Title: Haldane-like antiferromagnetic spin chain in the large anisotropy limit

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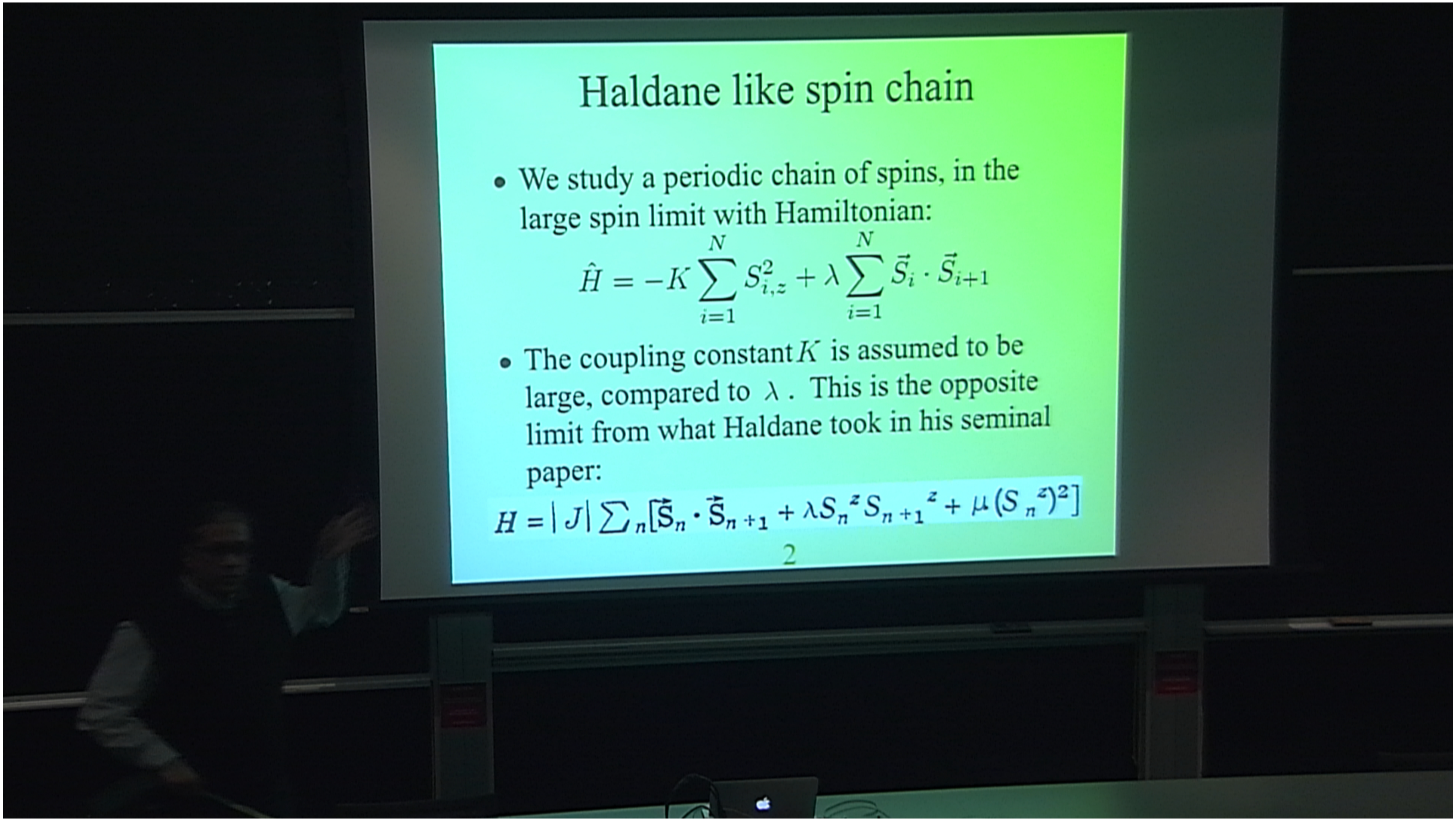
Abstract: <p>We consider the one dimensional, periodic spin chain with N sites, similar to the one studied by Haldane \cite{hal}, however in the opposite limit of very large anisotropy and small nearest neighbour, anti-ferromagnetic exchange coupling between the spins, which are of large magnitude s. For a chain with an even number of sites we show that actually the ground state is non degenerate and given by a superposition of the two NÃ©el states, due to quantum spin tunnelling. With an odd number of sites, the NÃ©el state must necessarily contain a soliton. The position of the soliton is arbitrary thus the ground state is N-fold degenerate. This set of states reorganizes into a band. We show that this occurs at order $2s$ in perturbation theory. The ground state is non-degenerate for integer spin, but degenerate for half-odd integer spin as is required by Kramer's theorem \cite{kram}. arXiv:1404.6706 , Phys.Lett. A378 (2014) 3066-3069; arXiv:1304.3734 Phys.Rev. B88 (2013) 22, 220403 </p>


