Title: Pinning of Fermionic Occupation Numbers

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URL: http://www.pirsa.org/13010105

Abstract: The problem of determining and describing the family of 1-particle reduced density operators (1-RDO) arising from N-fermion pure states (viapartial trace) is known as the fermionic quantum marginal problem. We present its solution, a multitude of constraints on the eigenvalues of the 1-RDO, generalizing the Pauli exclusion principle. To explore the relevance of these constraints we study an analytically solvable model of N fermions in a harmonic potential and determine the spectral `trajectory' corresponding to the ground state as function of the fermion-fermion interaction strength.Intriguingly, we find that the occupation numbers are almost, but not exactly, pinned to the boundary of the allowed region (quasi-pinned). Our findings suggest a generalization of the Hartree-Fock approximation.

see also: http://arxiv.org/abs/1210.5531

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Credits: M.Christandl & D.Gross

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Outline

1) Motivation
2) Generalized Pauli Constraints
3) Physical Model
4) Pinning Analysis
5) Physical Relevance of Pinning

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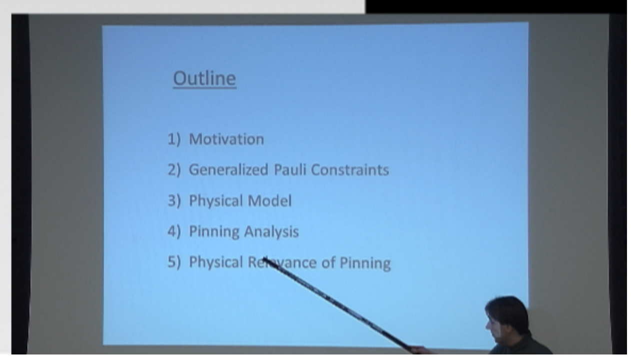

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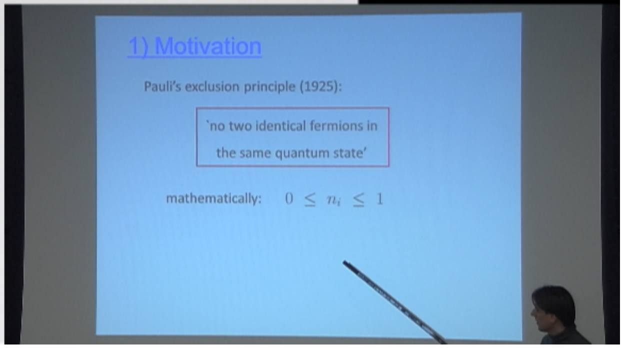

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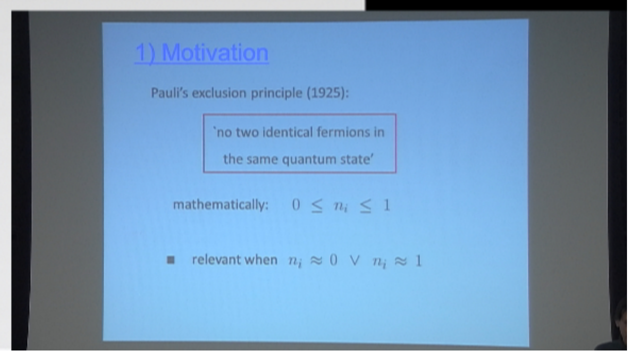

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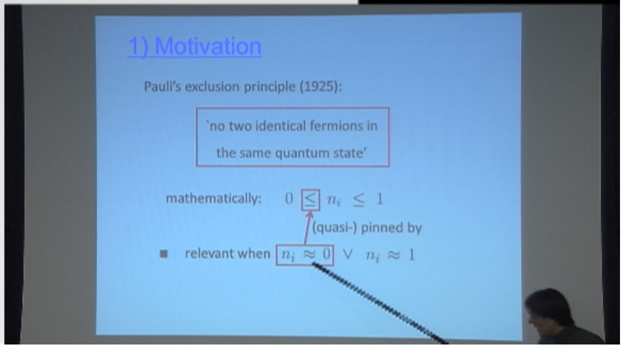

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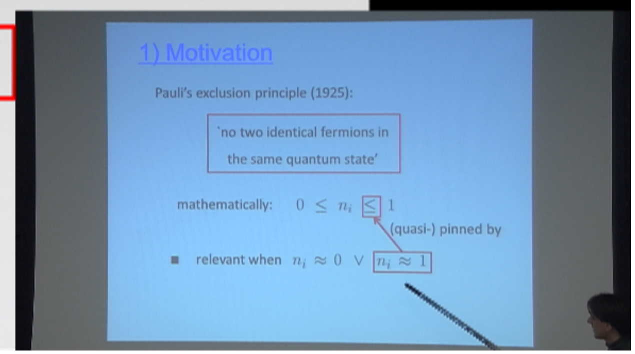

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mathematically: $0 \leq n_i \leq 1$

- relevant when $n_i \approx 0 \vee n_i \approx 1$
- $\longrightarrow$ Aufbau principle for atoms

strengthened by Dirac & Heisenberg in (1926):

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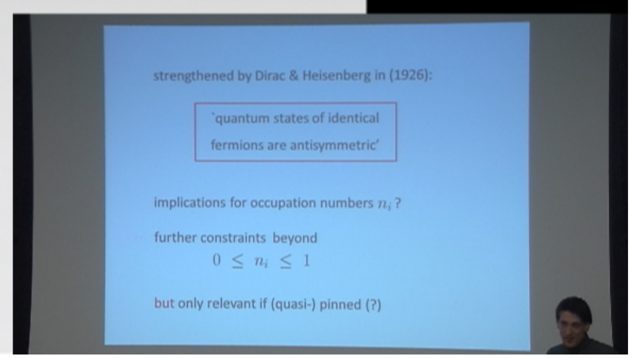
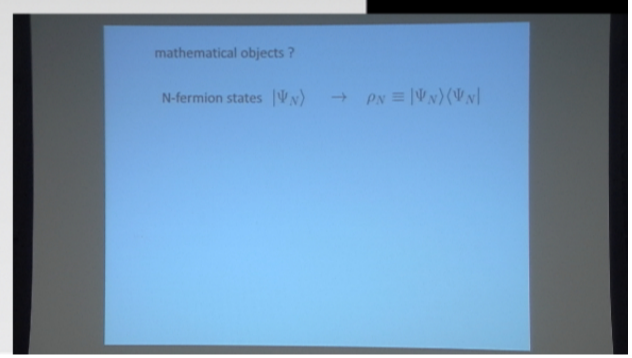
but only relevant if (quasi-) pinned (?)



mathematical objects ?

N-fermion states $|\Psi_N\rangle \quad \rightarrow \quad \rho_N \equiv |\Psi_N\rangle\langle\Psi_N|$



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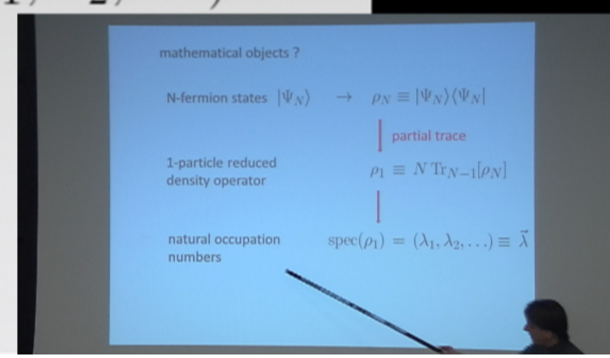
1-particle reduced density operator $\quad \rho_1 \equiv N\,\mathrm{Tr}_{N-1}[\rho_N]$

natural occupation numbers $\quad \mathrm{spec}(\rho_1) = (\lambda_1, \lambda_2, \ldots) \equiv \vec{\lambda}$



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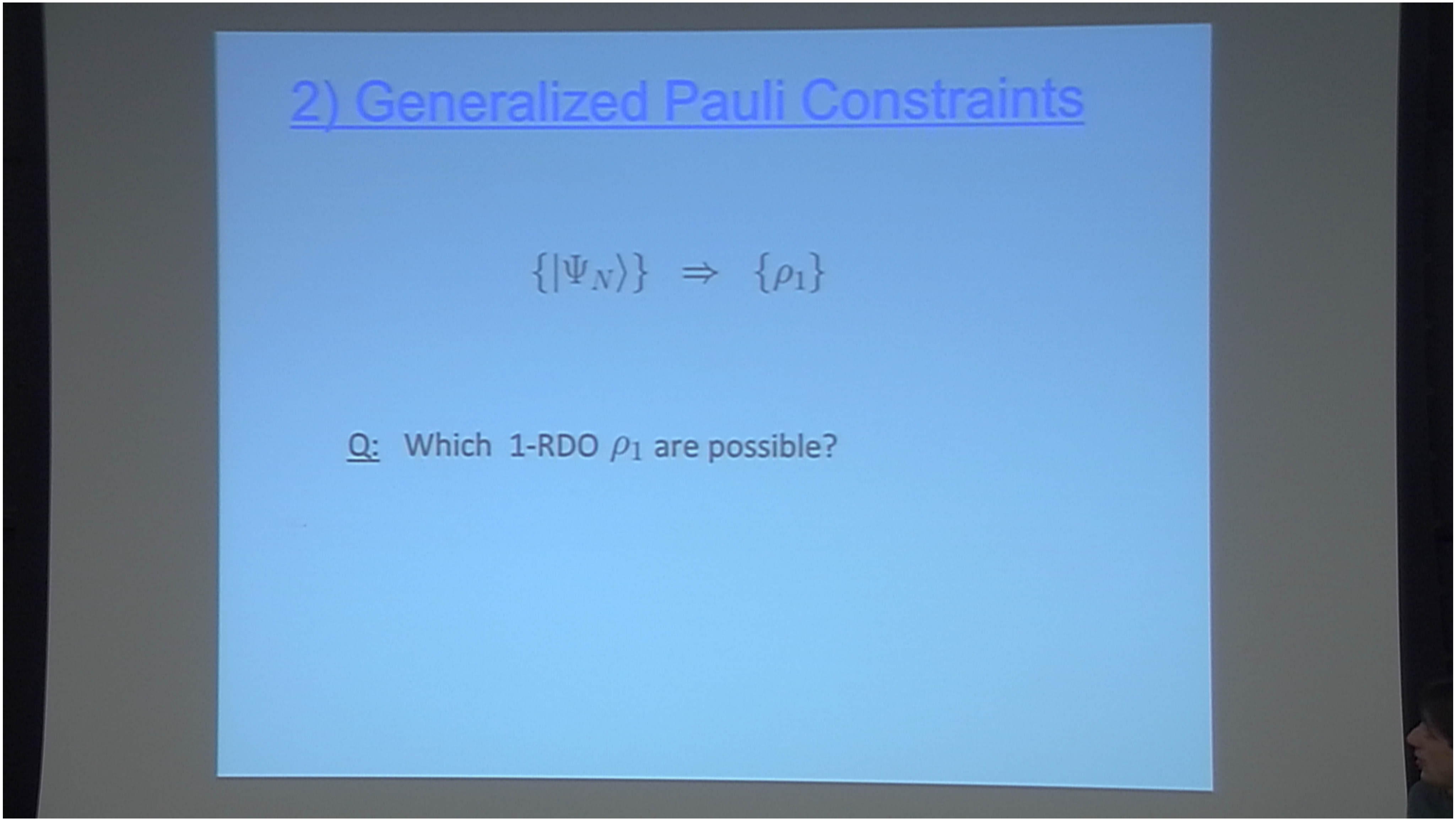
translate antisymmetry of $|\Psi_N\rangle$ to 1-particle picture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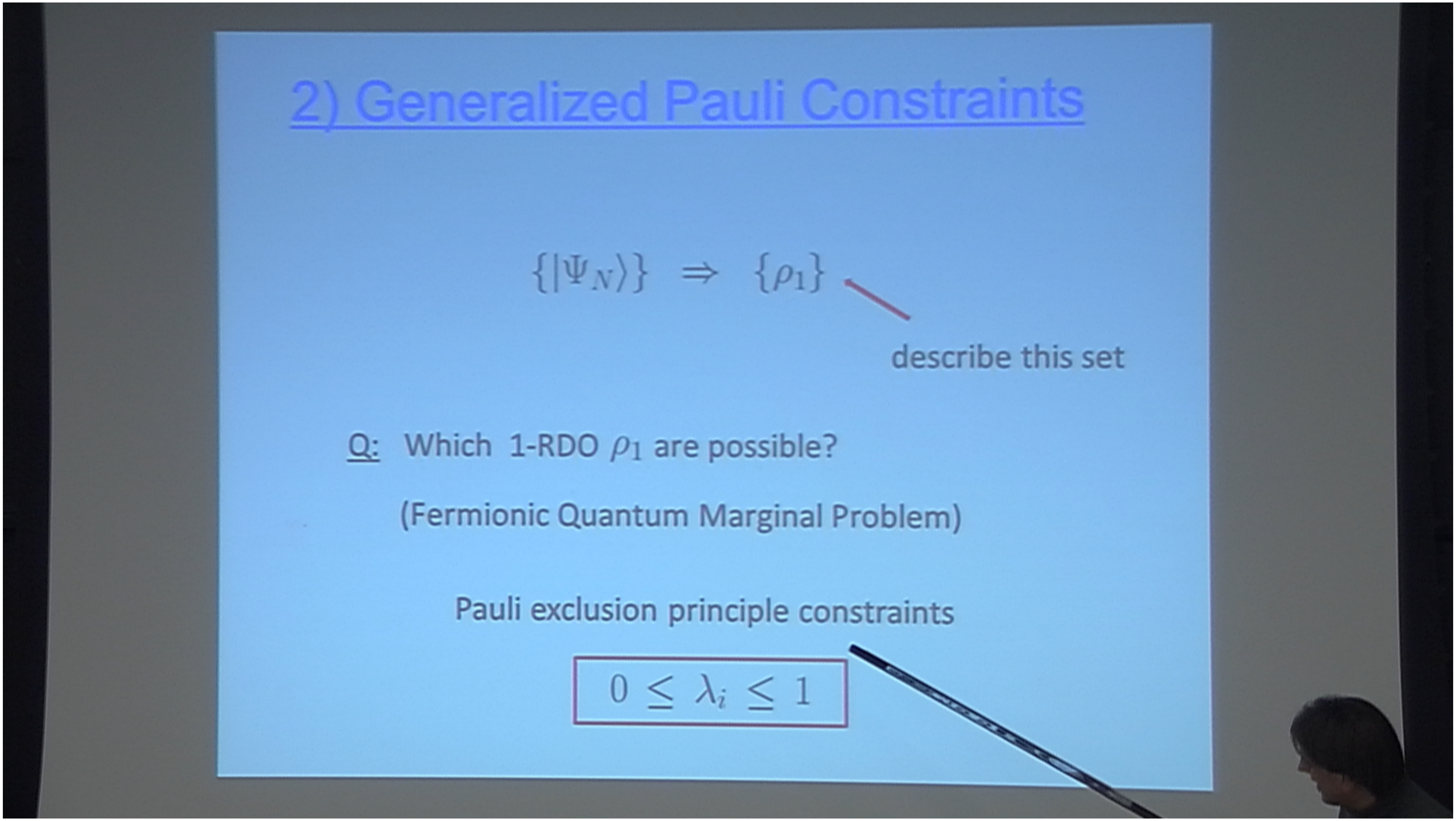
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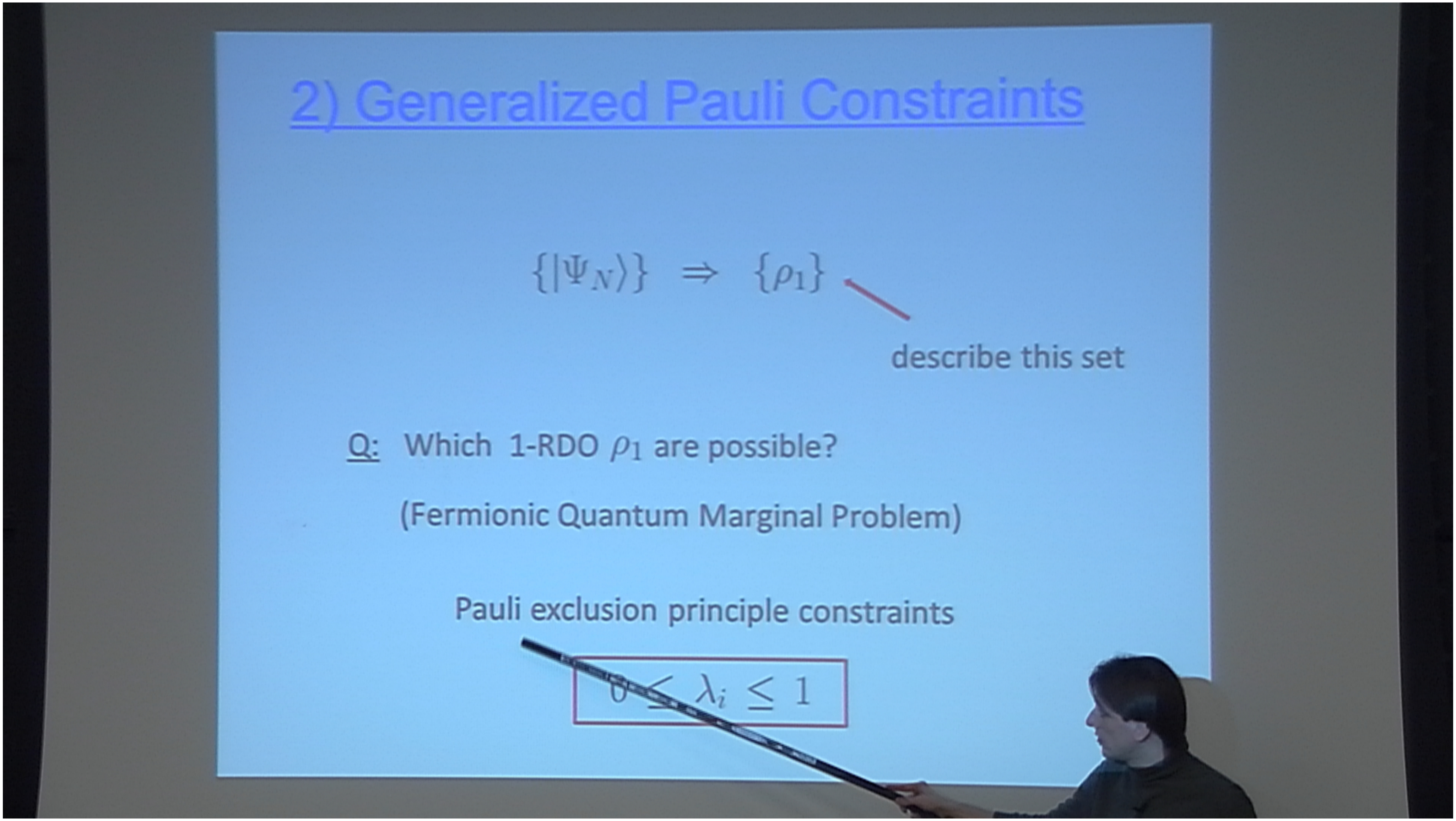
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A: ■ unitary equivalence:

$$\rho_1 \text{ arises from } |\Psi_N\rangle \quad \Rightarrow$$

$$U\,\rho_1\,U^\dagger \text{ can arise from } U^{\otimes^N}|\Psi_N\rangle$$

→ only natural occupation numbers $\vec{\lambda}$ relevant

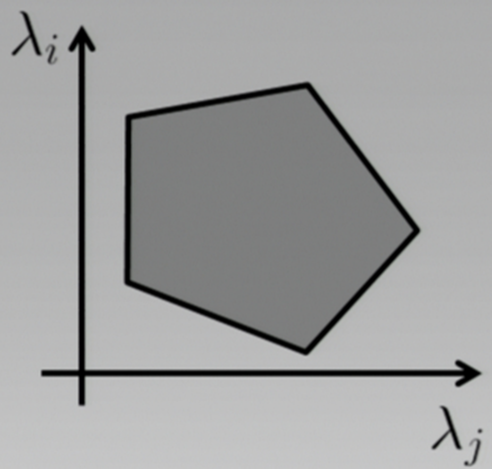
■ depends on N & d

N fermions & $\dim(\mathcal{H}_1) = d$

■ $\{\vec{\lambda}\} = \mathcal{P}_{N,d} \subset \mathbb{R}^d$

Polytope

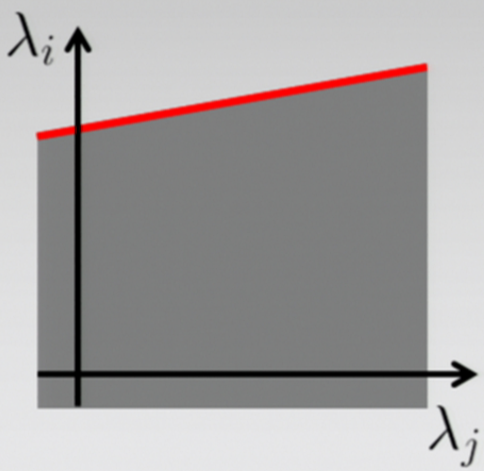
[A.Klyachko., CMP 282, p287-322, 2008]
[A.Klyachko, J.Phys 36, p72-86, 2006]



polytope

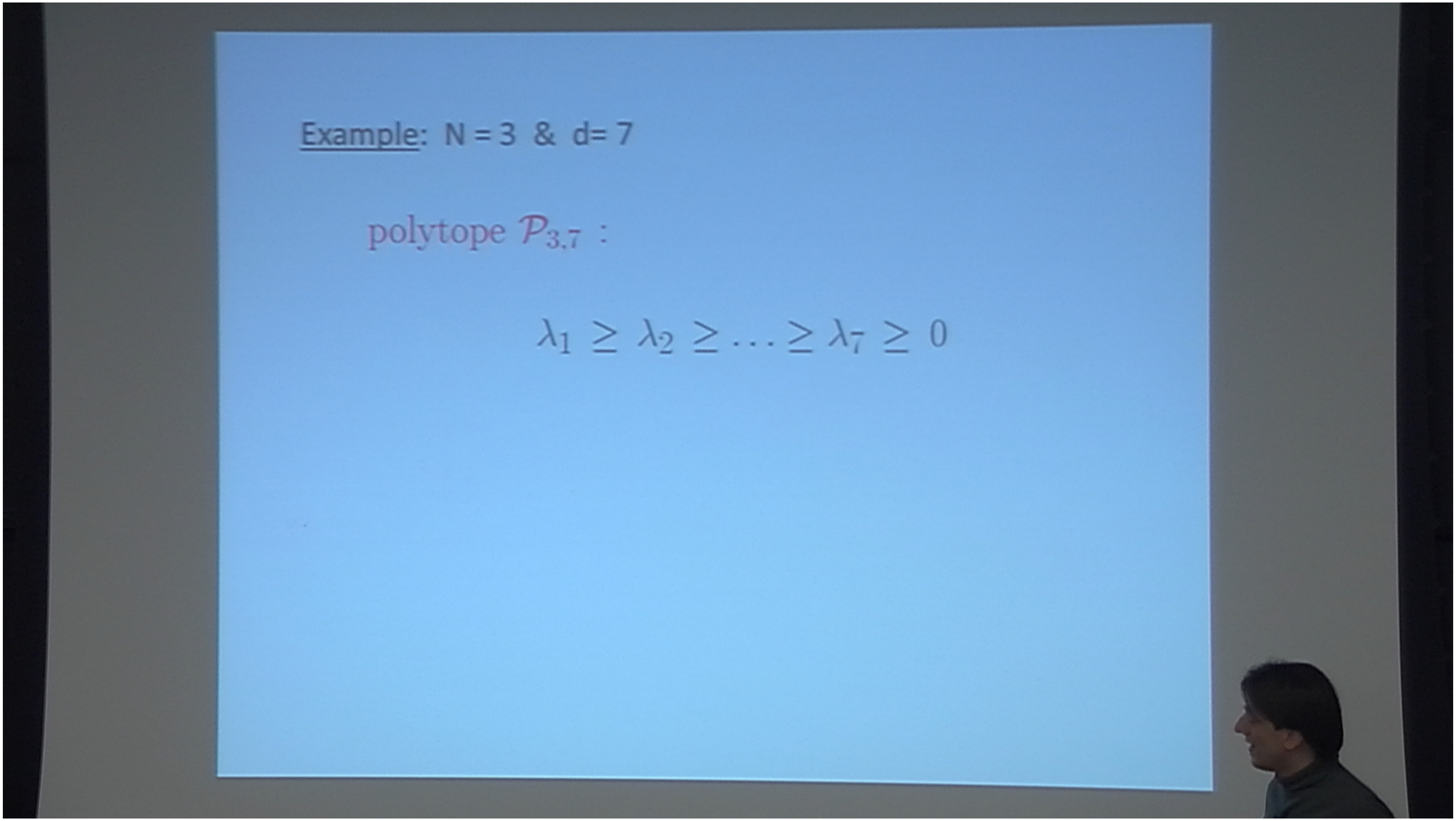
=

intersection of finitely many half spaces



facet: $c_1\,\lambda_1 + \ldots\, c_d\,\lambda_d = \kappa$

half space: $c_1\,\lambda_1 + \ldots\, c_d\,\lambda_d \leq \kappa$


Example: N = 3 & d= 7
polytope $\mathcal{P}_{3,7}$:
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$$
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\lambda_1 + \ldots + \lambda_7 = 3 \\
\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2 \\
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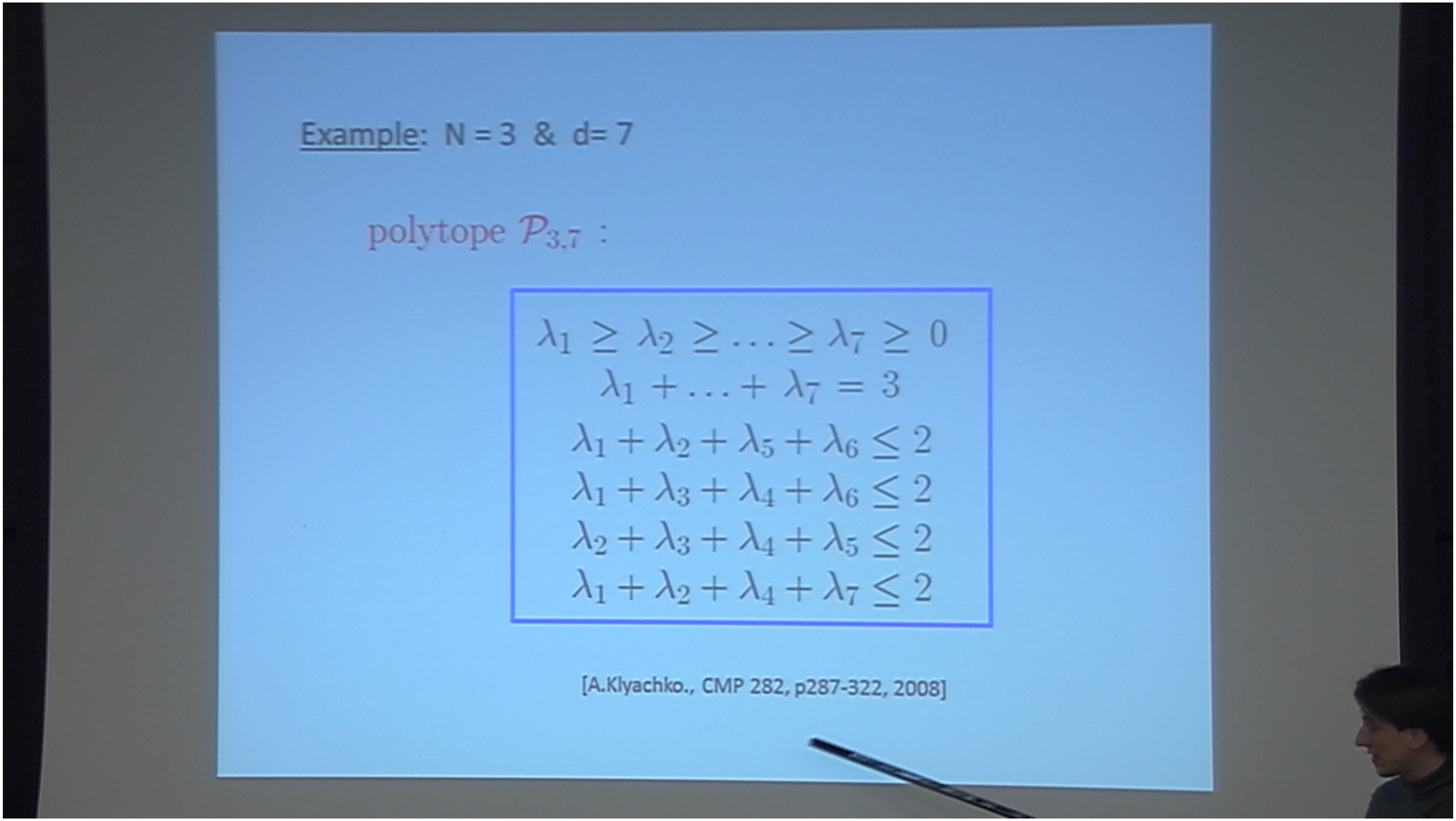
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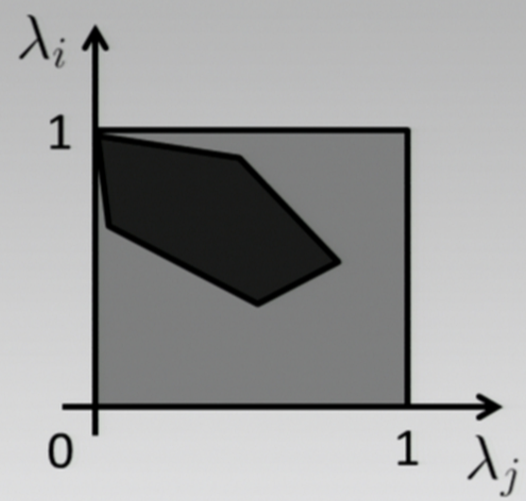
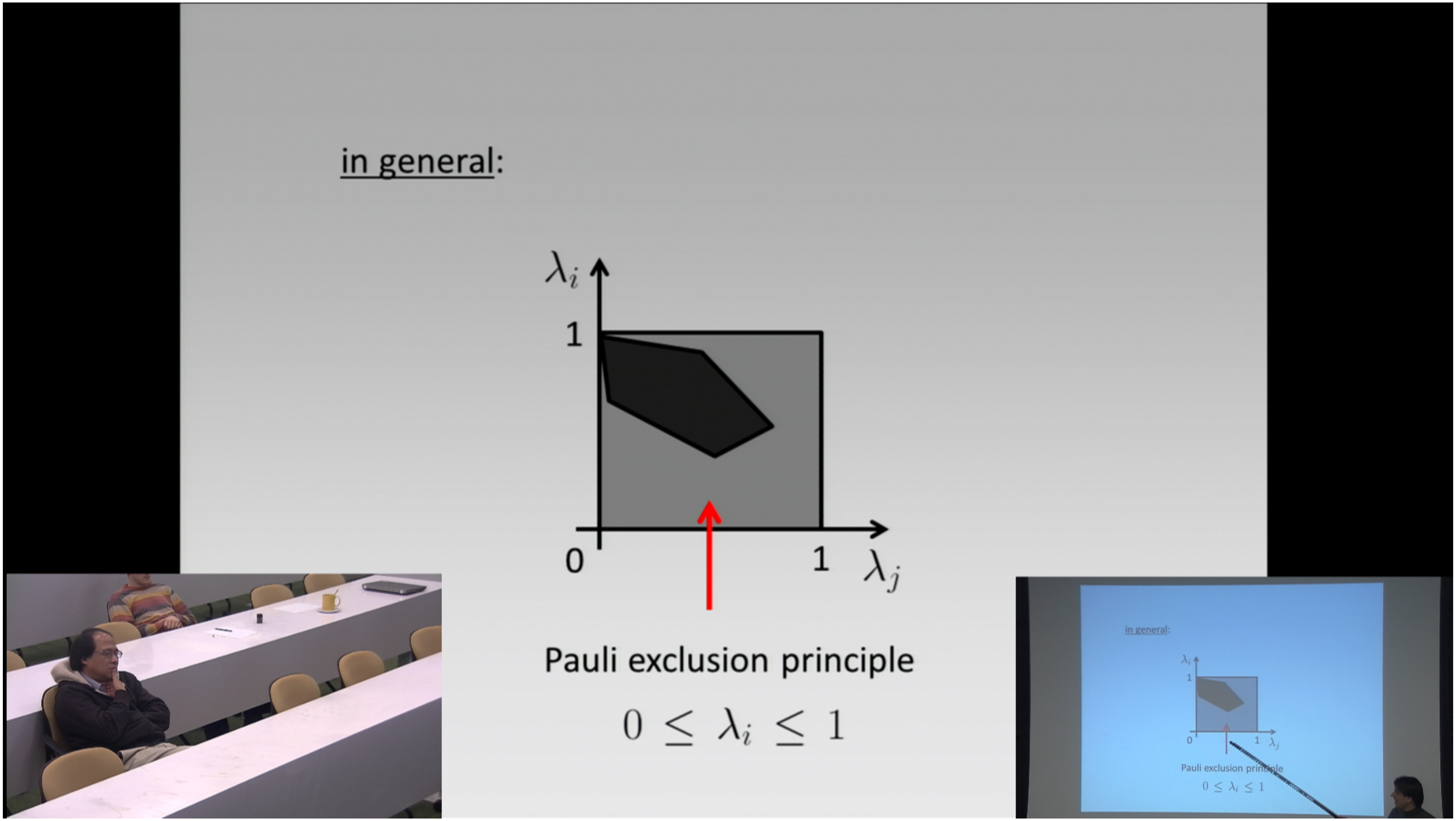
in general:




in general:
λ_i
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λ_j
Pauli exclusion principle
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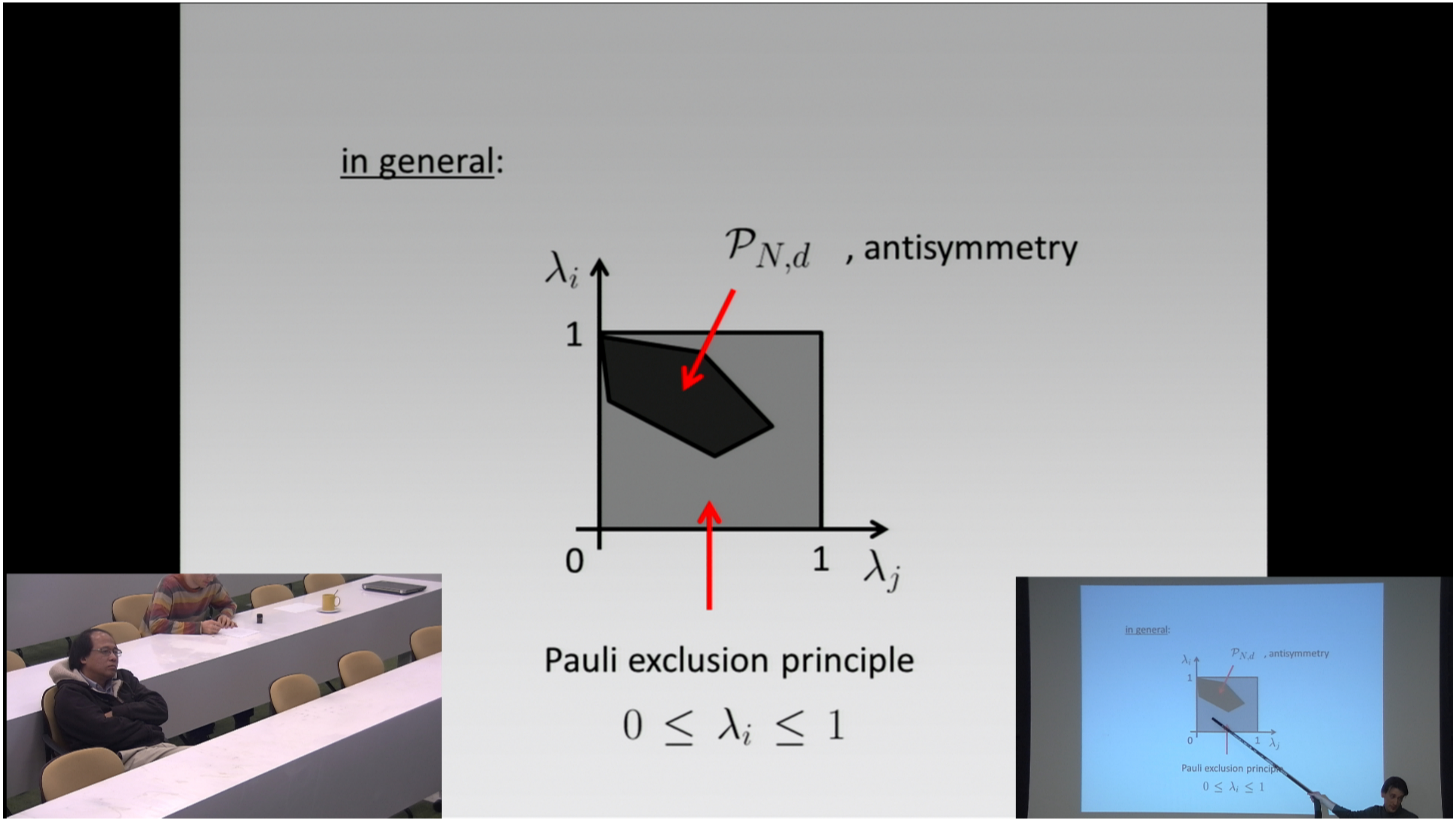
in general:
$\mathcal{P}_{N,d}$, antisymmetry
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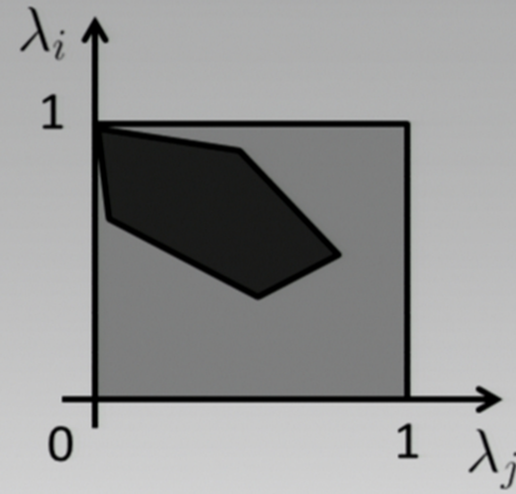
Position of relevant states

(e.g. ground state) ?



