Title: Rigorous adiabatic estimates using integration by parts

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Abstract:

Overview

- Adiabatic theorem with explicit error bound
- Traditional adiabatics versus adiabatic quantum computing: two different ways of looking at the theorem
- Sketch of proof following the lines of
  Avron, Seiler, Yaffe, CMP 1987
  & Klein, Seiler CMP 1990
  Reichardt STOC 2004
- Application to interpolating Hamiltonians: a simple example (search in unordered list)

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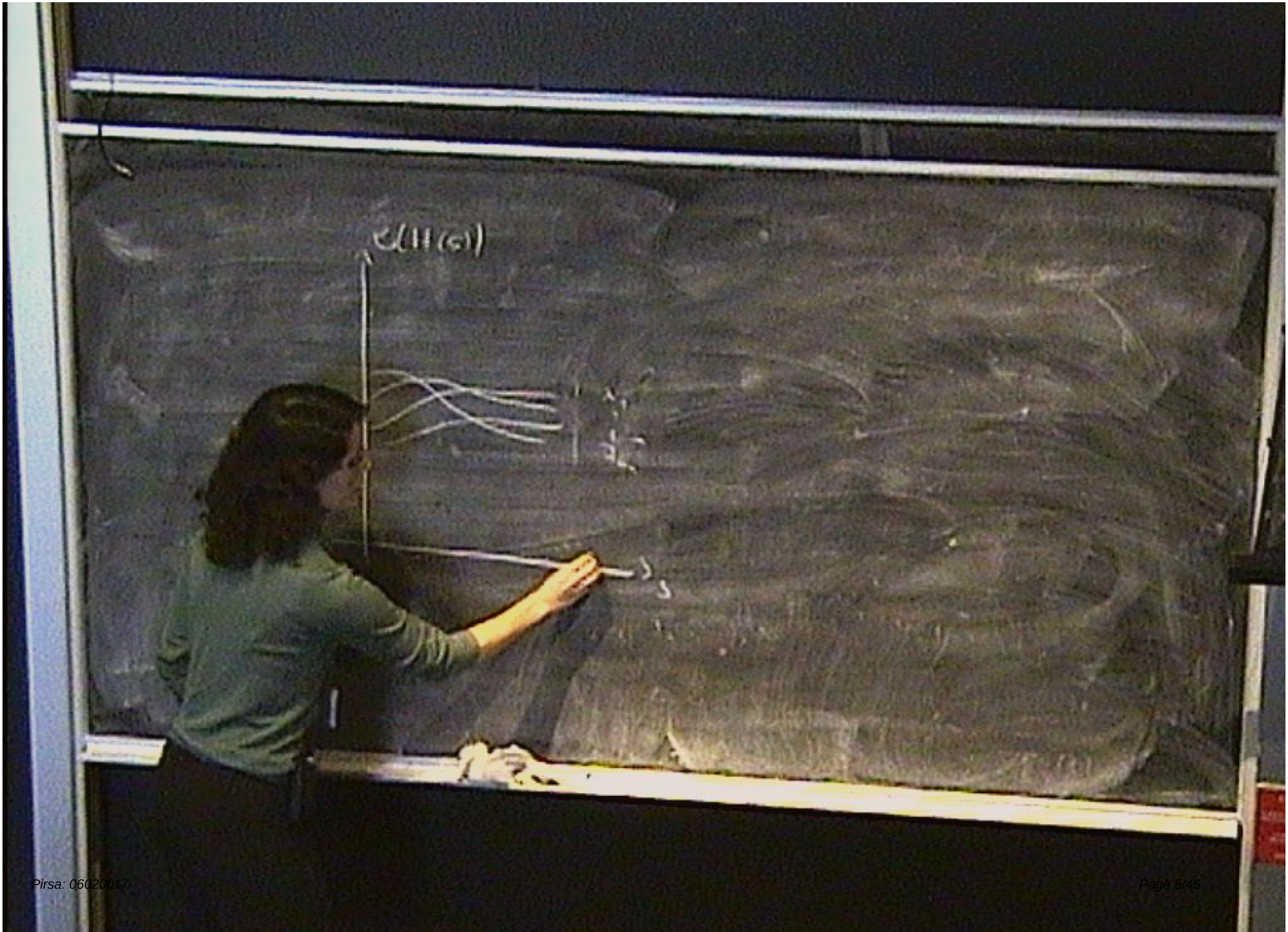
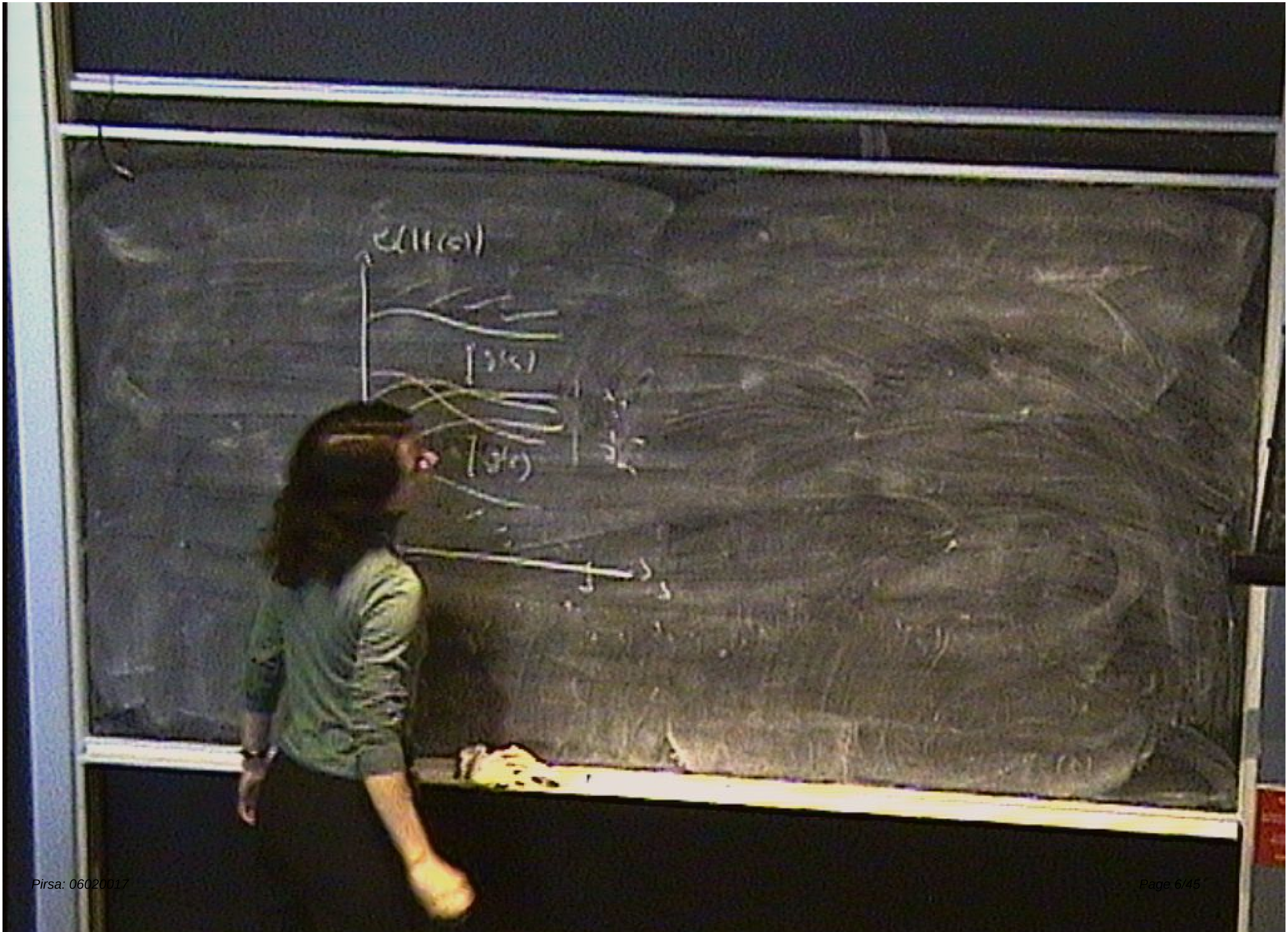
Setting

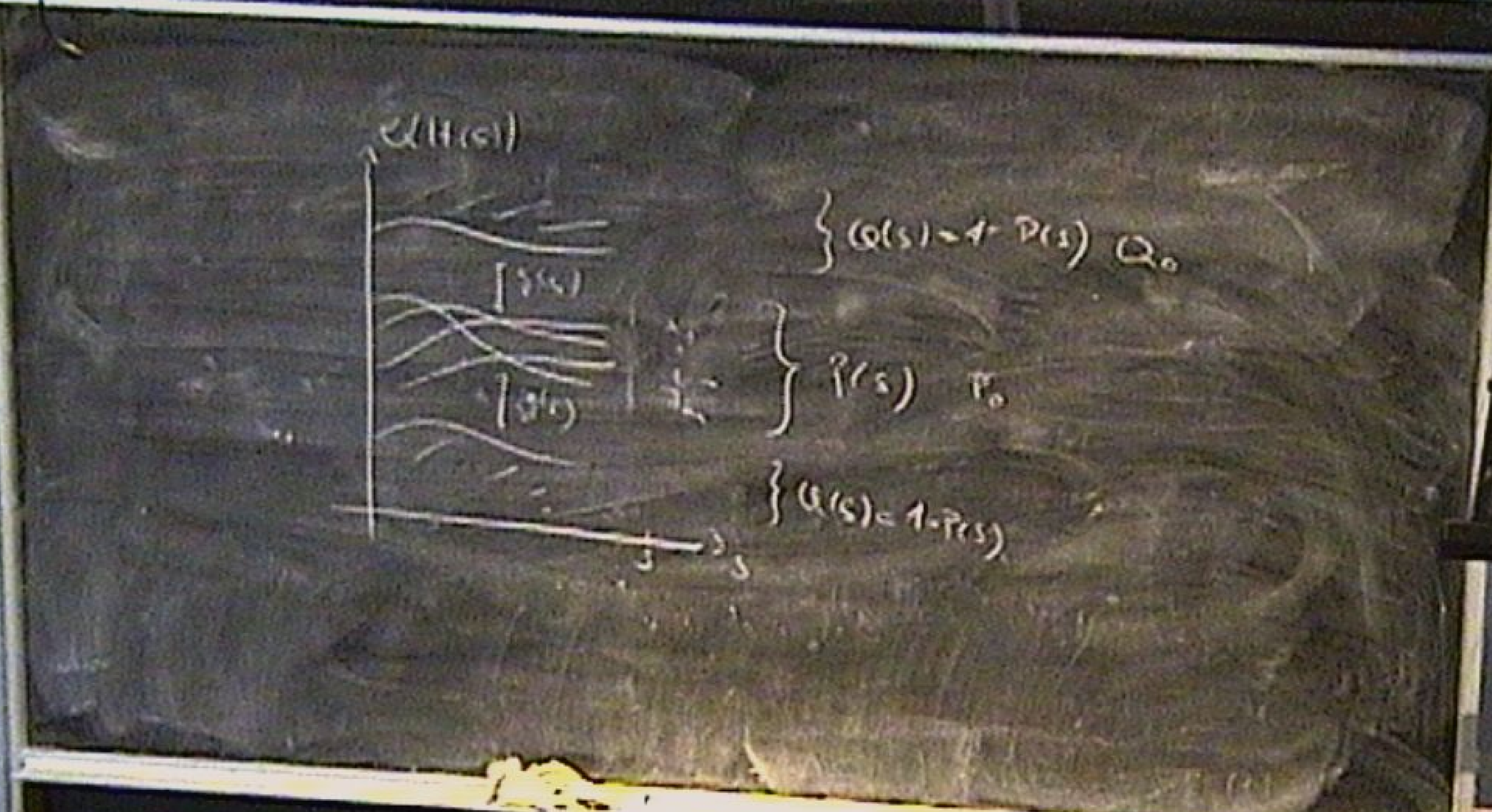
- Hilbert space $\mathcal{H}$, $\mathcal{B}(\mathcal{H})$ bounded operators in $\mathcal{H}$
- $s \in [0,1] \mapsto H(s) = H^*(s) \in \mathcal{B}(\mathcal{H})$ k-times differentiable map, $k \geq 2$
- $P(s)$ is the projection on the spectral subspace associated to finitely many eigenvalues $\lambda_1(s), ..., \lambda_m(s)$ (*but* possibly $\dim P = \infty$) separated from the rest of the spectrum by a gap $g(s)$