Haldane like spin chain
We study a periodic chain of spins, in the large spin limit with Hamiltonian:
$\hat{H} = -K \sum_{i=1}^{N} S_{i,z}^2 + \lambda \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}$
The coupling constant K is assumed to be large, compared to λ. This is the opposite limit from what Haldane took in his seminal paper:
$H = |J| \sum_n [\vec{S}_n \cdot \vec{S}_{n+1} + \lambda S_n^z S_{n+1}^z + \mu (S_n^z)^2]$
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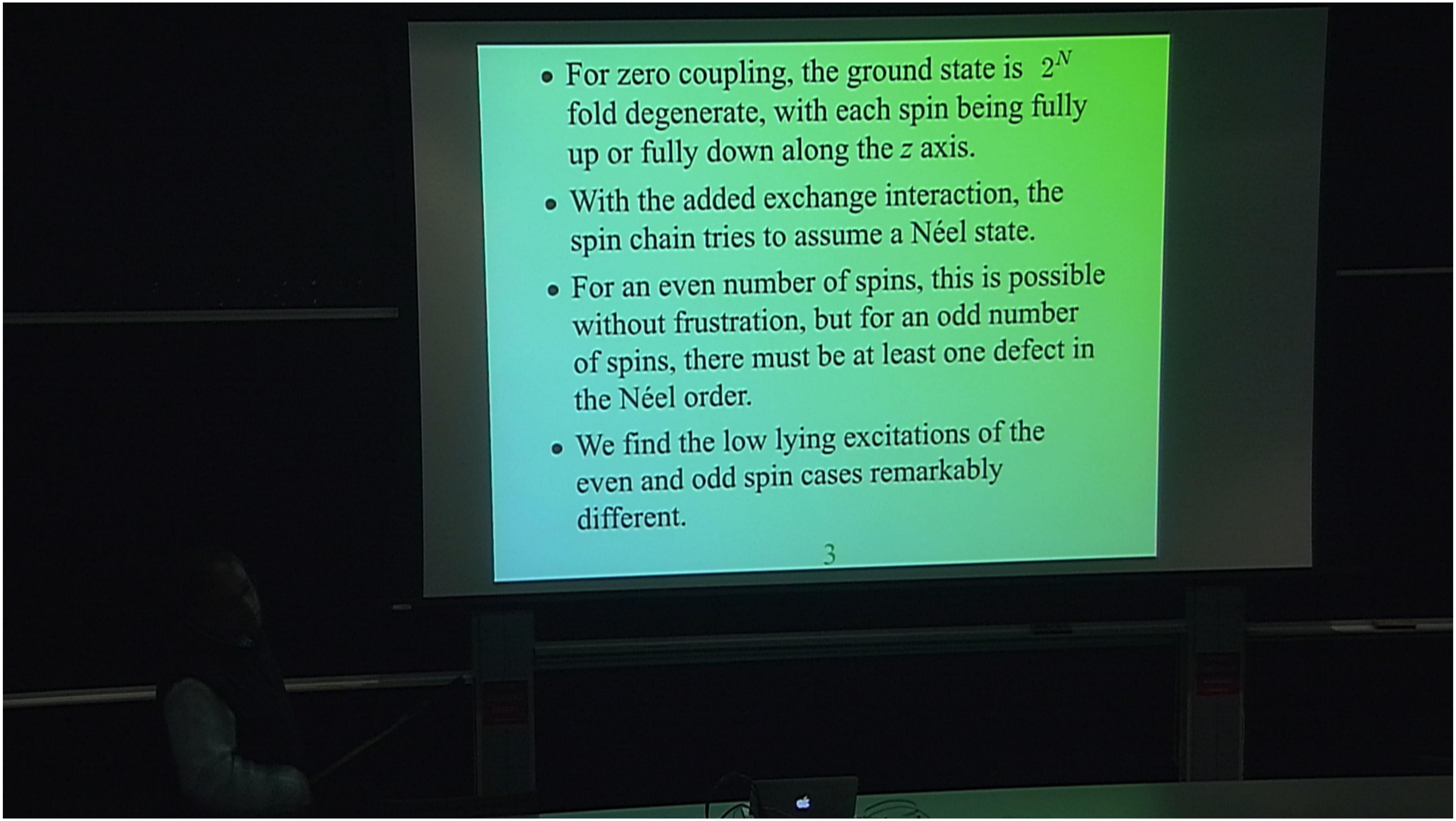
• For zero coupling, the ground state is 2^N fold degenerate, with each spin being fully up or fully down along the z axis.
• With the added exchange interaction, the spin chain tries to assume a Néel state.
• For an even number of spins, this is possible without frustration, but for an odd number of spins, there must be at least one defect in the Néel order.
• We find the low lying excitations of the even and odd spin cases remarkably different.
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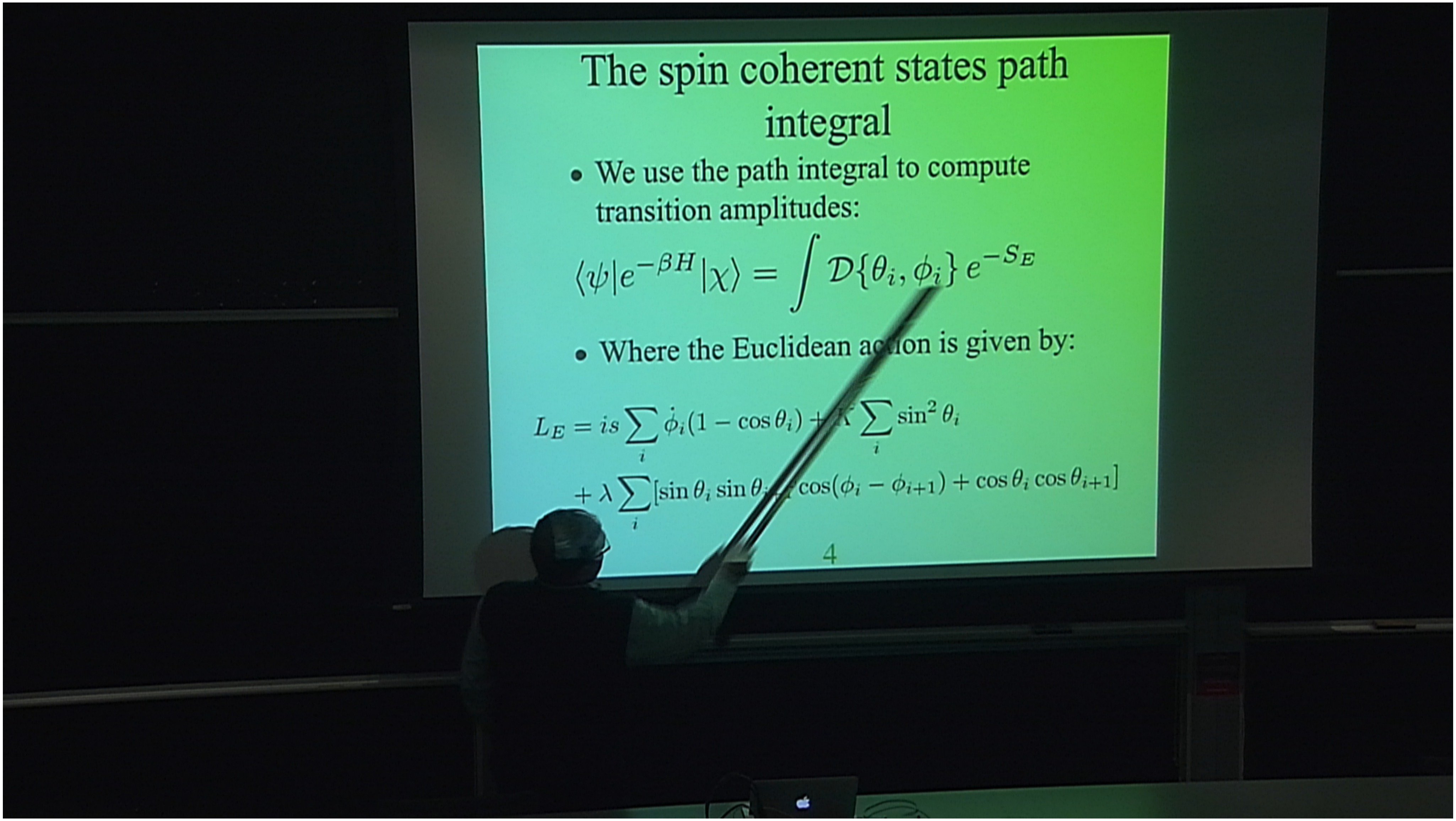
The spin coherent states path integral
We use the path integral to compute transition amplitudes:
$\langle\psi|e^{-\beta H}|\chi\rangle = \int \mathcal{D}\{\theta_i, \phi_i\}\, e^{-S_E}$
Where the Euclidean ac ion is given by:
$L_E = is\sum_i \dot{\phi}_i(1-\cos\theta_i)$
$\sum_i \sin^2\theta_i$
$+\lambda\sum_i[\sin\theta_i\sin\theta$
$\cos(\phi_i-\phi_{i+1})+\cos\theta_i\cos\theta_{i+1}]$
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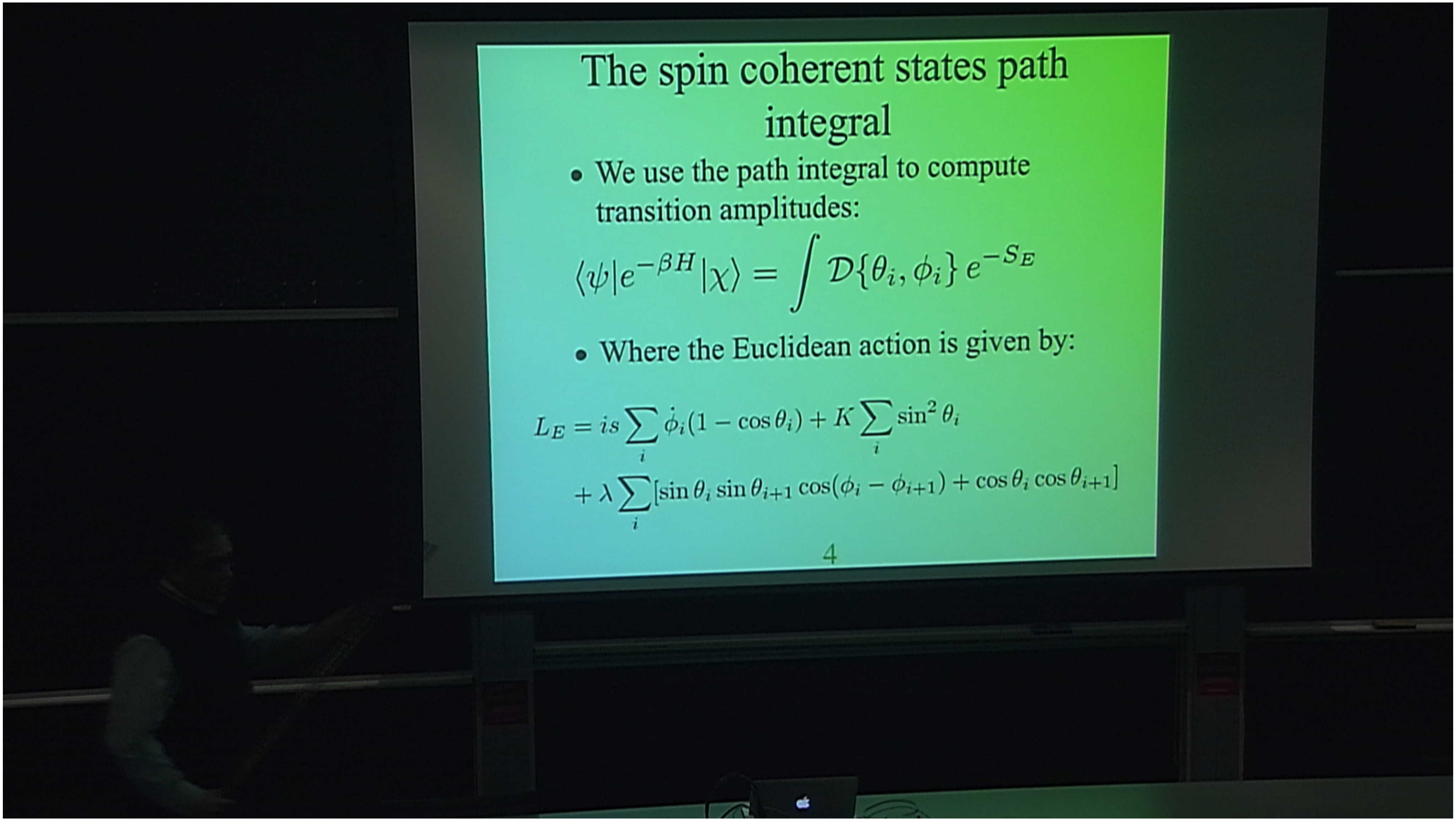
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• We use the path integral to compute transition amplitudes:
$\langle\psi|e^{-\beta H}|\chi\rangle = \int \mathcal{D}\{\theta_i, \phi_i\}\, e^{-S_E}$
• Where the Euclidean action is given by:
$L_E = is \sum_i \dot{\phi}_i (1 - \cos\theta_i) + K \sum_i \sin^2\theta_i$
$+ \lambda \sum_i [\sin\theta_i \sin\theta_{i+1} \cos(\phi_i - \phi_{i+1}) + \cos\theta_i \cos\theta_{i+1}]$
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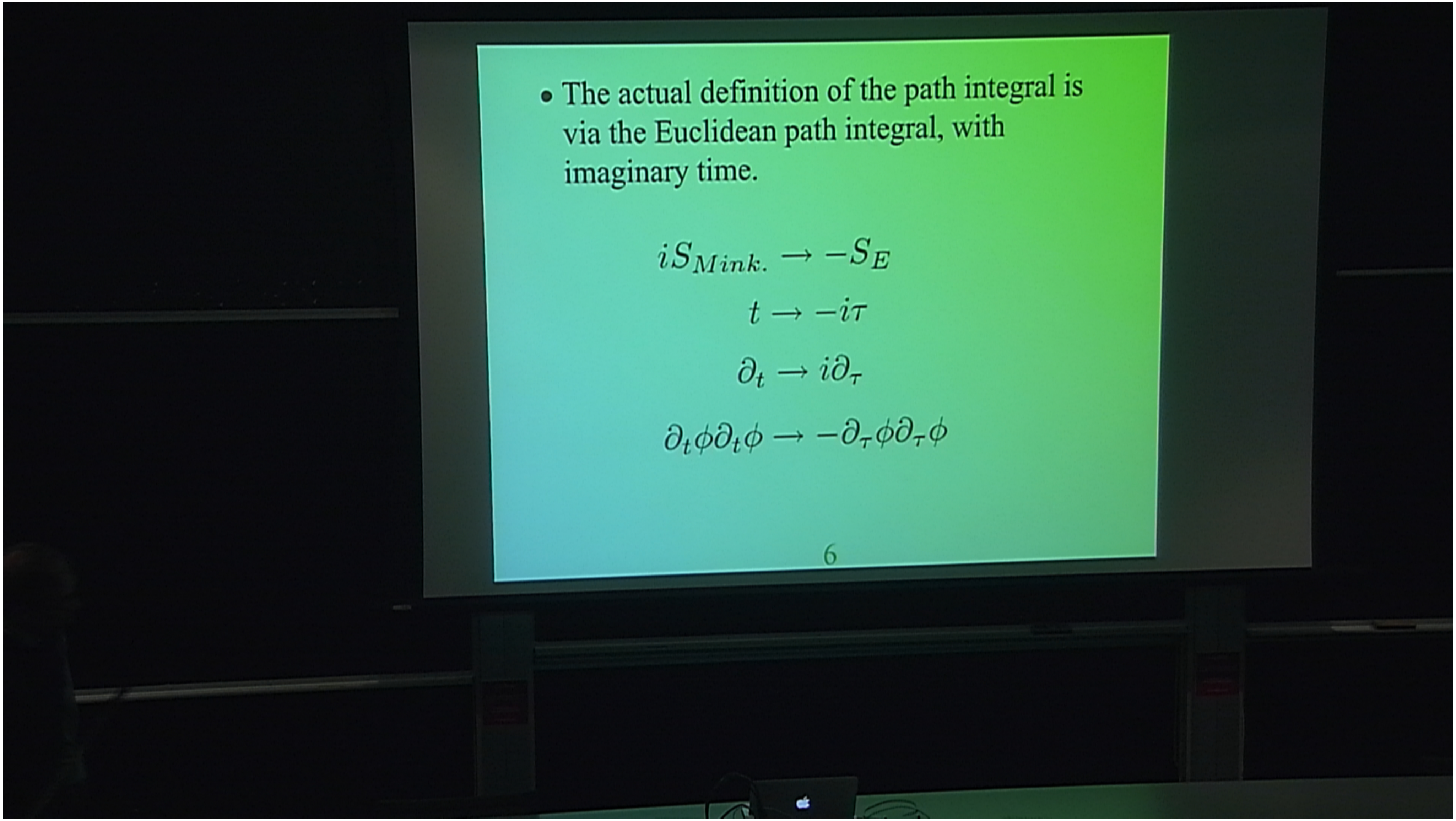
• The actual definition of the path integral is via the Euclidean path integral, with imaginary time.
$iS_{Mink.} \to -S_E$
$t \to -i\tau$
$\partial_t \to i\partial_\tau$
$\partial_t\phi\partial_t\phi \to -\partial_\tau\phi\partial_\tau\phi$
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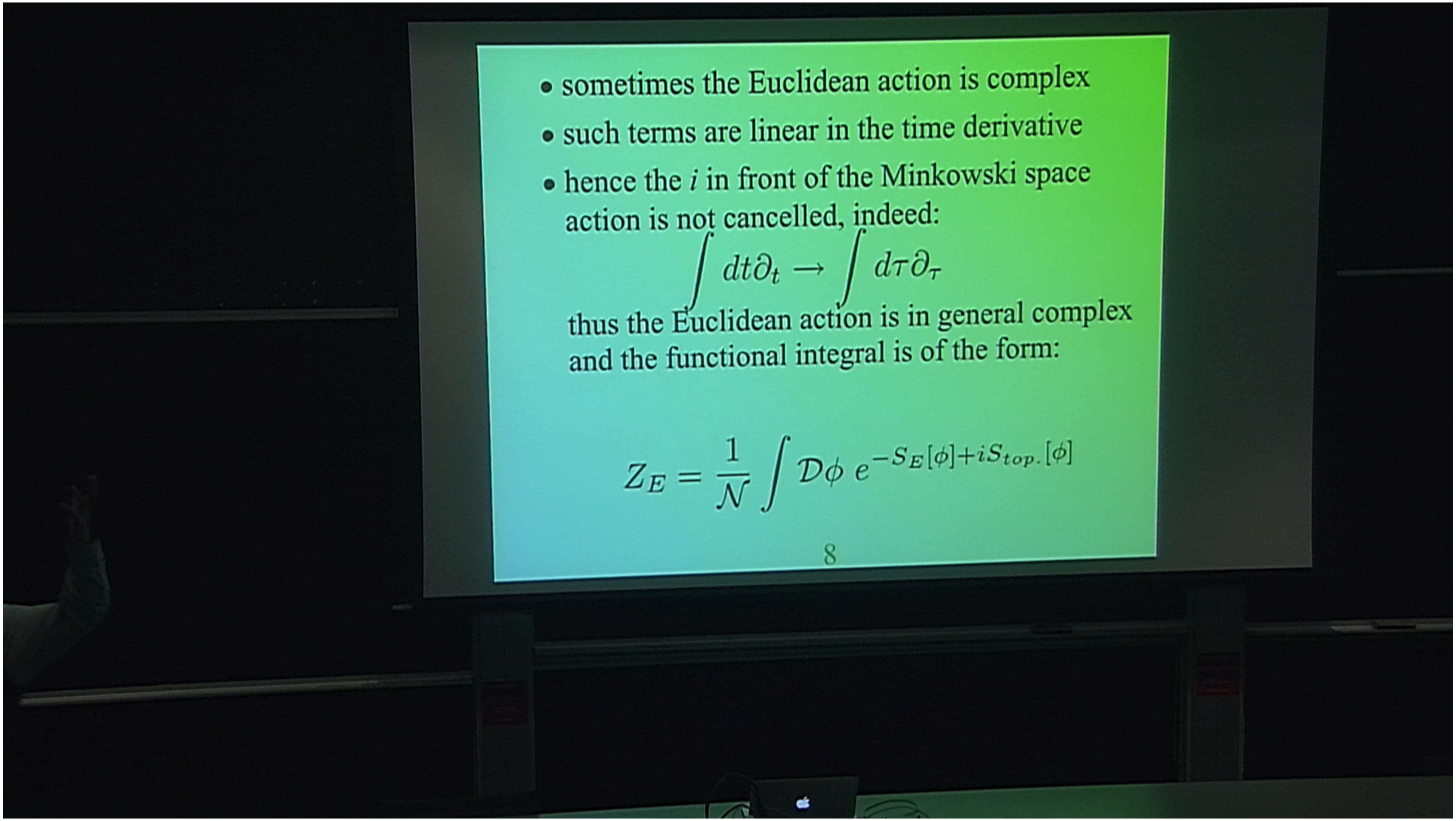
$iS_{Mink} = i\int dt d^3x (1/2)\partial_\mu\phi\partial^\mu\phi - V(\phi)$
$= i\int dt d^3x (1/2)\partial_t\phi\partial_t\phi - (1/2)\partial_i\phi\partial_i\phi - V(\phi)$
$\rightarrow i(-i)\int d\tau d^3x - (1/2)\partial_\tau\phi\partial_\tau\phi - (1/2)\partial_i\phi\partial_i\phi - V(\phi)$
$\equiv -S_E$
• Then the Euclidean functional integral defined by:
$Z_E[J] = \frac{1}{\mathcal{N}}\int \mathcal{D}\phi\ e^{-S_E[\phi]+\int J\phi}$
7


• sometimes the Euclidean action is complex
• such terms are linear in the time derivative
• hence the i in front of the Minkowski space action is not cancelled, indeed:
$\int dt\partial_t \rightarrow \int d\tau\partial_\tau$
thus the Euclidean action is in general complex and the functional integral is of the form:
$Z_E = \frac{1}{\mathcal{N}} \int \mathcal{D}\phi \, e^{-S_E[\phi]+iS_{top.}[\phi]}$
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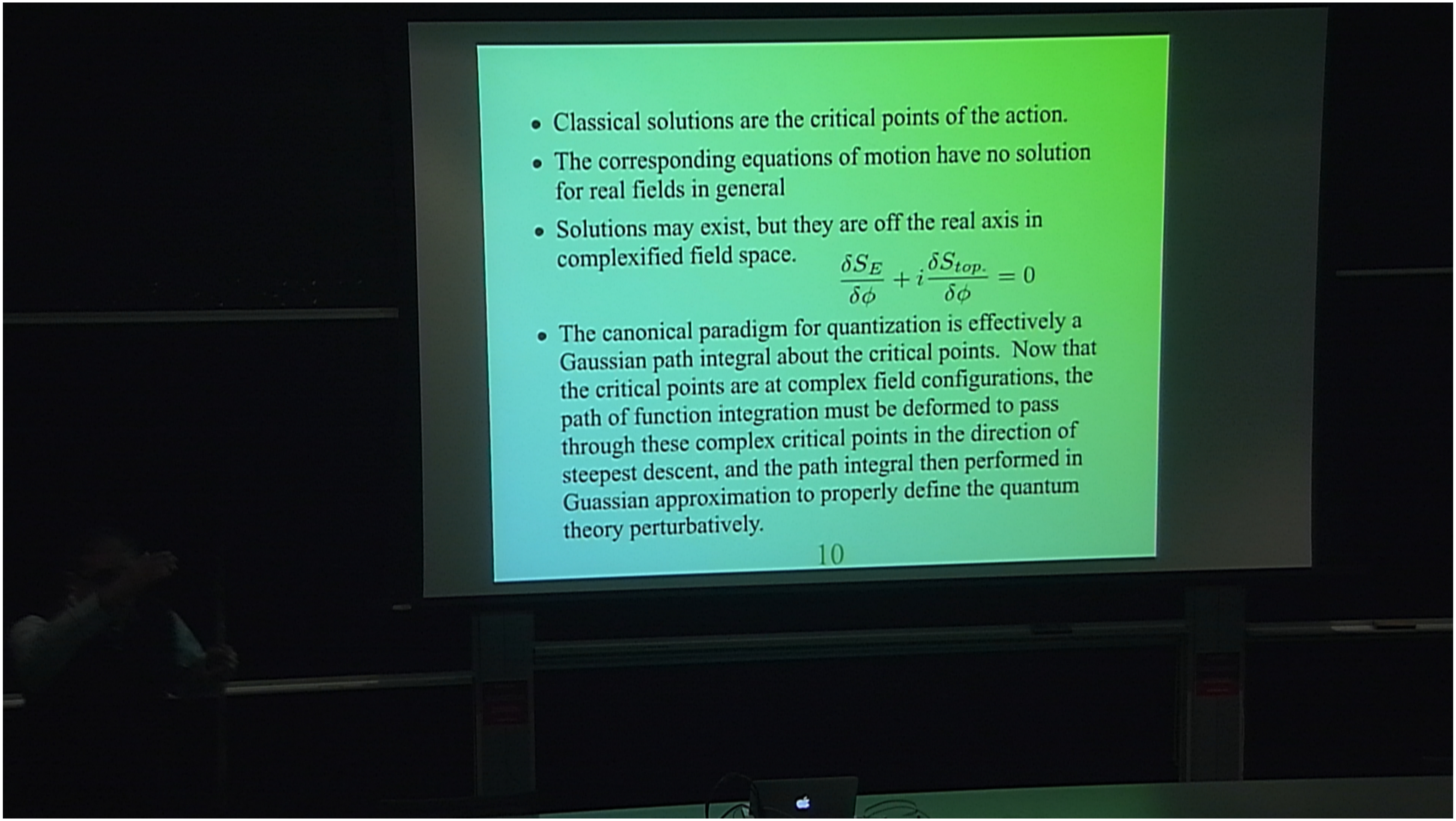

