle = \sum v(S) |S\rangle \in \mathcal{H}, \text{ e.g., } |V\rangle = v(1,2) |1,2\rangle + v(1,3) |1,3\rangle + \dots + v(3,4) |3,4\rangle : \begin{matrix} l=4 \\ n=2 \end{matrix}$$

Gaussian states

$$|G\rangle = \exp\left(\sum_{pq} \theta_{pq} \psi_q^\dagger \psi_p\right) |S_0\rangle$$

Properties:

Eigs of $H = \sum h_{pq} \psi_q^\dagger \psi_p$

Wick's rule: $\langle G | \psi_q^\dagger \psi_p | G \rangle = \det \left(\langle G | \psi_q^\dagger \psi_p | G \rangle \right)$

Purity of $(\rho_1) = \langle v | \psi_r^+ \psi_p | v \rangle : \omega_1 = \text{tr}[\rho_1 - \rho_1^2] = 0$
 \uparrow
 $\underline{1 \times 1}$

$\text{tr}[\rho_1] = n$

Plücker relations: $\Omega = \sum \psi_r \otimes \psi_r^+$ acts on $\mathfrak{g} \otimes \mathfrak{g}$

$\Omega |v\rangle \otimes |v\rangle = 0$

\uparrow
 $l \times l$

Plücker relations: $\Omega = \sum \psi_r \otimes \psi_r^+$ acts on $\mathfrak{g} \otimes \mathfrak{g}$ $\text{tr}[\rho, \cdot] = n$

$$\Omega |v\rangle \otimes |v\rangle = 0; \quad \begin{matrix} l=4, n=2 \\ v(1,2)v(3,4) - v(1,3)v(2,4) \\ + v(1,4)v(2,3) = 0 \end{matrix}$$



1-RDM

Purity of $(\rho_i) = \langle v | \psi_i^\dagger \psi_i | v \rangle : \omega_i = \text{tr}[\rho_i - \rho_i^2] = 0$

\uparrow
 $l \times l$

$i, j = n$

Plücker relations: $\Omega = \sum \psi_r \otimes \psi_r^\dagger$

$\omega_i = \text{tr}[\rho_i - \rho_i^2]$

$\Omega |v\rangle \otimes |v\rangle = 0 ;$ $l=4, n=2$
 $v(1,2) - v(3,4) - v(1,3) + v(2,4)$

$|\Omega |v\rangle \otimes |v\rangle|^2 = \omega_i$

Plücker relations. $\Omega = \sum_{i < j} \psi_i \psi_j$ acts on $\mathcal{H} \otimes \mathcal{H}$

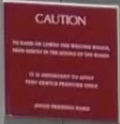
$$\Omega |v\rangle \otimes |v\rangle = 0; \quad \ell=4, n=2$$

$$v(1,2)v(3,4) - v(1,3)v(2,4)$$

$$+ v(1,4)v(2,3) = 0$$

$$|\Omega |v\rangle \otimes |v\rangle|^2 = \omega_1 = \sum_{p,q} \underbrace{\langle v | \psi_q^\dagger \psi_p | v \rangle}_{\delta_{pq}} \underbrace{\langle v | \psi_p \psi_q^\dagger | v \rangle}$$

$$\omega_1 =$$



Plücker relations: $\Omega = \sum \psi_r \otimes \psi_r^+$ acts on $\mathcal{P} \otimes \mathcal{P}$

$$\Omega |v\rangle \otimes |v\rangle = 0; \quad \ell=4, n=2$$

$$v(1,2)v(3,4) - v(1,3)v(2,4) + v(1,4)v(2,3) = 0$$

$$|\Omega |v\rangle \otimes |v\rangle|^2 = \omega_1 = \sum_{p,q} \underbrace{\langle v | \psi_q^+ \psi_p | v \rangle}_{\delta_{pq}} \underbrace{\langle v | \psi_q \psi_p^+ | v \rangle}_{\delta_{pq} - \delta_{q_1}} = \text{tr}[\rho, \rho_{1,c}]$$

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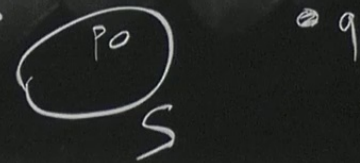
$$\omega_i = \text{tr}[\rho_i \rho_{i,c}] = 0$$

$$\int \Omega |v\rangle \langle v| = 0$$

Wick
for $\langle 0 \rangle$
and $v(s)$

$$|v\rangle = \exp(T_1) v(s) |S\rangle$$

$$T_1 = \sum_{\substack{p \in S \\ q \notin S}} \theta_{pq} \psi_q^+ \psi_p$$



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Always disconnect the power.

