Title: Symmetry Breaking and the Geometry of Reduced Density Matrices: About Convex Sets and Ruled Surfaces

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Abstract: <pre>The concept of symmetry breaking and the emergence of corresponding </pre>

<pre>local order parameters</pre>

<pre>constitute the pillars of modern day many body physics. I will </pre>

<pre>demonstrate that the existence of</pre>

<pre>symmetry breaking is a consequence of the geometric structure of the </pre>

<pre>convex set of reduced density</pre>

<pre>matrices of all possible many body wavefunctions. The surfaces of these </pre>

<pre>convex bodies exhibit</pre>

<pre>certain features, which signal the emergence of symmetry breaking and of </pre>

<pre>an associated order</pre>

<pre>parameter. I will illustrate this with a few paradigmatic examples of </pre>

<pre>many body systems exhibiting</pre>

<pre>symmetry breaking: the quantum Ising model, the classical Ising and </pre>

<pre>Potts model in 2D at finite</pre>

<pre>temperature and the ideal Bose gas in three dimensions at finite </pre>

<pre>temperature. This quantum state</pre>

<pre>based viewpoint on phase transitions provides a very intuitive and </pre>

<pre>informative new way of drawing phase diagrams</pre>

<pre>and constitutes a unique novel tool for studying exotic quantum phenomena.</pre>

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Symmetry Breaking and the Geometry of Reduced Density Matrices

About Convex Sets and Ruled Surfaces

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arXiv:1412.7642

SFB FoQuS Foundations and Applications of Quantum Science

Vienna Computational Materials Laboratory ViCoM

CoQuS Complex Quantum Systems

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Outline

- **Convex sets** of all possible (reduced) density matrices of a certain system and their lower dimensional projections
- Structure of **surface** tells about the occurrence of **symmetry breaking**
- Symmetry breaking is a **consequence of the geometry** of Hilbert space
- Examples:
  - Spin-1/2 on a lattice in 0,1,∞ dimensions
  - Classical statistical mechanics: 2d Ising and Potts model
  - Ideal Bose Gas in 3d at finite T: Bose Einstein Condensation
- Conclusions and Outlook

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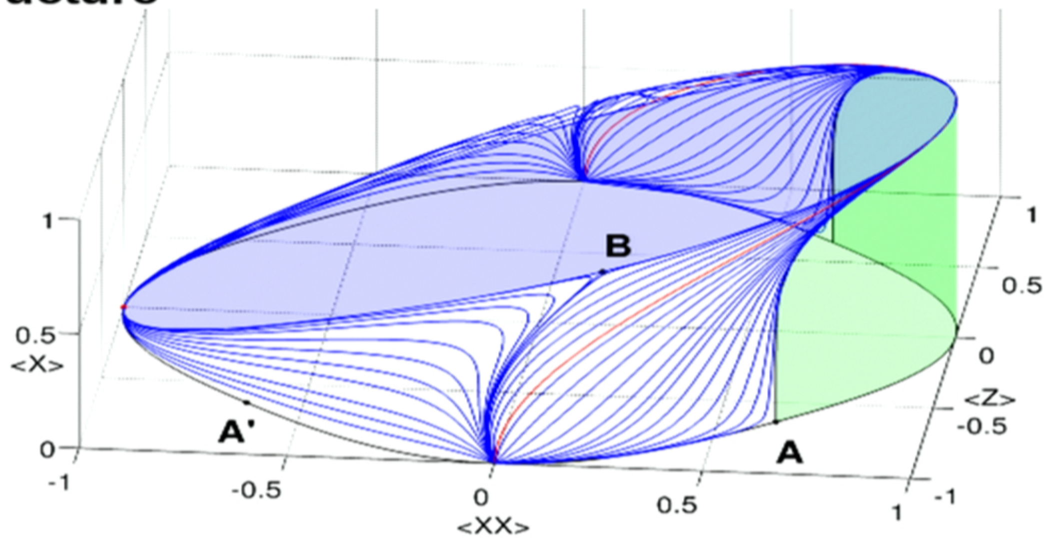
Infinite 1D spin-1/2 chain

Shape determined by **geometrical structure** of Hilbert space

Surface corresponds to ground states of a certain Hamiltonian



J. Gibbs (1867)
C. Coulson (1960)
R. Erdahl (1978)
D. Mazziotti (2004)
C. Schwerdtfeger, D. Mazziotti (2009)
...

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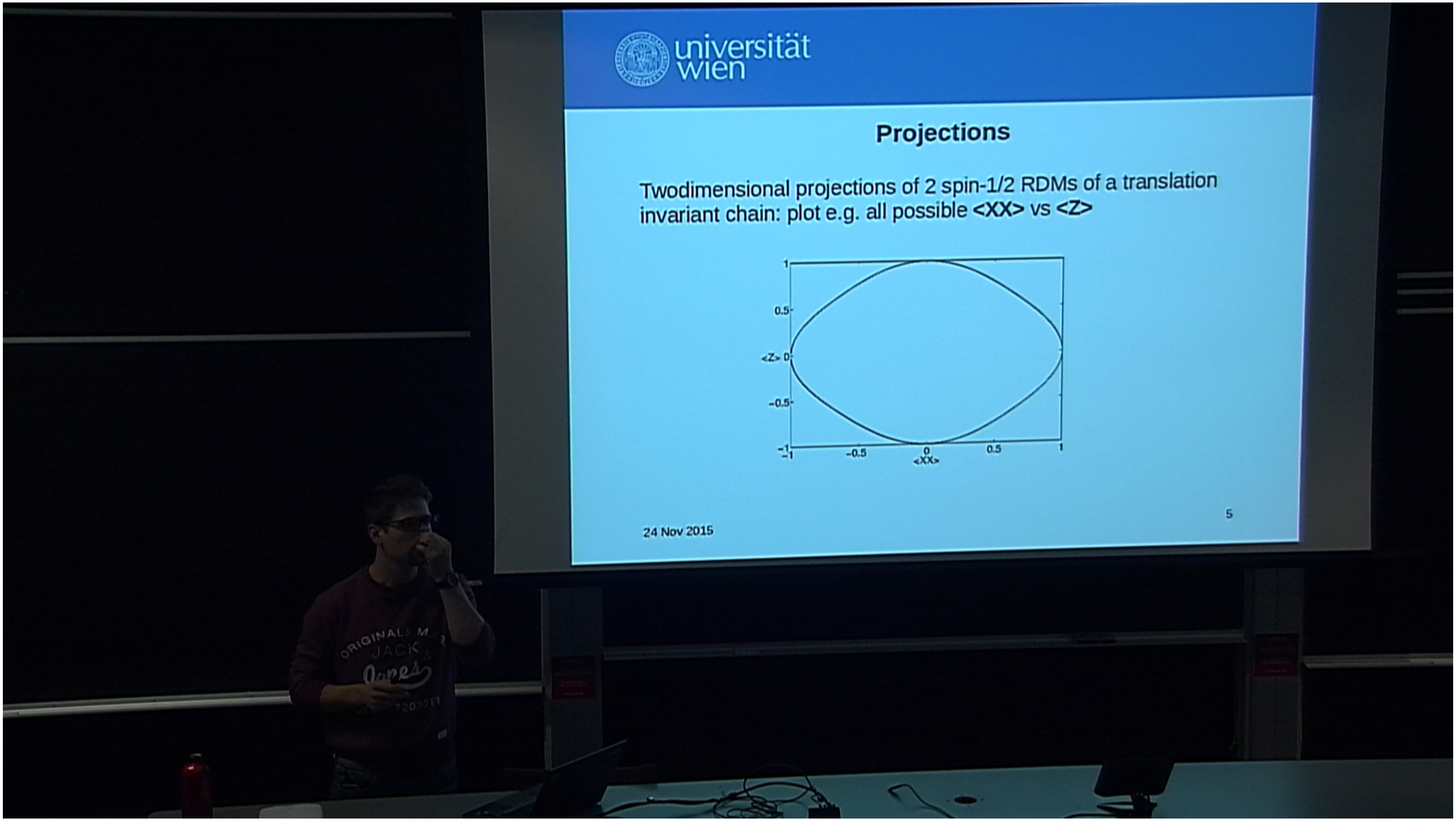
Two spin-1/2