• Classical solutions are the critical points of the action.
• The corresponding equations of motion have no solution for real fields in general
• Solutions may exist, but they are off the real axis in complexified field space.
$$\frac{\delta S_E}{\delta \phi} + i\frac{\delta S_{top.}}{\delta \phi} = 0$$
• The canonical paradigm for quantization is effectively a Gaussian path integral about the critical points. Now that the critical points are at complex field configurations, the path of function integration must be deformed to pass through these complex critical points in the direction of steepest descent, and the path integral then performed in Guassian approximation to properly define the quantum theory perturbatively.
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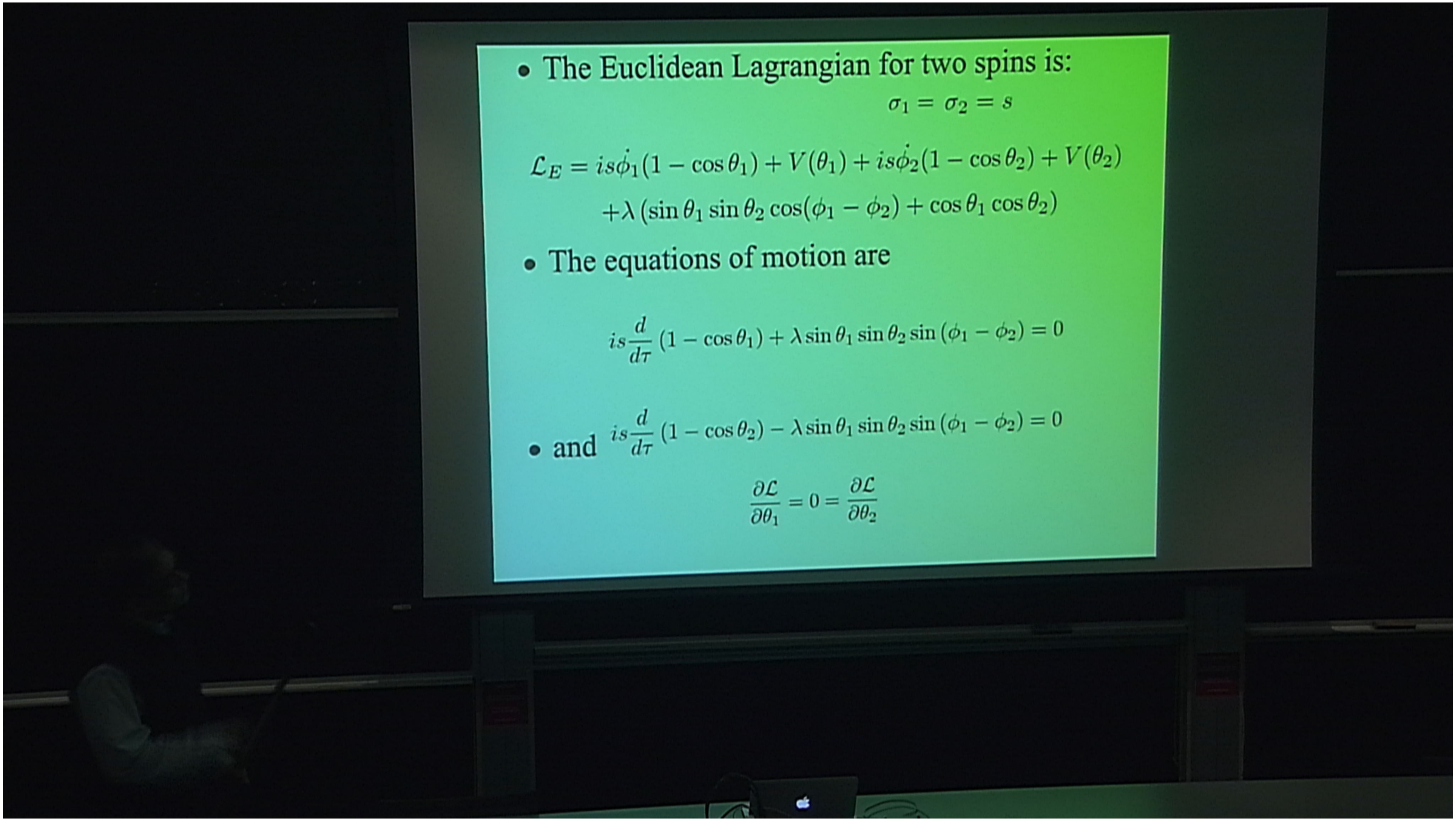
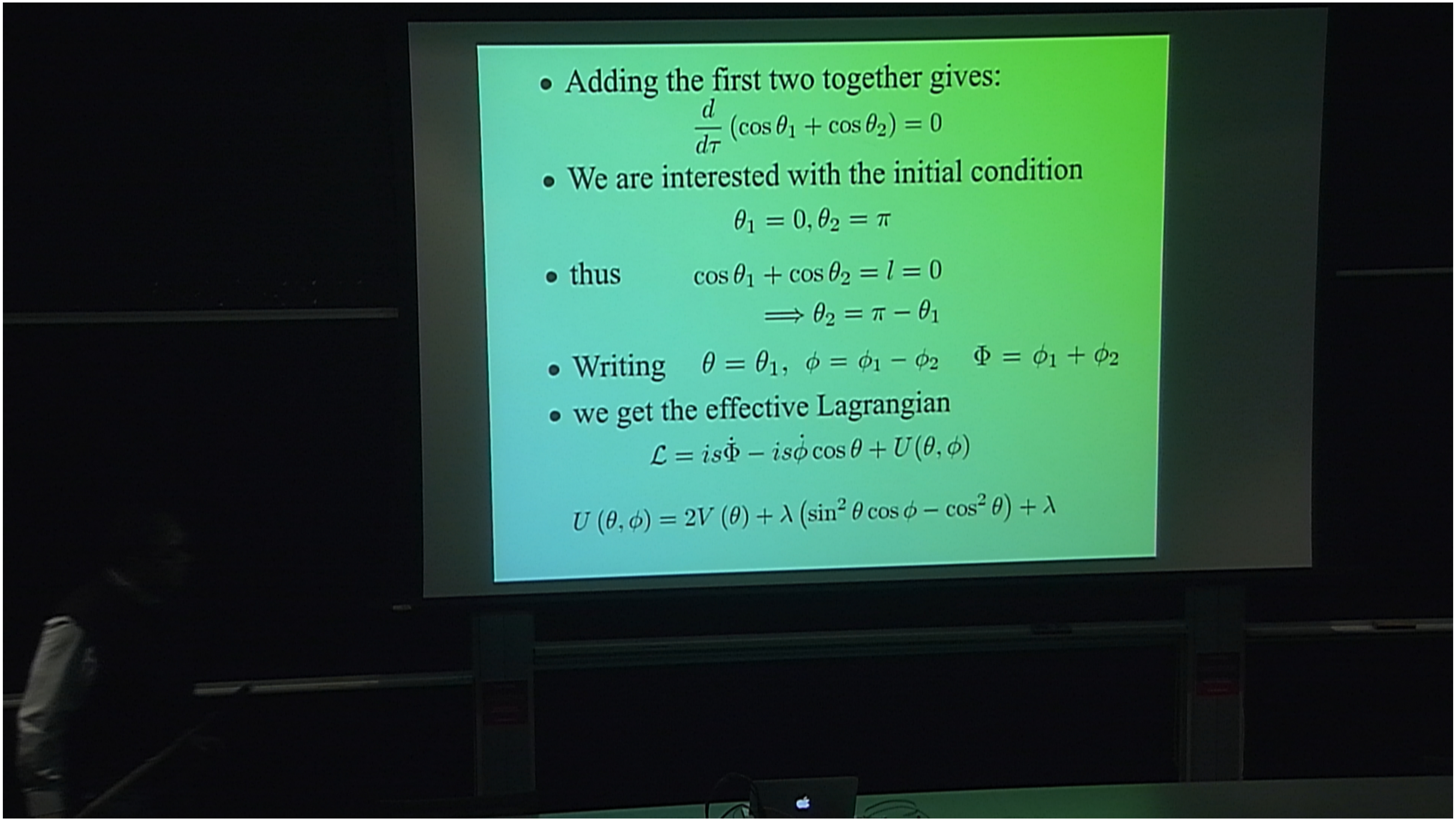
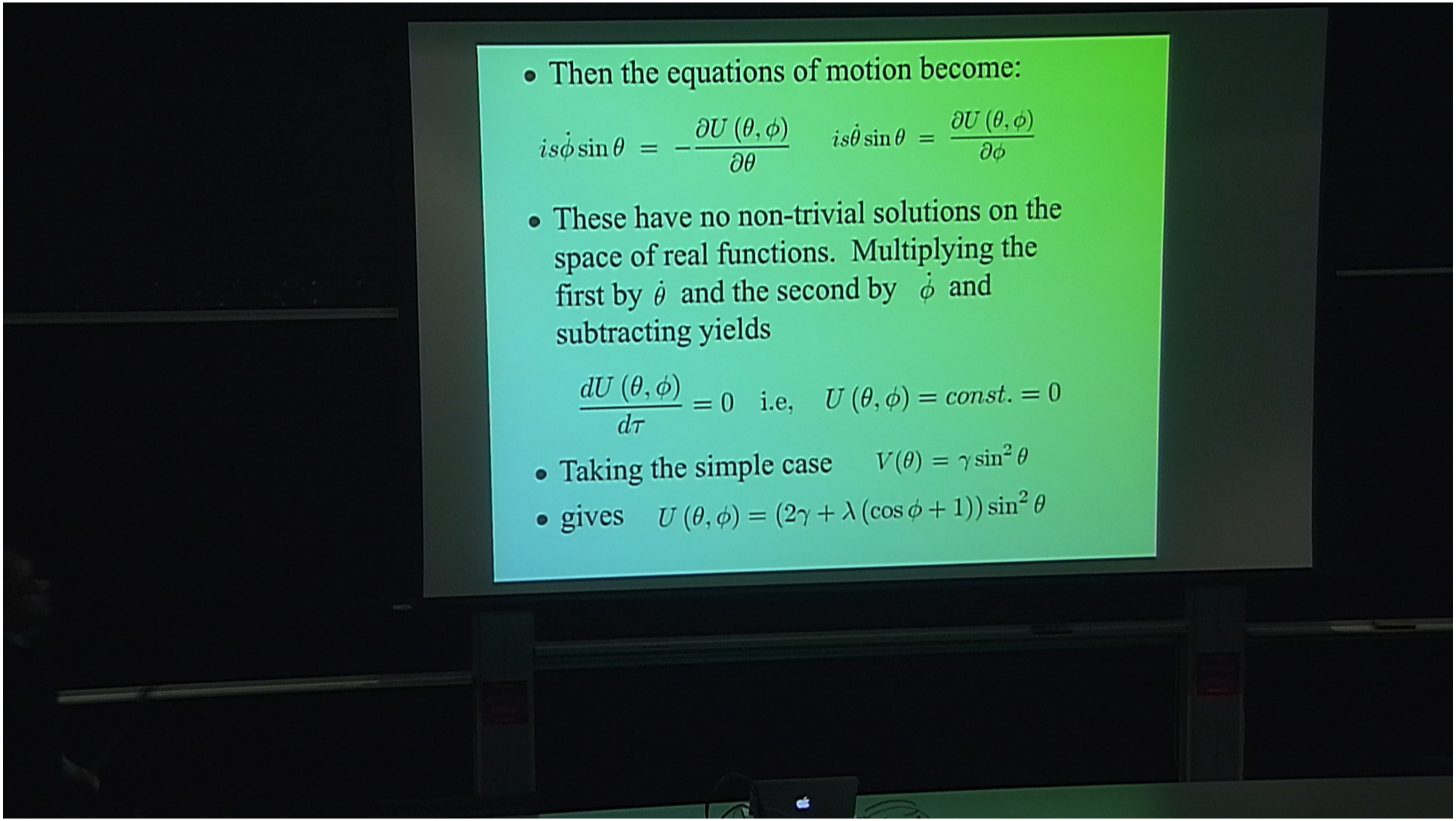
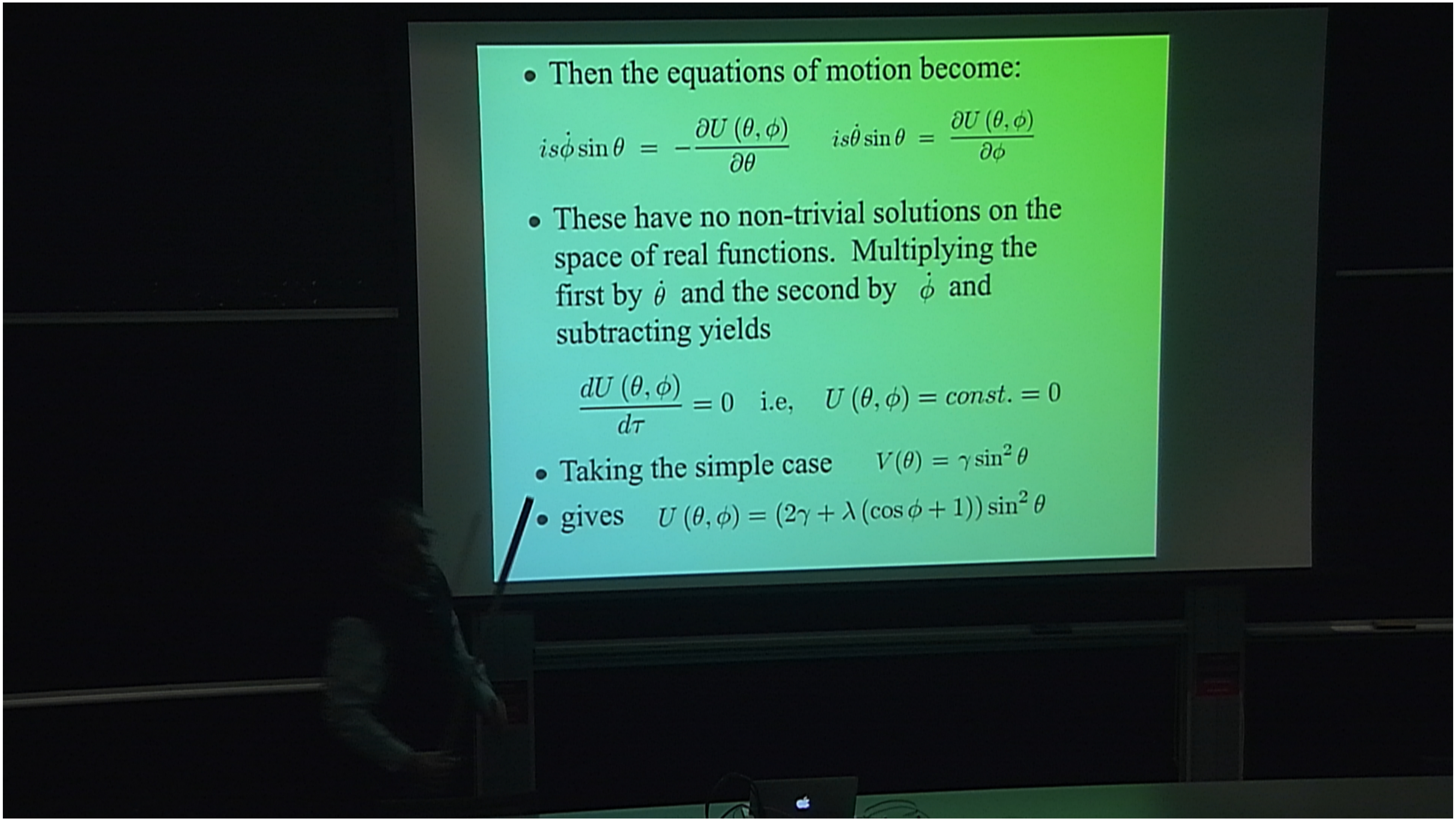