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$$\mathcal{H}_{k=n+1} = \mathcal{H}$$

\cup
 \mathcal{H}_k
 \cup
 \vdots
 \cup
 \mathcal{H}_1

$$\omega_k = \text{tr} [p_k \rho_k] = 0 \quad \text{Green. Wick}$$

$$\int \langle \psi | \psi \rangle = 0 \quad \Rightarrow \text{for } \psi(S)$$

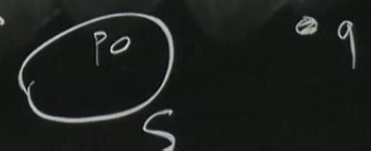
$$\omega_1 = \text{tr} [p_1 \rho_1] = 0$$

\updownarrow
 Wick
 for $\langle 0 \rangle$
 and $\psi(S)$

$$\int \langle \psi | \psi \rangle = 0$$

$$|\psi\rangle = \exp(T_1) \psi(S) |S\rangle$$

$$T_1 = \sum_{\substack{p \neq S \\ q \neq S}} \theta_{pq} \psi_q^+ \psi_p$$



$$\mathcal{H}_{k=n+1} = \mathcal{H}$$

$$\cup \mathcal{H}_k$$

$$\cup \mathcal{H}_1$$

$$\omega_k = \text{tr} [p_k p_{k,c}] = 0$$

$$\Omega^k |v\rangle |v\rangle = 0$$

$$\omega_1 = \text{tr} [p_1 p_{1,c}] = 0$$

$$\Omega |v\rangle |v\rangle = 0$$

Gren Wick

for $v(S)$

Wick

for $\langle 0 \rangle$

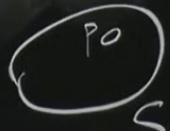
and $v(S)$

