Title: Statistical Mechanics (PHYS 602) - Lecture 3

Date: Sep 30, 2009 10:30 AM

URL: http://pirsa.org/09090113

Abstract:

Sums and Averages in Classical Mechanics

The probability distribution for a single particle in a weakly interacting gas as is given by

$$\rho(p,r) = (1/z)\exp(-\beta H)$$

$$H = [p_x^{\,2} + p_y^{\,2} + p_z^{\,2}]/2m + U(r)$$

Here, the potential holds the particles in a box of volume Ω, so that U is zero inside a box of this volume and infinite outside of it. The partition function, is

$$z = \Omega[\int dp \exp(-\beta p^2/(2m))]^3 = \Omega(2\pi m/\beta)^{3/2}$$

The average of any function of **p** and **r** is given by

$$\langle g(\mathbf{p},\mathbf{r})\rangle = \int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})\, g(\mathbf{p},\mathbf{r})$$

Since there are N particles in the system $N\, d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})$ is the number of particles which have position and momentum within $d\mathbf{p}\, d\mathbf{r}$ about the phase space point $\mathbf{p},\mathbf{r}$. The quantity $N\, \rho(\mathbf{p},\mathbf{r}) = f(\mathbf{p},\mathbf{r})$ is called the distribution function. The total amount of the quantity represented by $g(\mathbf{p},\mathbf{r})$ is given in terms of the distribution function as

$$\text{total amount of } g = \int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r})\, g(\mathbf{p},\mathbf{r})$$

Example: We calculated the average energy $\langle \mathbf{p}^2/(2m)\rangle = 3\,kT/2 = \int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r})\, \mathbf{p}^2/(2m)$

The total energy in the system is $\int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r})\, \mathbf{p}^2/(2m) = 3N\,kT/2$.

More sums and averages

The normalization condition for the probability is $\int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r}) = \langle 1 \rangle = 1$

The normalization for the distribution function is $\int d\mathbf{p}\, d\mathbf{r}\, f(\mathbf{p},\mathbf{r}) = N$

The pressure, P, is defined as the total momentum transfer to a wall per unit of area and unit time. Call these dA and dt. Since a low density gas is the same all over, the number hitting is the number within the distance $p_x/m\, dt$ of the area, for $p_x > 0$, and hence the number within th volume $p_x/m\, dt\, dA$ which is $\int d\mathbf{p}\, f(\mathbf{p},\mathbf{r})\, p_x/m\, dt\, dA$ with the integral covering all **p**'s with the condition that $p_x > 0$. If a particle hits the wall and bounces back it transfers momentum $2p_x$.
do we need specular reflection condition??

Therefore the total momentum transferred is $\int d\mathbf{p}\, f(\mathbf{p},\mathbf{r})\, p_x/m\, dt\, dA\, 2p_x$ once again with th condition that $p_x > 0$. An integral over all momenta would give a result twice as large. In the end we get that the pressure is

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which is then NkT as we knew it would be.

The partition function is the sum over all variables of $\exp(-\beta H)$. For large N, it can be interpreted as $W \exp(-\beta \langle H \rangle)$, where W is the number of configuration which enter. Boltzmann got W in terms of the entropy as $\ln W = S/k$. We put together previous results and find

$W \exp(-3N/2) = z^N = \Omega^N (2\pi\, m\, kT)^{3N/2}$ so that $S/k = N [\ln \Omega + 3 (\ln (2\pi\, e\, m\, kT))/2]$

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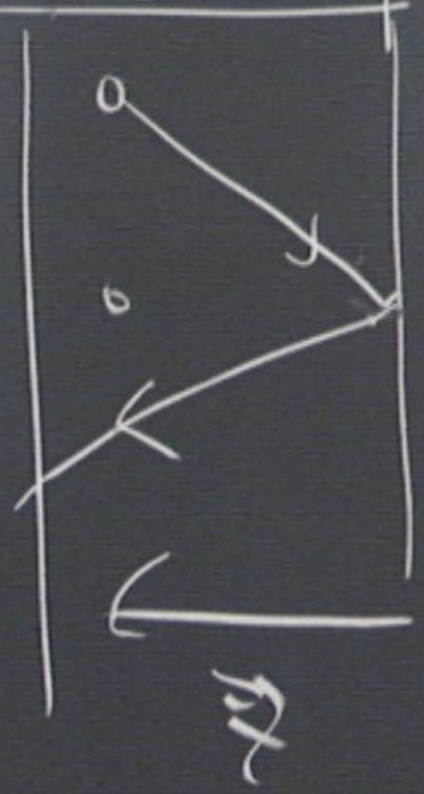
$$z \leq \frac{p_x}{m} dt$$

$$f = \frac{dp}{dt}$$



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connections with field theory, GR: pressure

connection with field theory

$T_{ij} = m\, v_i v_j + \delta_{ij}\, P$ + non-equilibrium terms

how come we find the pressure in thermodynamics?