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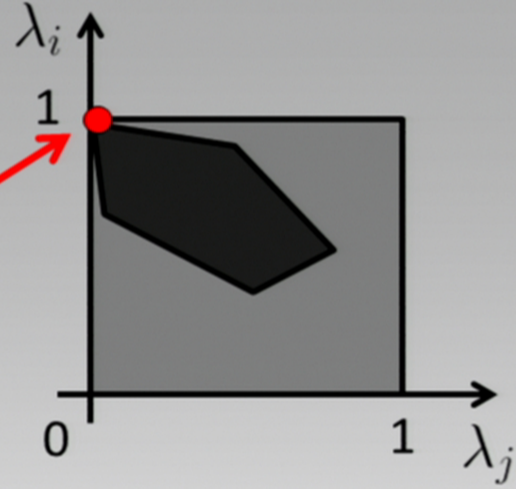
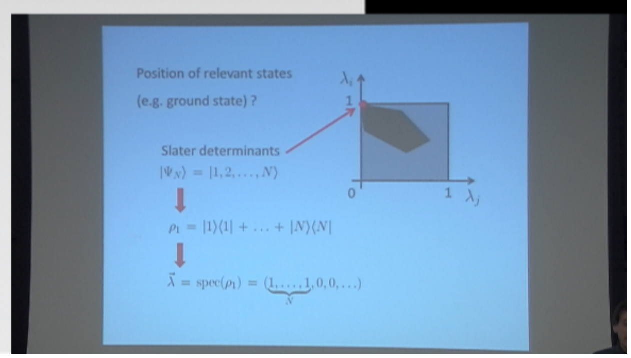


Slater determinants

$$|\Psi_N\rangle = |1, 2, \ldots, N\rangle$$

$$\rho_1 = |1\rangle\langle 1| + \ldots + |N\rangle\langle N|$$

$$\vec{\lambda} = \text{spec}(\rho_1) = (\underbrace{1, \ldots, 1}_{N}, 0, 0, \ldots)$$



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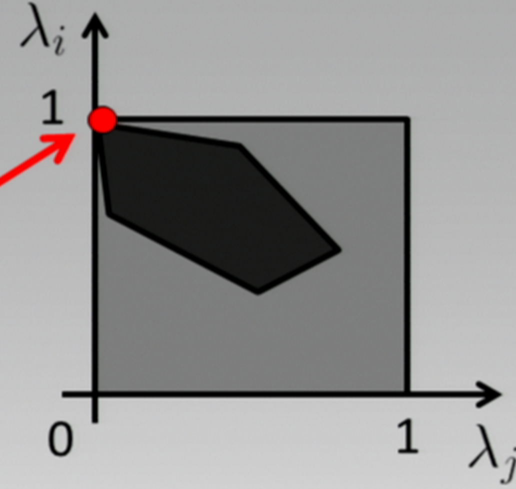

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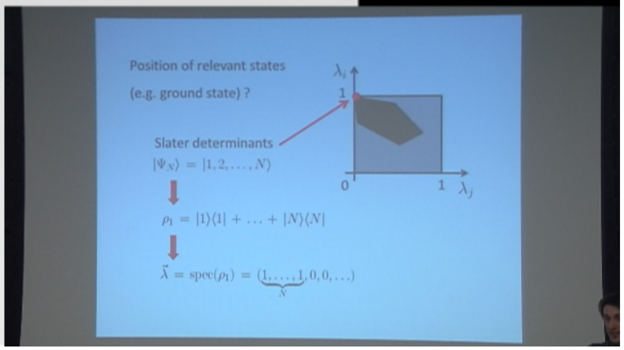

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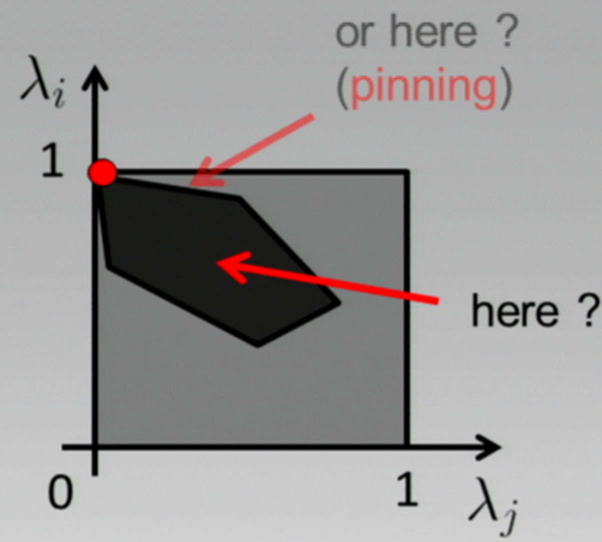

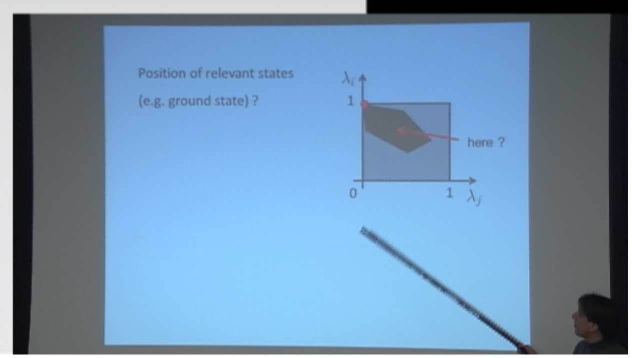

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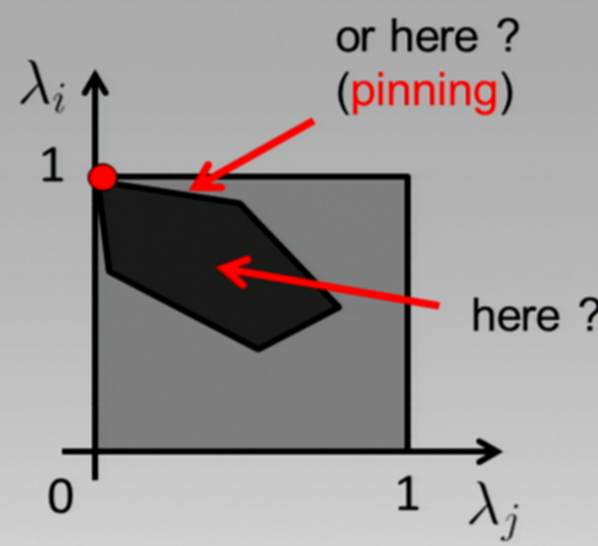
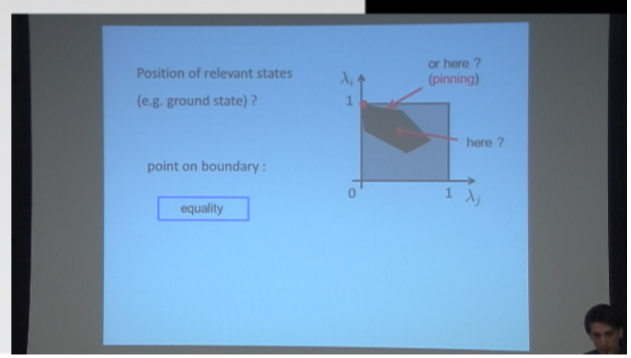


point on boundary :

equality



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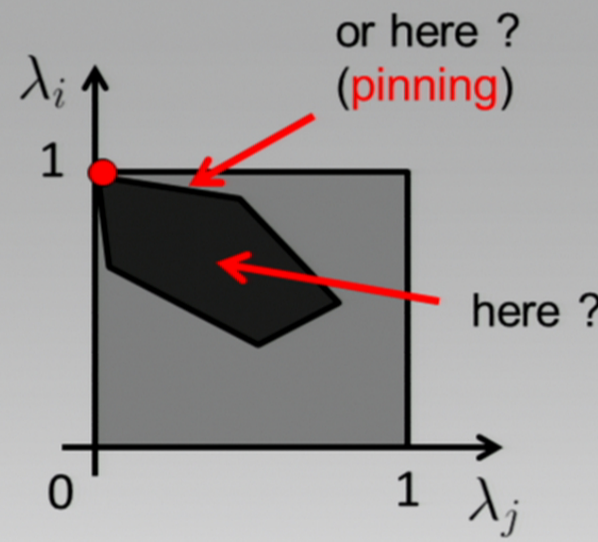

point on boundary :

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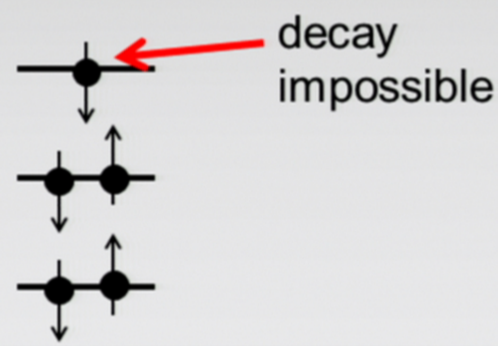
kinematical constraints

generalization of:



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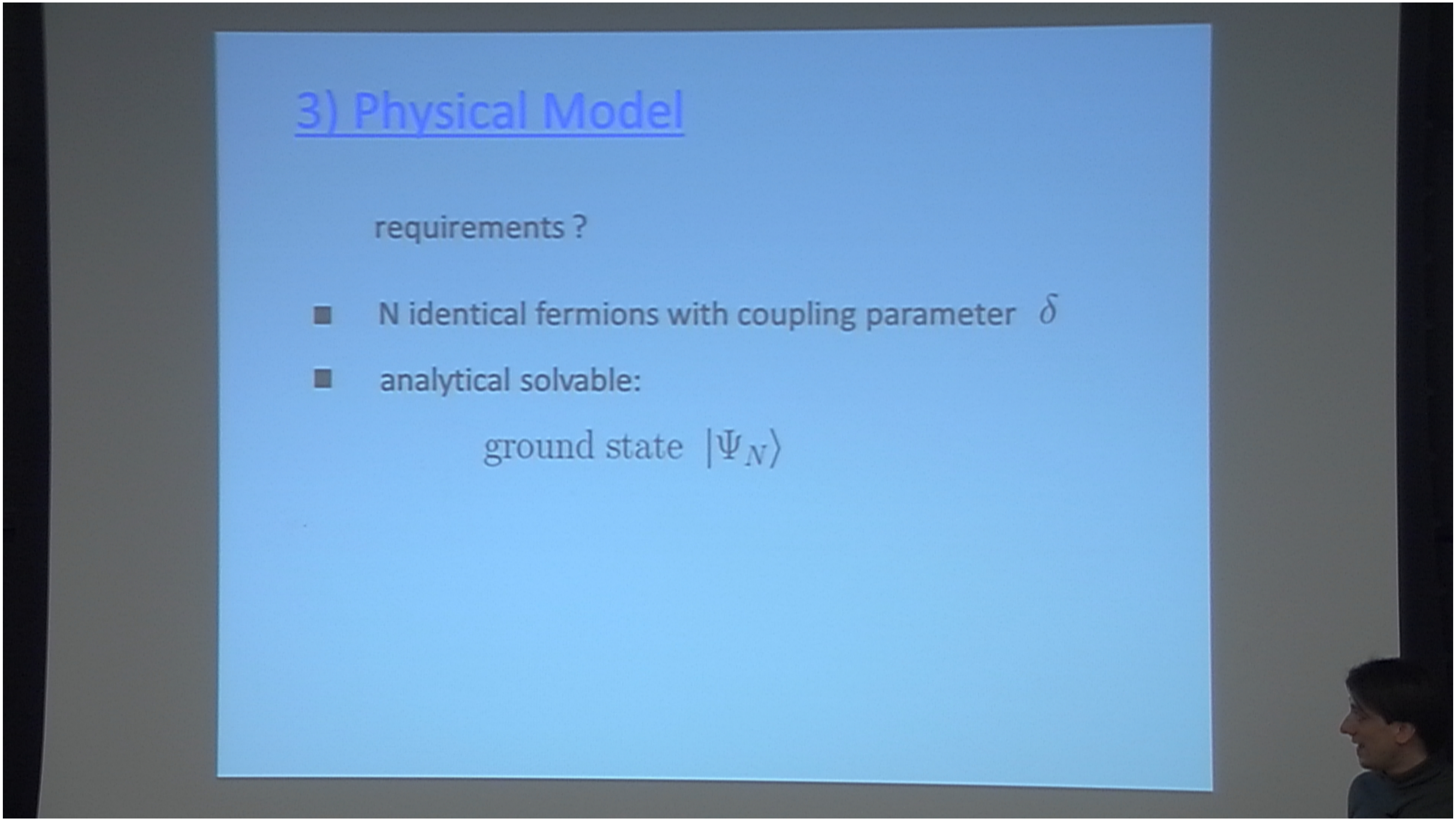
requirements ?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requirements ?