$$|v\rangle = v(S) F(T_1, \dots, T_k) |S\rangle$$

$$T_k = \sum_{\substack{p \in S \\ q \notin S}} \theta_{pq} \psi_q^+ \psi_p$$

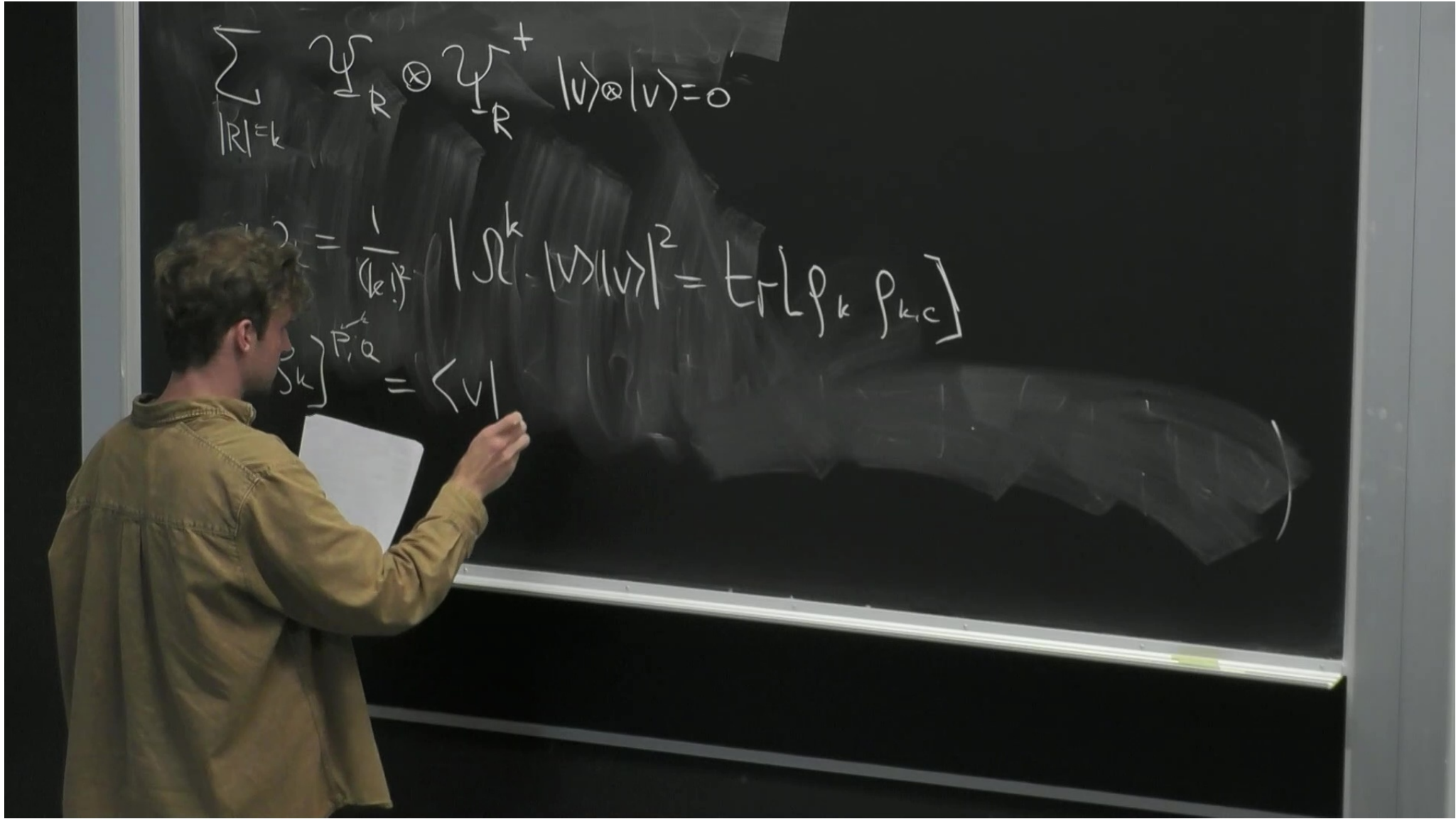
$$|v\rangle = \exp(T_1) v(S) |S\rangle$$

$$T_1 = \sum_{\substack{p \in S \\ q \notin S}} \theta_{pq} \psi_q^+ \psi_p$$



θ_{pq}

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$|R|^k$

$$\omega_k = \frac{1}{(k!)^2} |\Omega^k |v\rangle \langle v| |^2 = \text{tr}[\rho_k \rho_{k,c}] = \text{func}(\rho_k)$$

$$[\rho_k]^{P,Q} = \langle v | \Psi_Q^\dagger \Psi_P | v \rangle$$

$$[\rho_{k,c}]^{P,Q} = \langle v | \Psi_P \Psi_Q^\dagger | v \rangle$$

$$\rho_{k'} = \text{marg.}(\rho_k) \\ \downarrow k$$

$$\sum^k |v\rangle \otimes |v\rangle = 0$$

$$\sum_{|R|=k} \psi_{-R} \otimes \psi_{-R}^+ |v\rangle \otimes |v\rangle = 0$$

$$\omega_k = 0 \Rightarrow \omega_{k'} = 0 \quad k' > k$$

$$\omega_k = \frac{1}{(k!)^2} \left| \sum^k |v\rangle |v\rangle \right|^2 = \text{tr}[\rho_k \rho_{k,c}] = \text{func}(\rho_k)$$