• The Euclidean Lagrangian for two spins is:
$\sigma_1 = \sigma_2 = s$
$\mathcal{L}_E = is\dot{\phi}_1(1-\cos\theta_1) + V(\theta_1) + is\dot{\phi}_2(1-\cos\theta_2) + V(\theta_2)$
$+\lambda\left(\sin\theta_1 \sin\theta_2 \cos(\phi_1-\phi_2) + \cos\theta_1\cos\theta_2\right)$
• The equations of motion are
$is\frac{d}{d\tau}\left(1-\cos\theta_1\right) + \lambda\sin\theta_1\sin\theta_2\sin\left(\phi_1-\phi_2\right) = 0$
• and $is\frac{d}{d\tau}\left(1-\cos\theta_2\right) - \lambda\sin\theta_1\sin\theta_2\sin\left(\phi_1-\phi_2\right) = 0$
$\frac{\partial\mathcal{L}}{\partial\theta_1} = 0 = \frac{\partial\mathcal{L}}{\partial\theta_2}$


• Adding the first two together gives:
$$\frac{d}{d\tau}\left(\cos\theta_1 + \cos\theta_2\right) = 0$$
• We are interested with the initial condition
$$\theta_1 = 0, \theta_2 = \pi$$
• thus $\cos\theta_1 + \cos\theta_2 = l = 0$
$$\Longrightarrow \theta_2 = \pi - \theta_1$$
• Writing $\theta = \theta_1, \ \phi = \phi_1 - \phi_2 \quad \Phi = \phi_1 + \phi_2$
• we get the effective Lagrangian
$$\mathcal{L} = is\dot{\Phi} - is\dot{\phi}\cos\theta + U(\theta, \phi)$$
$$U(\theta, \phi) = 2V(\theta) + \lambda\left(\sin^2\theta\cos\phi - \cos^2\theta\right) + \lambda$$


Then the equations of motion become:
$is\dot{\phi}\sin\theta = -\frac{\partial U(\theta,\phi)}{\partial\theta}$ $is\dot{\theta}\sin\theta = \frac{\partial U(\theta,\phi)}{\partial\phi}$
These have no non-trivial solutions on the space of real functions. Multiplying the first by $\dot{\theta}$ and the second by $\dot{\phi}$ and subtracting yields
$\frac{dU(\theta,\phi)}{d\tau} = 0$ i.e, $U(\theta,\phi) = const. = 0$
Taking the simple case $V(\theta) = \gamma\sin^2\theta$
gives $U(\theta,\phi) = (2\gamma + \lambda(\cos\phi + 1))\sin^2\theta$



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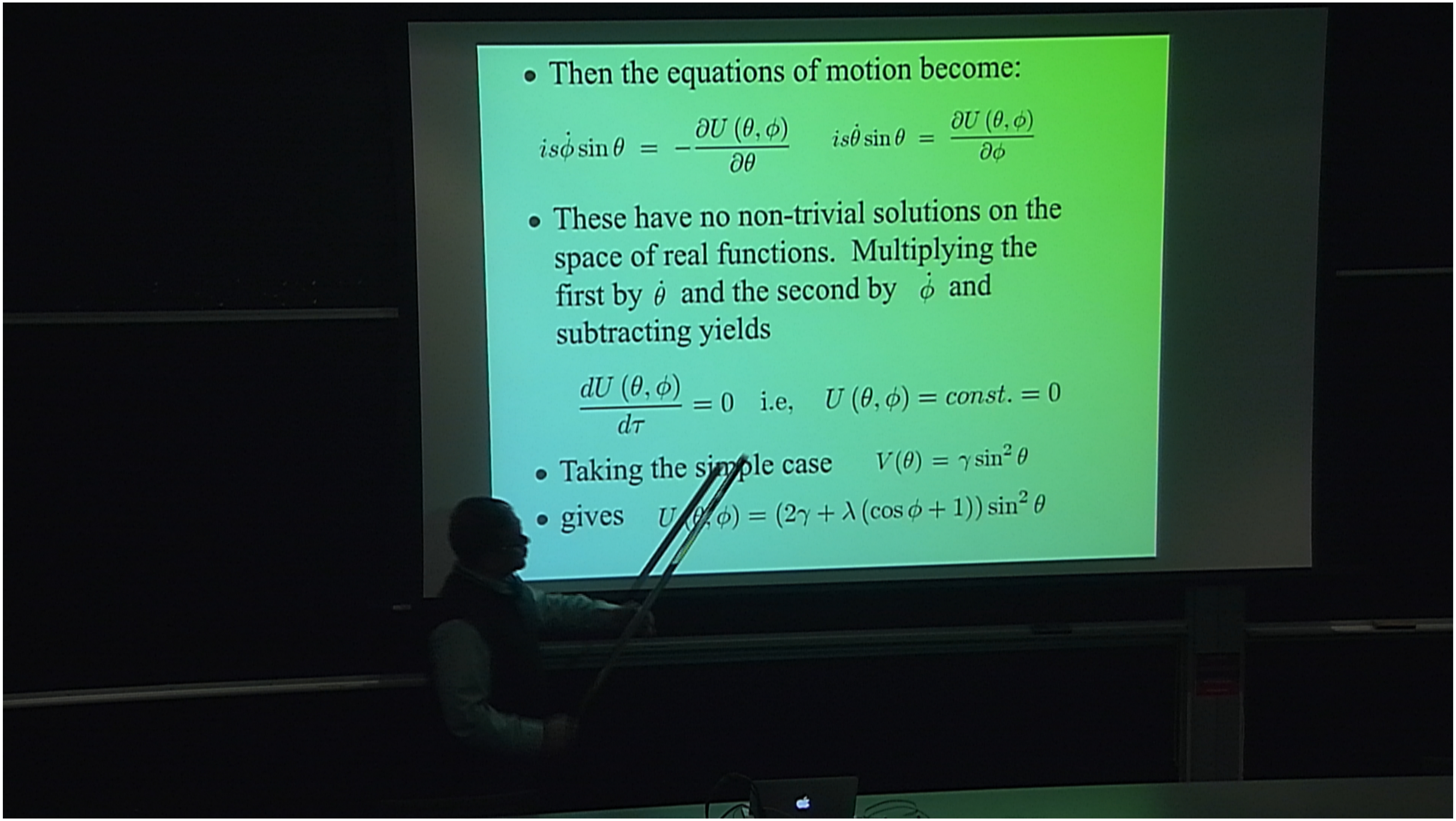

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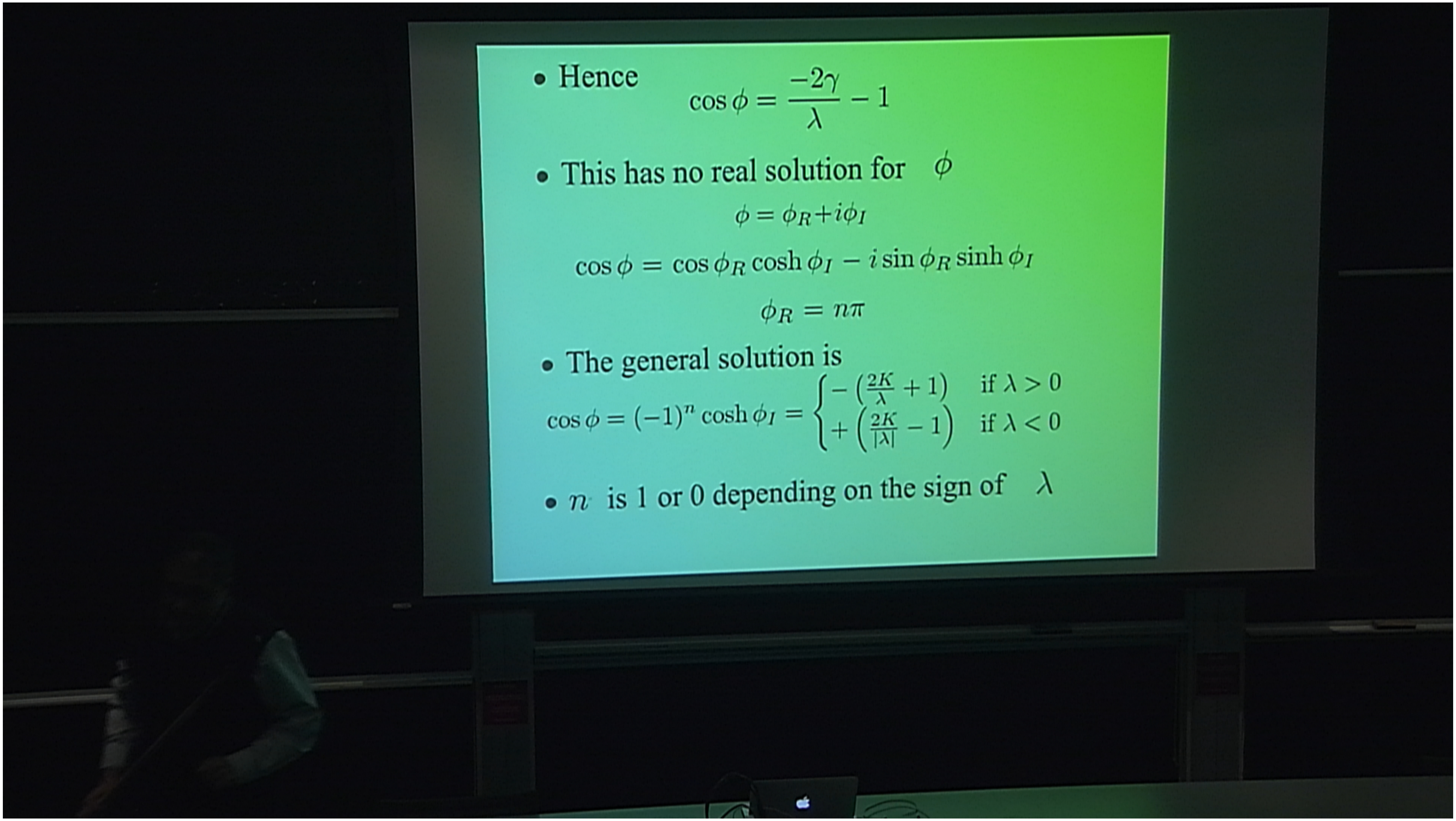
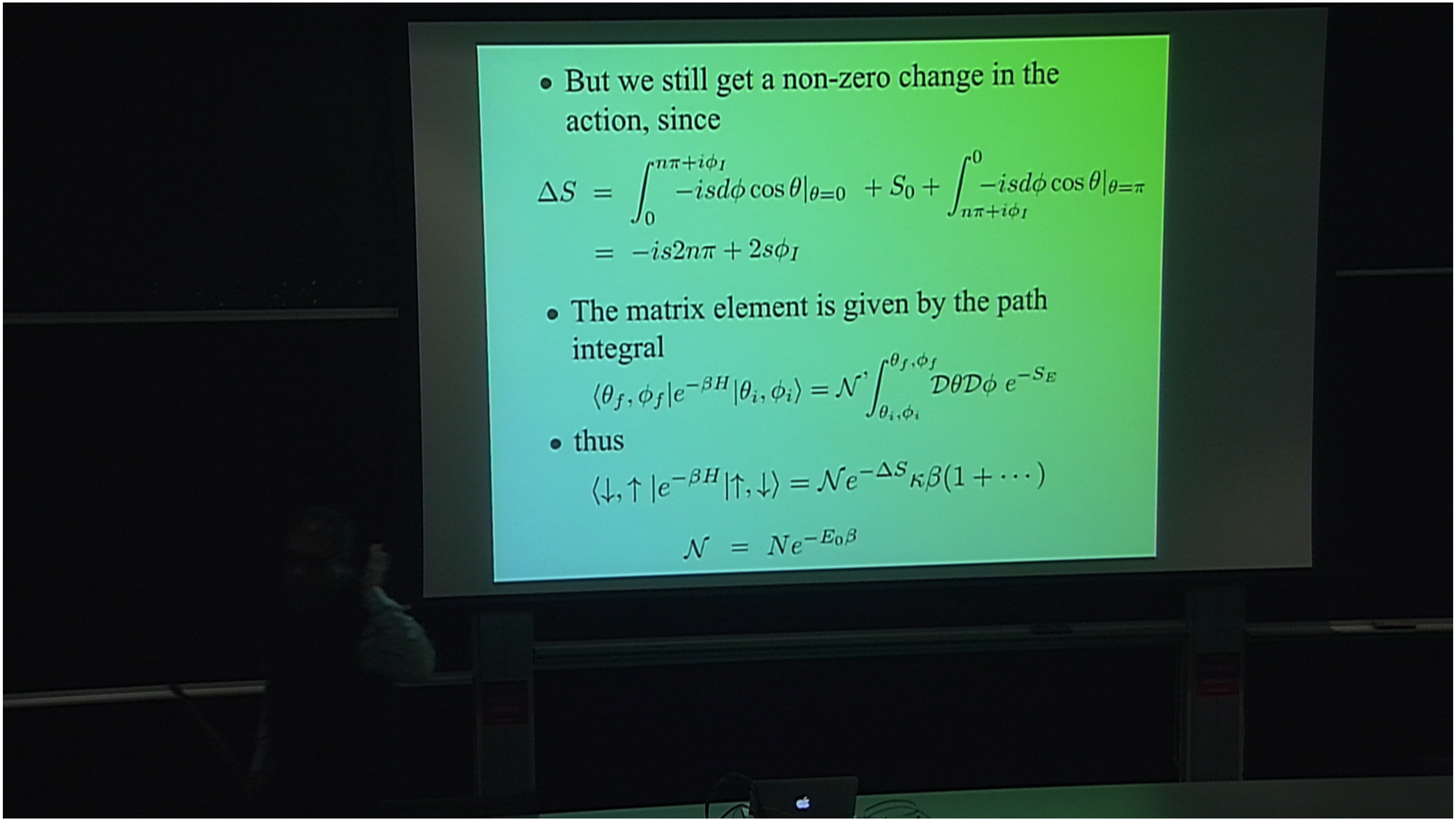
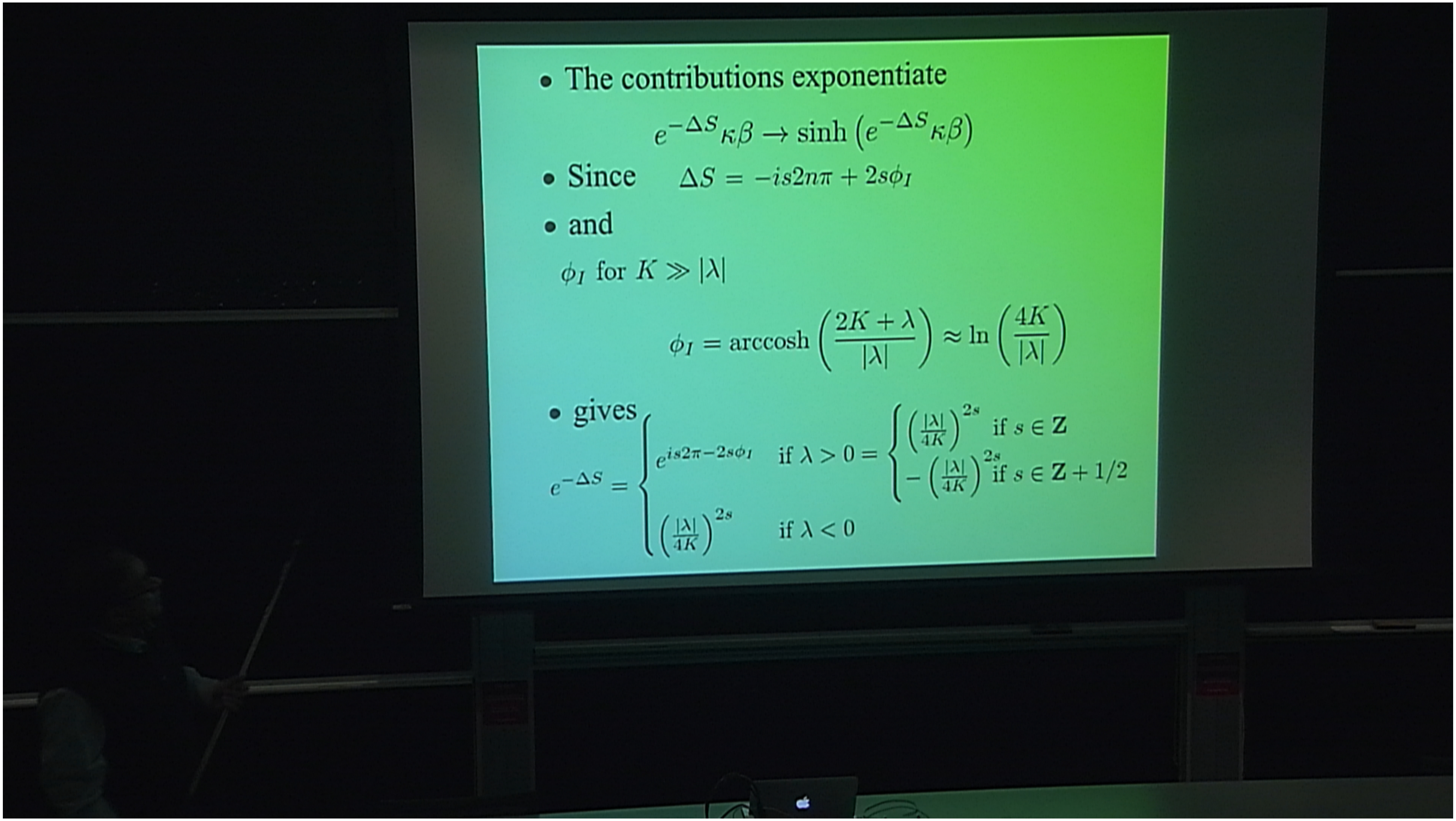
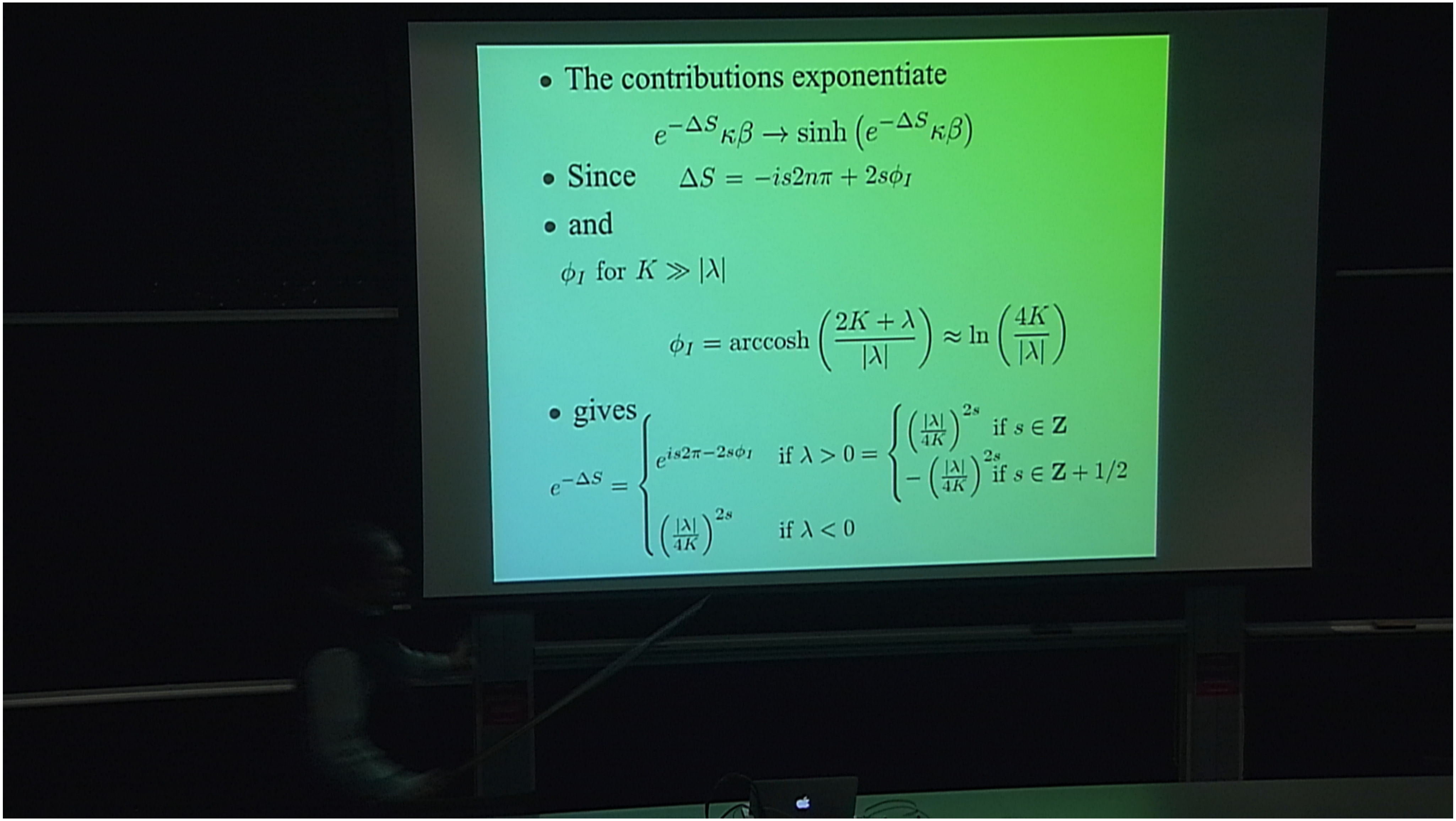