- Density matrices of two spin-1/2 parametrized by 15 real parameters
  $$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \alpha \mathbb{1} \otimes X + \beta \mathbb{1} \otimes Y + \ldots + \gamma X \otimes Z + \delta Y \otimes Y + \ldots\right)$$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Projections
Twodimensional projections of 2 spin-1/2 RDMs of a translation invariant chain: plot e.g. all possible <XX> vs <Z>
1
0.5
<Z> 0
−0.5
−1
−1
−0.5
0
0.5
1
<XX>
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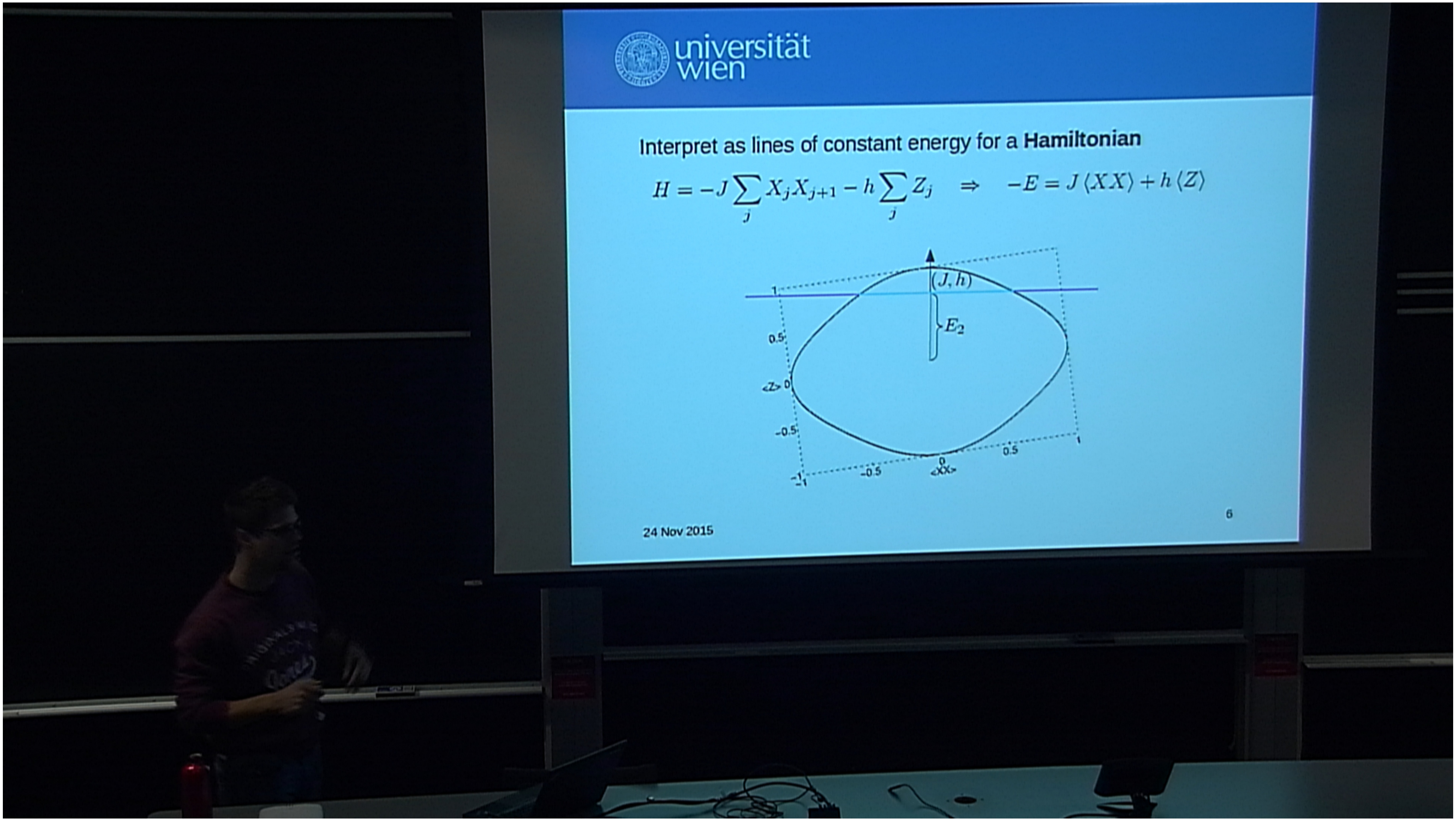
5
ORIGINALS
JACK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Interpret as lines of constant energy for a **Hamiltonian**