$$[\rho_k]^{P,Q} = \langle v | \psi_{-Q}^+ \psi_{-P} | v \rangle$$

$$[\rho_{k,c}]^{P,Q} = \langle v | \psi_{-P} \psi_{-Q}^+ | v \rangle$$

$$\rho_{k'} = \text{marg.} \quad k' < k$$

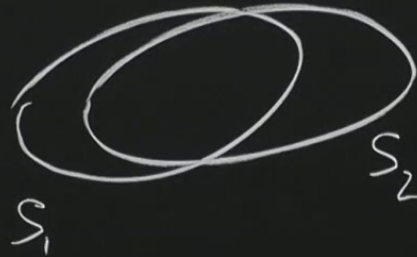
Plan

1. $|v\rangle \in \mathcal{H}_k$

2. Wick 2
ansatz

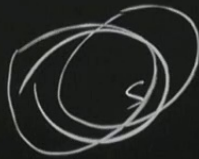
3. Discuss

$$\text{Any } |v\rangle = \sum v(s) |s\rangle$$



$$\frac{1}{2} |S_1 \Delta S_2| > k$$

$$\Rightarrow \begin{cases} v(S_1) = 0 \\ \text{or} \\ v(S_2) = 0 \end{cases}$$

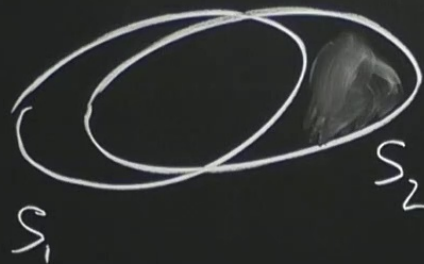


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1. $|v\rangle \in \mathcal{H}_k$

2. Wick 2
ansatz

3. Discuss



$$\frac{1}{2} |S_1 \Delta S_2| > k$$

$$\Rightarrow \begin{cases} v(S_1) = 0 \\ \text{or} \\ v(S_2) = 0 \end{cases}$$

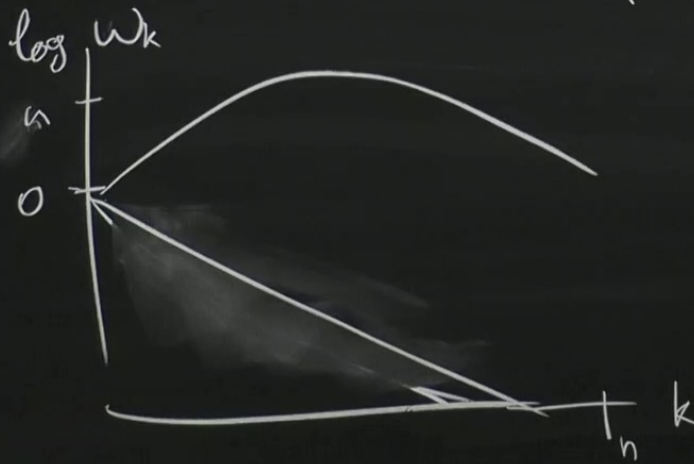
$$|v_1\rangle = \frac{1}{\sqrt{2}} (|1,2,3,4\rangle + |1,2,5,6\rangle) \quad \int^3 |v_1\rangle |v_1\rangle = 0,$$

$$|v_2\rangle = \frac{1}{\sqrt{2}} (|1,2,3,4\rangle + |5,6,7,8\rangle) \quad \int^3 |v_1\rangle |v_2\rangle \neq 0 \quad \int^5 |v_2\rangle |v_2\rangle = 0$$

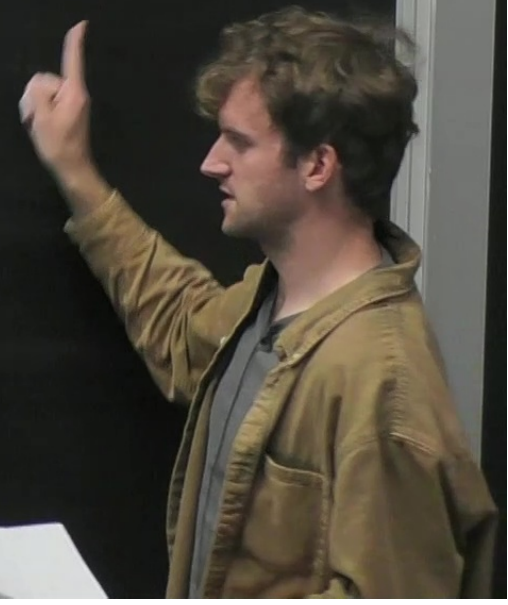
PT series:

$$|V) = v_0 |S_0) + \sum V(s) |S) \quad v(s) \propto \left(\frac{\sigma}{\Delta} \right)^{\frac{|s| |s_0|}{2 |s_0 s|}}$$