$$g(s) = \mathrm{dist}\left(\Lambda(s), \sigma(H(s)) \backslash \Lambda(s)\right) > 0,$$

$$\Lambda(s) = \{\lambda_1(s), ..., \lambda_m(s)\}$$







Q(H(s))
{ Q(s) = 1 - P(s) Q₀
P(s) P₀
{ Q(s) = 1 - P(s)

Adiabatic Theorem

- time-dependent Schrödinger equation

  $i\partial_t\psi = H(t/\tau)\psi$, $\tau > 0$ time scale

- Propagator $U_\tau(s)$ in rescaled time $s = t/\tau$

$$i\partial_s U_\tau(s) = \tau H(s) U_\tau(s), \quad U_\tau(0) = 1.$$

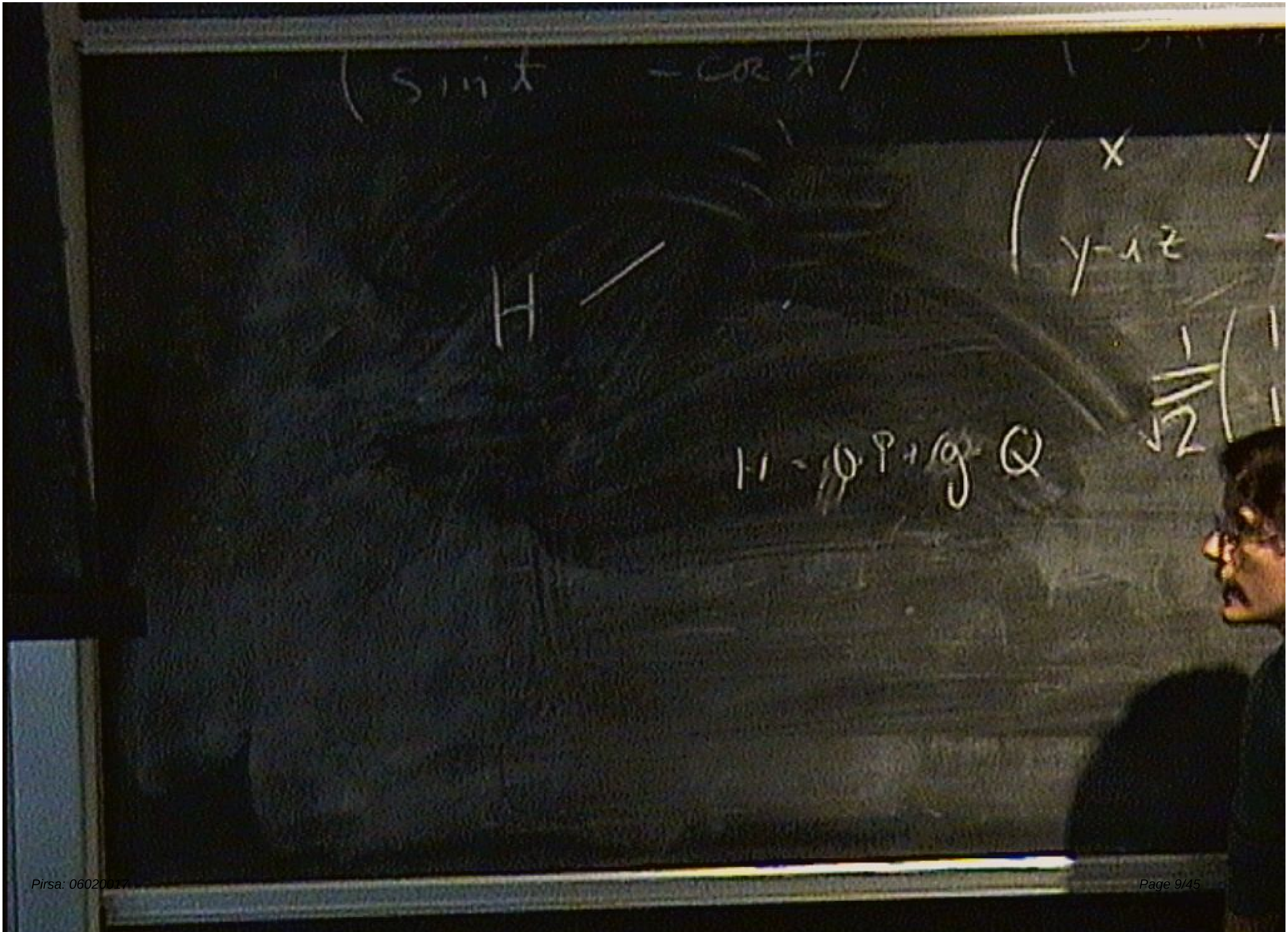
Theorem Transition amplitude $P(0) \rightsquigarrow Q(s)$

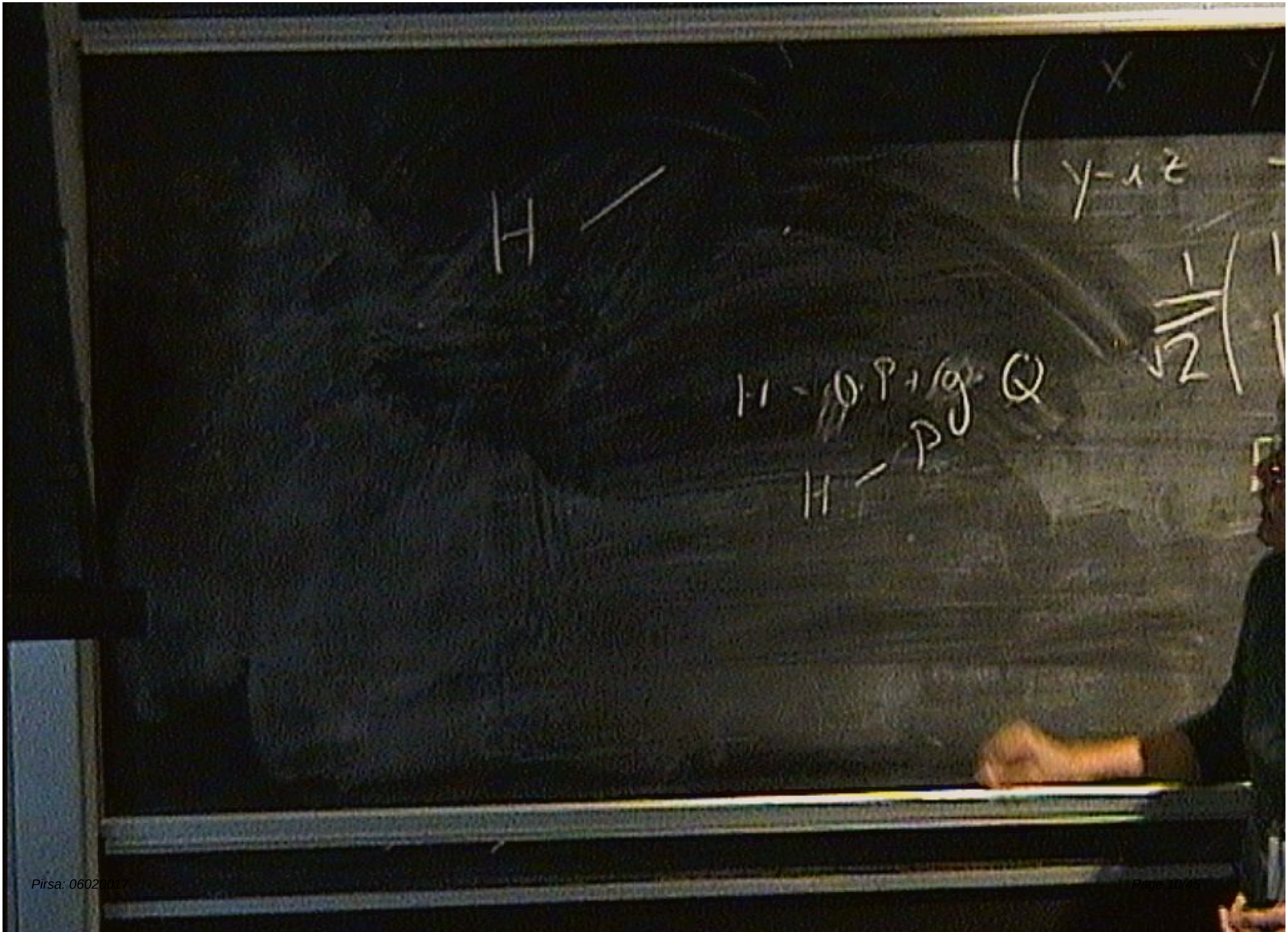
$$\|Q(s)U_\tau(s)P(0)\| \le \frac{1}{\tau}\left(\frac{m\|\dot{H}\|}{g^2}(0) + \frac{m\|\dot{H}\|}{g^2}(s)\right) + R$$