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$$\downarrow$$

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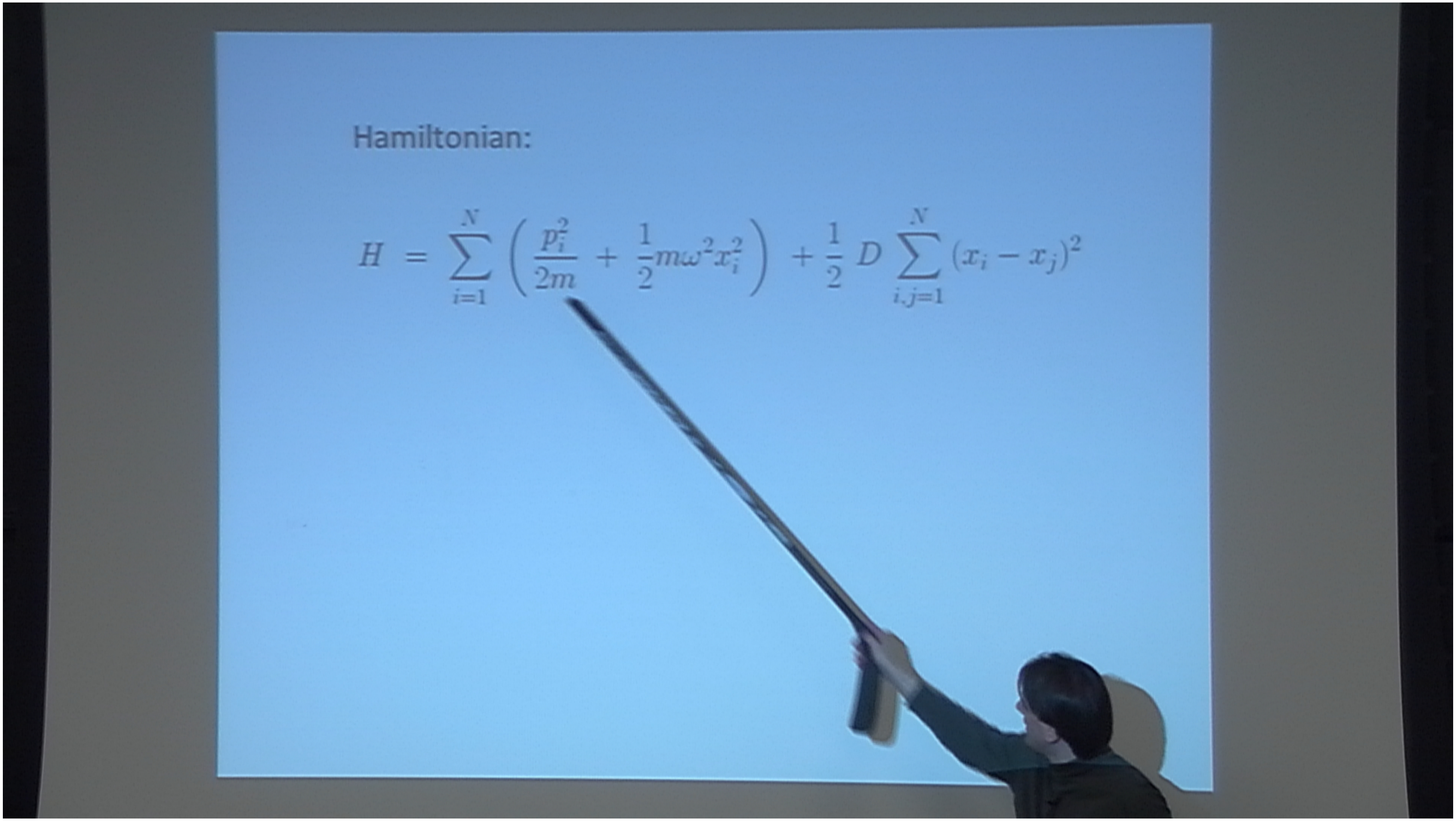
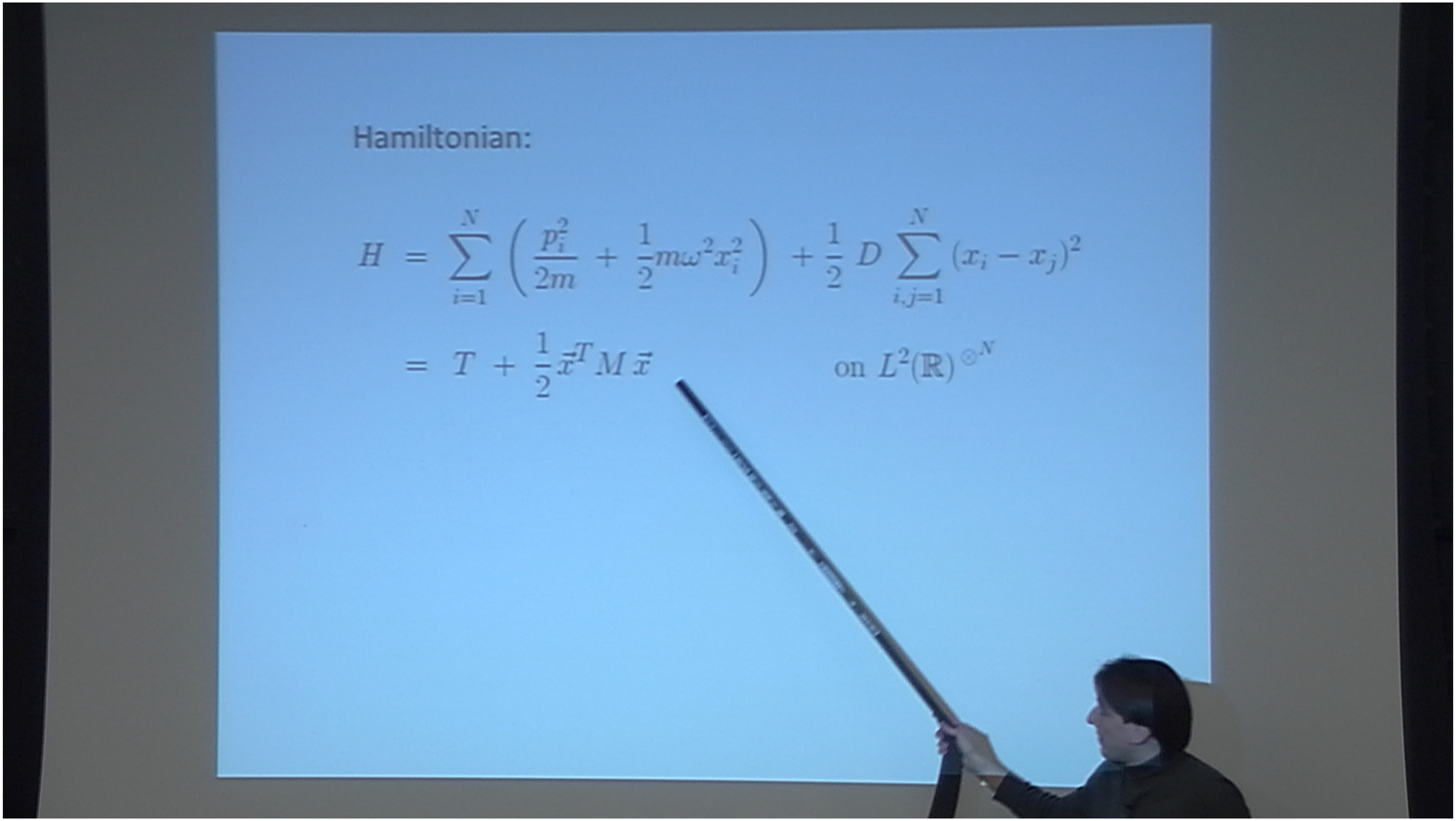
$$\vec{\lambda} = \mathrm{spec}(\rho_1)$$


Hamiltonian:
$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 x_i^2 \right) + \frac{1}{2} D \sum_{i,j=1}^{N} (x_i - x_j)^2$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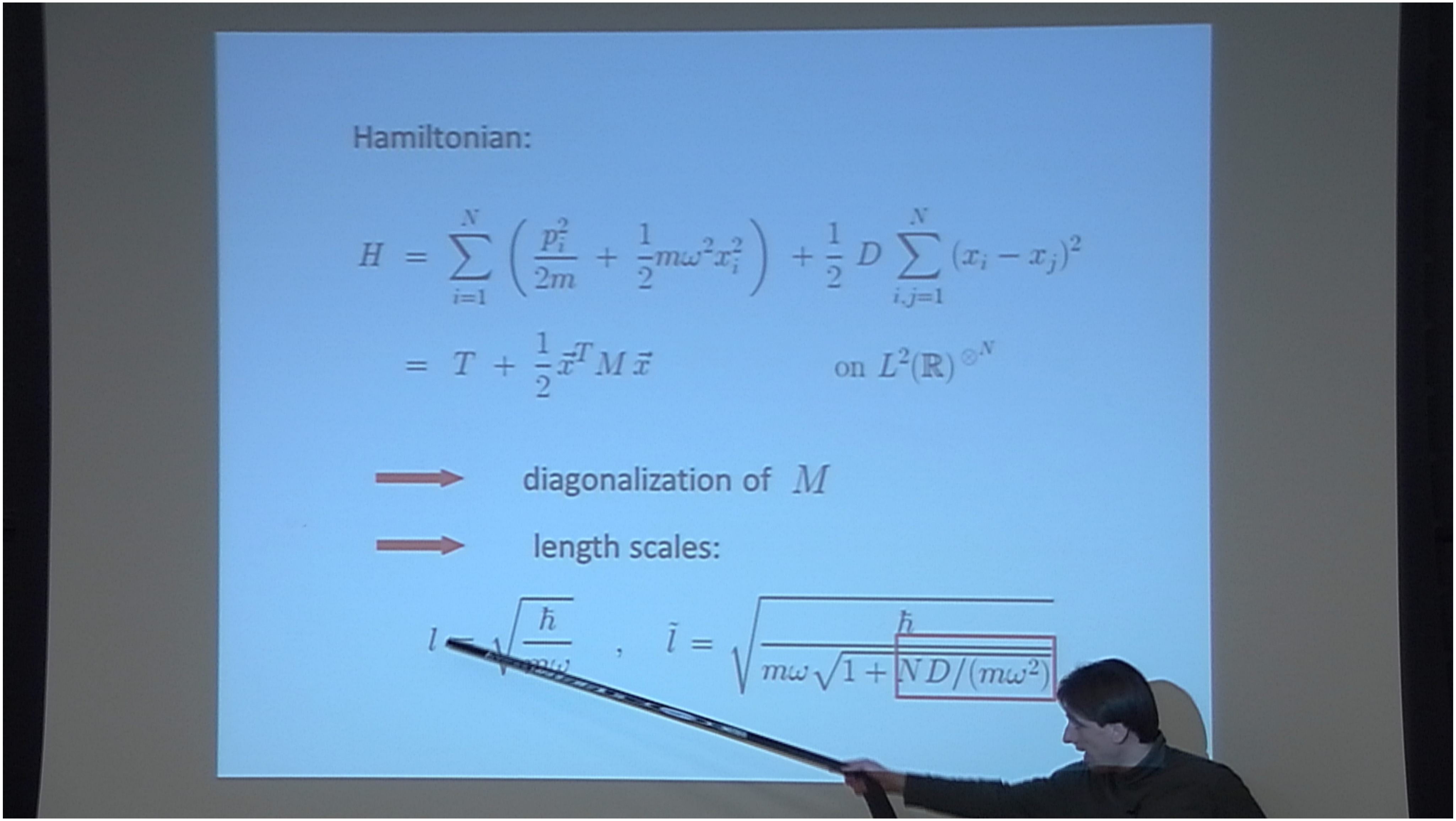
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Now: Fermions

→ restrict to $\wedge^N[L^2(\mathbb{R})] \leq L^2(\mathbb{R})^{\otimes^N}$

ground state: [Z.Wang et al., arXiv 1108.1607, 2011]

$$\Psi_N(\vec{x}) = \mathcal{N}\left(\prod_{1\leq i<j\leq N}(x_i - x_j)\right)\cdot\exp\left[-\frac{1}{2N}\left(\frac{1}{l^2}-\frac{1}{\tilde{l}^2}\right)(x_1+\ldots+x_N)^2 - \frac{1}{2}\frac{1}{\tilde{l}^2}\vec{x}^2\right]$$

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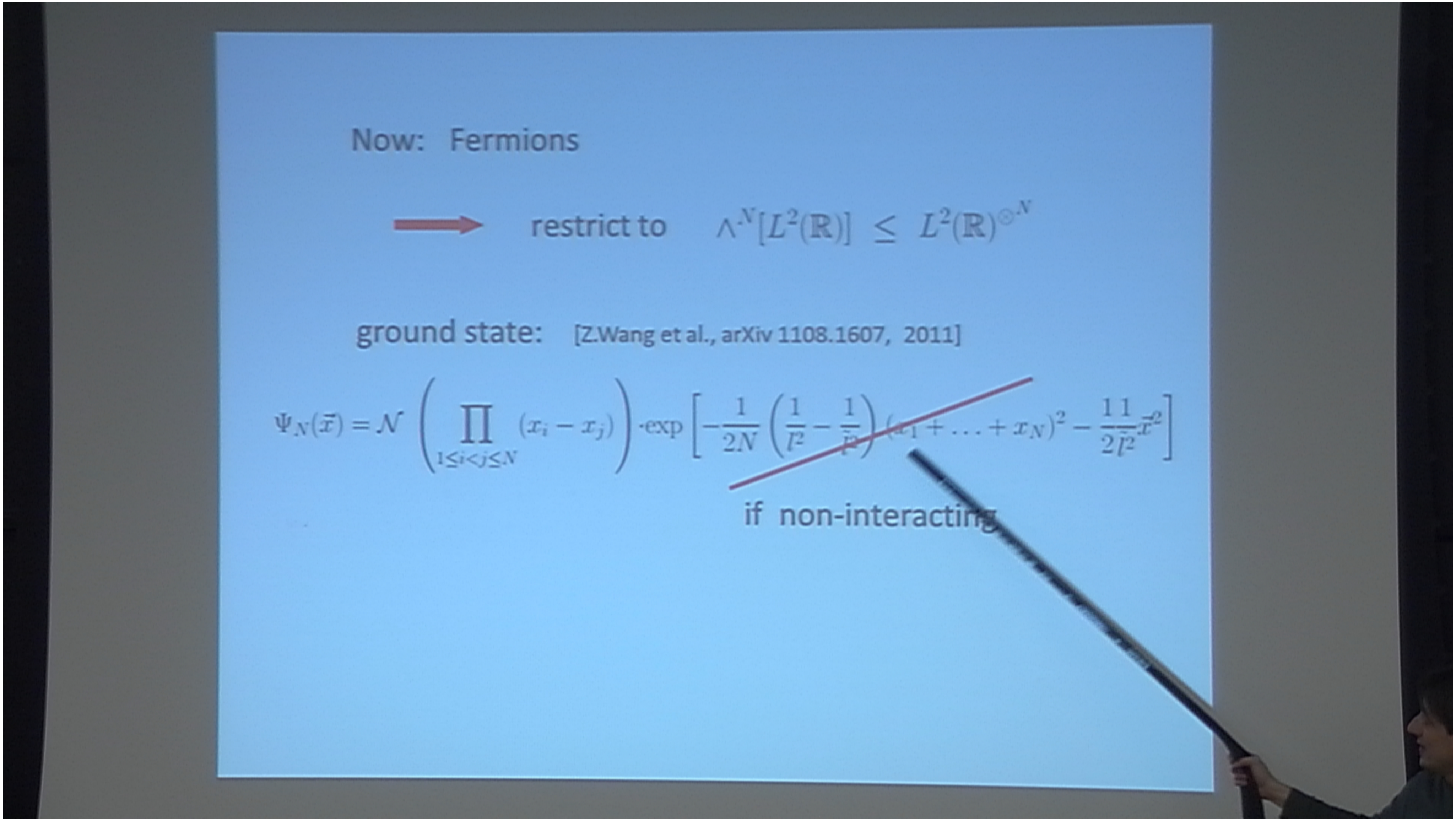
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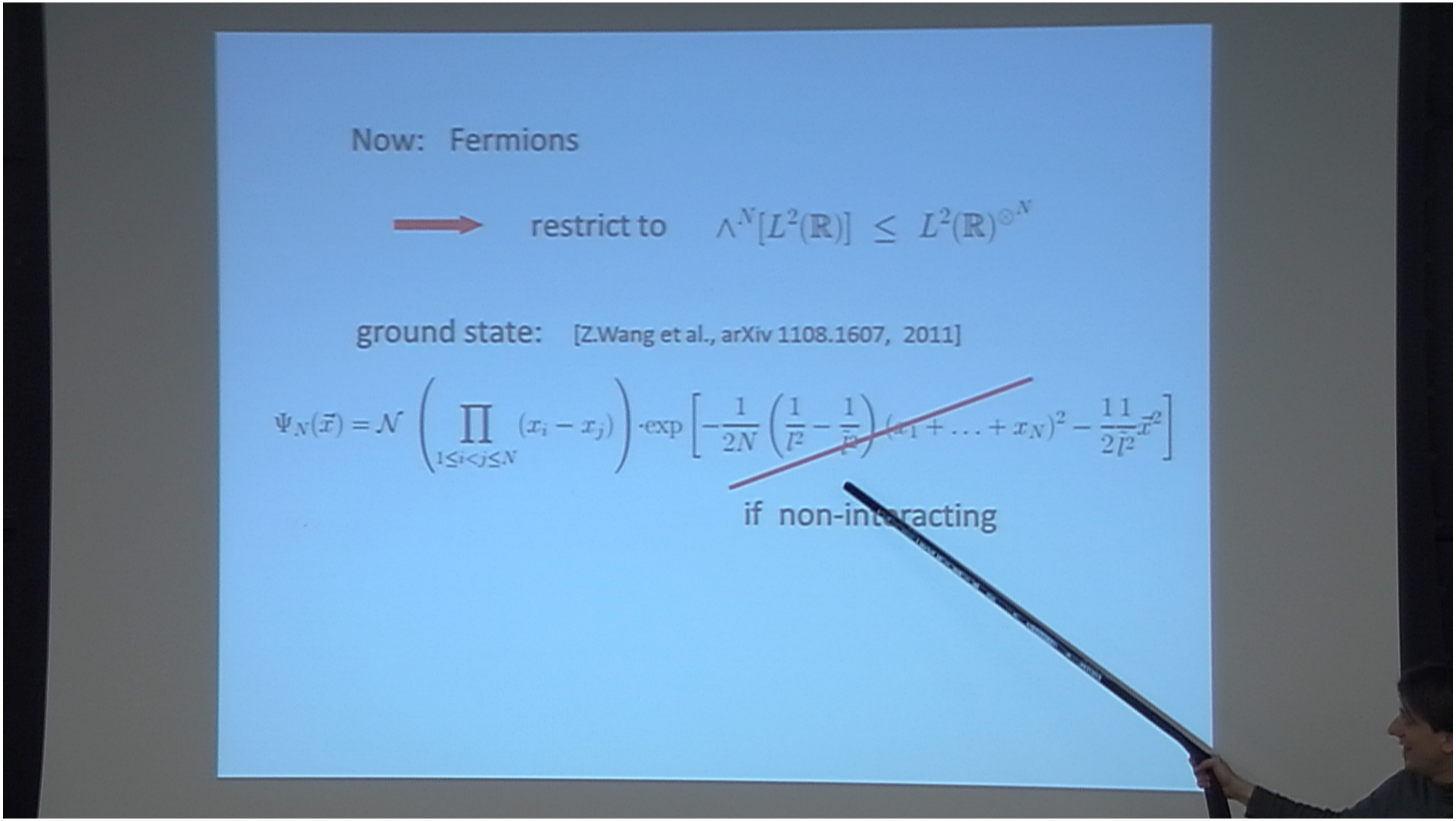
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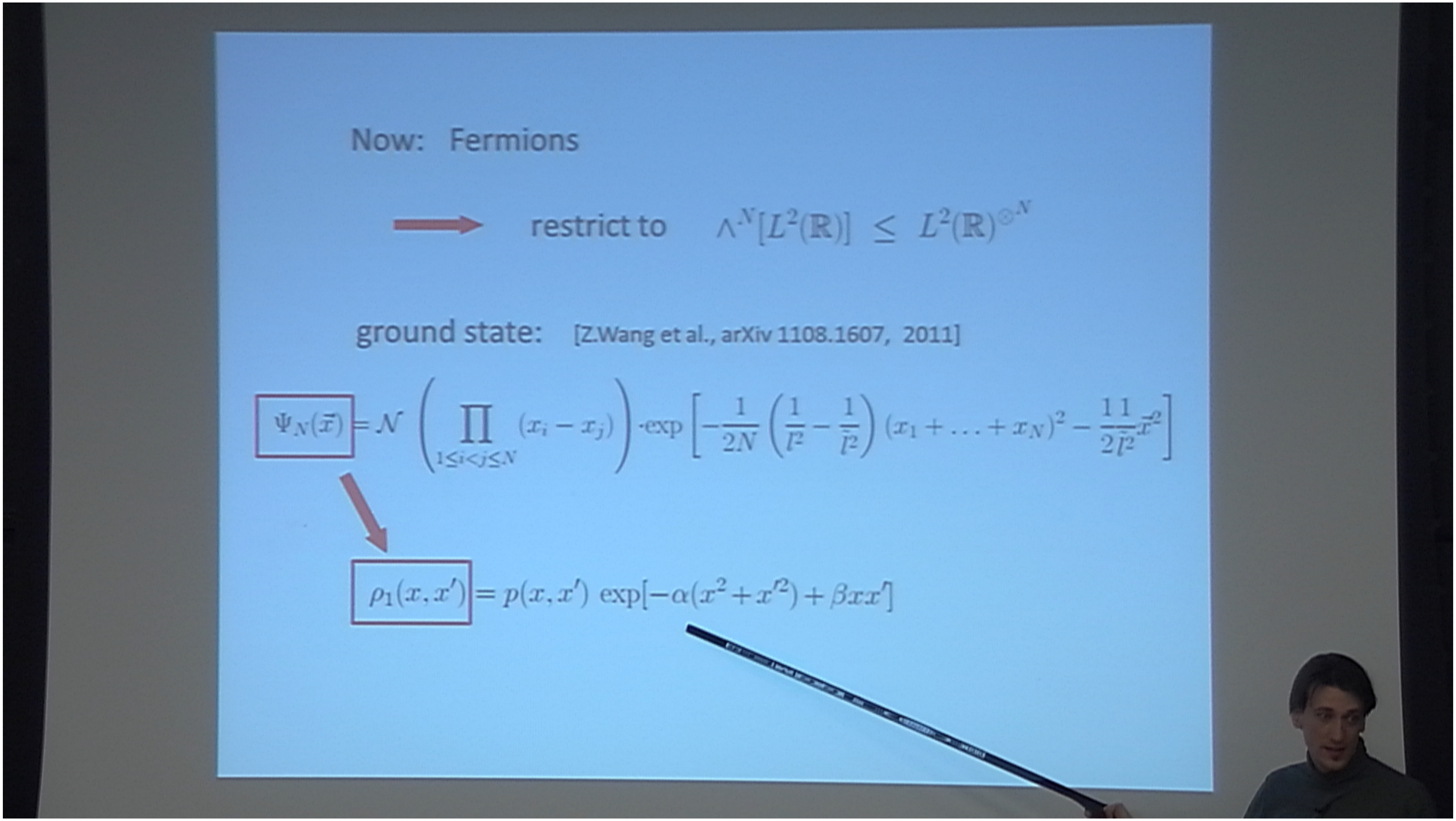
↓