$H = -J \sum_j X_j X_{j+1} - h \sum_j Z_j \quad \Rightarrow \quad -E = J \langle XX \rangle + h \langle Z \rangle$
(J, h)
E_2
<Z>
<XX>
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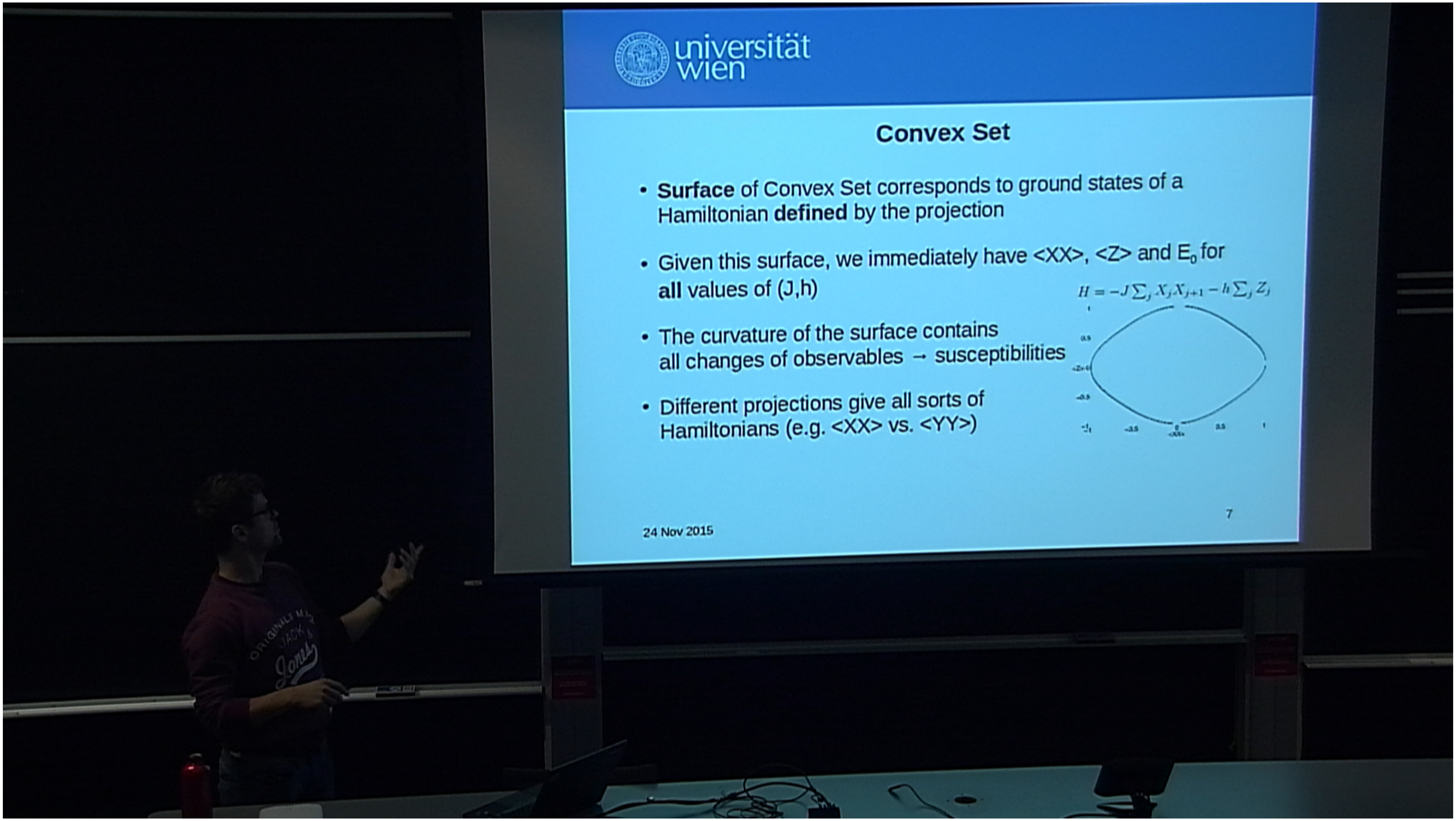
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Convex Set
• Surface of Convex Set corresponds to ground states of a Hamiltonian defined by the projection
• Given this surface, we immediately have <XX>, <Z> and E0 for all values of (J,h)
• The curvature of the surface contains all changes of observables → susceptibilities
• Different projections give all sorts of Hamiltonians (e.g. <XX> vs. <YY>)
H = −J ∑j Xj Xj+1 − h ∑j Zj
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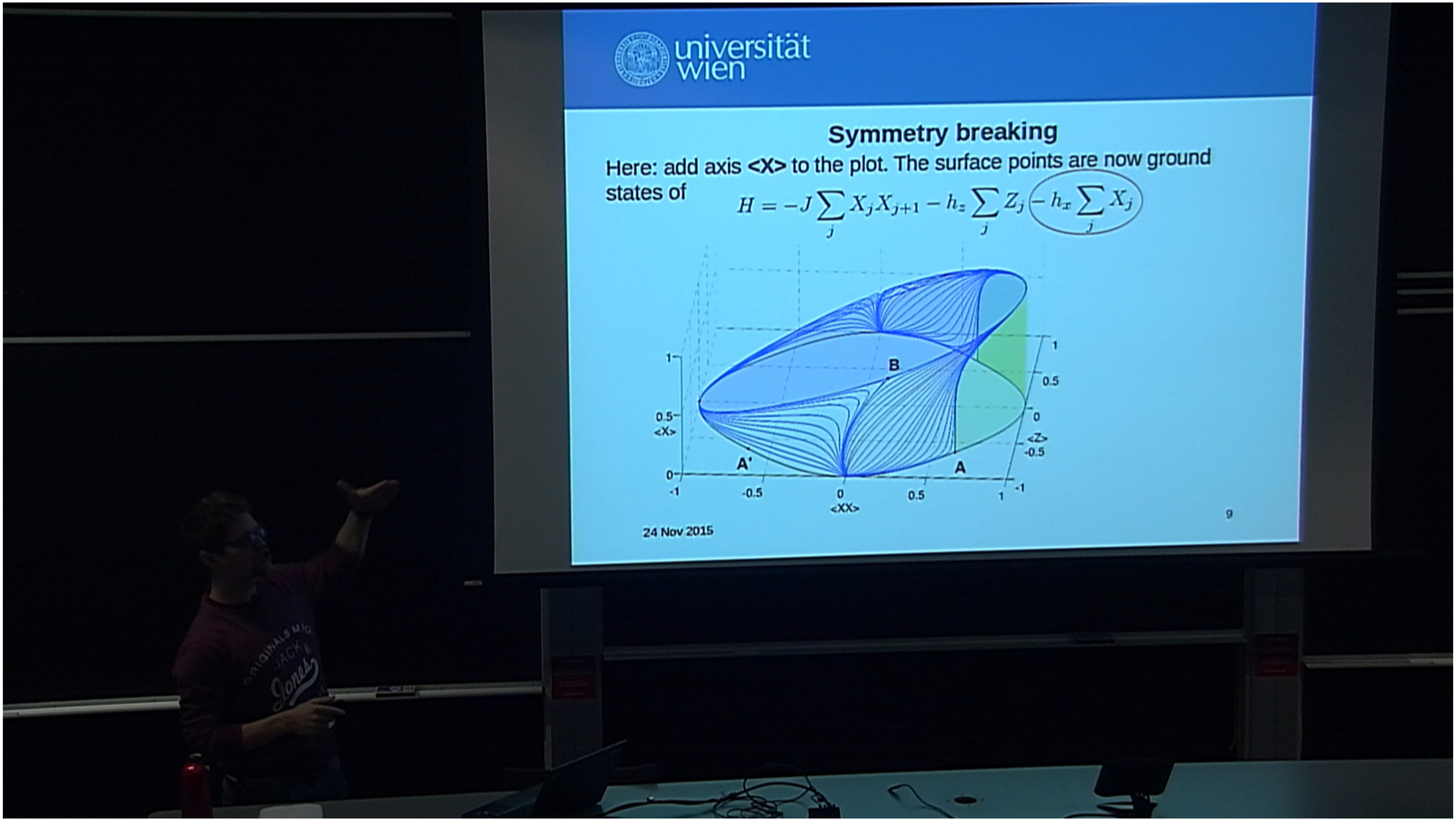