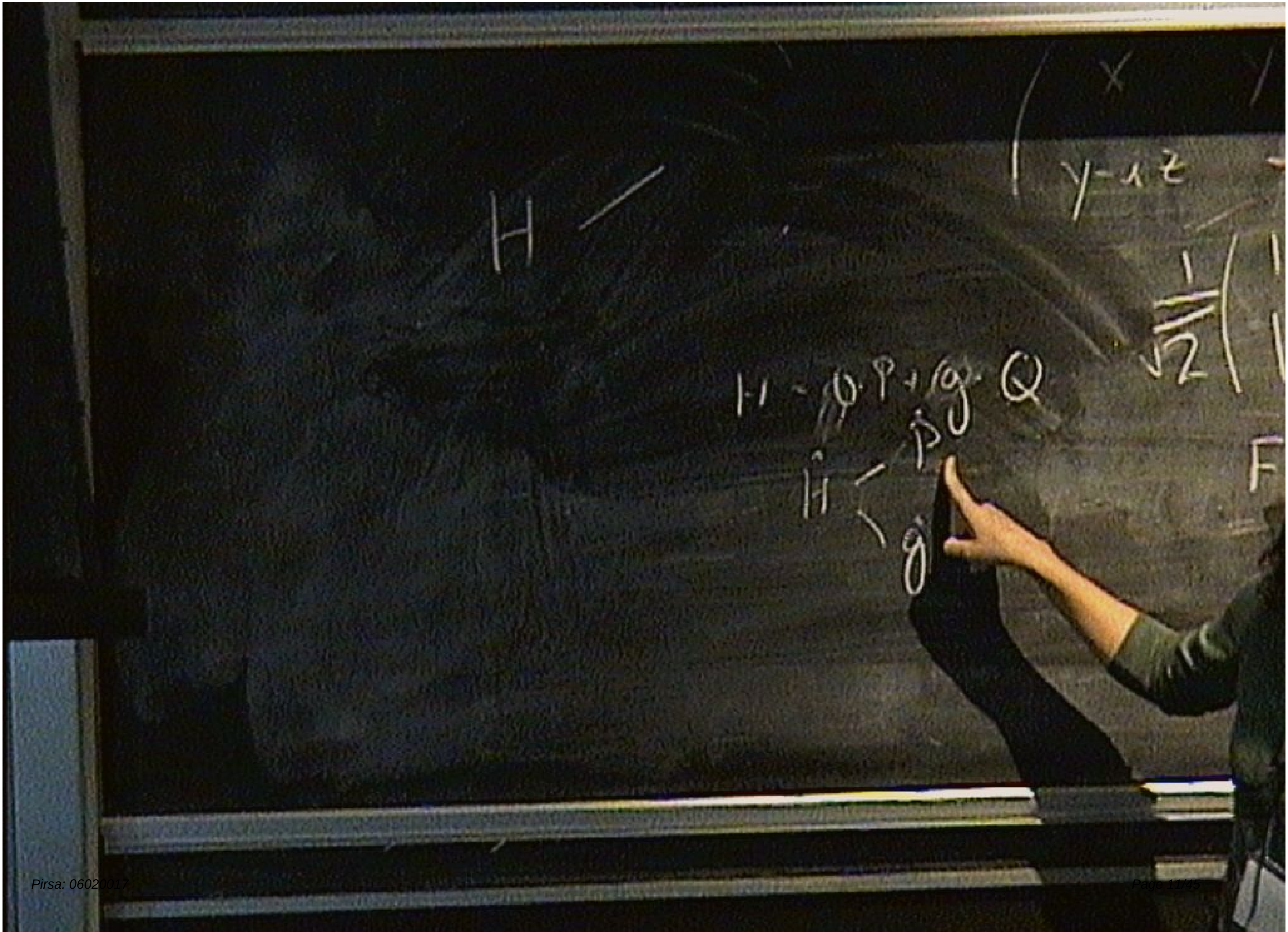
$$R \le \frac{1}{\tau}\int_0^s \left(\frac{m\|\ddot{H}\|}{g^2} + 7m\sqrt{m}\frac{\|\dot{H}\|^2}{g^3}\right)$$

If $k \ge 3$, $h(s) := \max(\|\dot{H}(s)\|, \|\ddot{H}(s)\|, \|\frac{d^3}{ds^3}H(s)\|)$

$$R \le \frac{C_m}{\tau^2}\Bigg(\frac{h^2}{g^4}(0) + \frac{h^2}{g^4}(s) + \frac{h}{g^2}(0)\int_0^s \frac{h^2}{g^3} + \int_0^s \frac{h^3}{g^5} + \int_0^s ds'\frac{h^2}{g^3}(s')\int_0^{s'} ds''\frac{h^2}{g^3}(s'')\Bigg)$$






H
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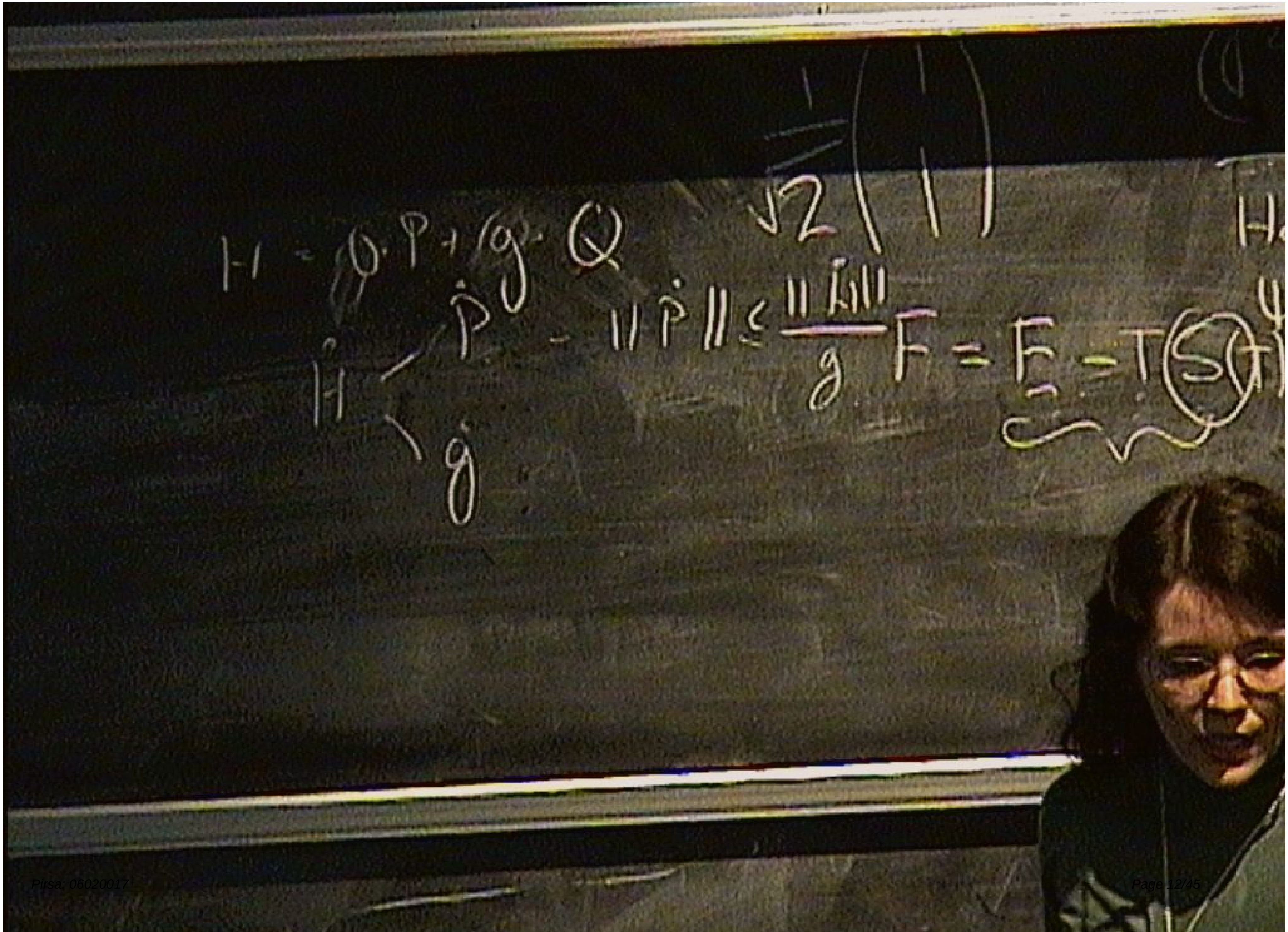

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Traditional adiabatics vs adiabatic quantum computing (AQC)

- Quantum mechanics textbook situation: fixed Hamiltonian, $\tau \to \infty$, $m = 1$, transition amplitude

$$\text{T.A.} \leq \frac{||\dot{H}||}{\tau g^2}(0) + \frac{||\dot{H}||}{\tau g^2}(s) + \frac{C(H)}{\tau^2}$$

  look only at first order term in $1/\tau$: integral remainder neglected

- AQC: additional parameter n (size of some problem), Hamiltonians $H_n(s)$. How should the sequence (τ_n) be chosen to keep the transition amplitude small, i.e.,

$$\text{T.A.}(n, \tau_n) \leq \text{const?}$$

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Sketch of proof: adiabatic time evolution

- idea of proof: compare real dynamics to idealized time evolution:

$$U^A_\tau(0) = \mathbf{1}, \quad i\partial_s U^A_\tau = \tau H^A_\tau U^A_\tau$$
$$H^A_\tau(s) = H(s) + \frac{i}{\tau}[\dot{P}(s), P(s)]$$

- intertwining property: $U^A_\tau(s)P(0) = P(s)U^A_\tau(s)$
- Example: 2-level system. $E_1(s) < E_2(s)$, $\psi_1(s), \psi_2(s)$ orthonormal and such that $\langle \dot{\psi}_j, \psi_j \rangle = 0$,

$$H = E_1|\psi_1\rangle\langle\psi_1| + E_2|\psi_2\rangle\langle\psi_2|.$$

Then

$$U^A_\tau(s)\psi_1(0) = e^{-i\tau\int_0^s E_1}\psi_1(s),$$
$$U^A_\tau(s)\psi_2(0) = e^{-i\tau\int_0^s E_2}\psi_2(s).$$

Wave operator

- Definition wave operator $\Omega_\tau(s) = U_\tau^A(s)^* U_\tau(s)$
  tool from scattering theory to compare dynamics

- transition amplitude $\leftrightarrow$ off-diagonal block of wave operator

$$||Q(s)U_\tau(s)P_0|| = ||Q_0\Omega_\tau(s)P_0||$$

- Volterra equation: $\Omega_\tau(s) = 1 - \int_0^s (U_\tau^A)^*[\dot{P}, P]U_\tau^A \Omega_\tau$

- 2-level system: kernel in basis $\psi_1(0), \psi_2(0)$:

$$(U_\tau^A)^*[\dot{P}, P]U_\tau^A = \begin{pmatrix} 0 & -e^{-i\tau \int_0^s (E_2 - E_1)}\bar{\alpha} \\ e^{i\tau \int_0^s (E_2 - E_1)}\alpha & 0 \end{pmatrix}$$

$$\alpha = \langle \psi_2, \dot{\psi}_1 \rangle$$

$\Rightarrow$ oscillating integrals !