$$\rho_1(x, x') = p(x, x') \; \exp[-\alpha(x^2 + x'^2) + \beta x x']$$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$\Psi_N(\vec{x}) = \mathcal{N} \left(\prod_{1 \leq i < j \leq N} (x_i - x_j) \right) \cdot \exp \left[-\frac{1}{2N} \left(\frac{1}{l^2} - \frac{1}{\tilde{l}^2} \right) (x_1 + \ldots + x_N)^2 - \frac{1}{2} \frac{1}{\tilde{l}^2} \vec{x}^2 \right]$
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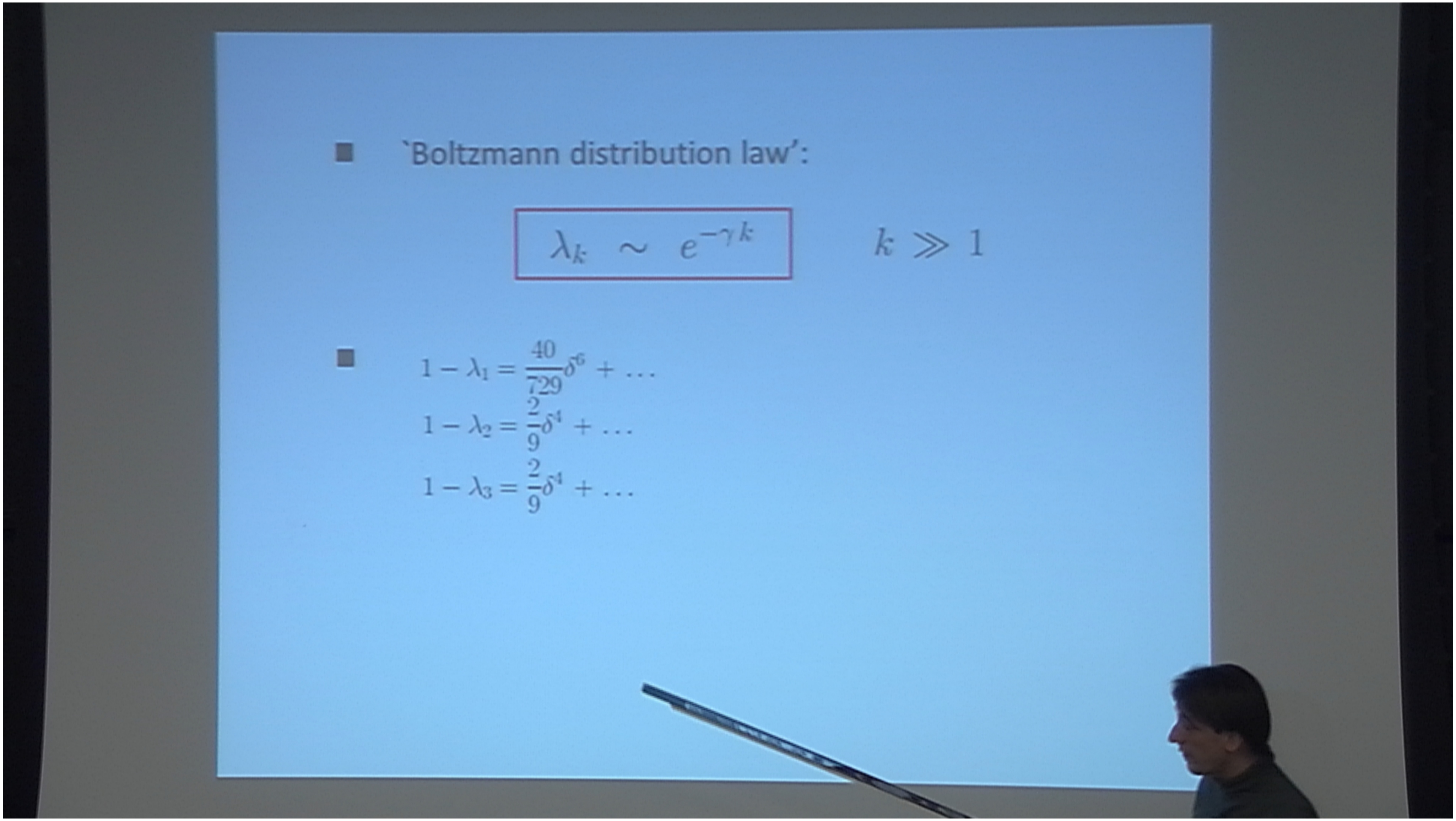
⟹ $\vec{\lambda}(\delta) \;=\; \vec{\lambda}(-\delta)$

⟹ weak-interacting $\;\widehat{=}\;$ $|\delta| \ll 1$


`Boltzmann distribution law':
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$1-\lambda_1 = \frac{40}{729}\delta^6 + \dots$
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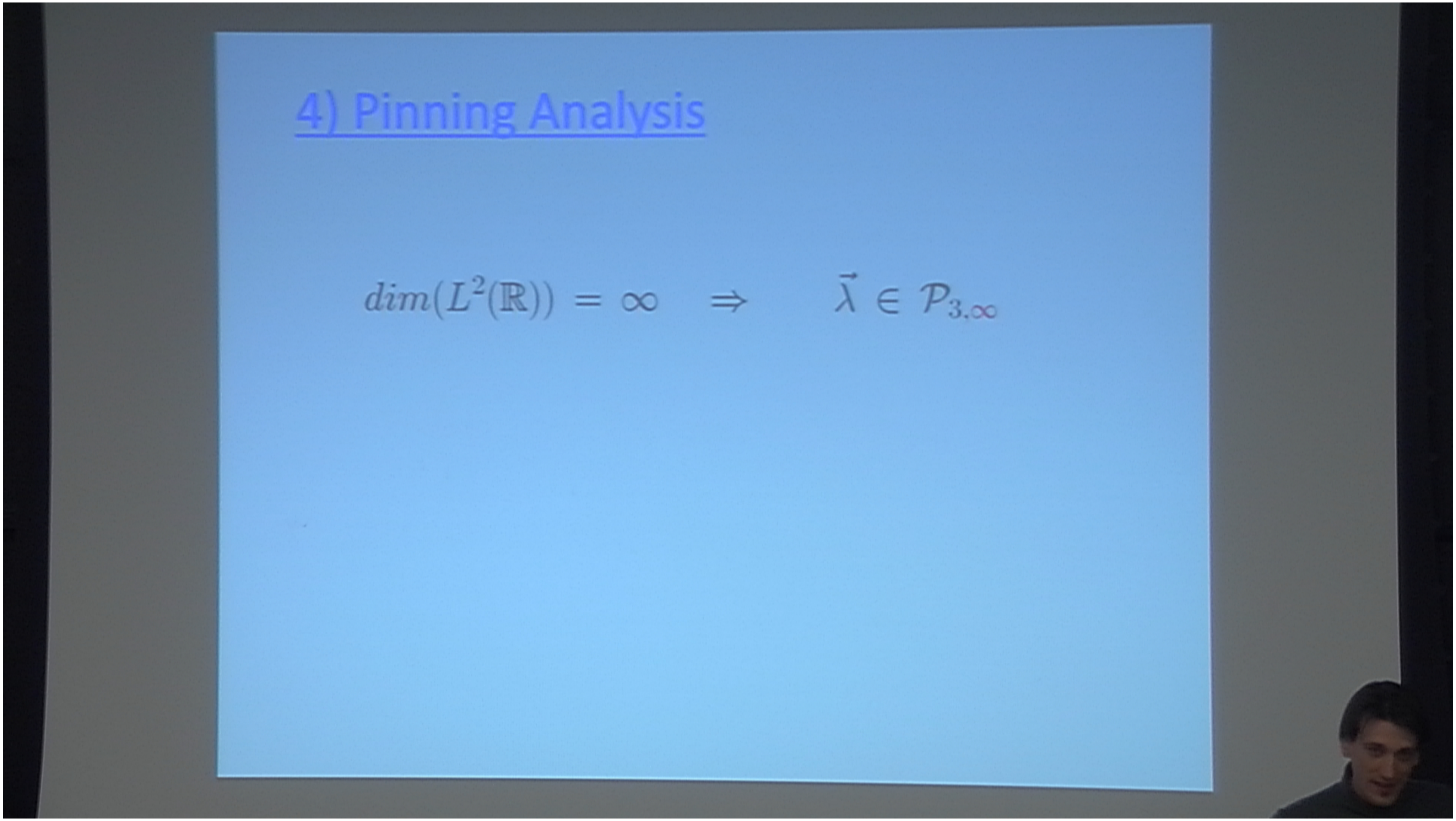
$$\lambda_4 = \frac{2}{9}\delta^4 + \dots \qquad \lambda_8 = O(\delta^{10})$$

- hierarchy:

$$\lambda_k \;=\; c_k\,\delta^{2k-6} \;+\; O(\delta^{2k-4}) \qquad ,\forall k \geq 5$$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$$\Leftrightarrow$$

(quasi-)pinning of $\mathcal{P}_{3,\infty}$ - constraint mod $O(\lambda_{d+1})$

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[Borland&Dennis, J.Phys. B, 5,1, 1972]
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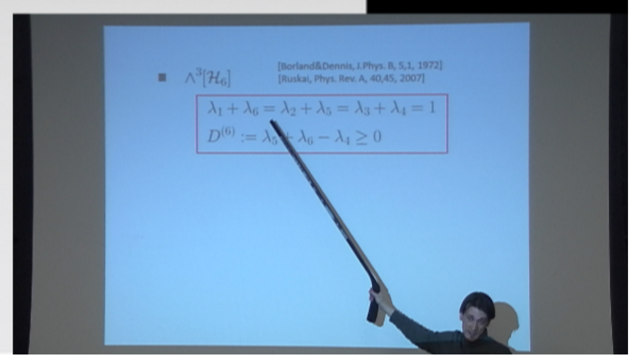

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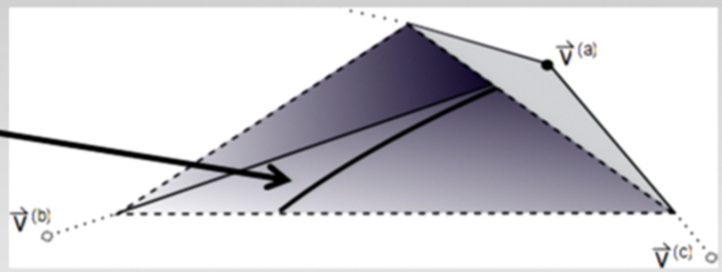

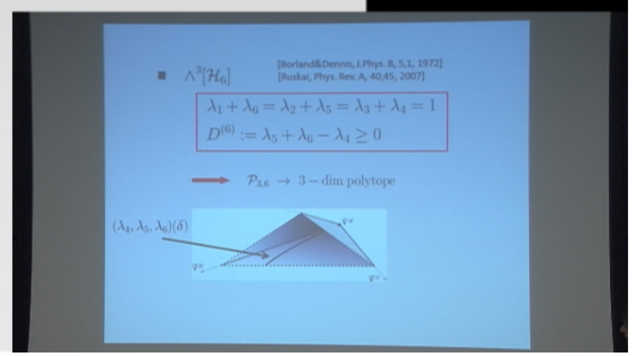

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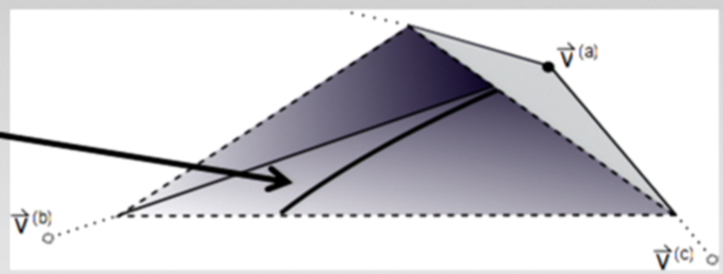

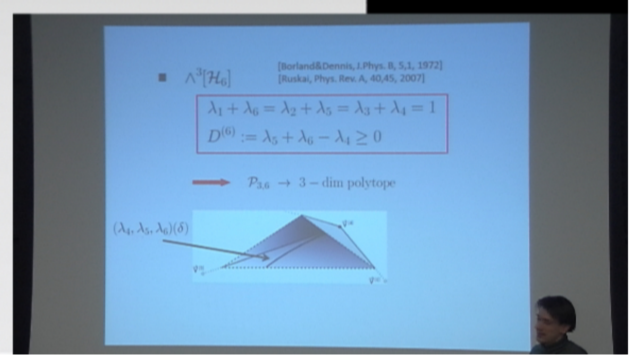

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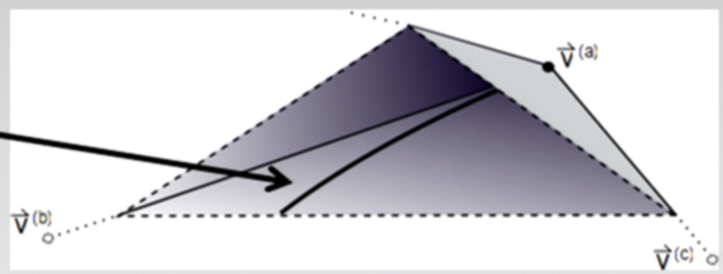
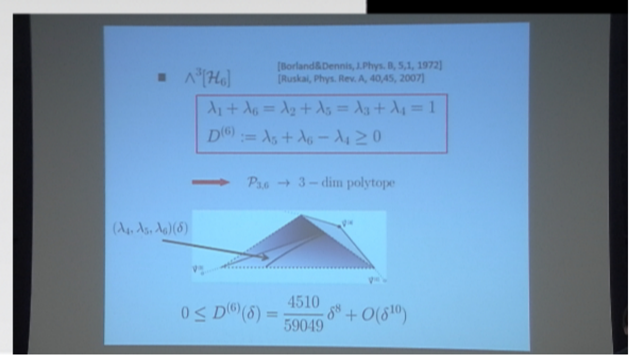


$$0 \leq D^{(6)}(\delta) = \frac{4510}{59049}\delta^8 + O(\delta^{10})$$



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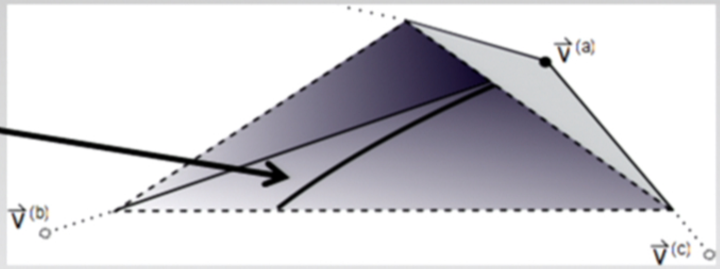

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lower bound on pinning order

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quasi-pinning

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saturated by $\vec{\lambda}_0$:

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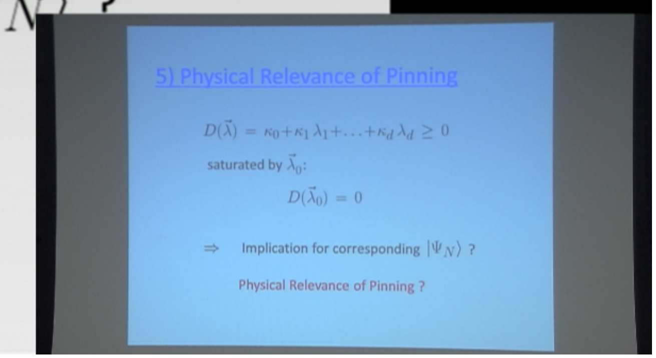
$\Rightarrow$ Implication for corresponding $|\Psi_N\rangle$?