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Symmetry breaking
Here: add axis <X> to the plot. The surface points are now ground states of
$H = -J\sum_j X_j X_{j+1} - h_z \sum_j Z_j - h_x \sum_j X_j$
B
A'
A
<X>
<XX>
<Z>
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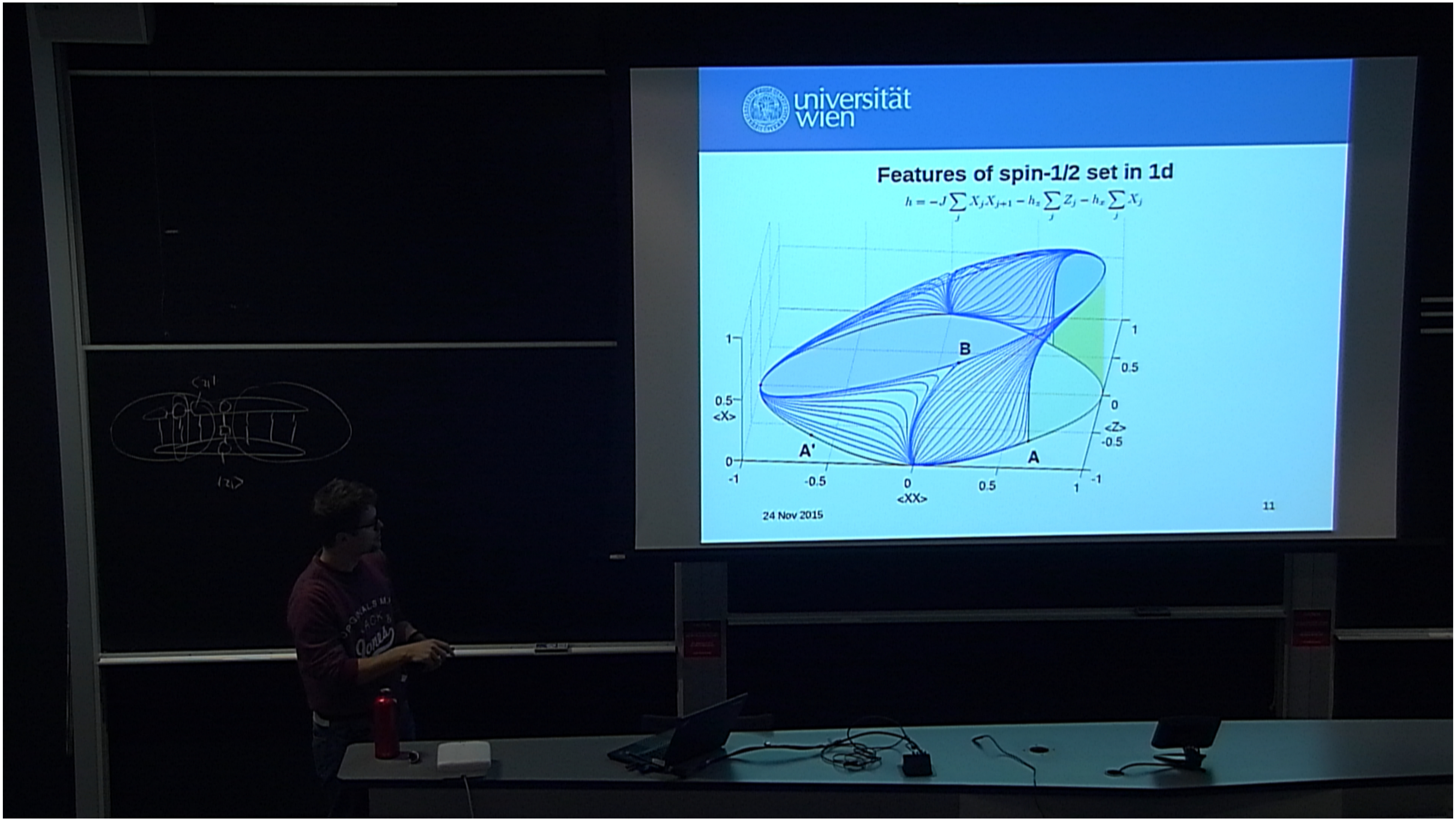
9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Features of spin-1/2 set in 1d
$h = -J \sum_j X_j X_{j+1} - h_z \sum_j Z_j - h_x \sum_j X_j$
B
A'
A
1
0.5
<X>
0
-1
-0.5
0
0.5
1
<XX>
1
0.5
0
<Z>
-0.5
-1
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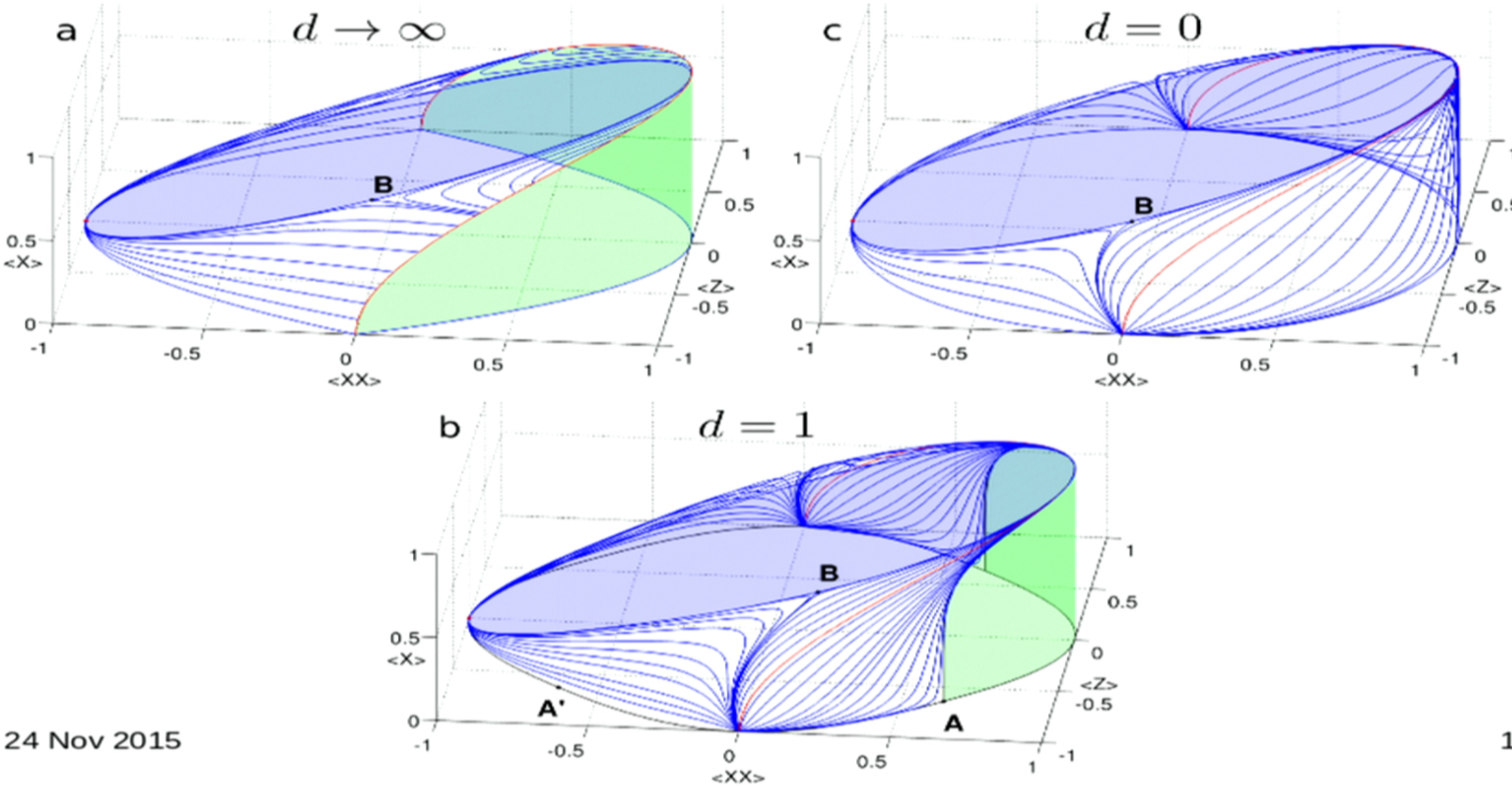
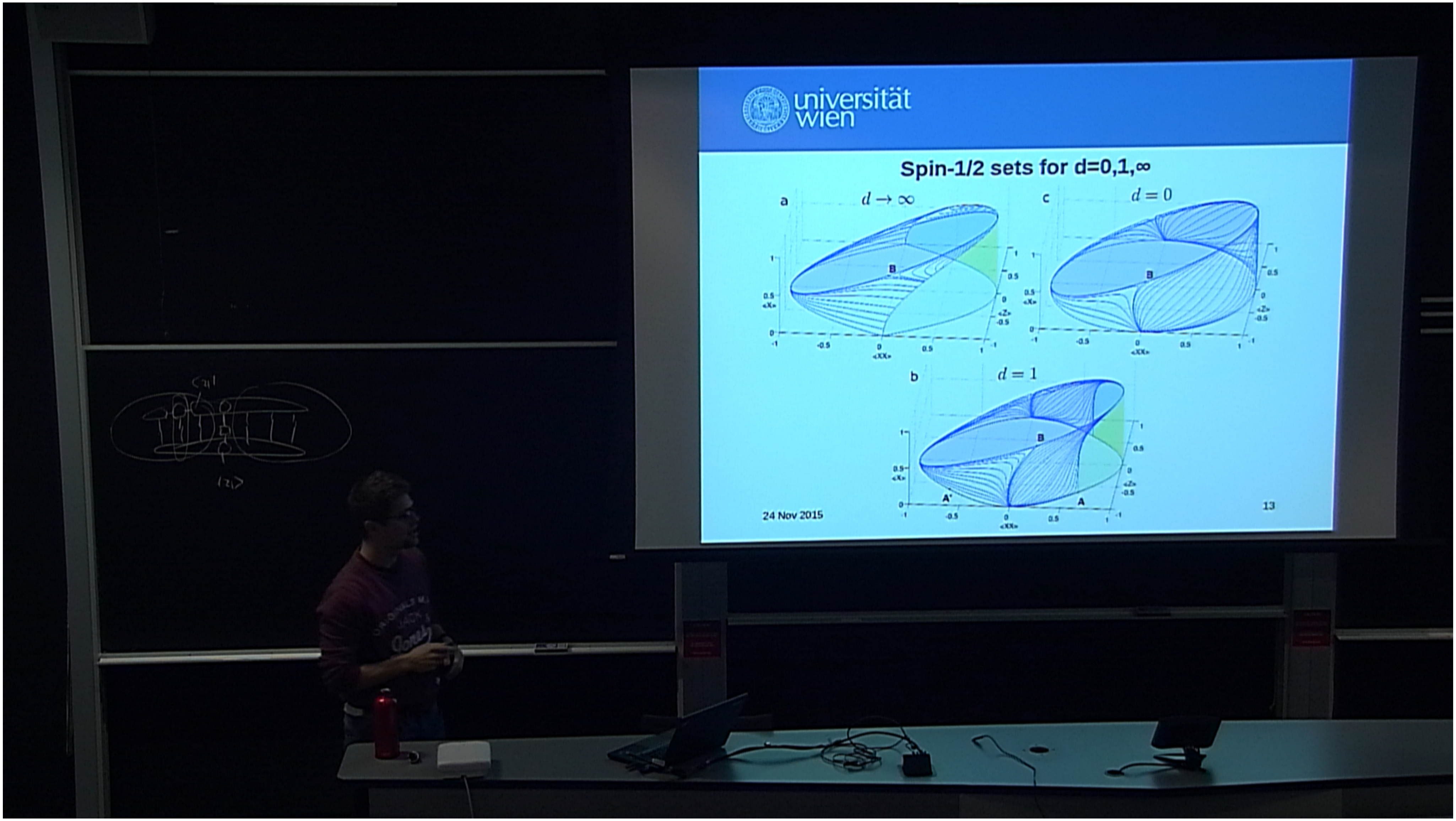
Spin-1/2 sets for d=0,1,∞