Integration by parts

- partial integration for functions: $\dot{G} = g \neq 0$

$$\int e^{i\tau G}\alpha f = -\frac{i}{\tau}\Big(e^{i\tau G}\frac{\alpha}{g}f| - \int e^{i\tau G}(\frac{\alpha}{g})' f - \int e^{i\tau G}\frac{\alpha}{g}\dot{f}\Big)$$

- operator version needs analogue of $\alpha \mapsto \frac{\alpha}{g}$

- Def. Twiddle operation

  $\Gamma(s)$ contour in $\mathbb{C}$ circling the band

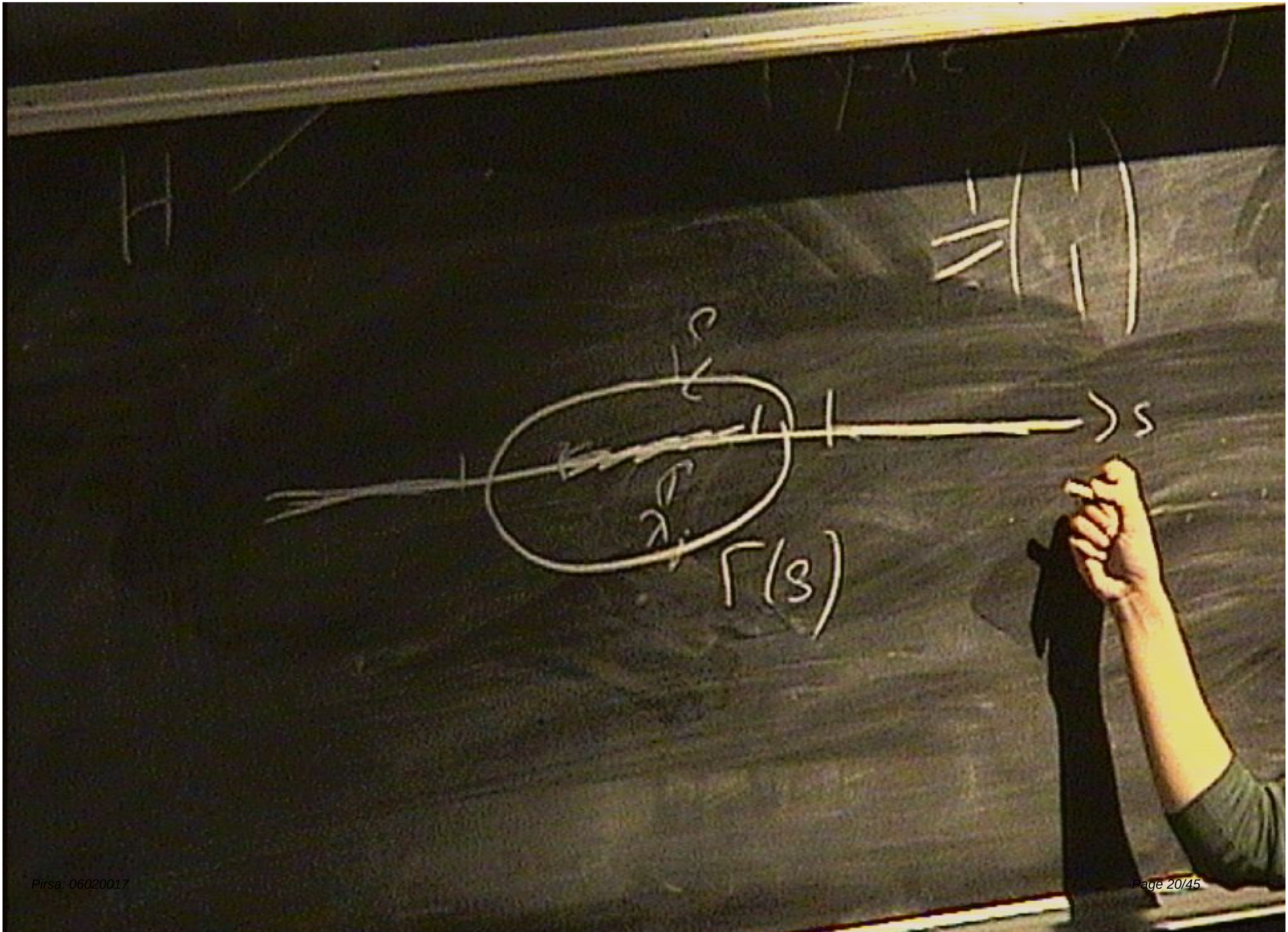
  $\tilde{X}(s) = \frac{1}{2\pi i}\oint_{\Gamma(s)}(H(s)-z)^{-1}X(s)(H(s)-z)^{-1}dz.$

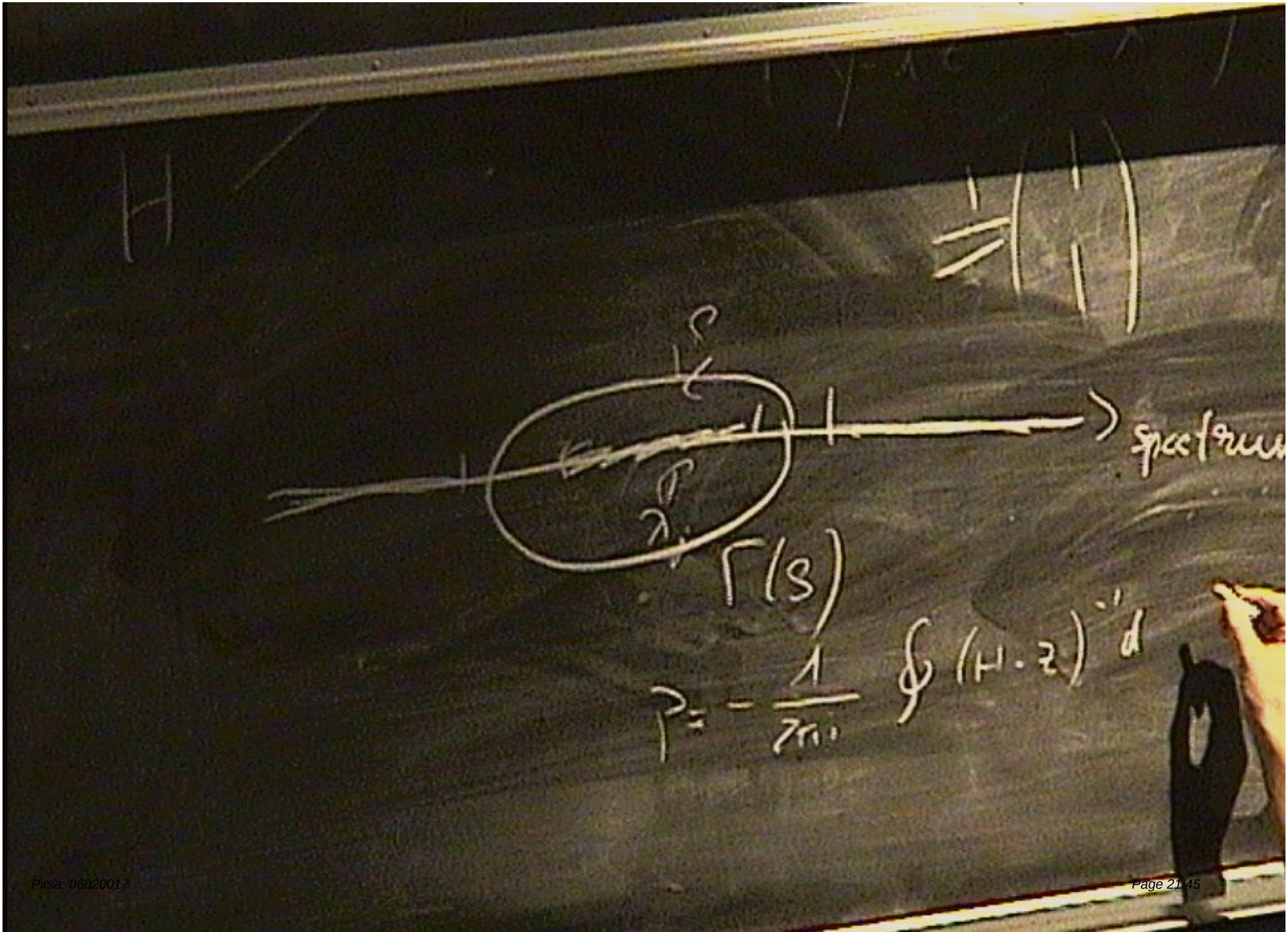
- integration by parts for wave operator

$$\begin{aligned} Q_0\Omega_\tau(s)P_0 &= -\int_0^s Q_0(U_\tau^A)^*\dot{P}U_\tau^A P_0\Omega_\tau P_0 \\ &= \frac{i}{\tau}\Big(Q_0(U_\tau^A)^*\tilde{\dot{P}}U_\tau^A P_0\Omega_\tau P_0|_0^s - \int_0^s Q_0(U_\tau^A)^*\dot{\tilde{\dot{P}}}U_\tau^A P_0\Omega_\tau P_0 \\ &\qquad - \int_0^s Q_0(U_\tau^A)^*\tilde{\dot{P}}U_\tau^A P_0\dot{\Omega}_\tau P_0\Big), \end{aligned}$$

$$P_0\dot{\Omega}_\tau = P_0(U_\tau^A)^*\dot{P}U_\tau^A Q_0\Omega_\tau$$

$\Rightarrow$ trans. ampl. $O(1/\tau)$.