Physical Relevance of Pinning ?



generalization of:

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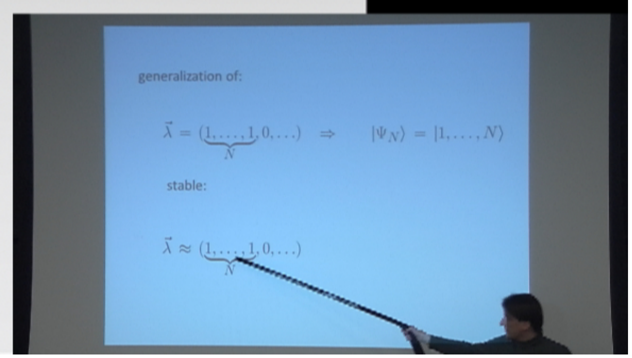

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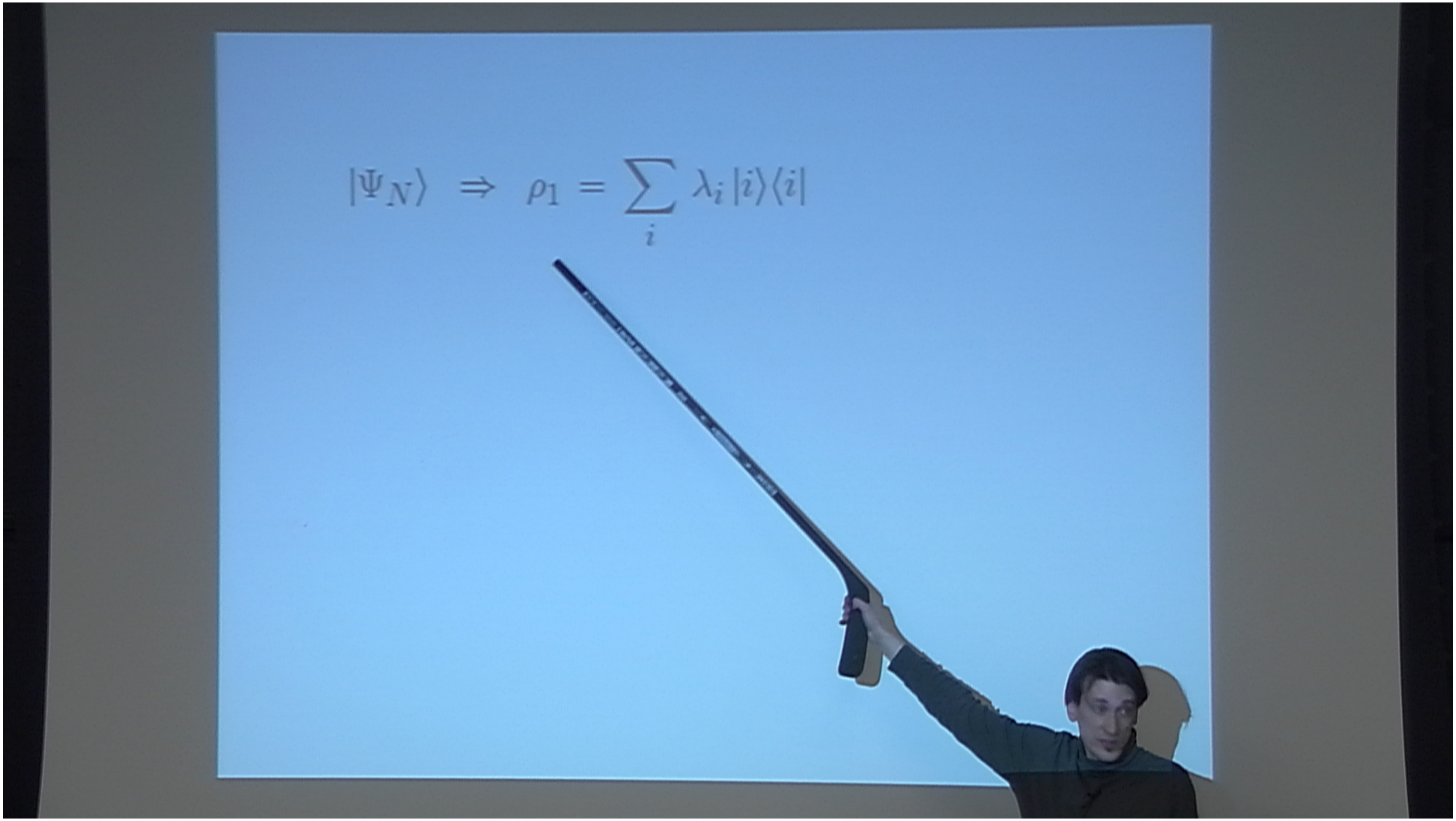
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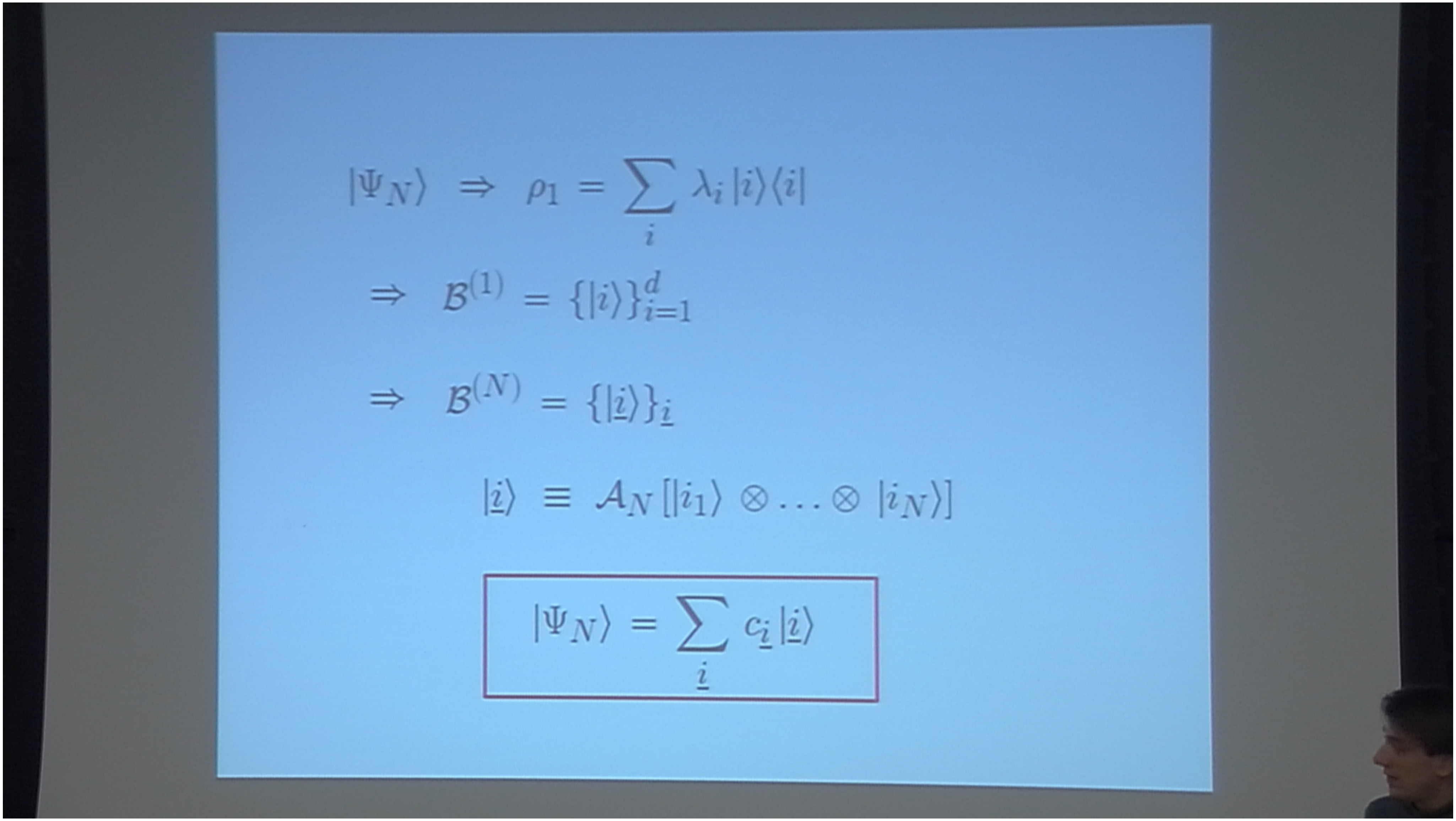
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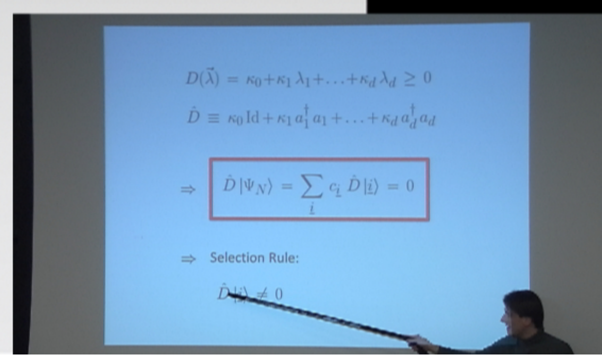

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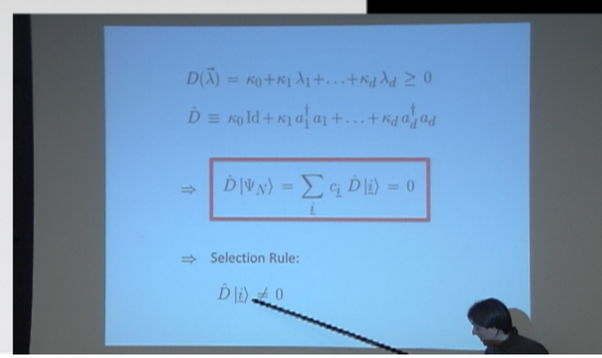
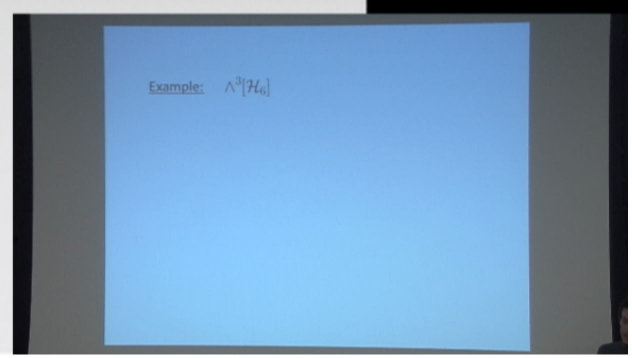


Example: $\wedge^3[\mathcal{H}_6]$



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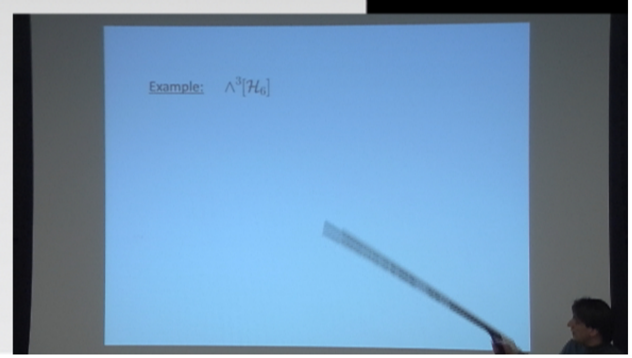

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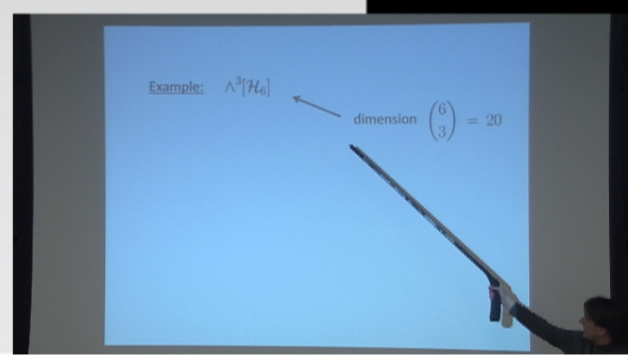