1D Kub. model

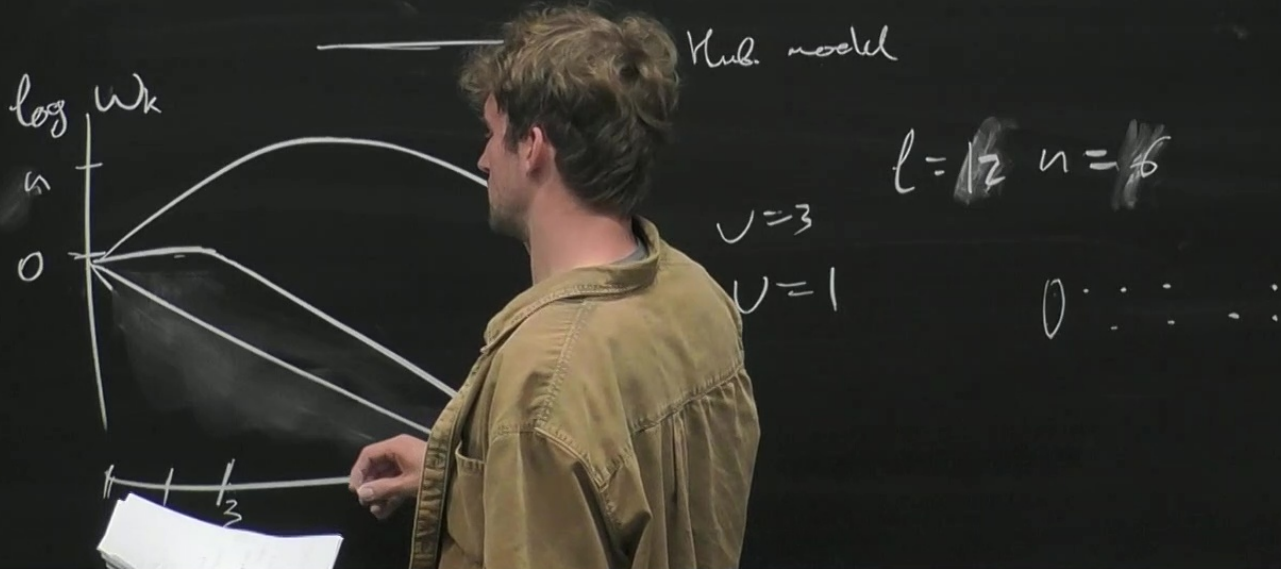


$v=1$



PT series:

$$|V\rangle = v_0 |S_0\rangle + \sum V(s) |S\rangle \quad v(s) \propto \left(\frac{\sigma}{\Delta}\right)^{\frac{|S| |S_0|}{2}} \frac{|S| |S_0|}{2} \frac{1}{|S| |S_0|}$$

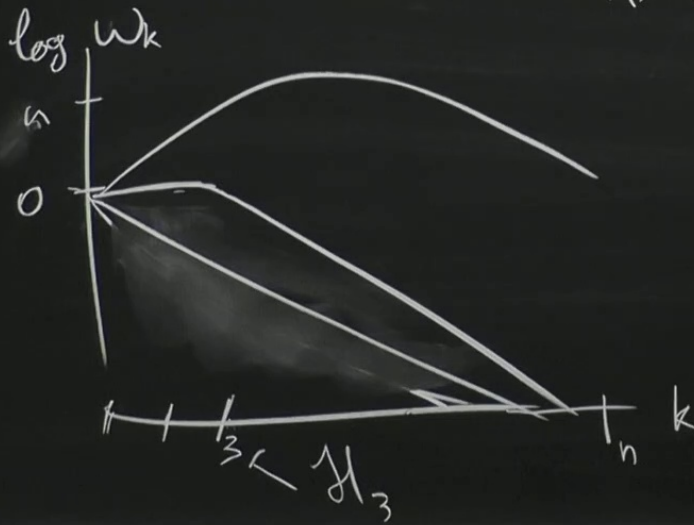


PT series:

$$|V\rangle = v_n |S_0\rangle + \sum V(s) |S\rangle$$

$$v(s) \propto \left(\frac{\sigma}{\Delta} \right)^{\frac{|s|}{|S_0|}} \approx \frac{1}{2} |s| |S_0|$$