Hence
$\cos\phi = \frac{-2\gamma}{\lambda} - 1$
This has no real solution for ϕ
$\phi = \phi_R + i\phi_I$
$\cos\phi = \cos\phi_R \cosh\phi_I - i\sin\phi_R \sinh\phi_I$
$\phi_R = n\pi$
The general solution is
$\cos\phi = (-1)^n \cosh\phi_I = \begin{cases} -\left(\frac{2K}{\lambda}+1\right) & \text{if } \lambda > 0 \\ +\left(\frac{2K}{|\lambda|}-1\right) & \text{if } \lambda < 0 \end{cases}$
n is 1 or 0 depending on the sign of λ


• But we still get a non-zero change in the action, since
$\Delta S = \int_0^{n\pi+i\phi_I} -isd\phi \cos\theta|_{\theta=0} + S_0 + \int_{n\pi+i\phi_I}^{0} -isd\phi \cos\theta|_{\theta=\pi}$
$= -is2n\pi + 2s\phi_I$
• The matrix element is given by the path integral
$\langle\theta_f,\phi_f|e^{-\beta H}|\theta_i,\phi_i\rangle = \mathcal{N}'\int_{\theta_i,\phi_i}^{\theta_f,\phi_f}\mathcal{D}\theta\mathcal{D}\phi\, e^{-S_E}$
• thus
$\langle\downarrow,\uparrow|e^{-\beta H}|\uparrow,\downarrow\rangle = \mathcal{N}e^{-\Delta S}\kappa\beta(1+\cdots)$
$\mathcal{N} = Ne^{-E_0\beta}$



• The contributions exponentiate
$e^{-\Delta S}\kappa\beta \to \sinh\left(e^{-\Delta S}\kappa\beta\right)$
• Since $\Delta S = -is2n\pi + 2s\phi_I$
• and
ϕ_I for $K \gg |\lambda|$
$\phi_I = \text{arccosh}\left(\frac{2K+\lambda}{|\lambda|}\right) \approx \ln\left(\frac{4K}{|\lambda|}\right)$
• gives
$e^{-\Delta S} = \begin{cases} e^{is2\pi - 2s\phi_I} & \text{if } \lambda > 0 = \begin{cases} \left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } s \in \mathbf{Z} \\ -\left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } s \in \mathbf{Z}+1/2 \end{cases} \\ \left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } \lambda < 0 \end{cases}$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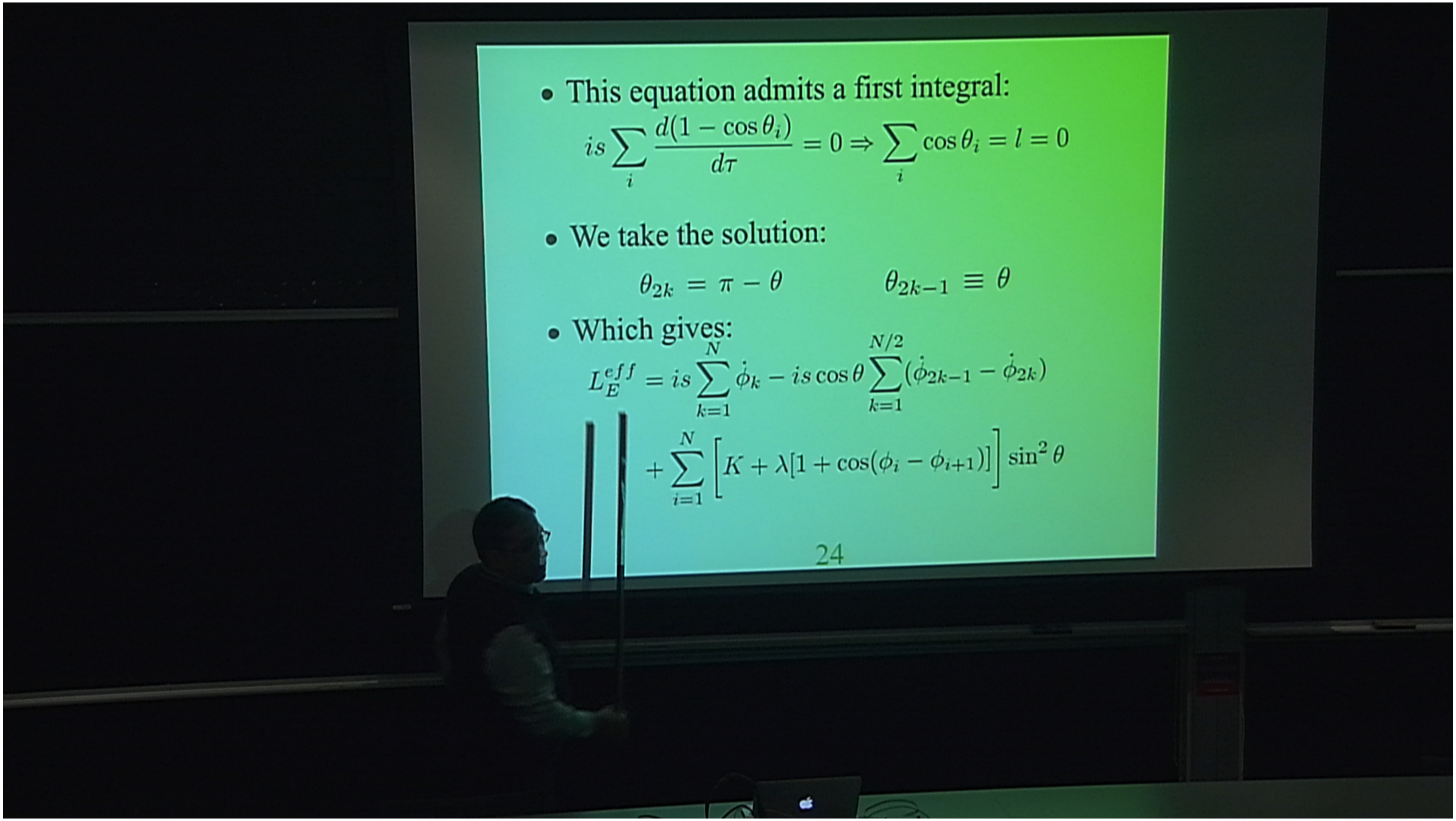