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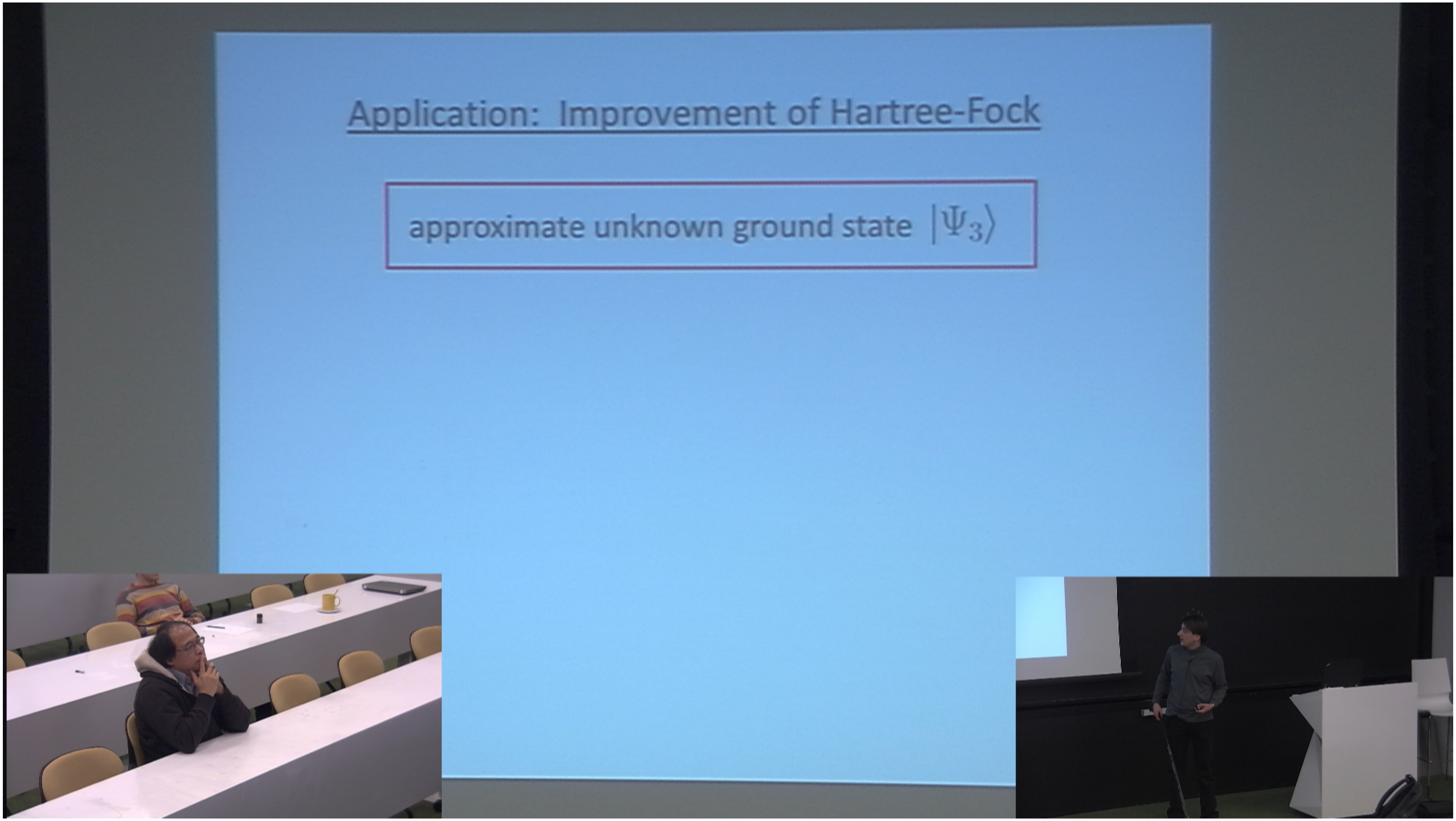
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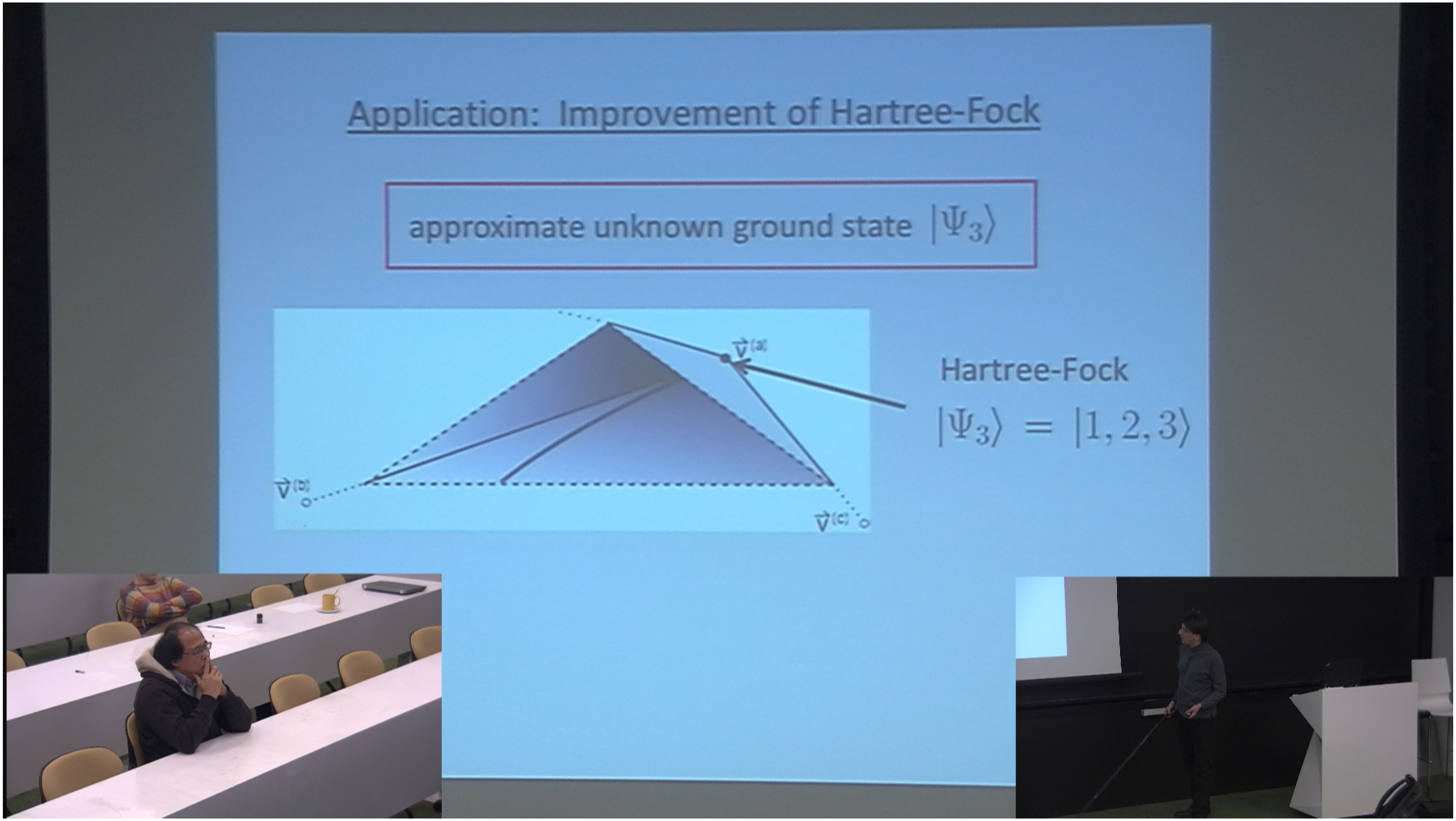
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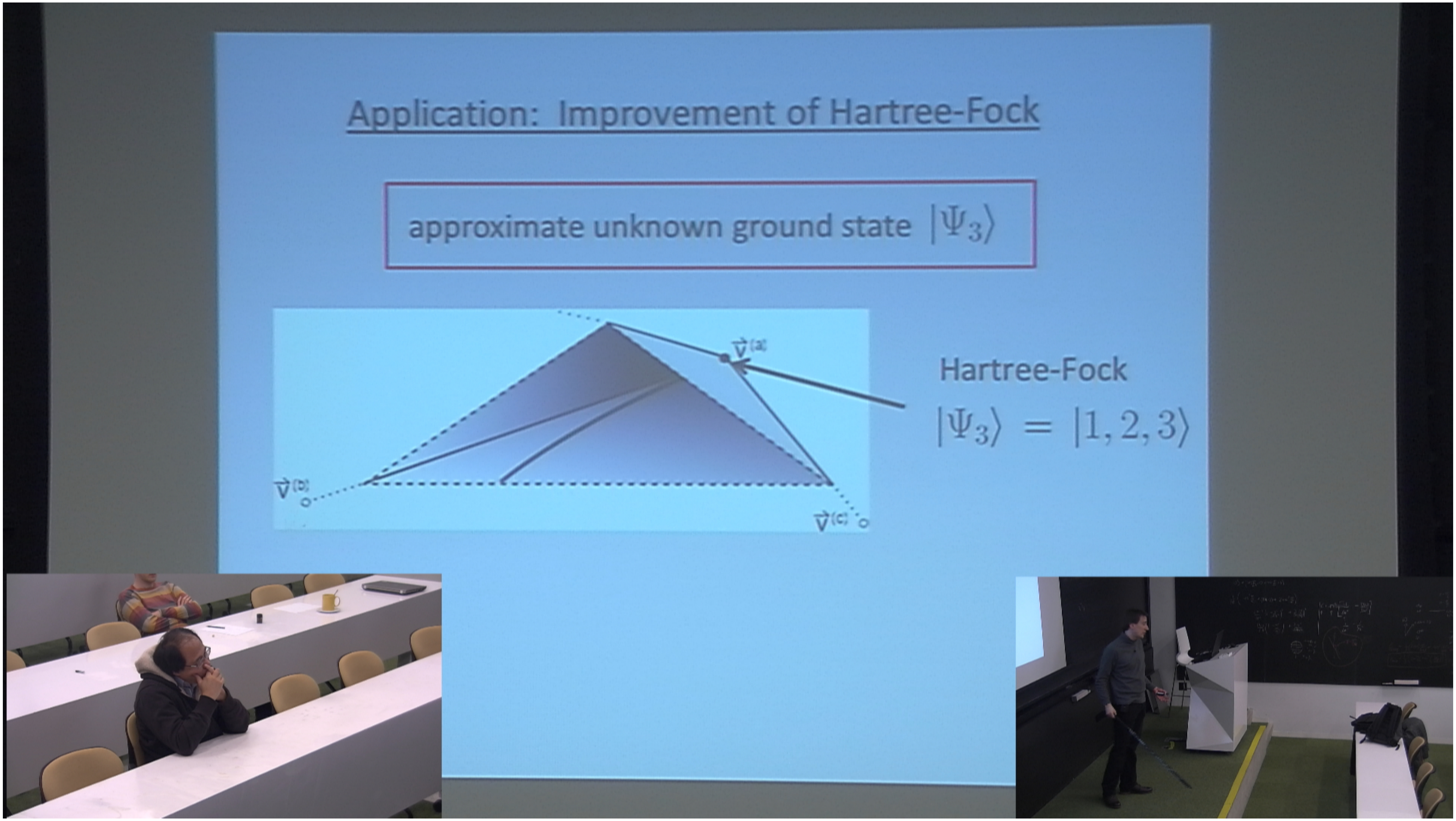
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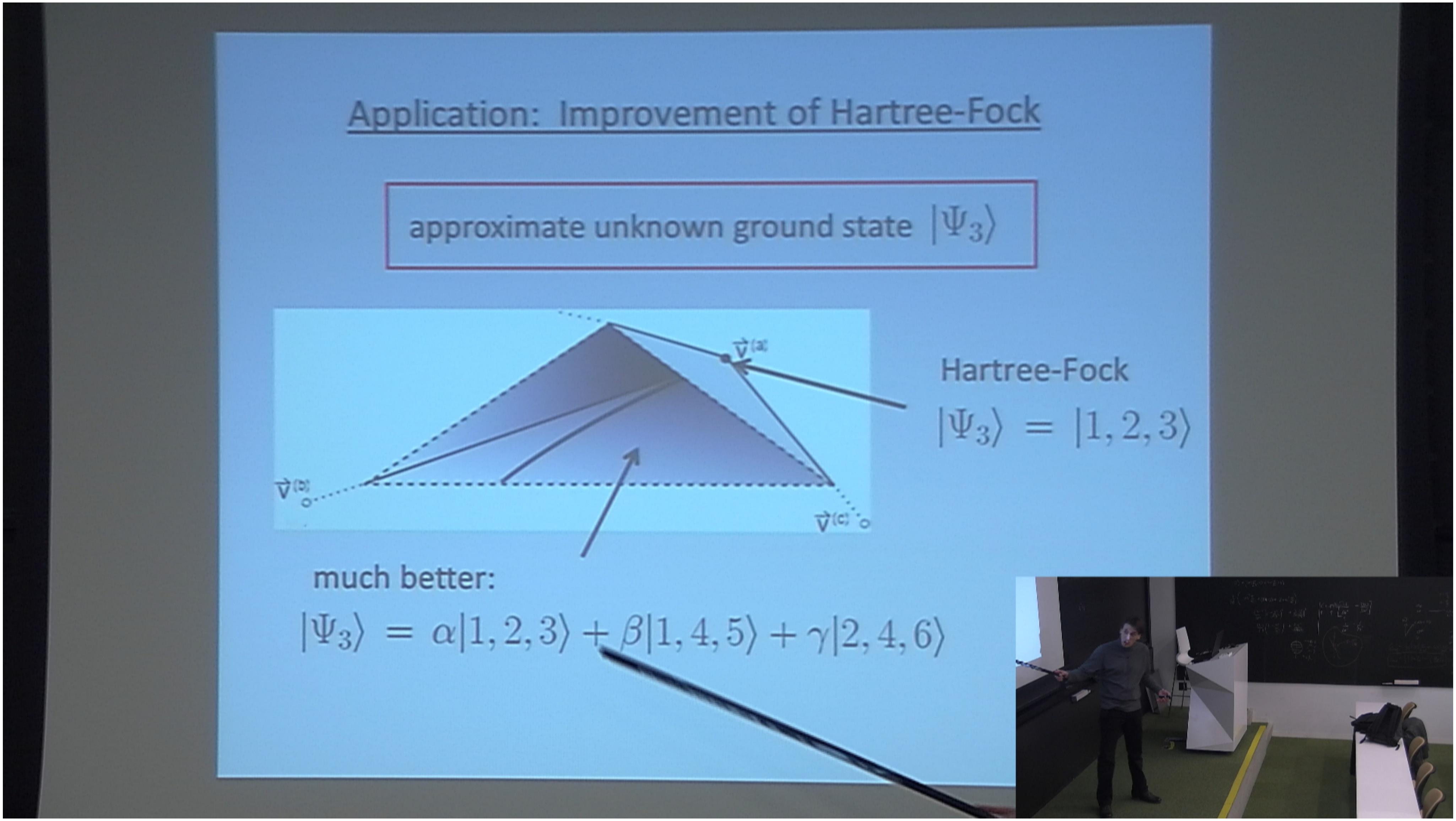
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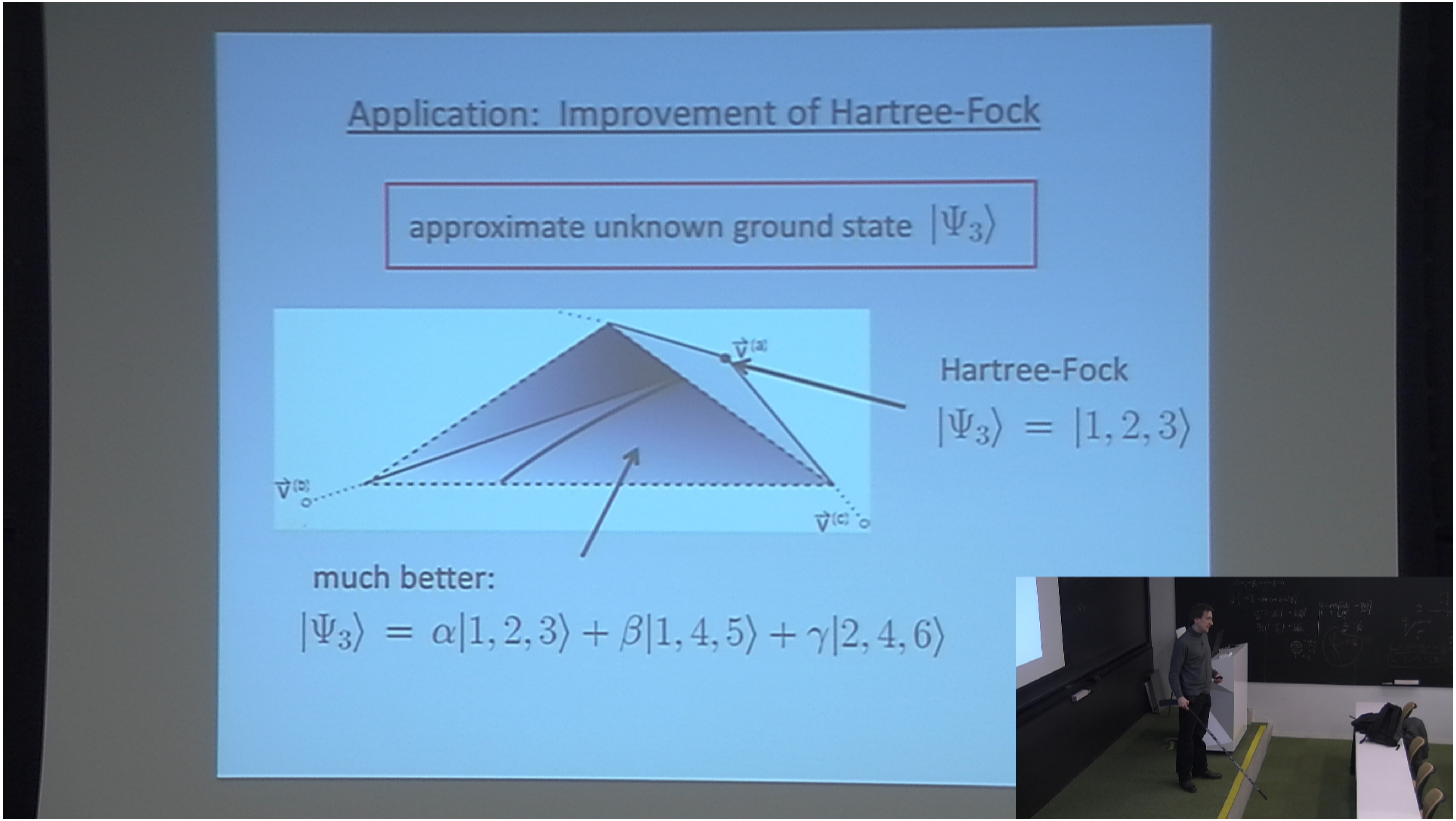
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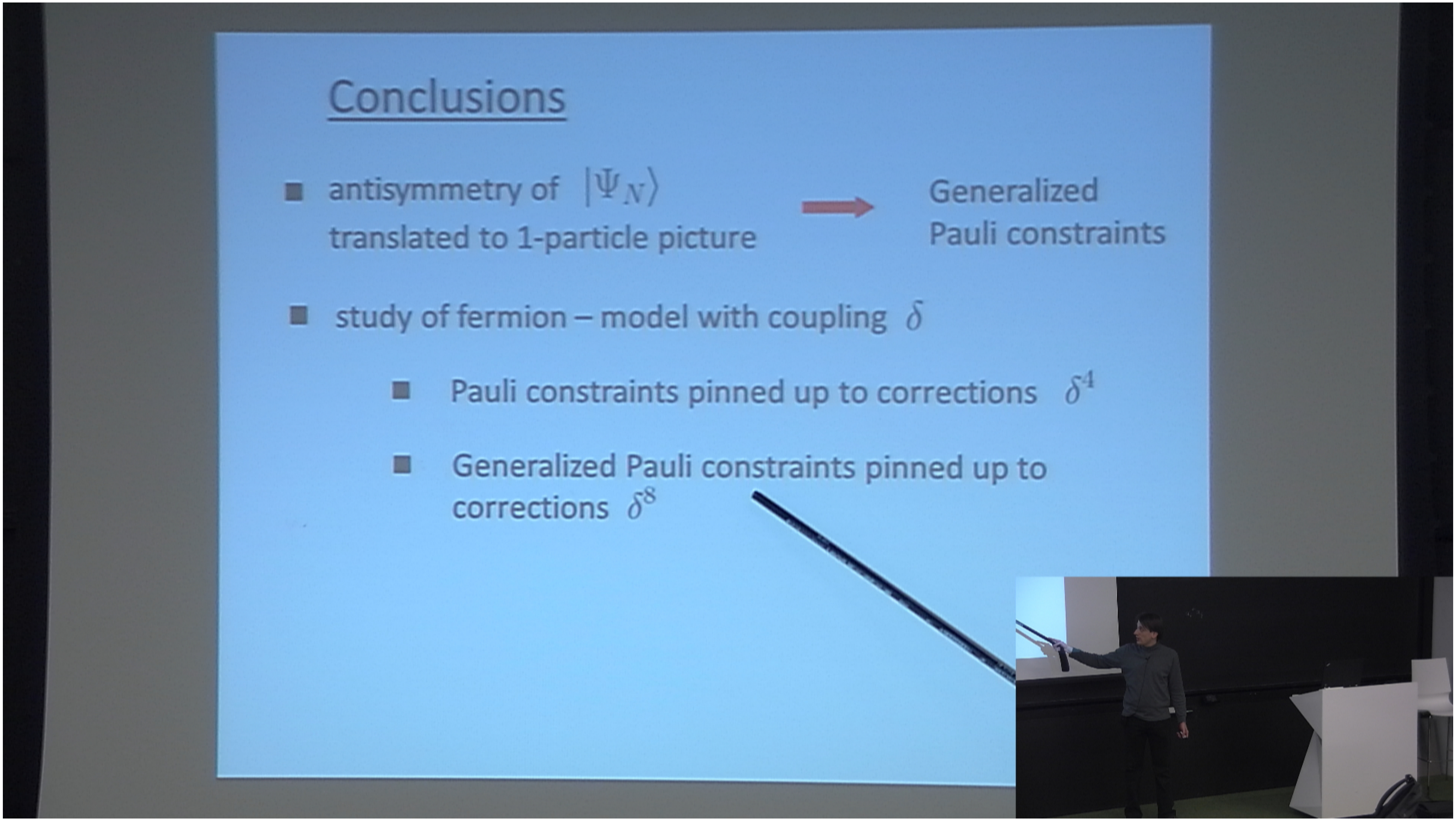
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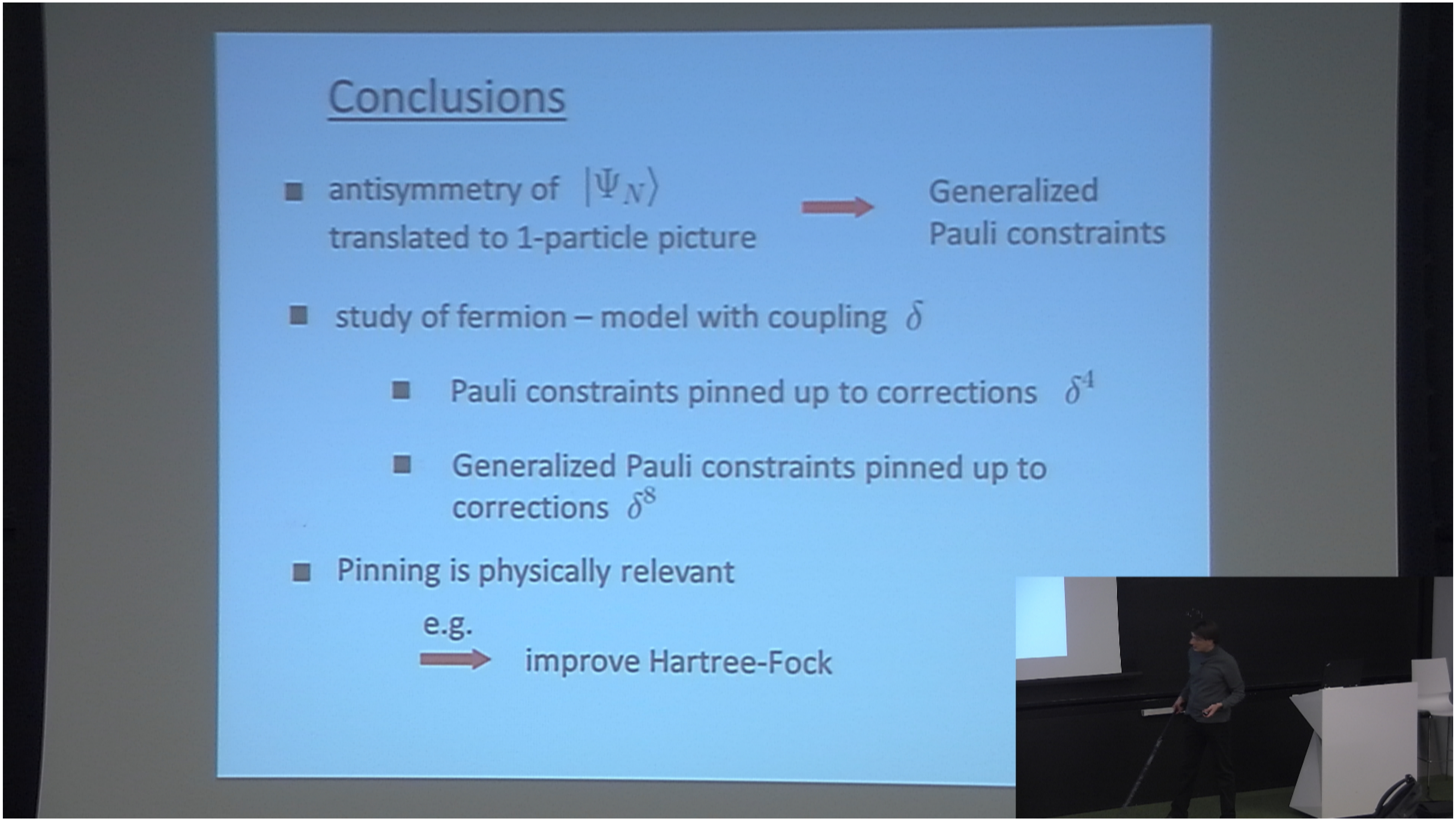
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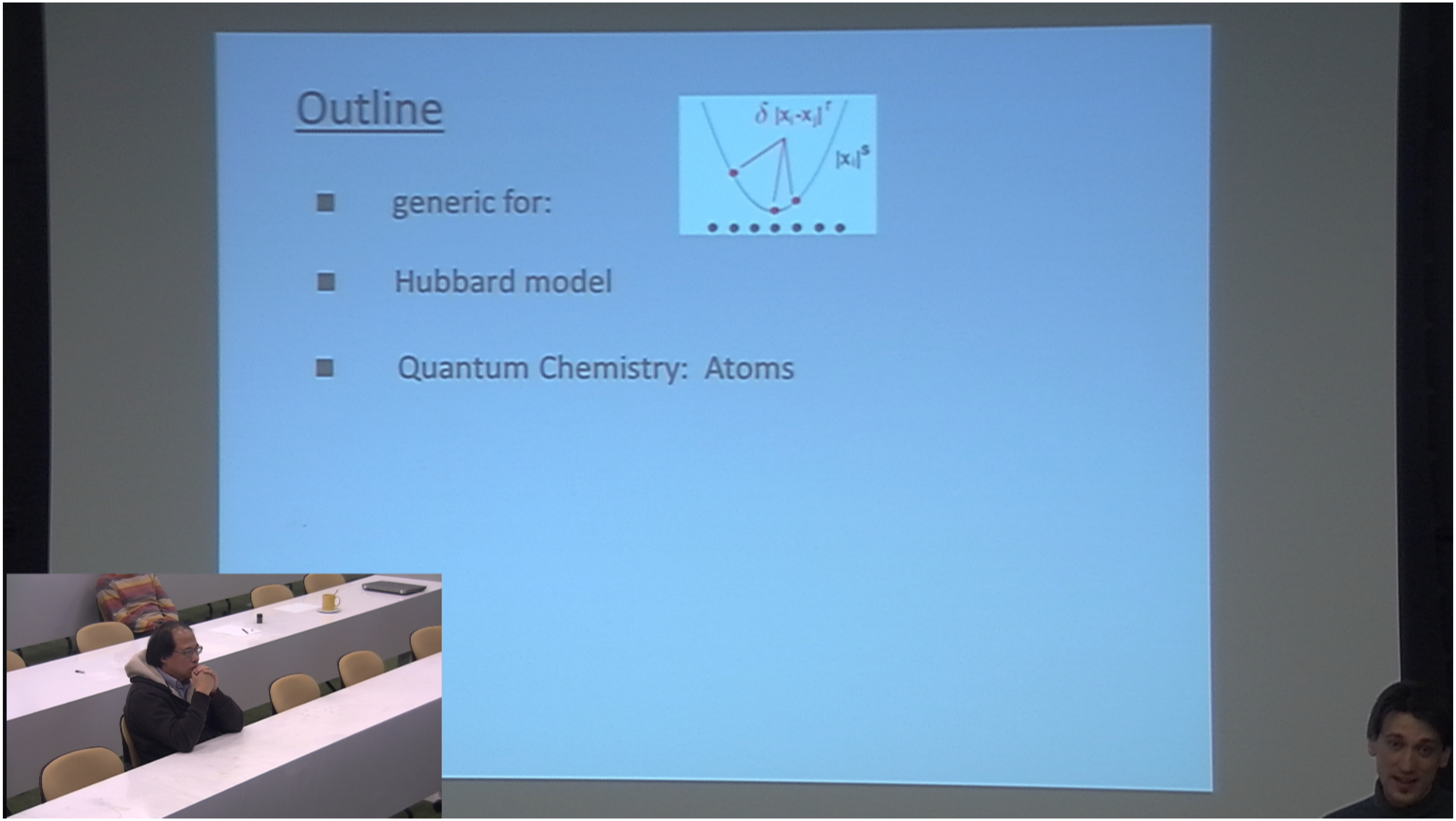
Outline
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Quantum Chemistry: Atoms
$\delta\ |x_i - x_j|^r$
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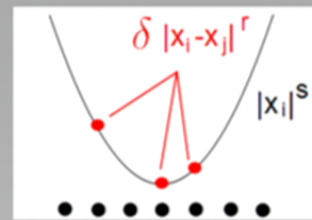
Outline