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Spin-1/2 sets for d=0,1,∞
a
$d \to \infty$
c
$d = 0$
b
$d = 1$
B
A'
A
<XX>
<X>
<Z>
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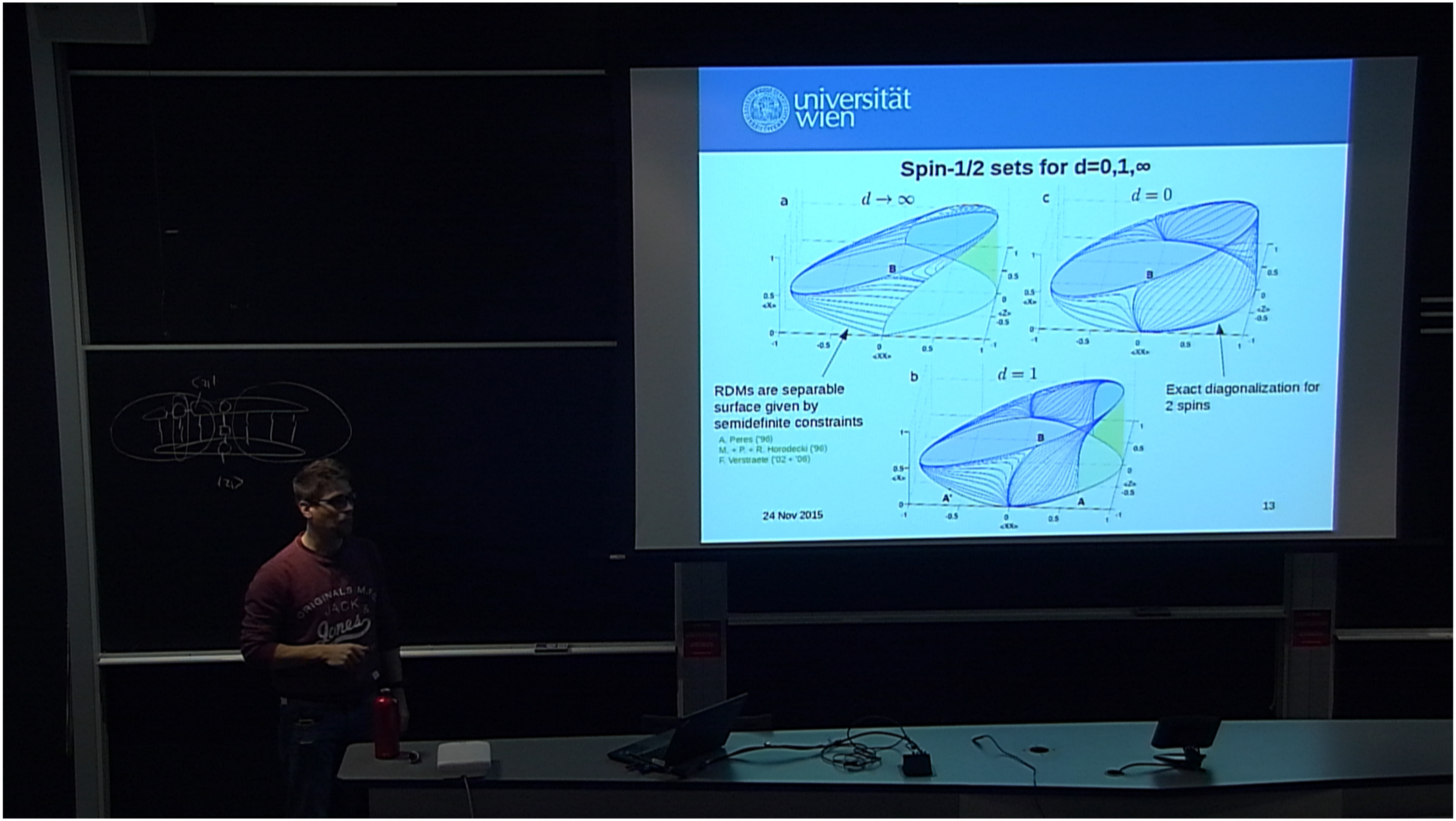
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Spin-1/2 sets for d=0,1,∞
a
$d \to \infty$
c
$d = 0$
b
$d = 1$
RDMs are separable
surface given by
semidefinite constraints
A. Peres ('96)
M. + P. + R. Horodecki ('96)
F. Verstraete ('02 + '06)
Exact diagonalization for
2 spins
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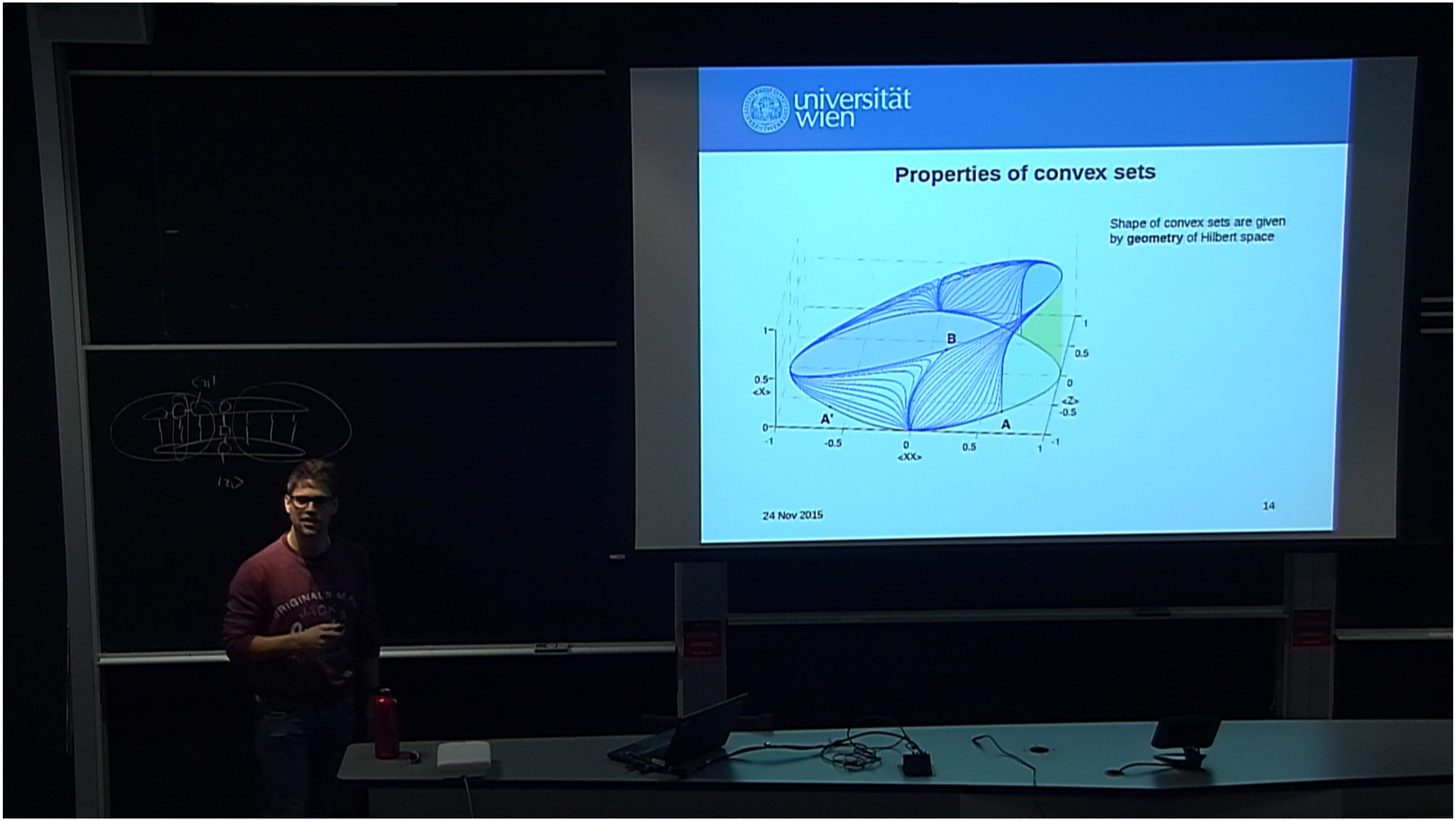
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Properties of convex sets
Shape of convex sets are given by **geometry** of Hilbert space
B
A'
A
<X>
<XX>
<Z>