This equation admits a first integral:
$is \sum_i \frac{d(1-\cos\theta_i)}{d\tau} = 0 \Rightarrow \sum_i \cos\theta_i = l = 0$
We take the solution:
$\theta_{2k} = \pi - \theta \qquad \theta_{2k-1} \equiv \theta$
Which gives:
$L_E^{eff} = is \sum_{k=1}^{N} \dot{\phi}_k - is\cos\theta \sum_{k=1}^{N/2} (\dot{\phi}_{2k-1} - \dot{\phi}_{2k})$
$+ \sum_{i=1}^{N} \Big[K + \lambda[1 + \cos(\phi_i - \phi_{i+1})] \Big] \sin^2\theta$
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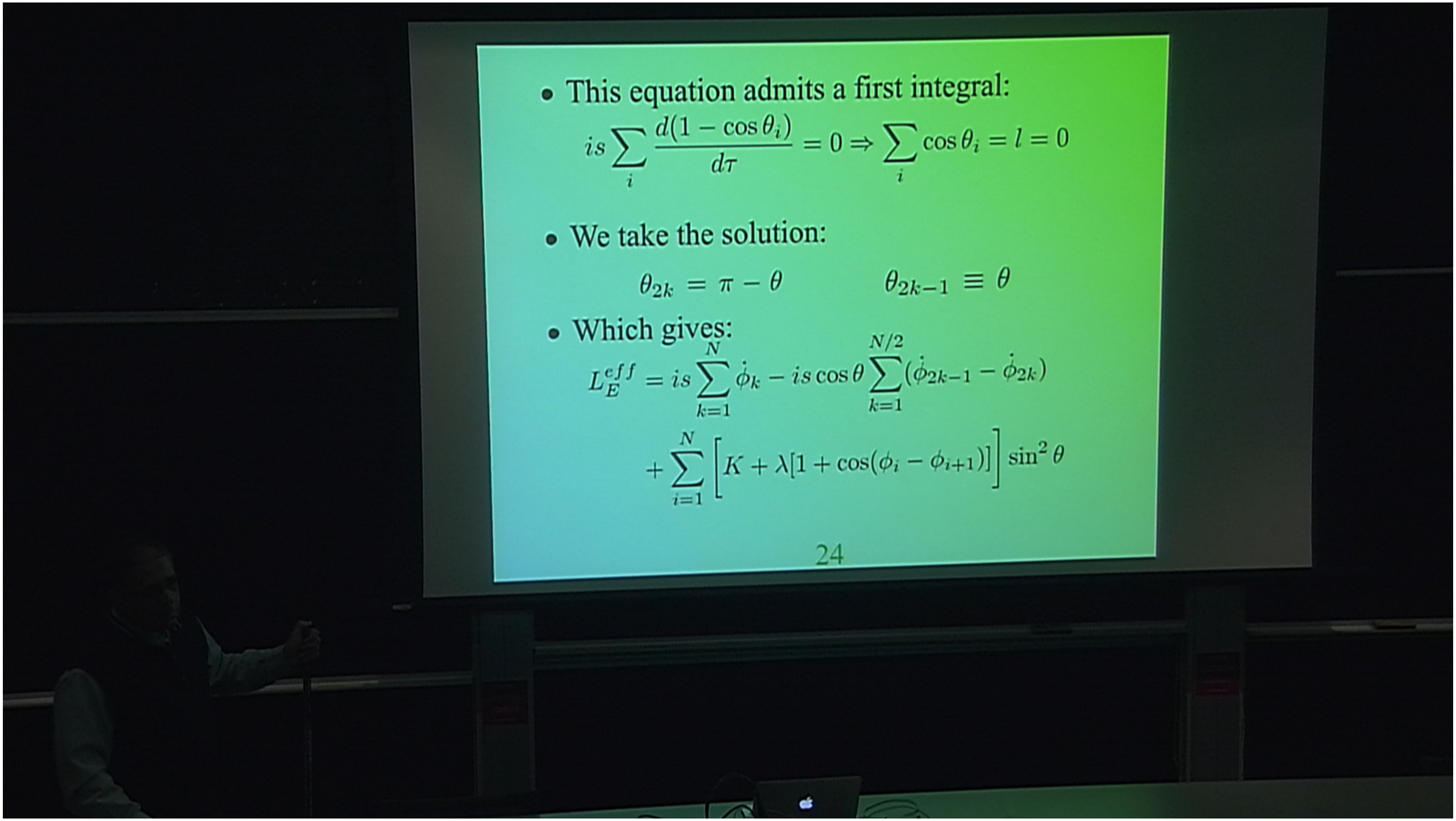
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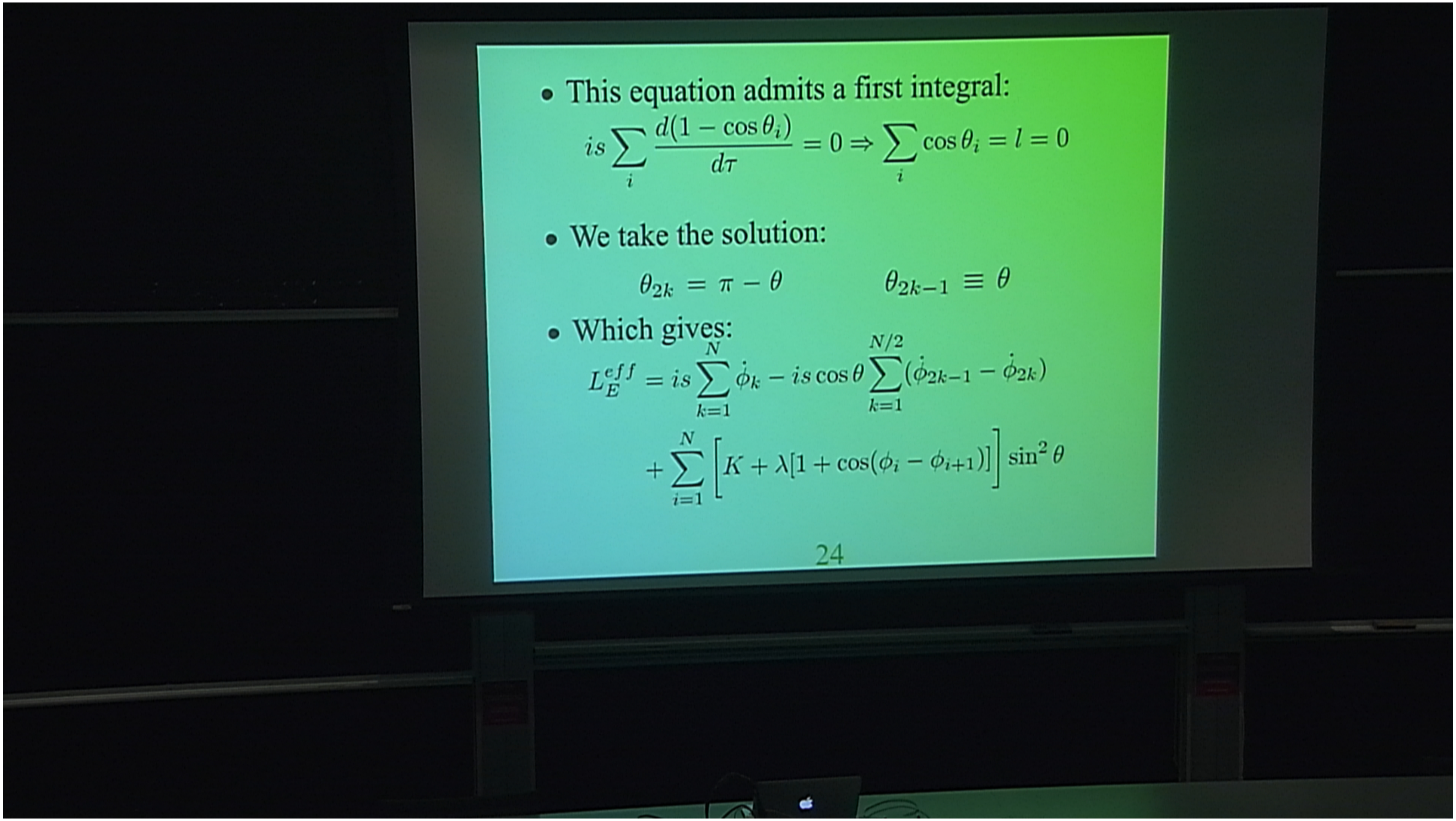
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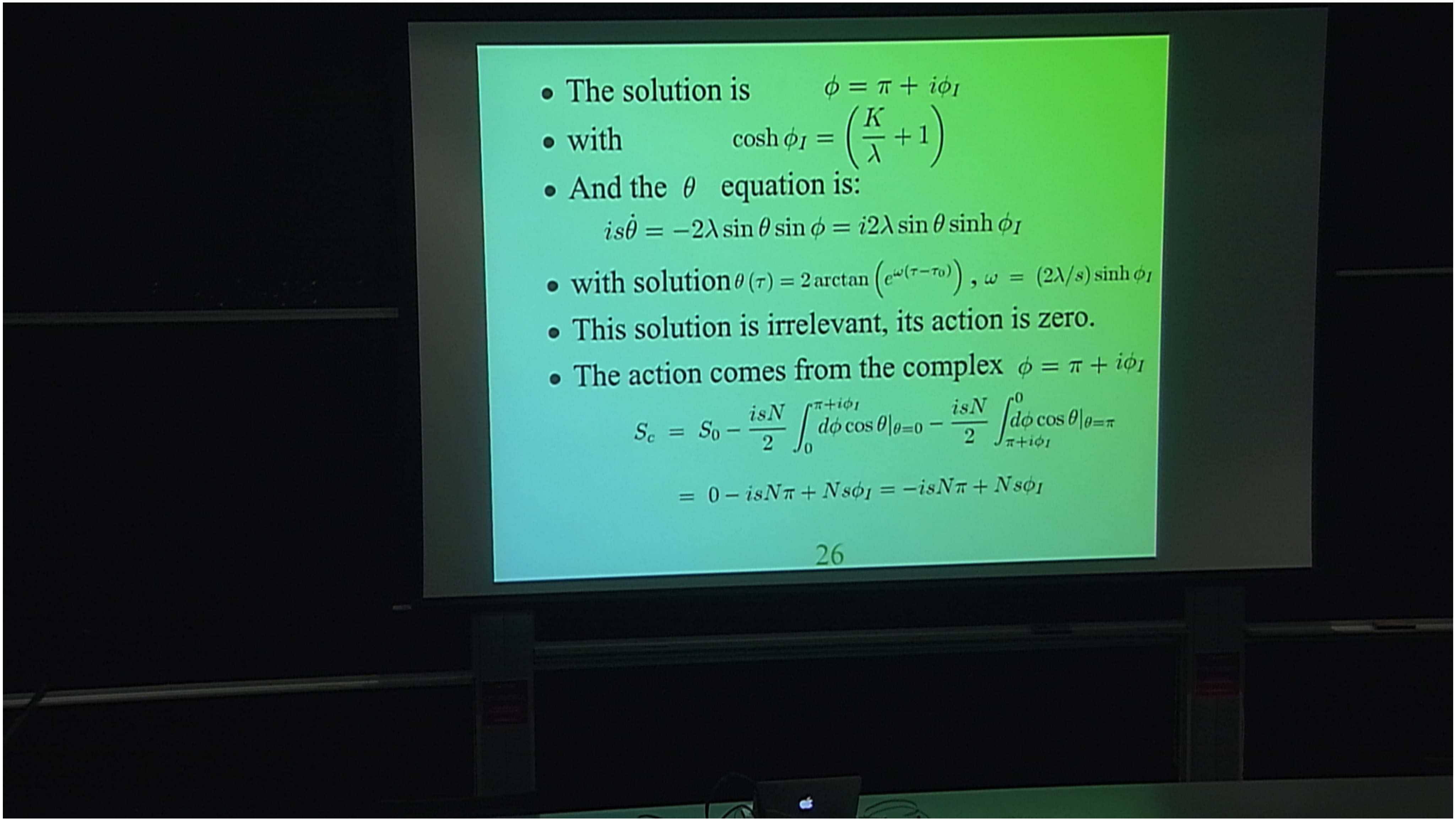
The solution is $\phi = \pi + i\phi_I$
with $\cosh \phi_I = \left(\frac{K}{\lambda} + 1 \right)$
And the θ equation is:
$is\dot{\theta} = -2\lambda \sin\theta \sin\phi = i2\lambda \sin\theta \sinh\phi_I$
with solution $\theta(\tau) = 2 \arctan\left(e^{\omega(\tau-\tau_0)}\right)$, $\omega = (2\lambda/s)\sinh\phi_I$
This solution is irrelevant, its action is zero.
The action comes from the complex $\phi = \pi + i\phi_I$
$S_c = S_0 - \frac{isN}{2}\int_0^{\pi+i\phi_I} d\phi \cos\theta|_{\theta=0} - \frac{isN}{2}\int_{\pi+i\phi_I}^{0} d\phi \cos\theta|_{\theta=\pi}$
$= 0 - isN\pi + Ns\phi_I = -isN\pi + Ns\phi_I$
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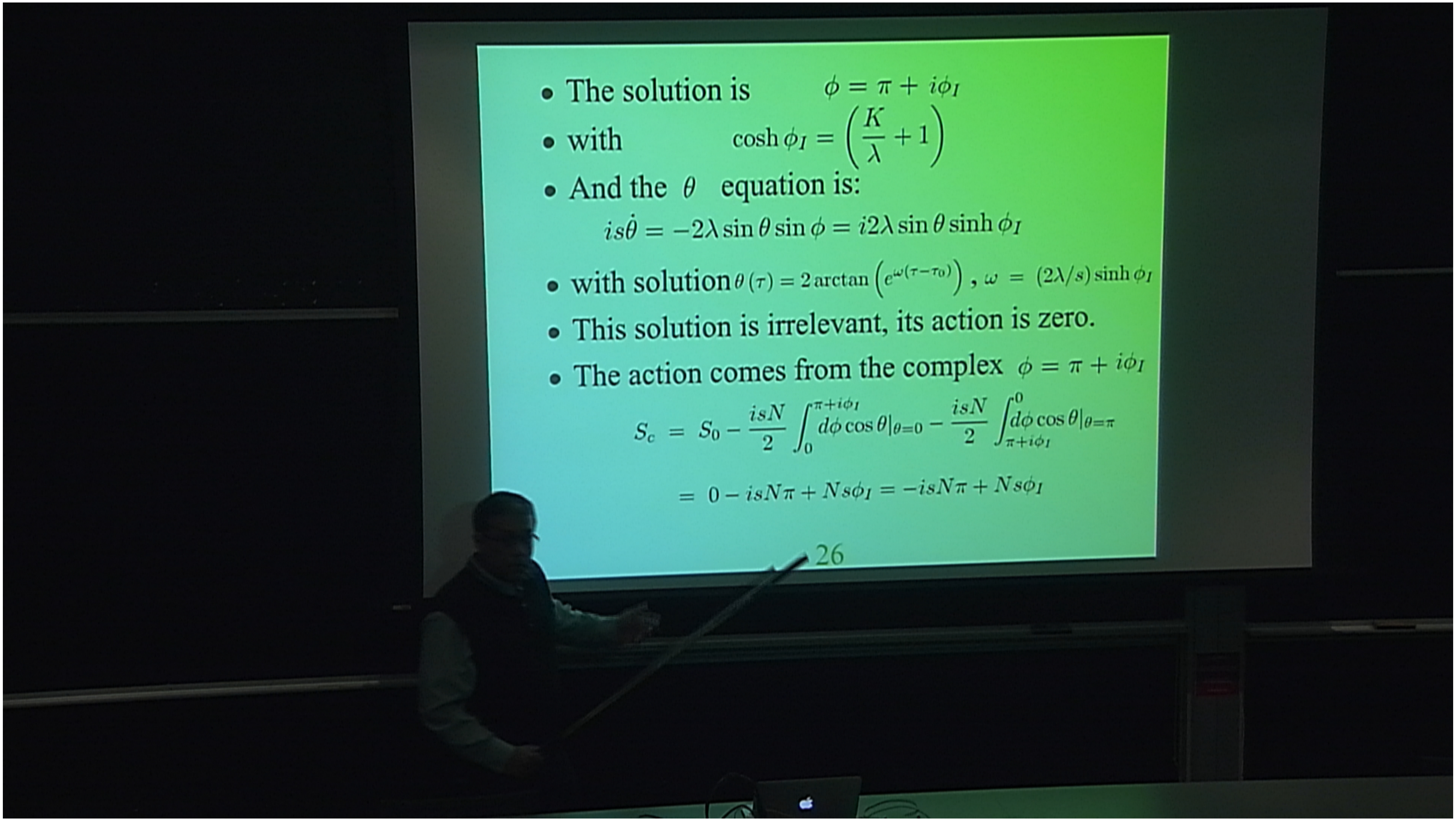
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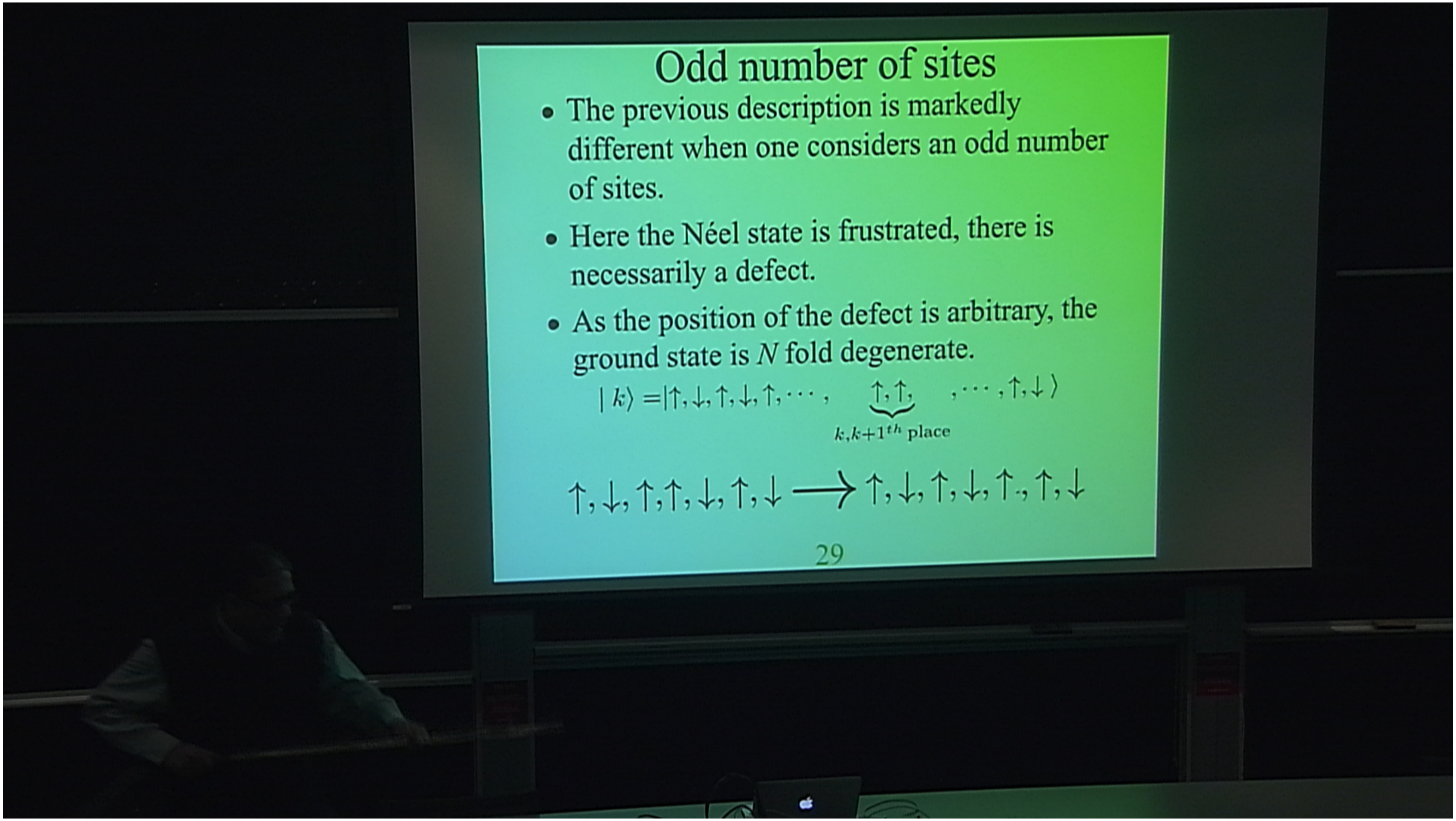
Odd number of sites
• The previous description is markedly different when one considers an odd number of sites.
• Here the Néel state is frustrated, there is necessarily a defect.
• As the position of the defect is arbitrary, the ground state is N fold degenerate.
$| k\rangle = |\uparrow,\downarrow,\uparrow,\downarrow,\uparrow,\cdots, \underbrace{\uparrow,\uparrow,}_{k,k+1^{th}\text{ place}} ,\cdots,\uparrow,\downarrow\rangle$