s
Γ(s)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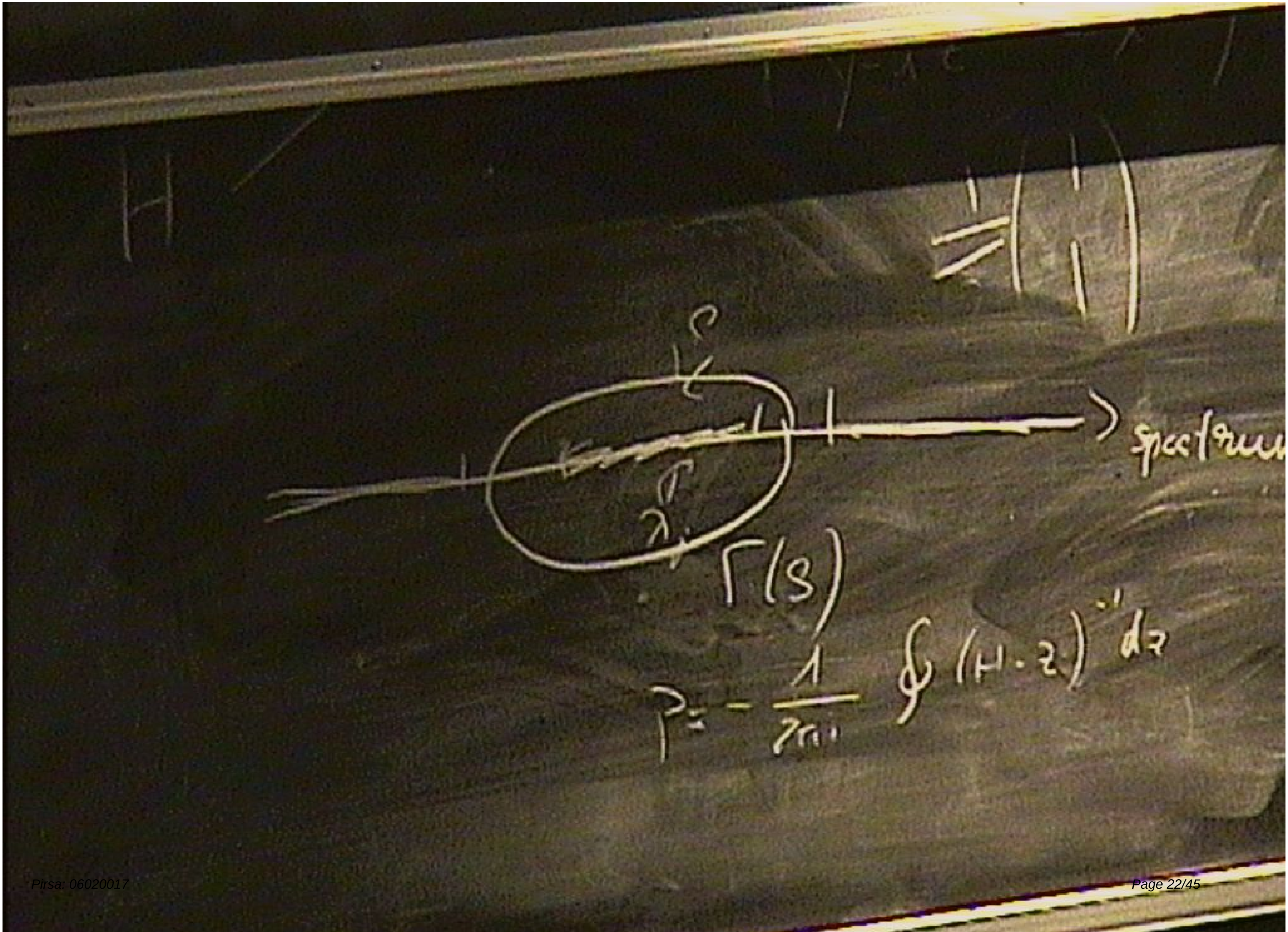
H
spectrum
Γ(s)
P = - 1/2πi ∮ (H - z)^-1 dz

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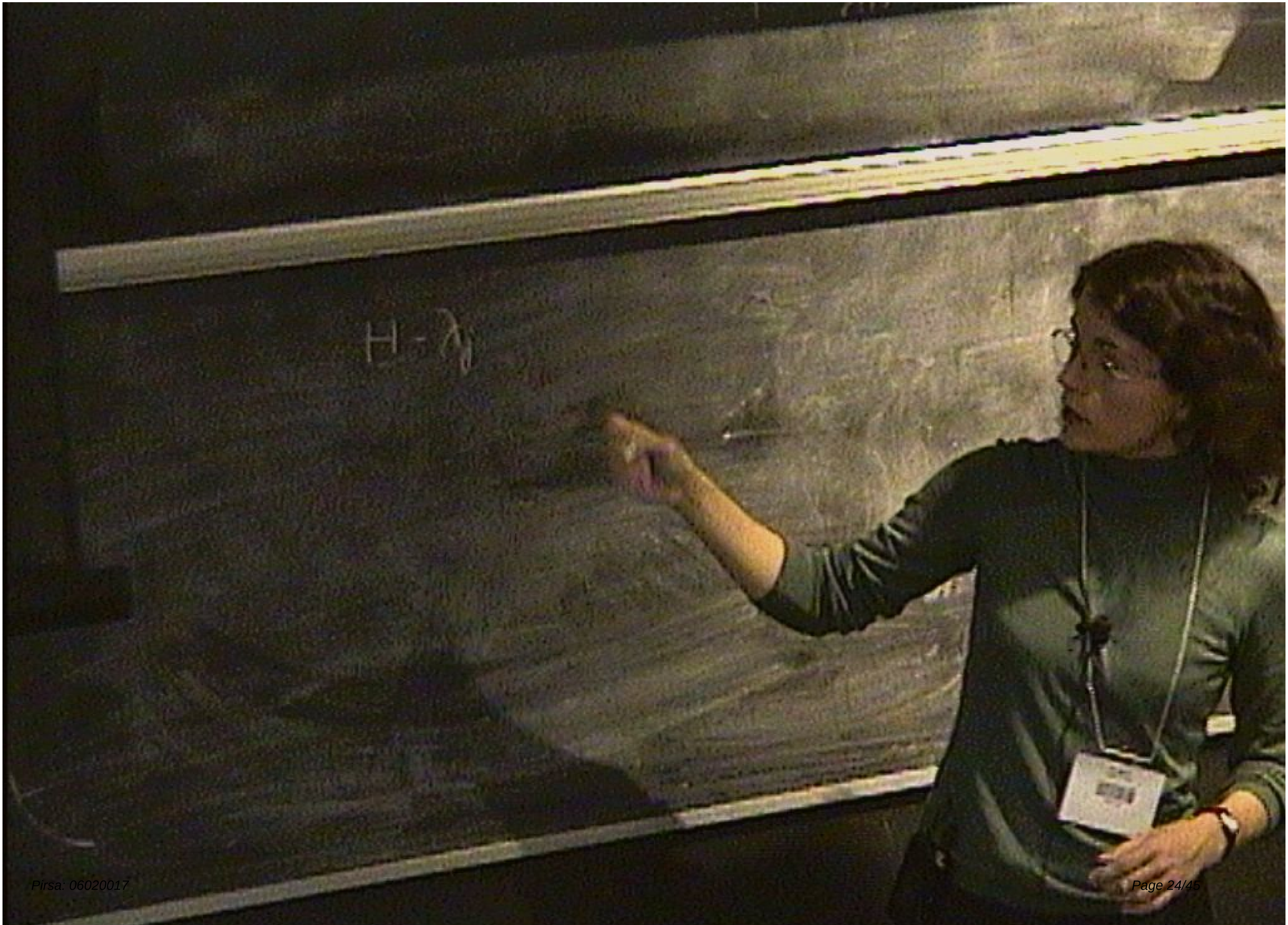
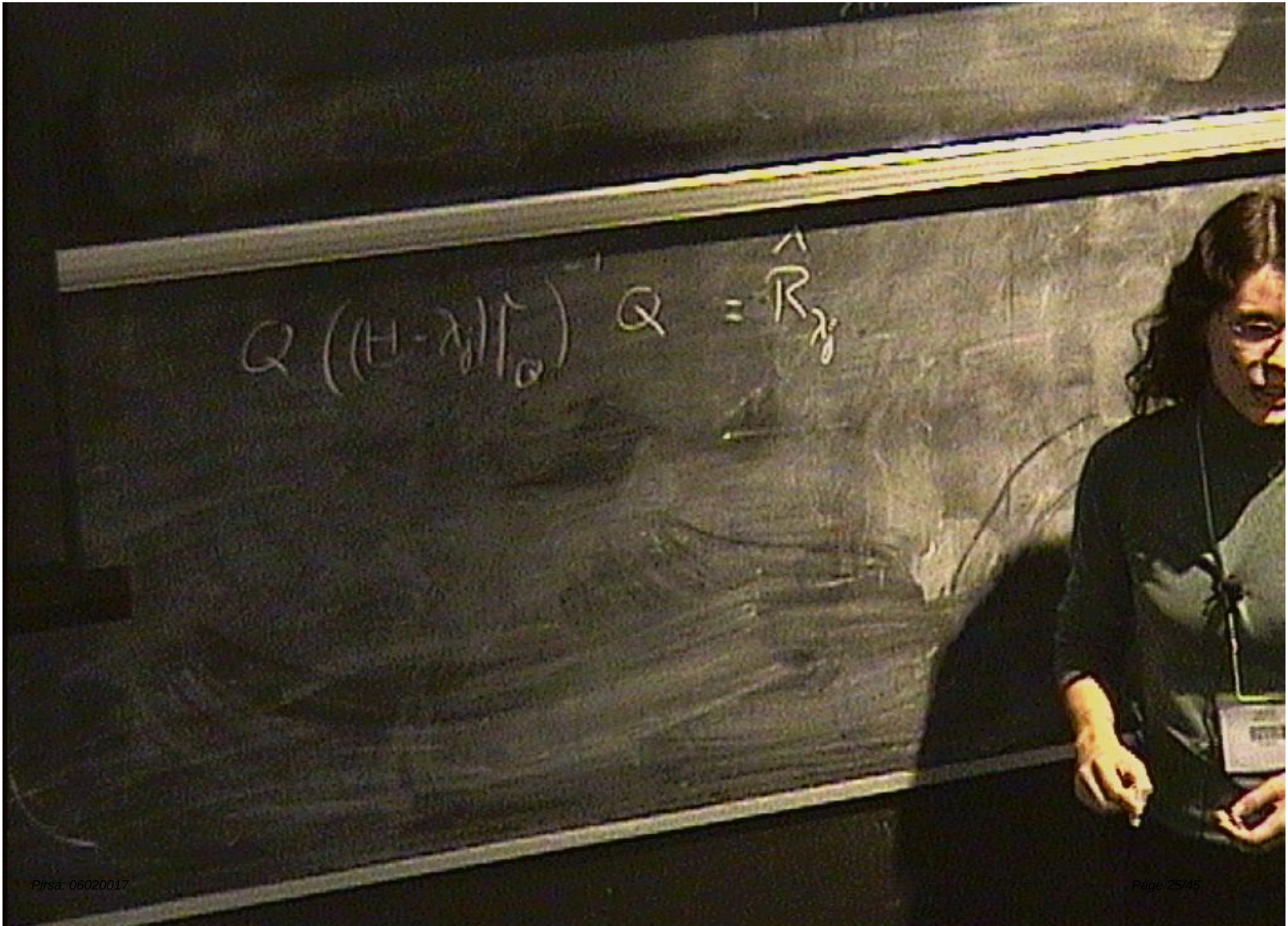