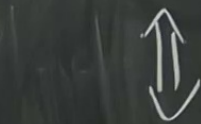
—————: 1D Kub. model



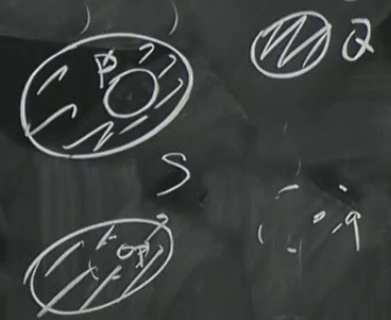
$l = 6$
 $v = 3$
 $v = 1$

$k=1$ exercise RUM

$$\frac{v(S \setminus pUq)}{v(S)} = \det \left(\frac{v(S \setminus pUq)}{v(S)} \right)$$



$$v(S) = v(S) \exp \left(\sum_{p \in S} q \cdot 4S \right)$$



CAUTION
DO NOT TOUCH THE BOARD WHEN
IT IS BEING USED BY ANYONE
OTHER THAN THE PRESENTER

$$\bigwedge^k |v\rangle \otimes |v\rangle = 0$$

A, B

$$\sum_{|R|=k} \Psi_{-R} \otimes \Psi_{-R}^+ |v\rangle \otimes |v\rangle = 0$$

$$\sum v(A|UR) v(B|R) \times \text{sign} = 0$$

$$\omega_k = \frac{1}{(k!)^2} \left| \bigwedge^k |v\rangle |v\rangle \right|^2 = \text{tr}[\rho_k \rho_{k,c}] = \text{func}(\rho_k)$$

$$[\rho_k]^{P,Q} = \langle v | \Psi_{-Q}^+ \Psi_{-P} | v \rangle$$

$$[\rho_{k,c}]^{P,Q} = \langle v | \Psi_{-P} \Psi_{-Q}^+ | v \rangle$$

$$\rho_{k'} = \text{marg.}(\rho_k)$$

$k' < k$

$$\frac{V(S|P \cup Q)}{V(S)} = \sum \# \frac{V(S|P \cup Q)}{V(S)} \frac{V(S|\bar{P} \cup \bar{Q})}{V(S)}$$



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 this space at the service of our clients
 or in compliance to other
 applicable regulations.