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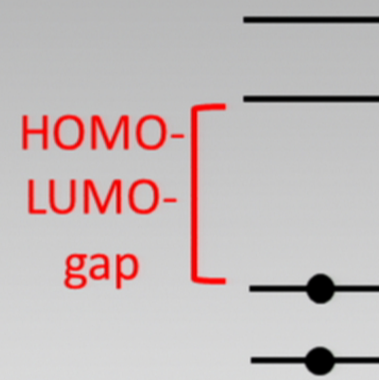
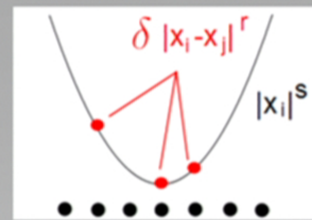


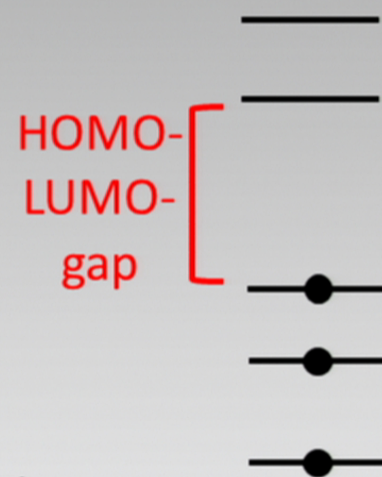
Outline

- generic for:



- Hubbard model
- Quantum Chemistry: Atoms
- Physical & mathematical Intuition

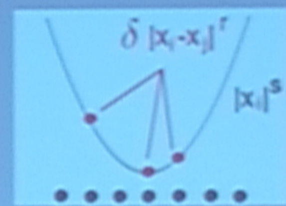
  for Pinning



- Future Research: Condensed Matter Theory

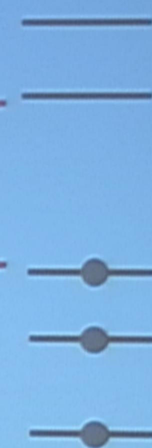
Outline

- generic for:

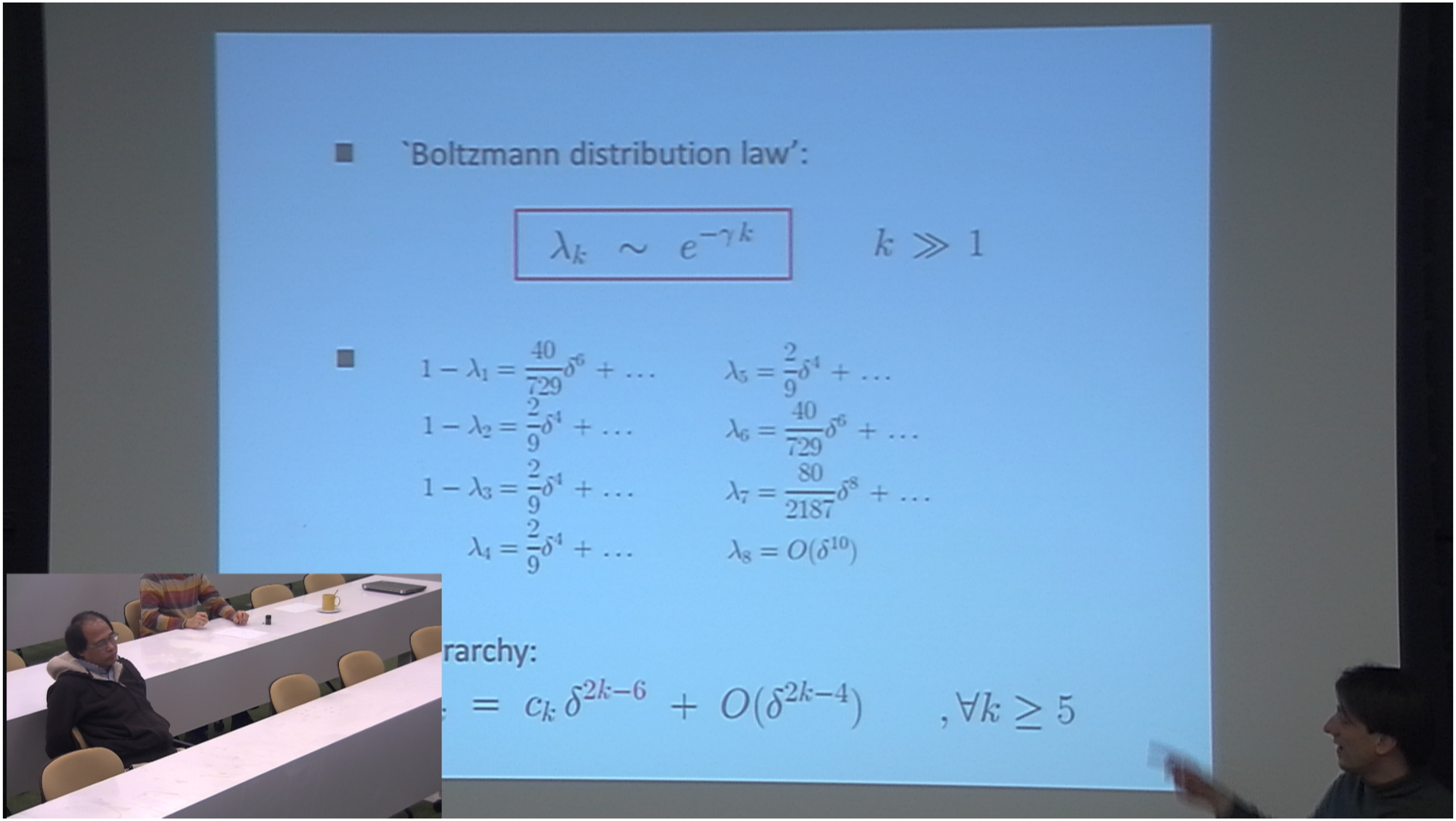


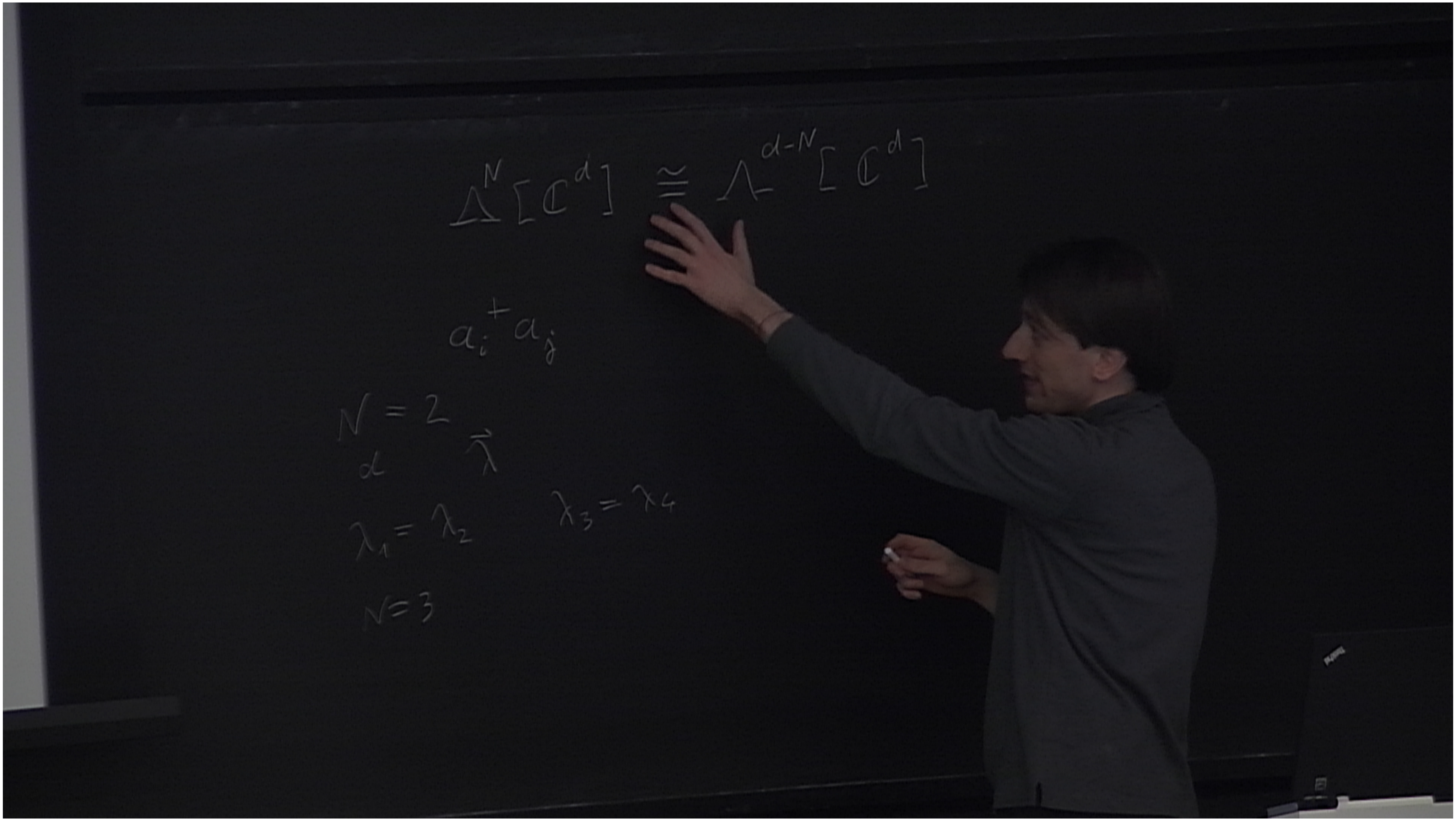
- Hubbard model
- Quantum Chemistry: Atoms
- Physical & mathematical Intuition
  for Pinning

HOMO-
LUMO-
gap



- Future Research: Condensed Matter Theory
- Antisymmetry ⚡ Energy Minimization


`Boltzmann distribution law':
$\lambda_k \sim e^{-\gamma k}$ $k \gg 1$
$1-\lambda_1 = \frac{40}{729}\delta^6 + \dots$
$\lambda_5 = \frac{2}{9}\delta^4 + \dots$
$1-\lambda_2 = \frac{2}{9}\delta^4 + \dots$
$\lambda_6 = \frac{40}{729}\delta^6 + \dots$
$1-\lambda_3 = \frac{2}{9}\delta^4 + \dots$
$\lambda_7 = \frac{80}{2187}\delta^8 + \dots$
$\lambda_4 = \frac{2}{9}\delta^4 + \dots$
$\lambda_8 = O(\delta^{10})$
rarchy:
$= c_k\,\delta^{2k-6} + O(\delta^{2k-4})$ $,\forall k \geq 5$


$\Lambda^N[\mathbb{C}^d] \cong \Lambda^{d-N}[\mathbb{C}^d]$
$a_i^+ a_j$
$N = 2$
d
$\vec{\lambda}$
$\lambda_1 = \lambda_2$
$\lambda_3 = \lambda_4$
$N=3$