how come we calculate pressure at the walls of the container?
how come we calculate the electrical current at the end of a wire?

connections with field theory, GR: pressure

connection with field theory

T_{ij}= m density $v_i v_j$ + δ_{ij} P + non-equilibrium terms

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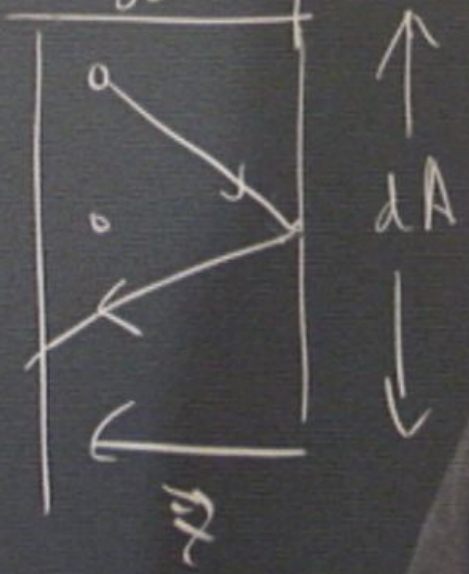
how come we calculate the electrical current at the end of a wire?

$$dz \leq \frac{p_x}{m} dt$$

$$\delta h z = - \frac{P S \Omega}{k T}$$

$$f = N \frac{dA}{\Omega}$$



connections with field theory, GR: pressure

connection with field theory

T_{ij}= m density $v_i v_j$ + δ_{ij} P + non-equilibrium terms

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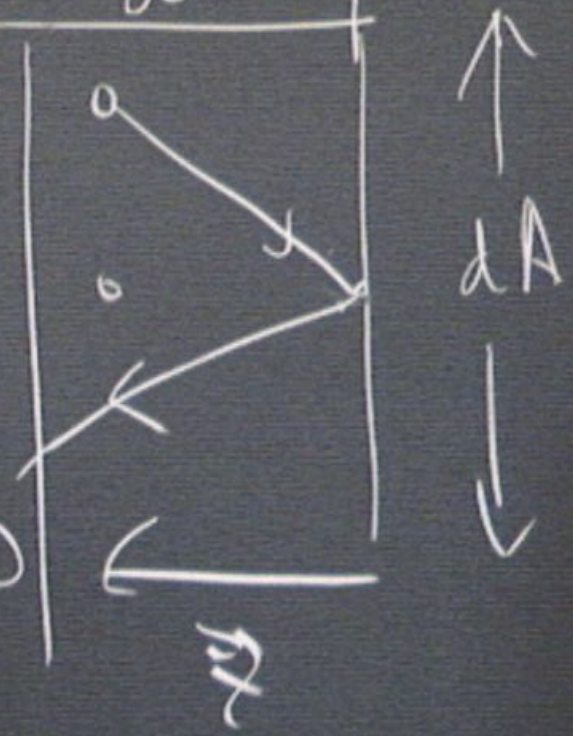

$$\frac{\partial p}{\partial t} + \nabla \cdot T = 0$$

More sums and averages

The normalization condition for the probability is $\int d\mathbf{p}\, d\mathbf{r}\, \rho(\mathbf{p},\mathbf{r}) = \langle 1 \rangle = 1$

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From Classical Stat Mech to Quantum to RG

All of quantum mechanics on one slide

To do quantum mechanics, one starts with a complete set of states $|q)$ and $(p|$ which have the ortho-normality property $(q|q') = \delta_{q,q'}$ and a completeness relation

$$\sum_q |q)(q| = 1 \qquad (4.1)$$

and a trace operation

$$\text{trace } \mathcal{P} = \sum_q (q|\mathcal{P}|q) \qquad (4.2)$$

Heisenberg representation $P(t)=e^{-iHt}\, P\, e^{iHt}$. Let $T(t) = e^{-iHt}$

Partition Function $Z(\beta)$ = trace $T(-i\beta)=\sum_\alpha \exp(-\beta\epsilon_\alpha)$

Average $\langle Q\rangle = [\text{trace}\, T(-i\beta)\, Q]/\, Z(\beta)$

Two Times $\langle Q(s)\, P(t)\rangle = [\text{trace}\, T(-i\beta)\, Q(s)\, P(t)\,]/\, Z(\beta)$

For grand canonical ensemble use $T(t)= exp[-i(H-\mu N)t]$

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Nearest Neighbor Interactions in Stat Mech on a One-Dimensional Lattice

Imagine that we wished to understand a problem involving nearest neighbor interactions one a one dimensional lattice which looks like