$\uparrow,\downarrow,\uparrow,\uparrow,\downarrow,\uparrow,\downarrow \longrightarrow \uparrow,\downarrow,\uparrow,\downarrow,\uparrow,\uparrow,\downarrow$
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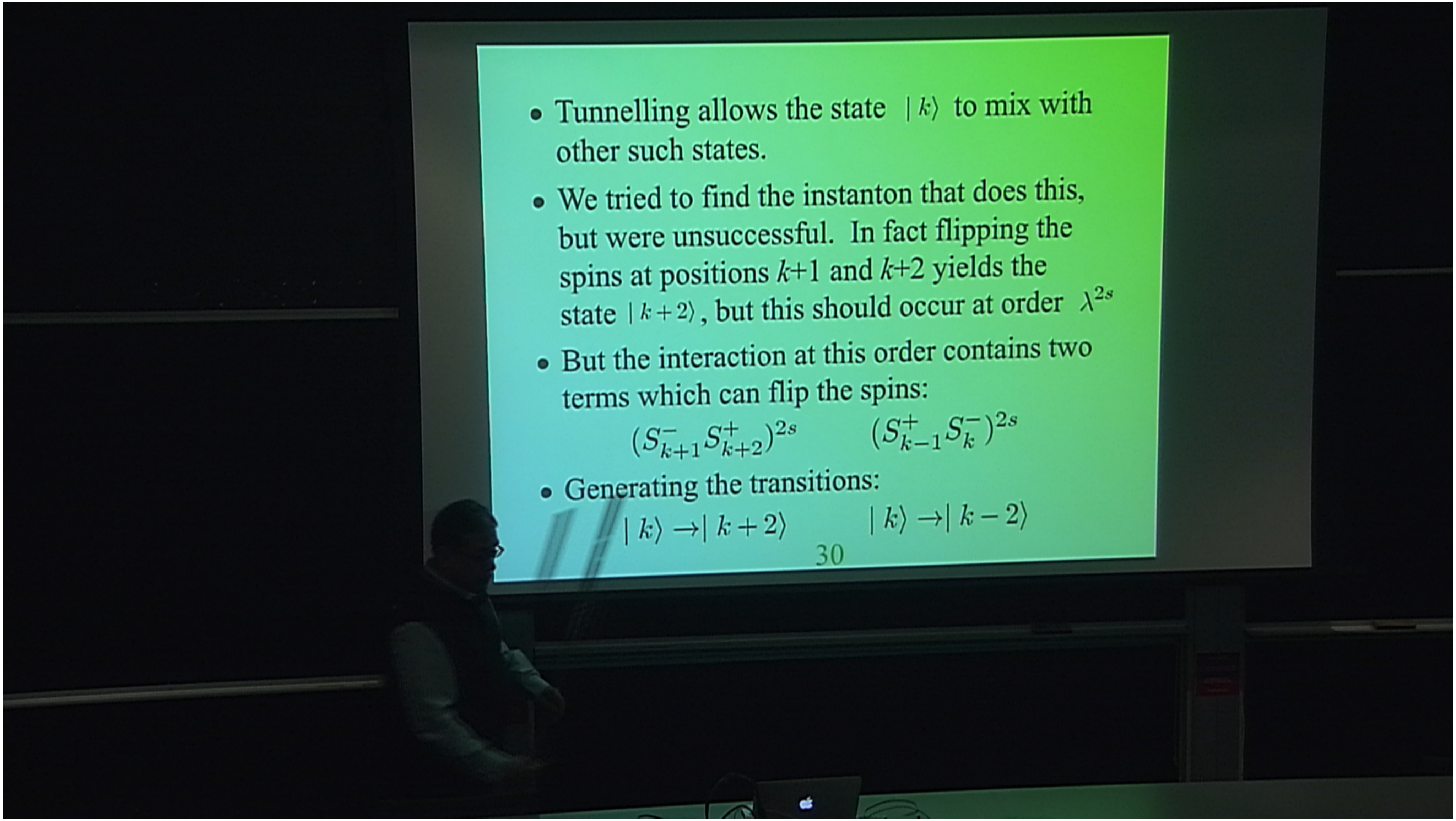
Tunnelling allows the state $|k\rangle$ to mix with other such states.
We tried to find the instanton that does this, but were unsuccessful. In fact flipping the spins at positions $k+1$ and $k+2$ yields the state $|k+2\rangle$, but this should occur at order λ^{2s}
But the interaction at this order contains two terms which can flip the spins:
$(S^-_{k+1}S^+_{k+2})^{2s}$ $(S^+_{k-1}S^-_k)^{2s}$
Generating the transitions:
$|k\rangle \rightarrow |k+2\rangle$ $|k\rangle \rightarrow |k-2\rangle$
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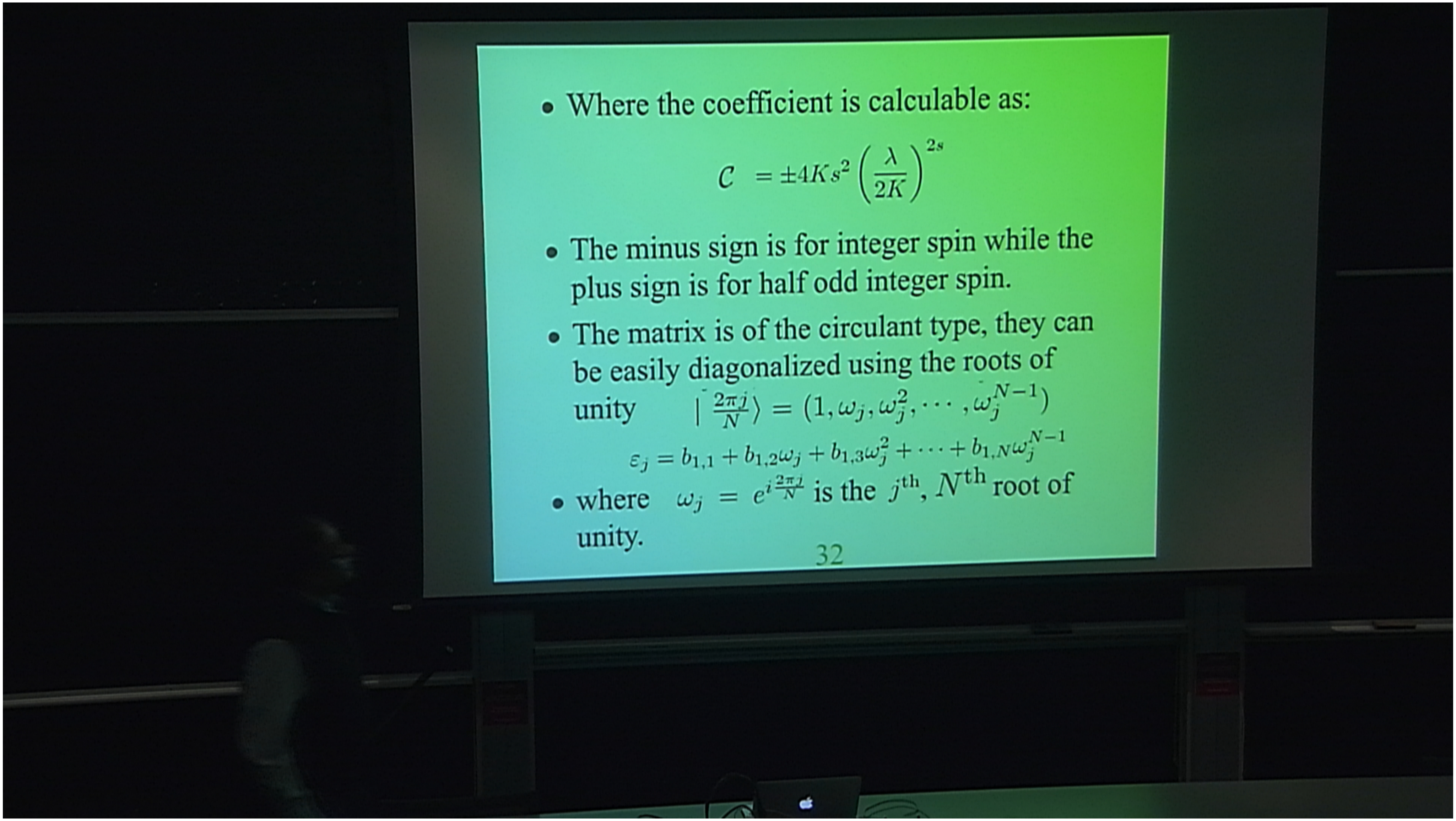
• Where the coefficient is calculable as:
$\mathcal{C} = \pm 4Ks^2 \left(\frac{\lambda}{2K}\right)^{2s}$
• The minus sign is for integer spin while the plus sign is for half odd integer spin.
• The matrix is of the circulant type, they can be easily diagonalized using the roots of unity $|\frac{2\pi j}{N}\rangle = (1, \omega_j, \omega_j^2, \cdots, \omega_j^{N-1})$
$\varepsilon_j = b_{1,1} + b_{1,2}\omega_j + b_{1,3}\omega_j^2 + \cdots + b_{1,N}\omega_j^{N-1}$
• where $\omega_j = e^{i\frac{2\pi j}{N}}$ is the j^{th}, N^{th} root of unity.
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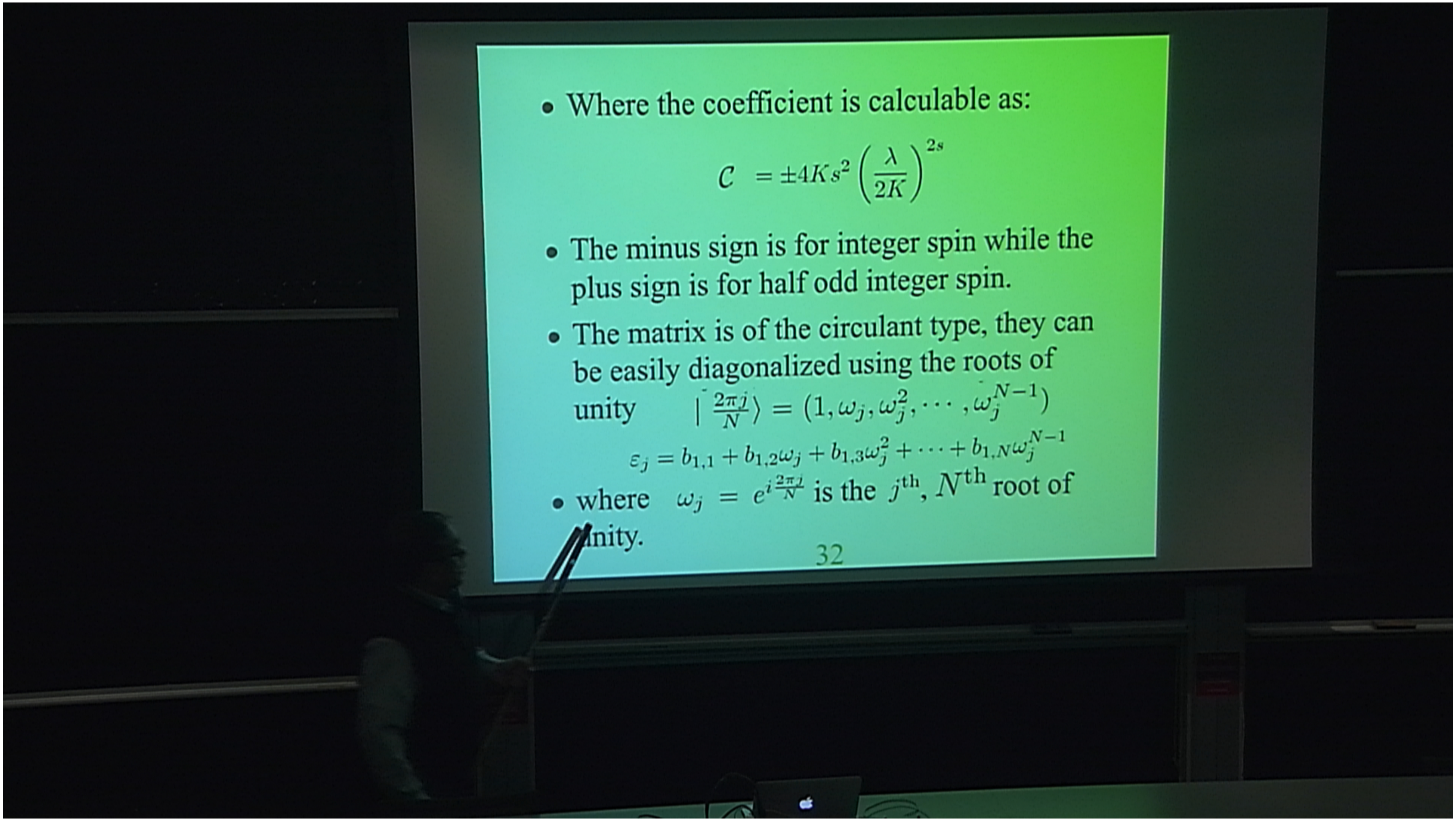
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• The matrix is of the circulant type, they can be easily diagonalized using the roots of unity $|\frac{2\pi j}{N}\rangle = (1, \omega_j, \omega_j^2, \cdots, \omega_j^{N-1})$
$\varepsilon_j = b_{1,1} + b_{1,2}\omega_j + b_{1,3}\omega_j^2 + \cdots + b_{1,N}\omega_j^{N-1}$