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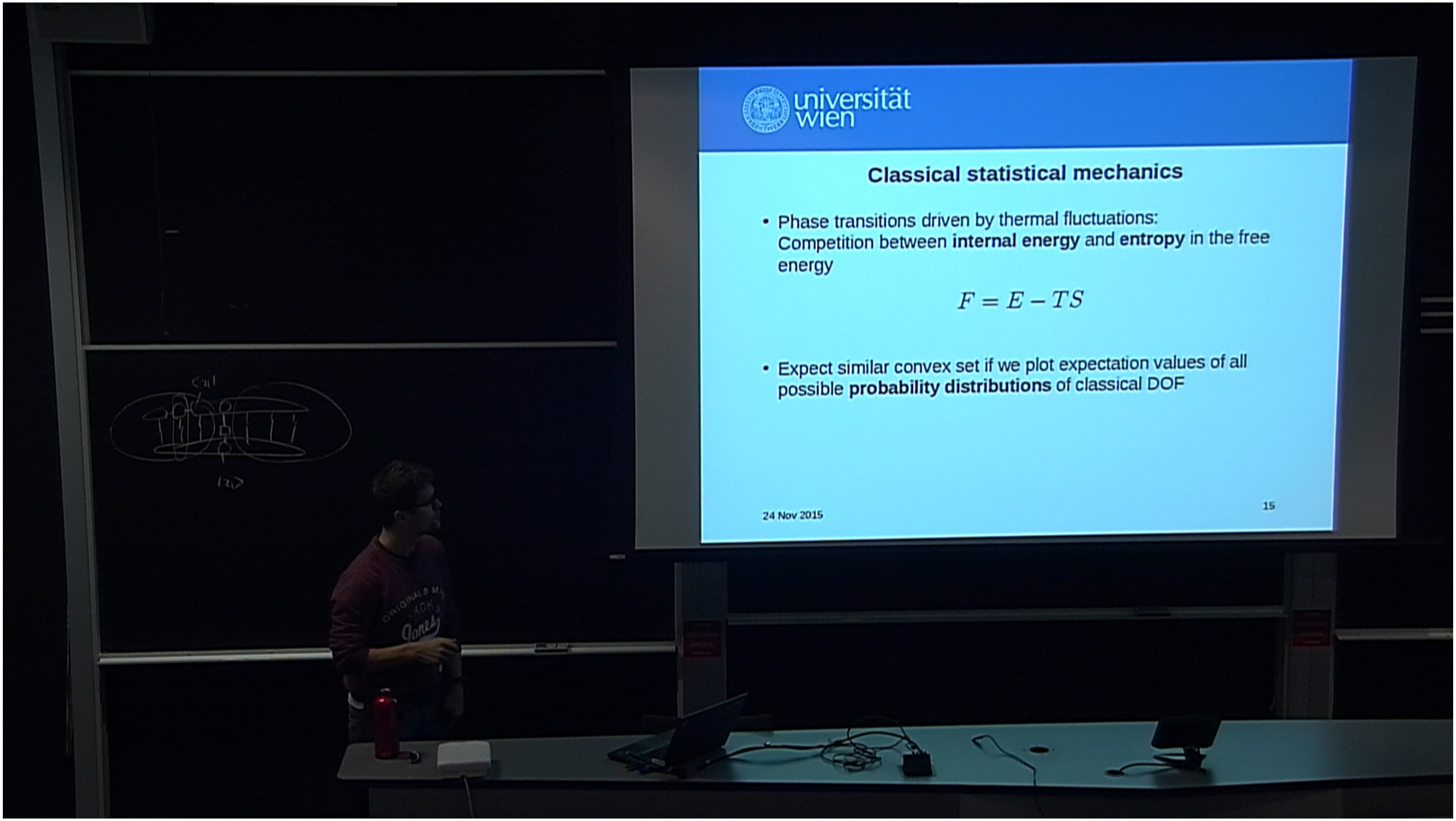
14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Classical statistical mechanics
• Phase transitions driven by thermal fluctuations:
Competition between internal energy and entropy in the free energy
$F = E - TS$
• Expect similar convex set if we plot expectation values of all possible probability distributions of classical DOF
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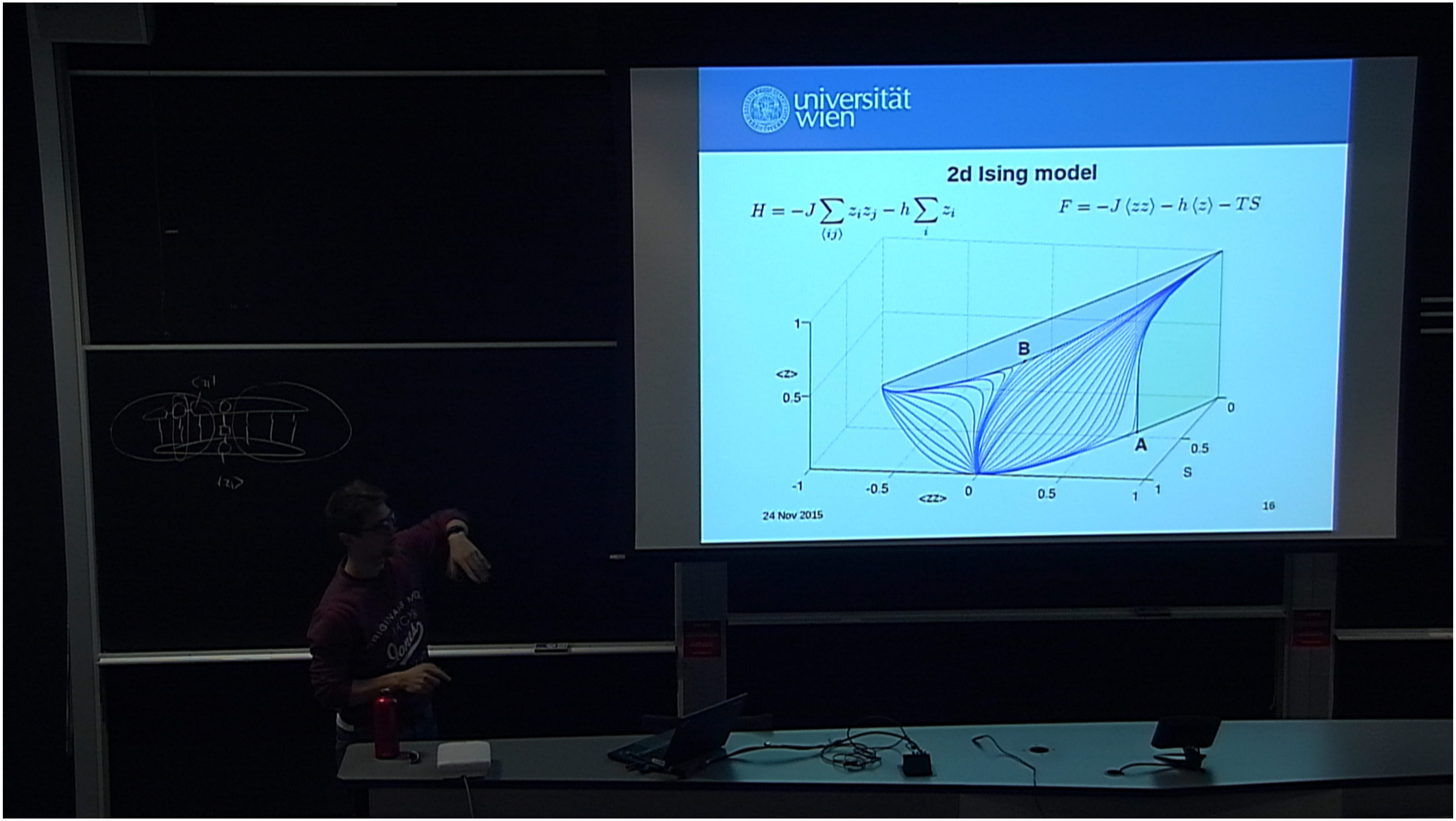
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2d Ising model
$H = -J \sum_{\langle ij \rangle} z_i z_j - h \sum_i z_i$
$F = -J \langle zz \rangle - h \langle z \rangle - TS$
B
A
<Z>
<ZZ>
S
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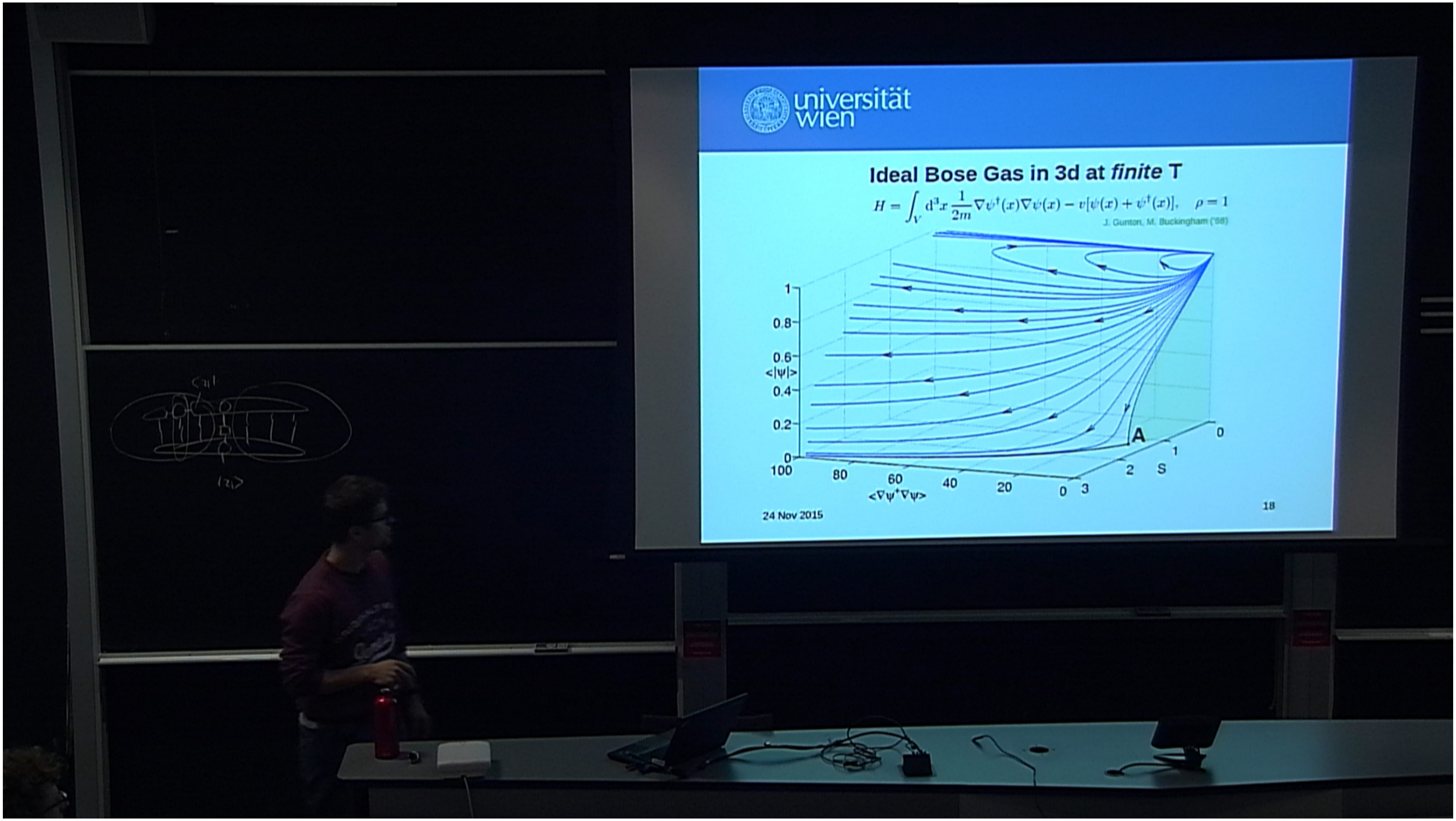