H - λ


Q ((H - λ_j) Γ_0)^{-1} Q = R̂_{λ_j}

$$Q\left((H-\lambda_j)|_Q\right)^{-1} Q = \hat{R}_{\lambda_j}$$

$$\tilde{X} = -\sum_{j=1}^{m} \hat{R}_{\lambda_j} X P_j + P_j X \hat{R}_{\lambda_j}$$

$$Q\left((H-\lambda_j)|_Q\right)^{-1} Q = \hat{R}_{\lambda_j}$$

$$\|\hat{R}_{\lambda_j}\| \leq \frac{1}{g(s)}$$

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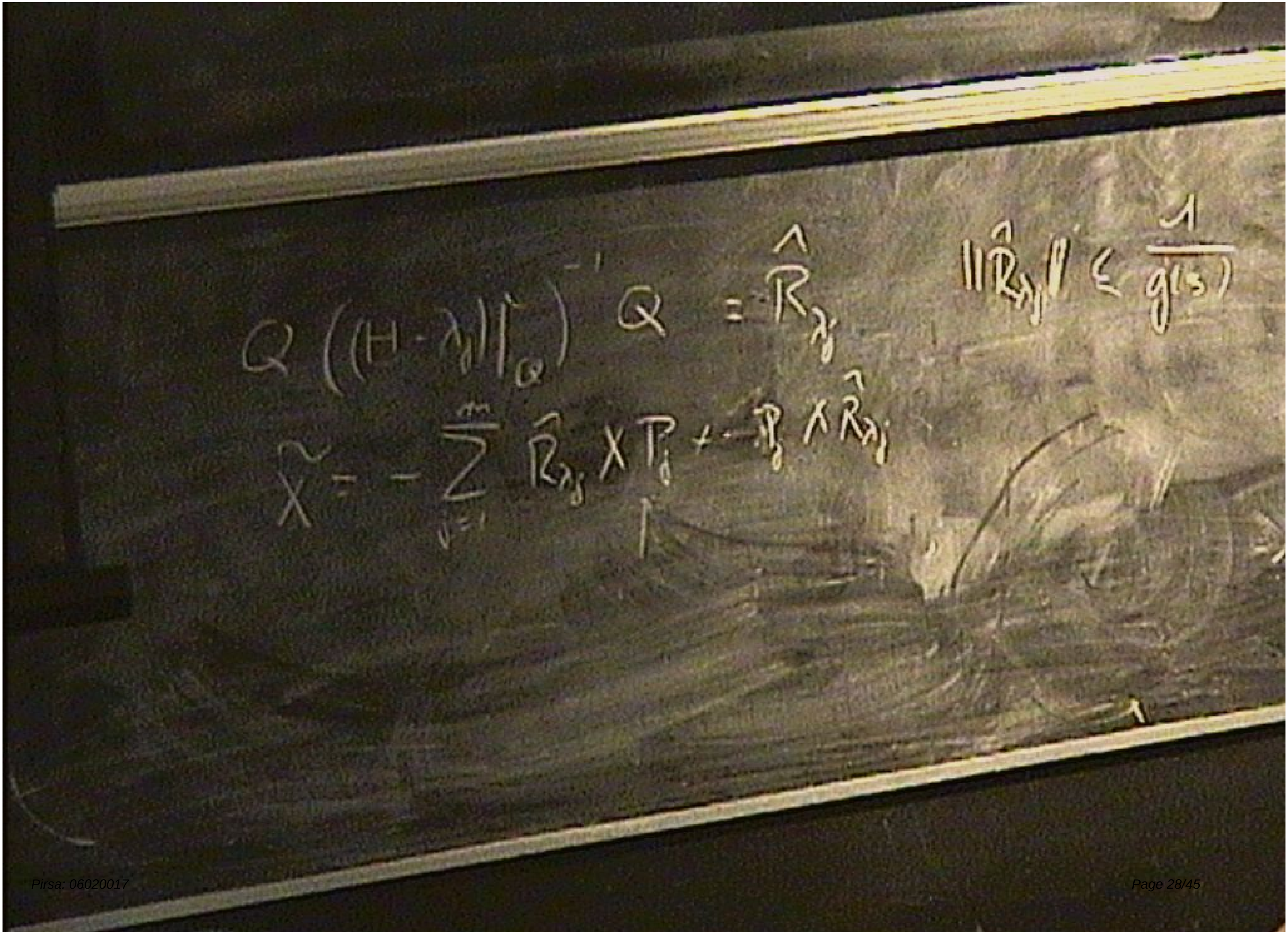

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$$P_0\dot\Omega_\tau = P_0(U_\tau^A)^*\dot P U_\tau^A Q_0\Omega_\tau$$

$\Rightarrow$ trans. ampl. $O(1/\tau)$.

Explicit estimates & iterating the ibp

- Lemma: m number of eigenvalues in the band, $g(s)$ gap

$$||\dot{P}|| \leq \sqrt{m}\frac{||\dot{H}||}{g}, \quad ||\dot{\tilde{P}}|| \leq m\frac{||\dot{H}||}{g^2},$$
$$||Q\ddot{\tilde{P}}P|| \leq \frac{m||\ddot{H}||}{g^2} + 6\frac{m\sqrt{m}||\dot{H}||^2}{g^3}.$$

$\Rightarrow$ leads to explicit estimates of transition amplitude:

$$\text{T.A.} \leq \frac{1}{\tau}\Big(\frac{m||\dot{H}||}{g^2}(0) + \frac{m||\dot{H}||}{g^2}(s)\Big)$$
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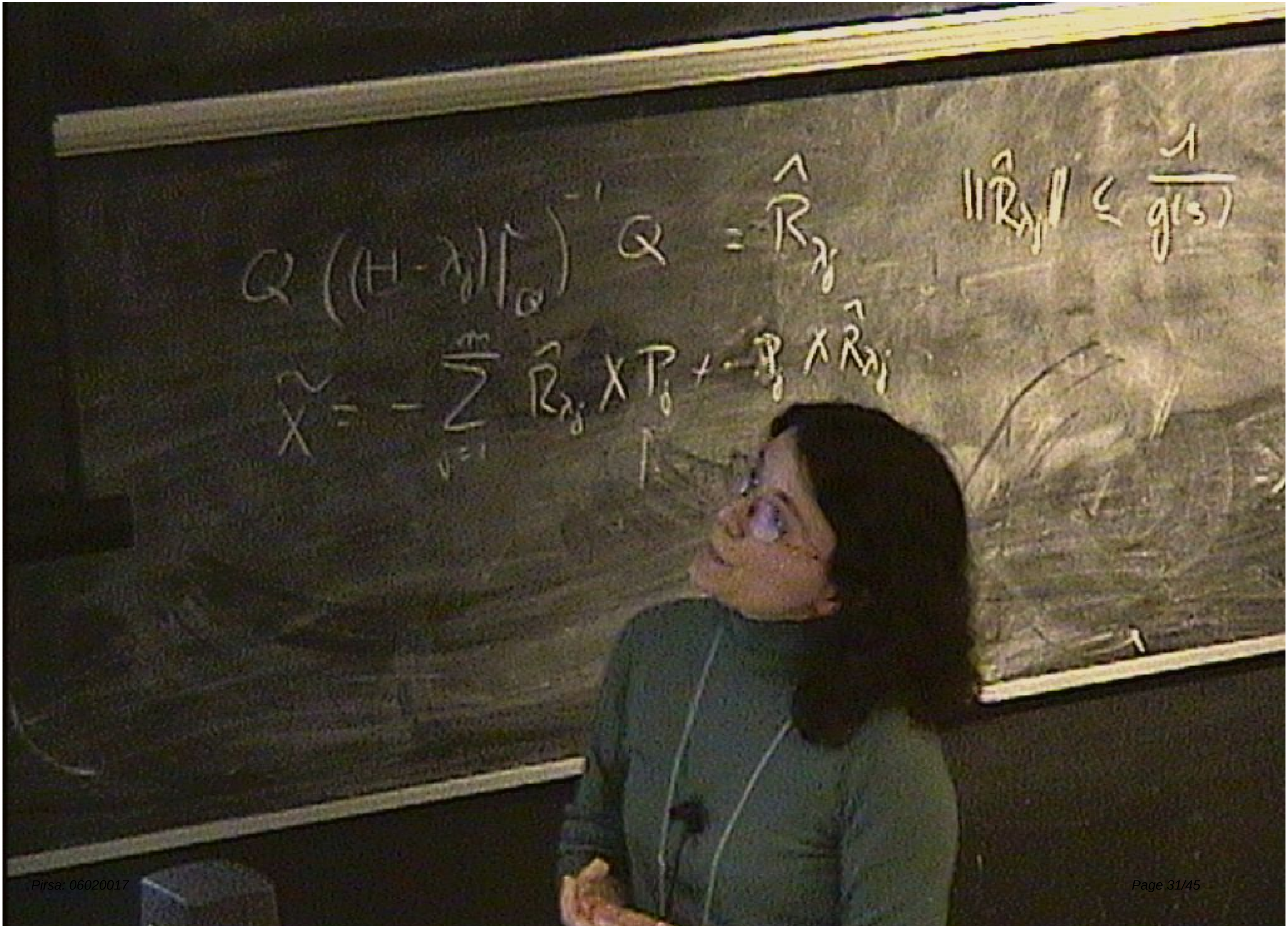
- Pitfall in iteration of integration by parts: differentiaton of $\dot{\Omega}_\tau$ generates powers of τ! Correct procedure leads to multiple integrals, does not a priori improve gap dependence of bound.

- What about "traditional criterion" $\tau \gg ||\dot{H}||/\mathrm{gap}^2$?