• where $\omega_j = e^{i\frac{2\pi j}{N}}$ is the $j^{\rm th}$, $N^{\rm th}$ root of nity.
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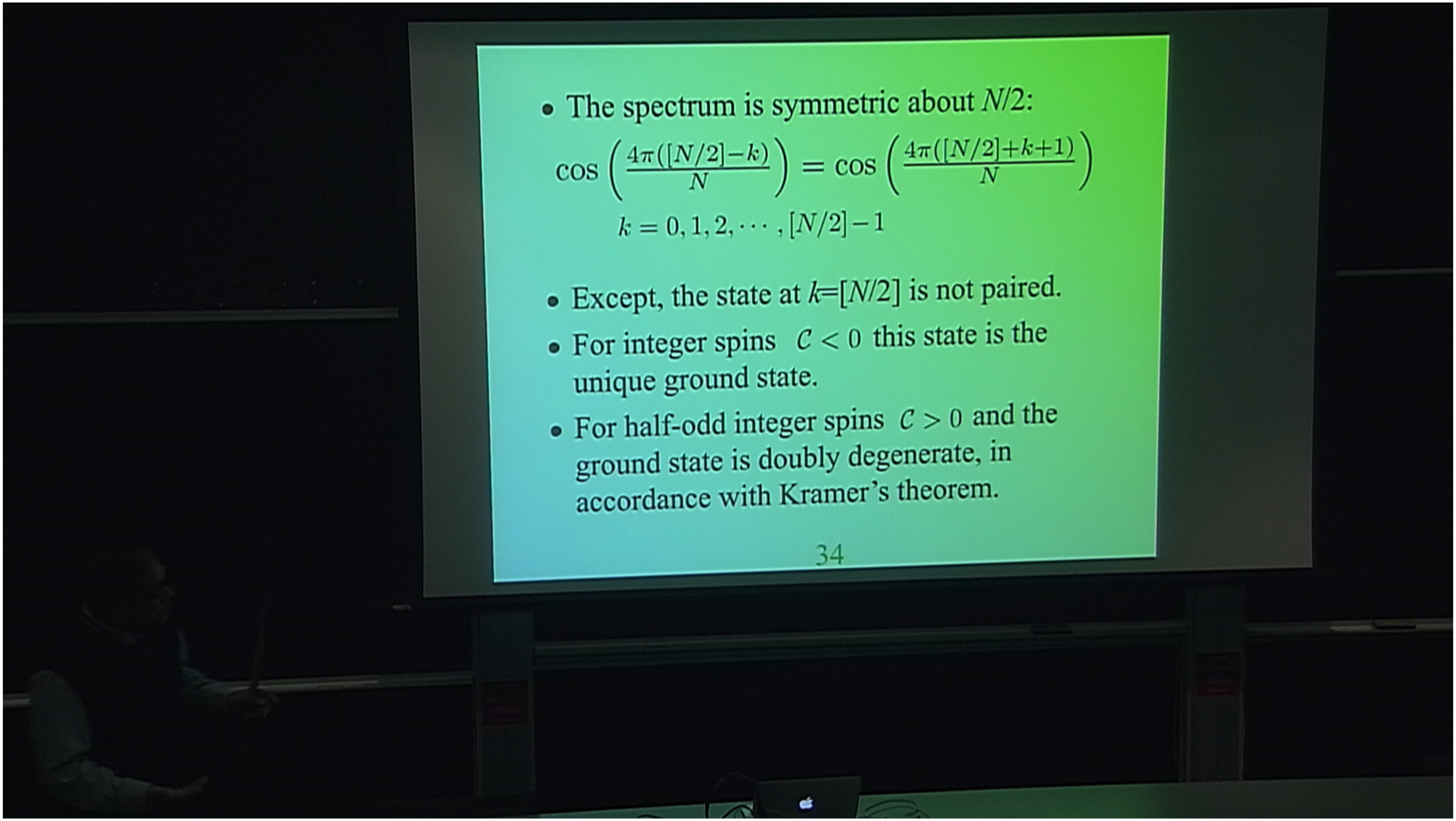
The spectrum is symmetric about N/2:
$\cos\left(\frac{4\pi([N/2]-k)}{N}\right) = \cos\left(\frac{4\pi([N/2]+k+1)}{N}\right)$
$k = 0, 1, 2, \cdots, [N/2]-1$
Except, the state at k=[N/2] is not paired.
For integer spins $C < 0$ this state is the unique ground state.
For half-odd integer spins $C > 0$ and the ground state is doubly degenerate, in accordance with Kramer's theorem.
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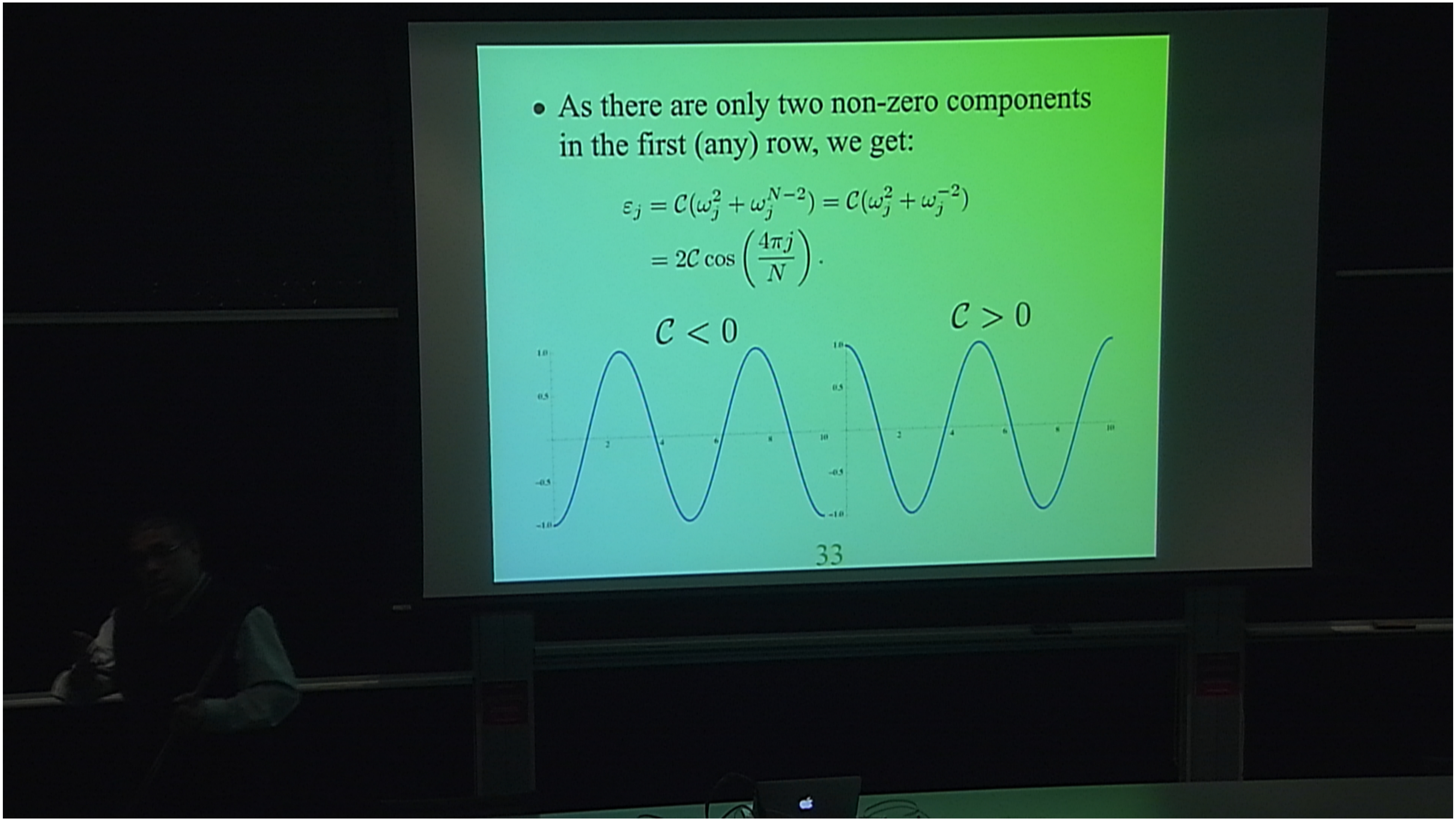
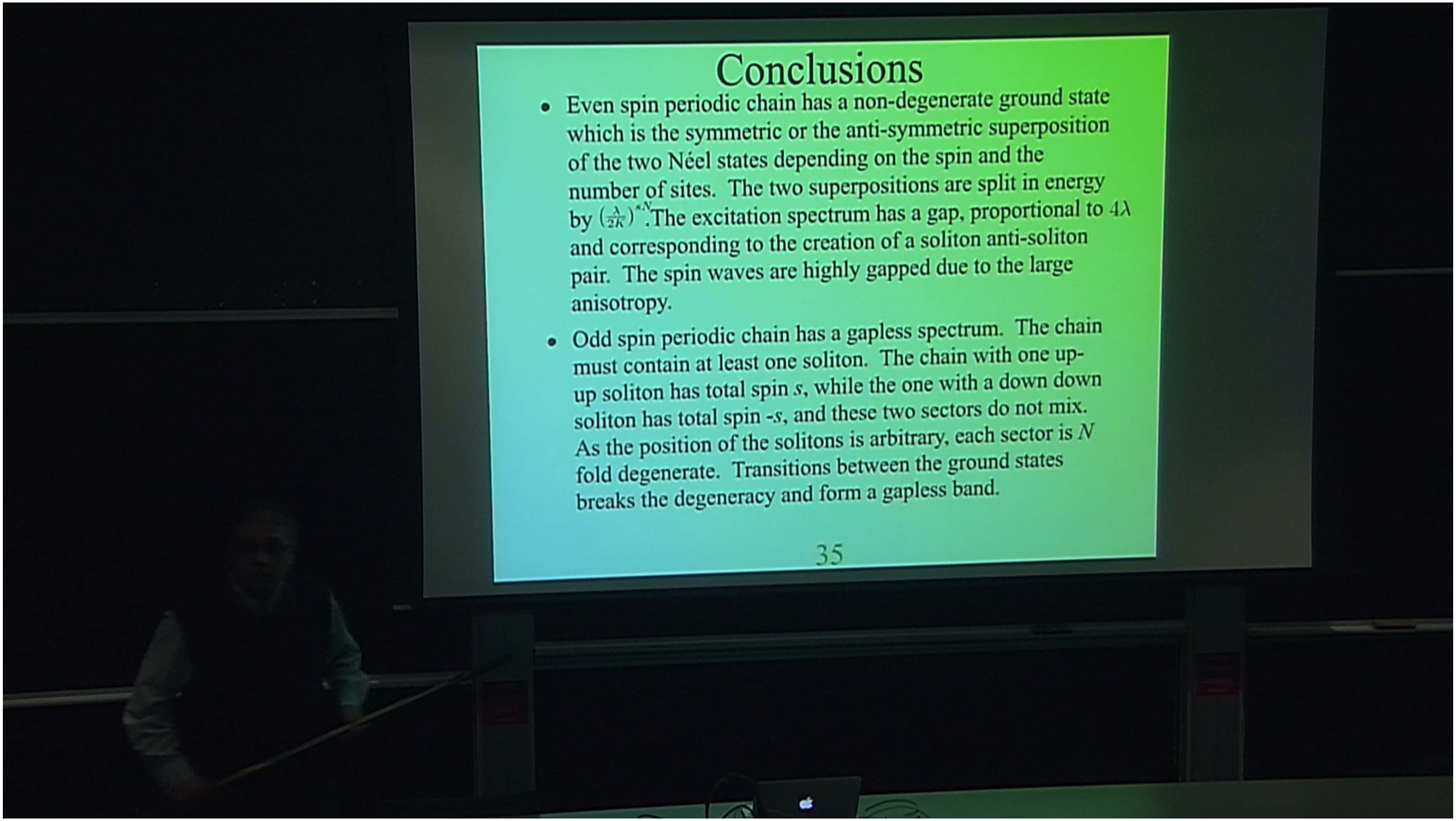

As there are only two non-zero components in the first (any) row, we get:
$\varepsilon_j = \mathcal{C}(\omega_j^2 + \omega_j^{N-2}) = \mathcal{C}(\omega_j^2 + \omega_j^{-2})$
$= 2\mathcal{C} \cos\left(\frac{4\pi j}{N}\right).$
$\mathcal{C} < 0$
$\mathcal{C} > 0$
33


Conclusions
• Even spin periodic chain has a non-degenerate ground state which is the symmetric or the anti-symmetric superposition of the two Néel states depending on the spin and the number of sites. The two superpositions are split in energy by $(\frac{\lambda}{2k})^{sN}$. The excitation spectrum has a gap, proportional to 4λ and corresponding to the creation of a soliton anti-soliton pair. The spin waves are highly gapped due to the large anisotropy.
• Odd spin periodic chain has a gapless spectrum. The chain must contain at least one soliton. The chain with one up-up soliton has total spin s, while the one with a down down soliton has total spin $-s$, and these two sectors do not mix. As the position of the solitons is arbitrary, each sector is N fold degenerate. Transitions between the ground states breaks the degeneracy and form a gapless band.
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