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Ideal Bose Gas in 3d at finite T
$H = \int_V d^3x \frac{1}{2m} \nabla\psi^\dagger(x)\nabla\psi(x) - v[\psi(x) + \psi^\dagger(x)], \quad \rho = 1$
J. Gunton, M. Buckingham ('68)
<|ψ|>
<∇ψ⁺∇ψ>
S
A
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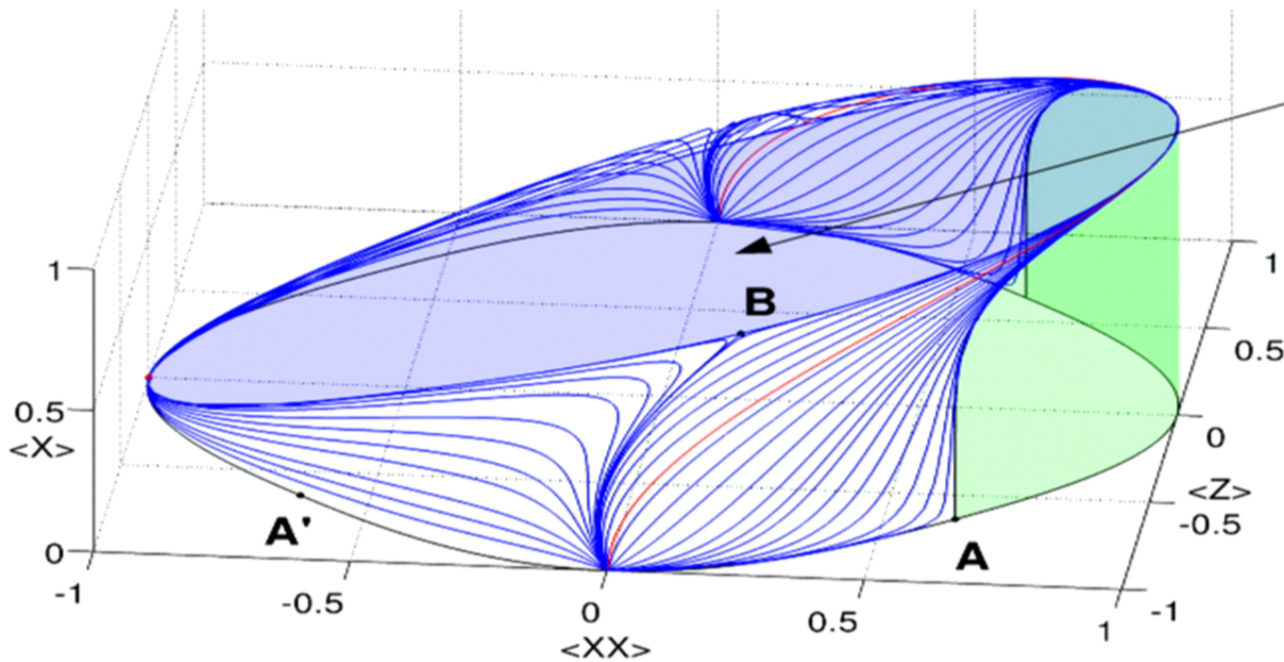
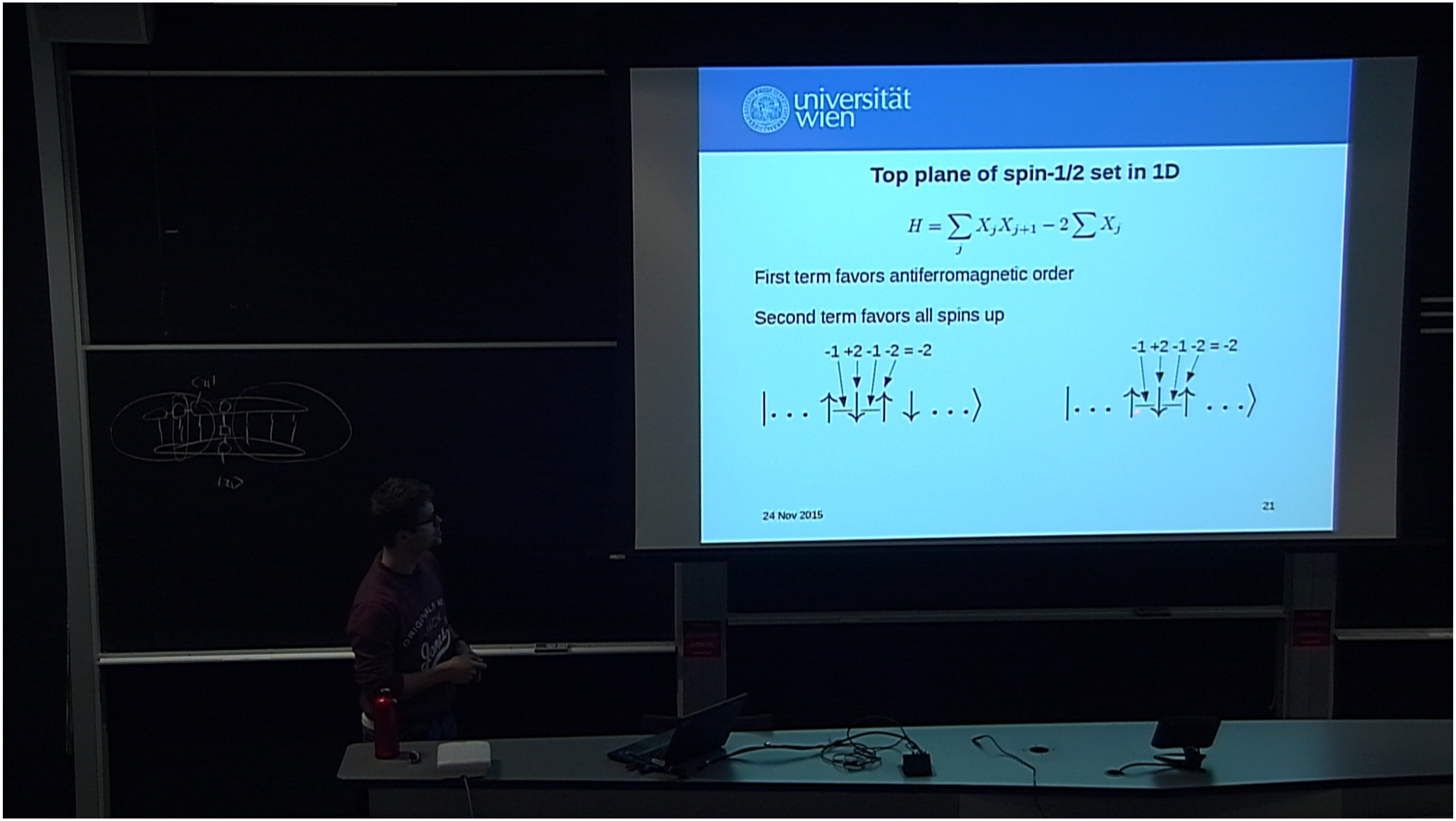
Top Planes