Q ((H - λj) |Q)^-1 Q = R̂λj
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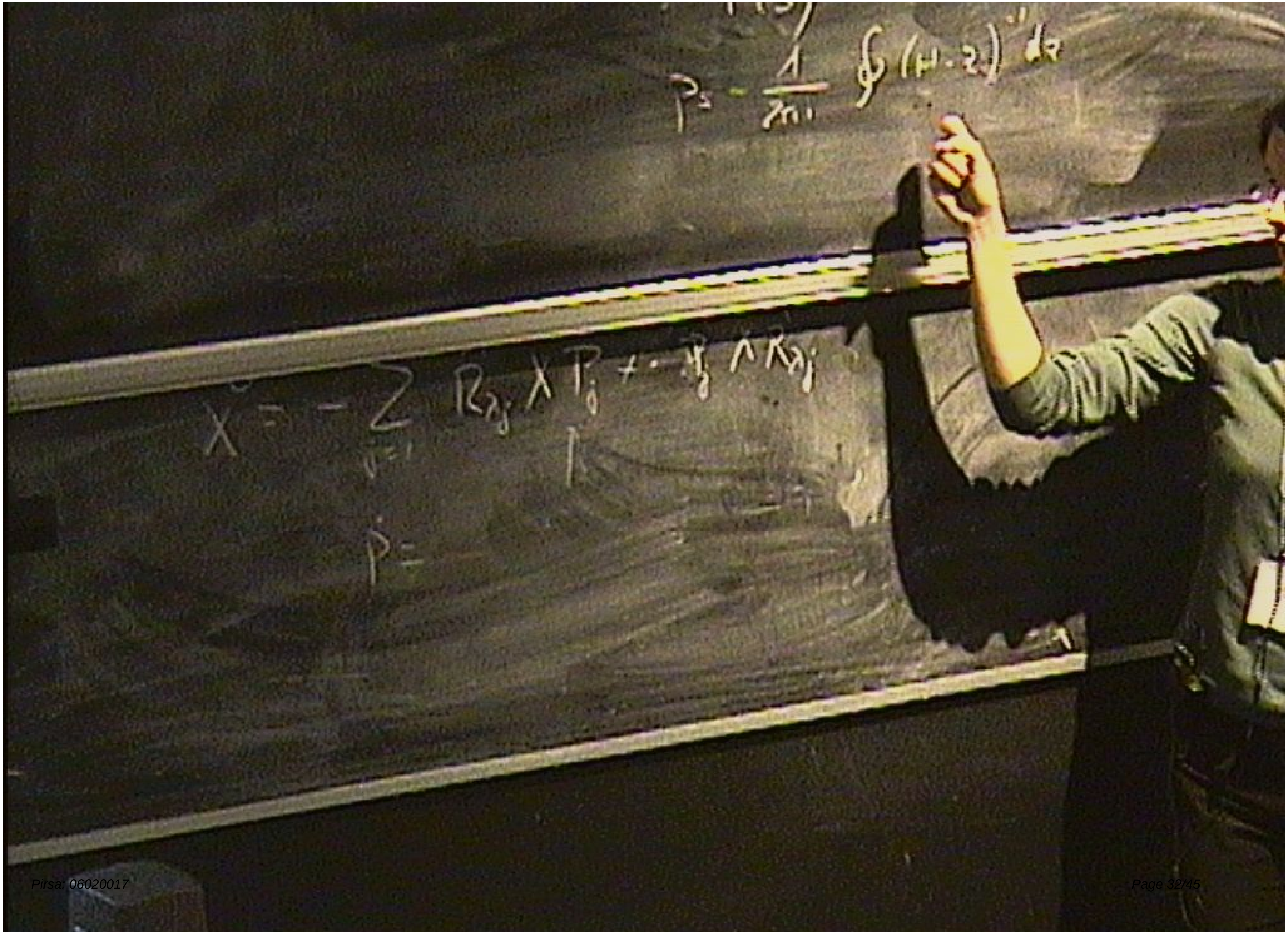

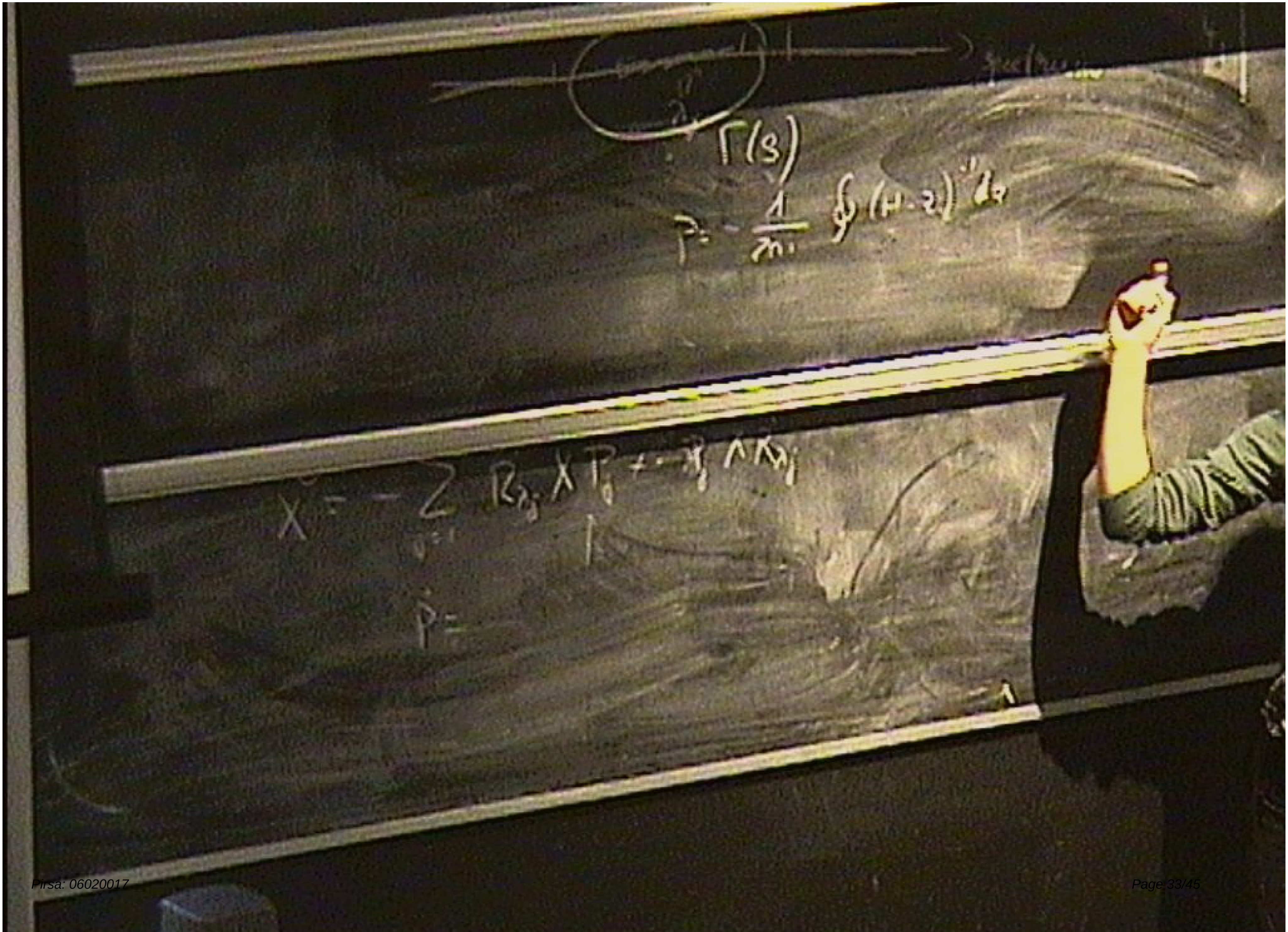
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Application to interpolating Hamiltonians: a simple example

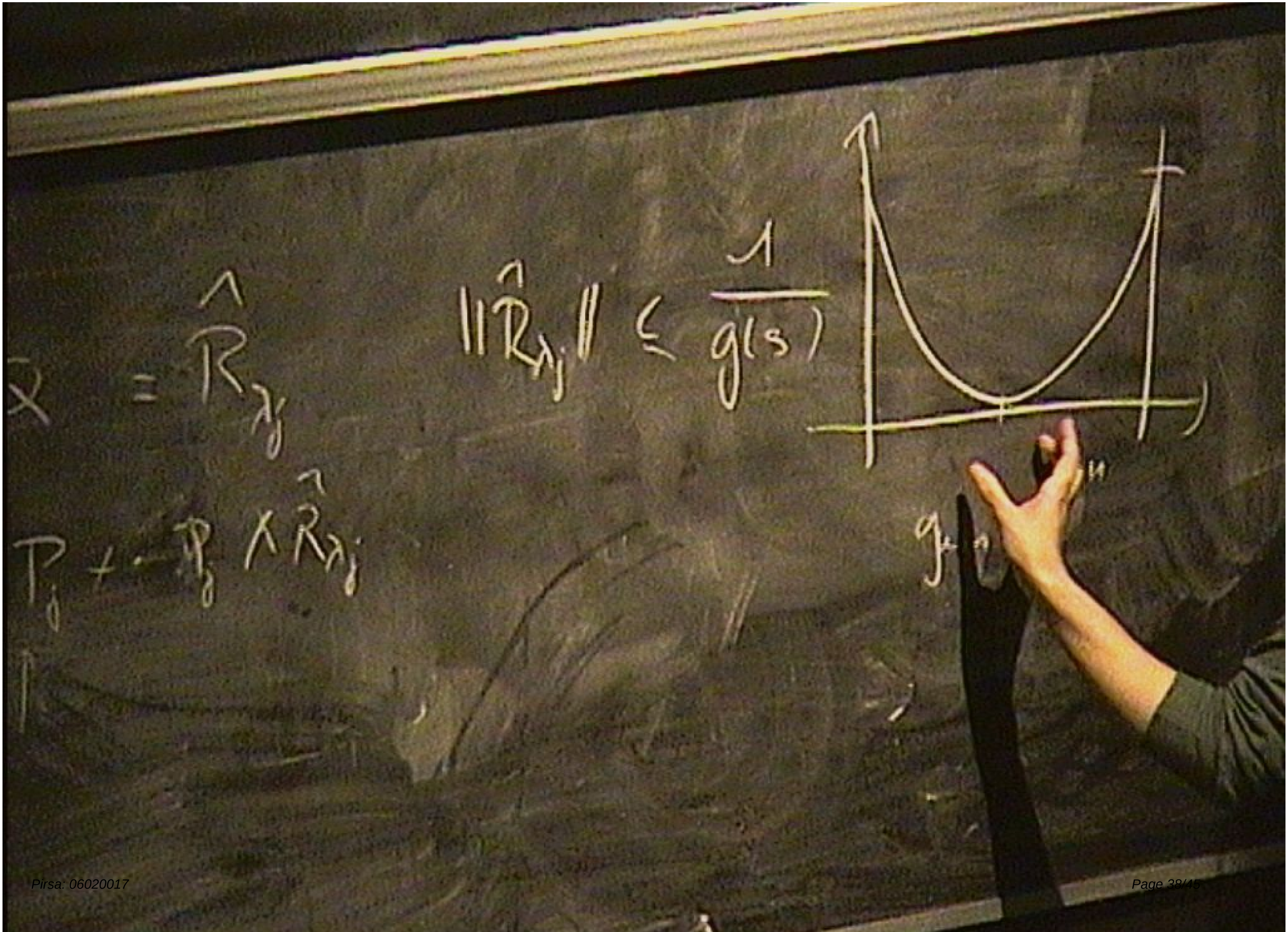
- Notation: $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$. $|0\rangle, |1\rangle$ a basis of $\mathbb{C}^2$, $|x\rangle = |x_1\rangle \otimes .. \otimes |x_n\rangle \in \mathcal{H}$ for $x \in \{0,1\}^n$.
- Path of Hamiltonians: $u \in \mathcal{H}$

$$H(s) = (1-s)(1 - |\hat{0}\rangle\langle\hat{0}|) + s(1 - |u\rangle\langle u|),$$
$$u \in \mathcal{H}, \quad |\hat{0}\rangle = \frac{1}{2^{n/2}} \sum_{x \in \{0,1\}^n} |x\rangle.$$

- $P(s)$ projection on ground state, gap to the rest of the spectrum

$$g(s) = \sqrt{2^{-n} + 4(1-2^{-n})(s - \frac{1}{2})^2}.$$

- $\int_0^1 g^{-3} = O(g_{\min}^{-2})$, $||\dot{H}|| = O(1)$, $\Rightarrow$ previous bounds show: T.A. $\leq C/(\tau g_{\min}^2)$, C *n-independent.*
- Remark: integral remainder bigger than boundary terms!