$$\mathcal{L}_1: \omega_1 = \text{tr}(p_i p_{i^c}) = 0$$

$$\uparrow$$

$$\Omega |v\rangle \otimes |v\rangle = 0$$

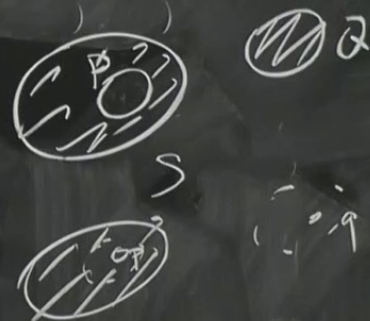
Wick
for $\langle 0 \rangle$
and $v(s)$

$$|v\rangle = \exp(T_1) v(s) |s\rangle$$

$$T_1 = \sum_{p \neq q} \theta_{pq} \psi_p^+ \psi_q$$

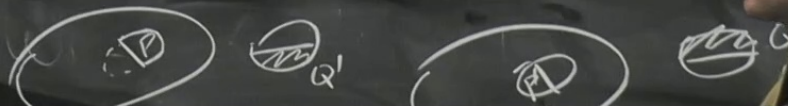
$k=1$ exercise RUM

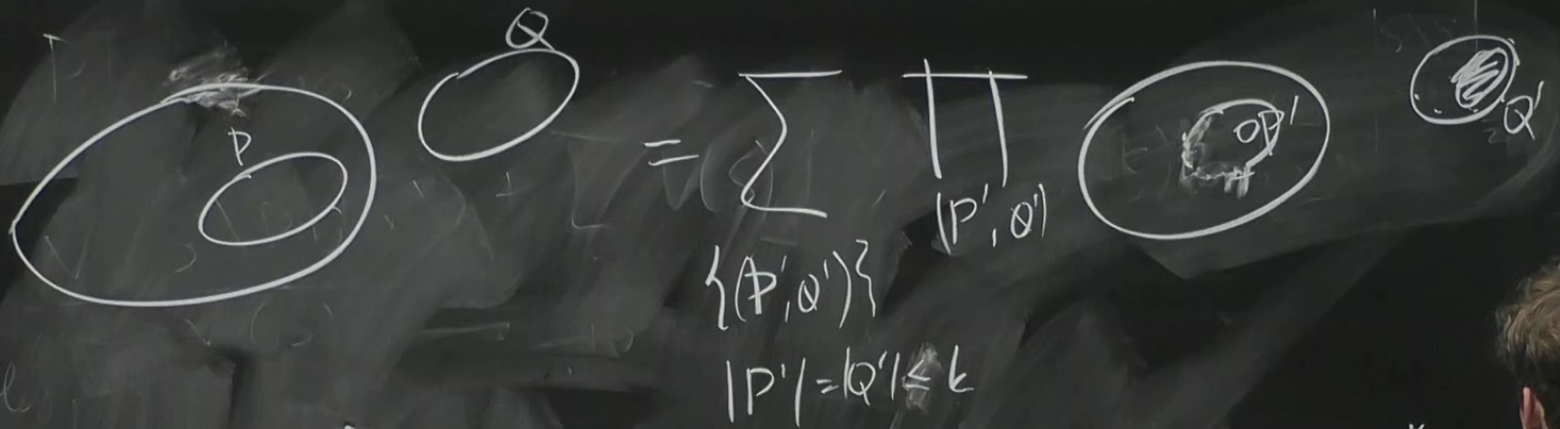
$$\frac{v(S \setminus P U Q)}{v(S)} = \det \left(\frac{v(S \setminus P U Q)}{v(S)} \right)$$



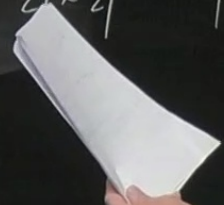
$$\frac{v(S \setminus P U Q)}{v(S)} = \sum_{\#} \frac{v(S \setminus P' U' Q')}{v(S)} \frac{v(S \setminus \bar{P}' U' \bar{Q}')}{v(S)}$$