Top plane of spin-1/2 set in 1D



$$H = \sum_j X_j X_{j+1} - 2 \sum X_j$$

- Classical Hamiltonian!
- Eigenstates are product states
- Ground state is exponentially degenerate



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Top plane of spin-1/2 set in 1D
$H = \sum_j X_j X_{j+1} - 2 \sum X_j$
First term favors antiferromagnetic order
Second term favors all spins up
-1 +2 -1 -2 = -2
-1 +2 -1 -2 = -2
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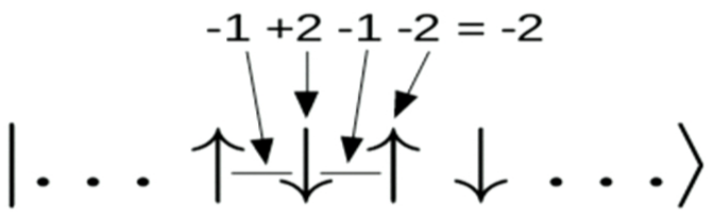
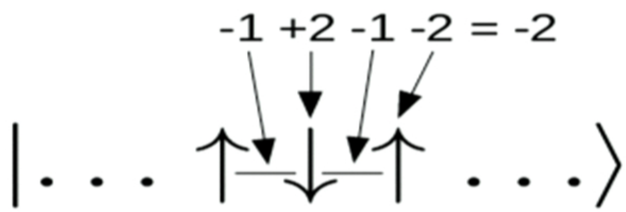
Top plane of spin-1/2 set in 1D

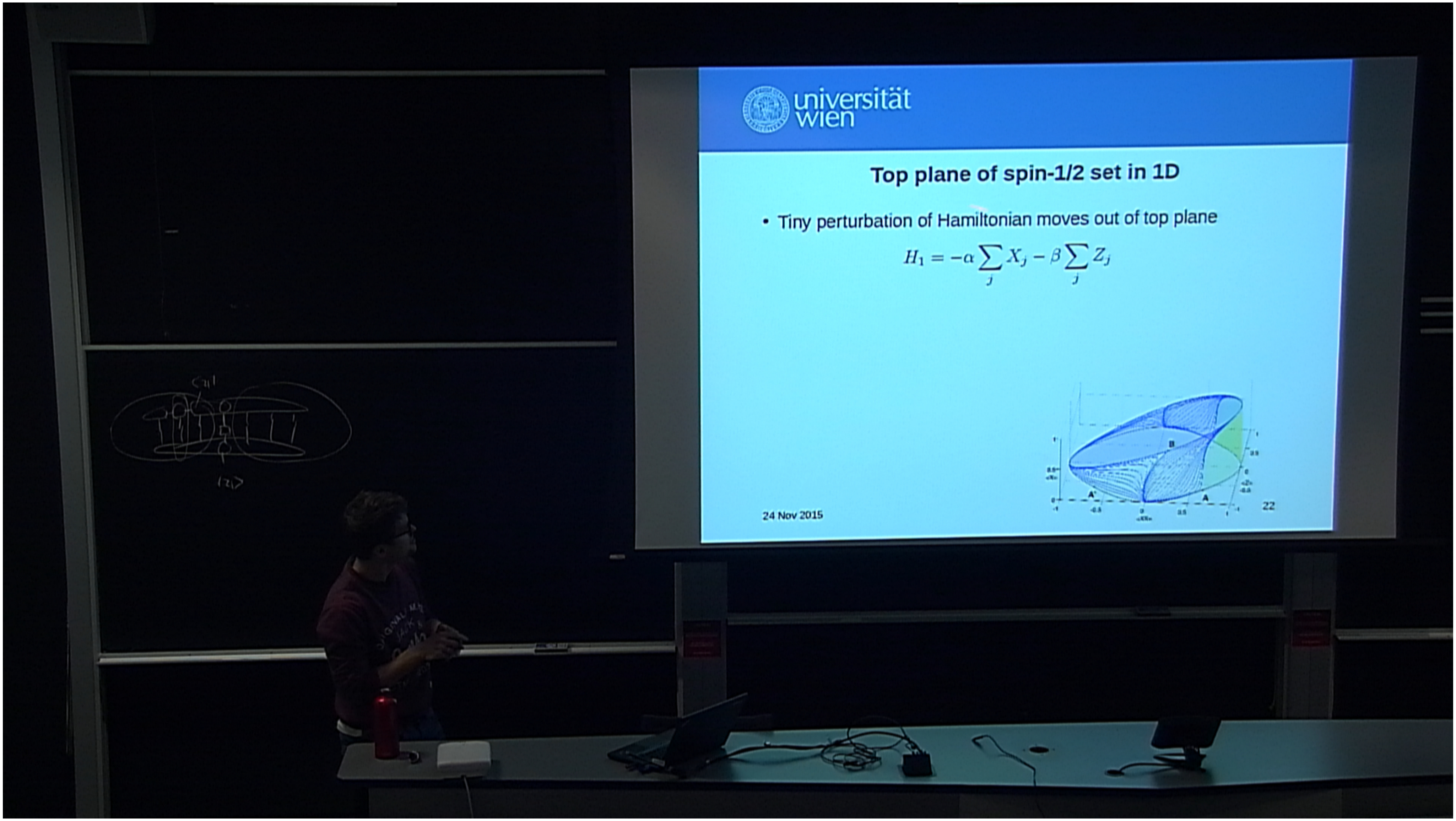
$$H = \sum_j X_j X_{j+1} - 2 \sum X_j$$

First term favors antiferromagnetic order

Second term favors all spins up



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Top plane of spin-1/2 set in 1D
• Tiny perturbation of Hamiltonian moves out of top plane
$H_1 = -\alpha \sum_j X_j - \beta \sum_j Z_j$
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Side plane for Potts model
• only configurations without equal neighboring spins are allowed → coloring problem
• For h=0 all of these configurations are equally probable
For q=3 exact solution:
$Z^{1/N} = (4/3)^{3/2}, \quad s = (3/2)\log(4/3) \approx 0.4315$
Baxter ('70), Lieb ('67)
B
A
C
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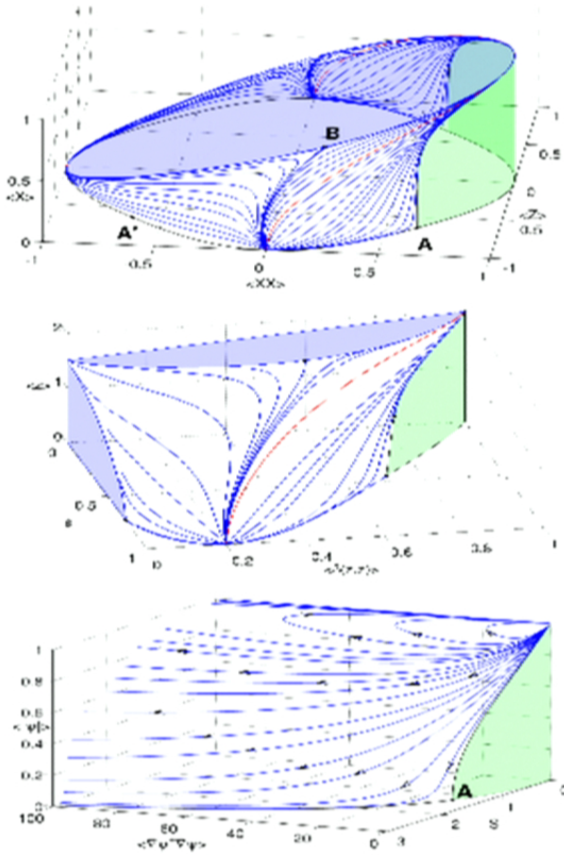
To wrap up

- **Convex sets** of reduced density matrices and marginal probability distributions
- **Surfaces** correspond to ground states and Gibbs states
- **Ruled surfaces** signal symmetry breaking (ground/Gibbs state is not unique)
- Symmetry breaking is a consequence of the **geometrical structure** of Hilbert space



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