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- Idea (e.g. van Dam, Mosca, Vazirani et al. 2005): adapting the interpolation to gap function improves running time τ to $O(g_{\min}^{-1})$. Here:

$$H_f(s) = (1 - f(s))H_0 + f(s)H_1$$
$$\dot{f}(s) = kg^p(f(s)), 1 < p < 2,$$

k chosen such that $f(1) = 1$, $1 < p < 2$.

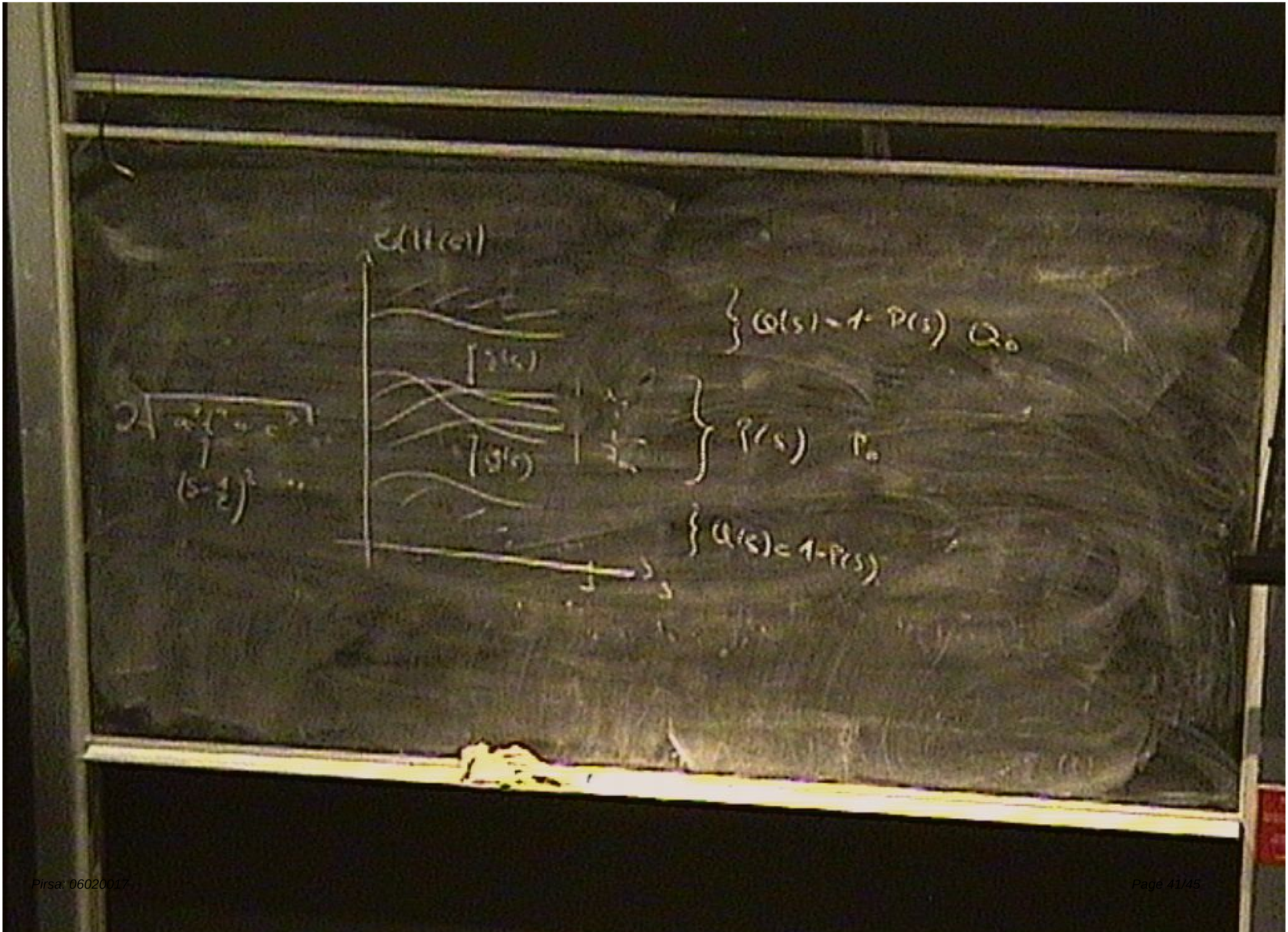
$$\Rightarrow \text{T.A.} \leq C/(\tau g_{min})$$

by the theorem & special features of gap function.

- Remark: reminiscent of problem treated in context of Landau-Zener transition (Hagedorn, CMP 1991):

$$i\varepsilon\partial_t\psi = H(t, \varepsilon^{1/2})\psi, \quad \varepsilon \to 0$$

Mitchell et al., Phys. Rev. A 2005: evaluate probability of a transition with Landau-Zener formula


Q(s) = 1 - P(s)   Q₀
P(s)   P₀
Q(s) = 1 - P(s)

- Idea (e.g. van Dam, Mosca, Vazirani et al. 2005): adapting the interpolation to gap function improves running time τ to $O(g_{\min}^{-1})$. Here:

$$H_f(s) = (1 - f(s))H_0 + f(s)H_1$$
$$\dot{f}(s) = kg^p(f(s)), 1 < p < 2,$$

k chosen such that $f(1) = 1$, $1 < p < 2$.

$$\Rightarrow \text{T.A.} \leq C/(\tau g_{min})$$

by the theorem & special features of gap function.

- Remark: reminiscent of problem treated in context of Landau-Zener transition (Hagedorn, CMP 1991):

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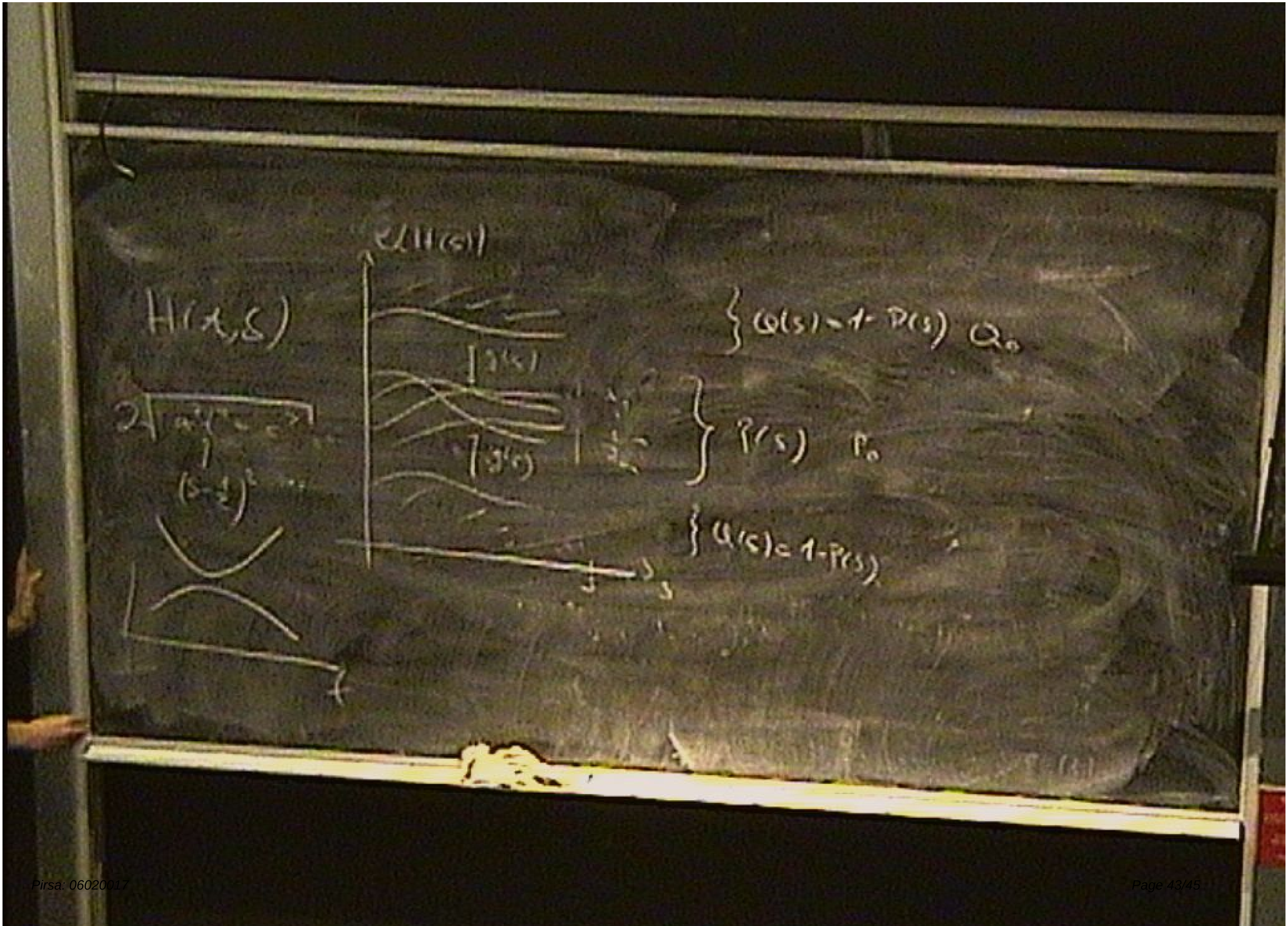
H(x,s)
Q(s) = 1 - P(s) Q0
P(s) P0
Q(s) = 1 - P(s)

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Conclusion

- AQC setting slightly different from traditional quantum adiabatics (fixed Hamiltonian) setting
- "Folk theorem" transition amplitude $\sim ||\dot{H}||/(\tau\, gap^2)$ not necessarily true when problem size gets big
- rigorous justification of criterion $\tau \geq g_{\min}^{-2}$ using partial integration proof requires extra look at gap function.