$$|P| = |Q| > k$$

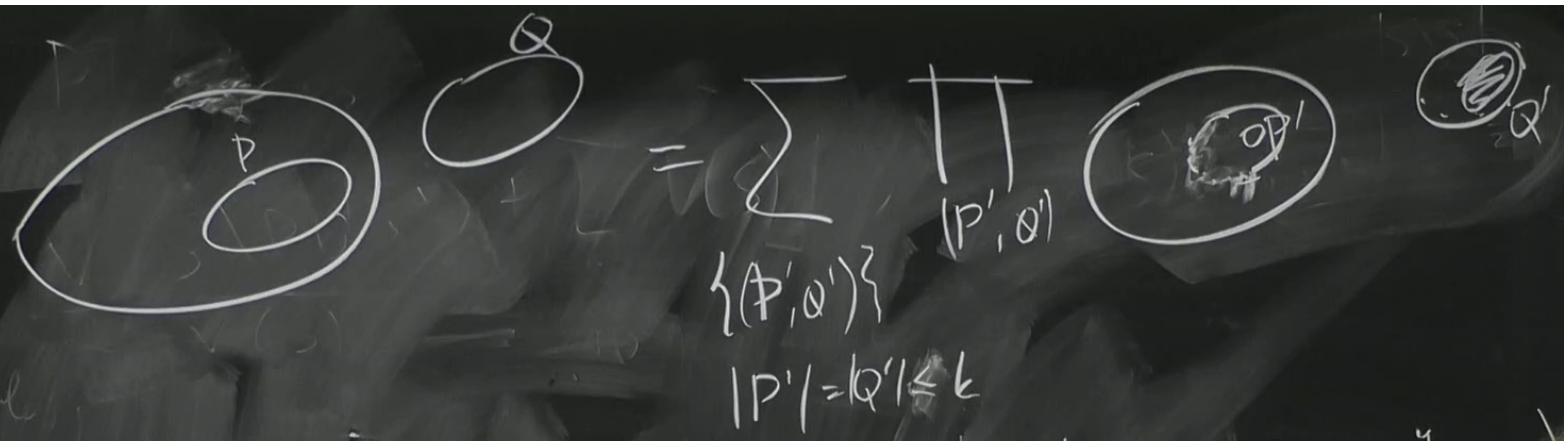




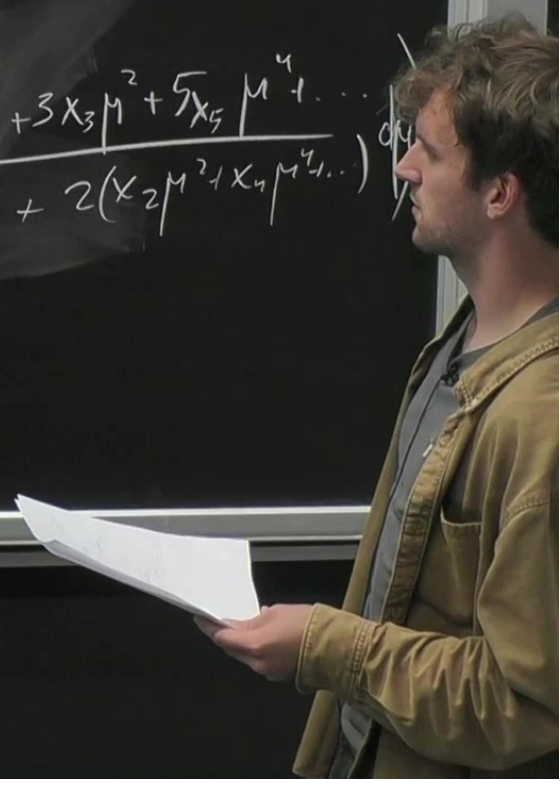
$$F(x_1, x_2, \dots) = \sqrt{1 + 2(x_2 + x_4 + \dots)} \exp\left(\frac{\int_0^1 x_1 + 3x_3 m^2 + 5x_5 m^4 + \dots}{e - 1 + 2(x_2 m^2 + x_4 m^4 + \dots)}\right)$$



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 IT IS RECOMMENDED BY ANOVA
 THAT YOU USE THE PROVIDED MARKERS.
 WHITE BOARD MARKERS



$$F(x_1, x_2, \dots) = \sqrt{1 + 2(x_2 + x_4 + \dots)} \exp\left(\int_0^1 \frac{x_1 + 3x_3 M^2 + 5x_5 M^4 + \dots}{1 + 2(x_2 M^2 + x_4 M^4 + \dots)} dM\right)$$



CAUTION
 DO NOT TOUCH THE BOARD SURFACE.
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 OF PROTECTIVE FILM.
 PLEASE BE CAREFUL.

$$\bigwedge^k |v\rangle \otimes |v\rangle = 0$$

$$\sum_{|R|=k} \psi_{\perp R} \otimes \psi_{\perp R}^+ |v\rangle \otimes |v\rangle = 0$$

A, B

$$Z(\beta) = \sum \omega_k \beta^{2k}$$

$$\sum_{|R|=k} v(A \cup R) v(B \setminus R) \times \text{sign} = 0$$

$$\omega_k = \frac{1}{(k!)^2} \left| \bigwedge^k |v\rangle |v\rangle \right|^2 = \text{tr}[\rho_k \rho_{k,c}] = \text{func}(\rho_k)$$

$$[\rho_k]^{P,Q} = \langle v | \psi_{\perp Q}^+ \psi_{\perp P} | v \rangle$$

$$[\rho_{k,c}]^{P,Q} = \langle v | \psi_{\perp P} \psi_{\perp Q}^+ | v \rangle$$

$$\rho_{k,c} = \text{marg.}(\rho_k)$$

$k' < k$