The variables at the different lattice sites are $q_1, q_2, \ldots\ldots, q_N$. The statistical weight is a product of terms depending on variables at the nearest neighboring lattice sites of the form $w(q_j, q_{j+1})$ so that the entire calculation of the partition function is*

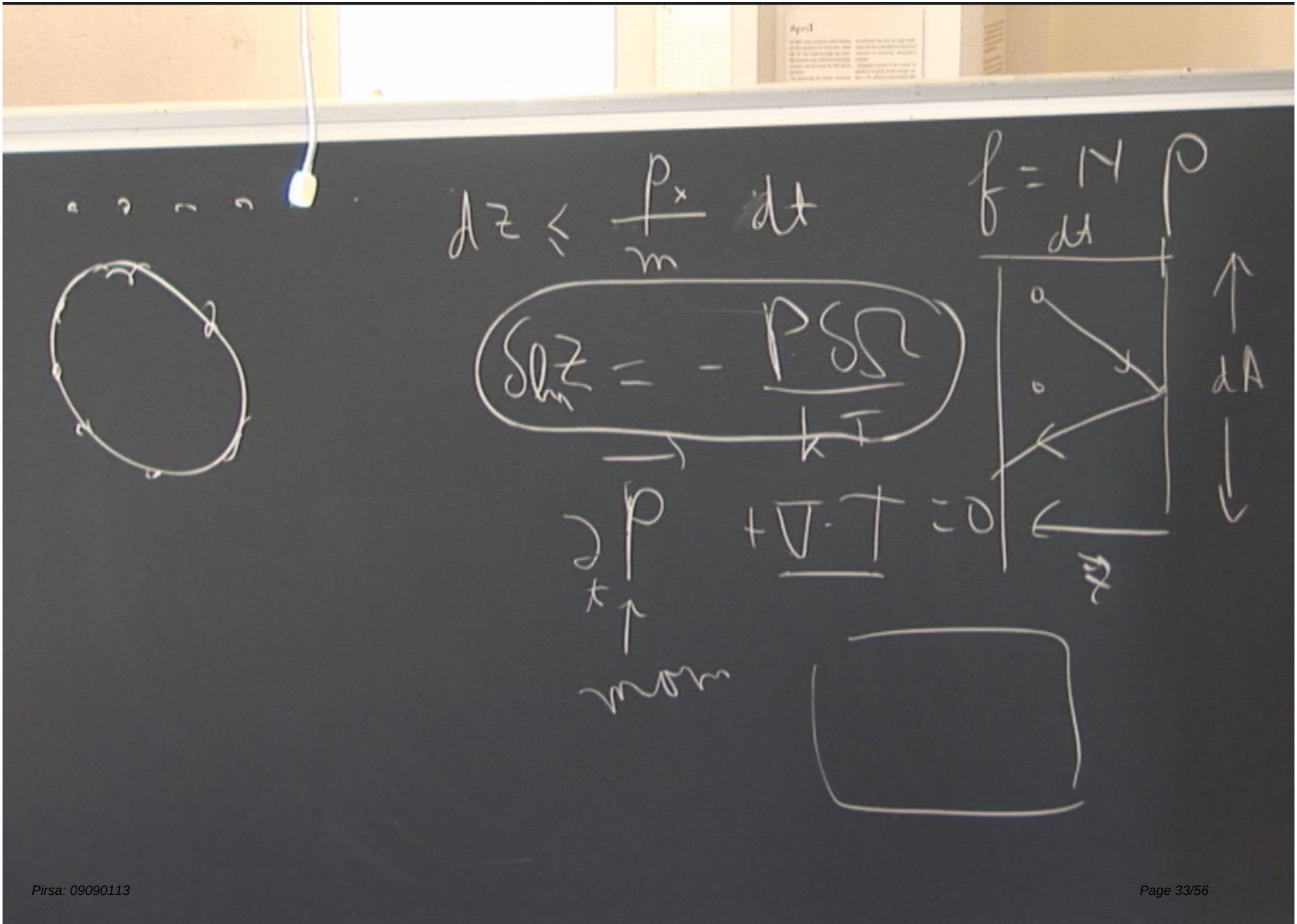
$$Z = \sum_{q_1, q_2, \cdots, q_N} exp[w(q_1, q_2) + w(q_2, q_3) + \cdots + w(q_{N-1}, q_N) + w(q_N, q_1)] \qquad \text{iii.1}$$

Notice that we have tied the two ends of the lattice to one another via a coupling $w(q_N, q_1)$. We have essentially used periodic boundary conditions. This calculation can be converted into a quantum mechanics calculation using a quantum mechanical operator, *T*, defined by its matrix elements

$\langle q|T|p\rangle = exp[w(q,p)]$

Now substitute this expression into the partition function calculation. We then have,

*We shall not describe the nearest neighbor problem in terms of a statistical mechanical Hamiltonian since we are saving the wor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dA

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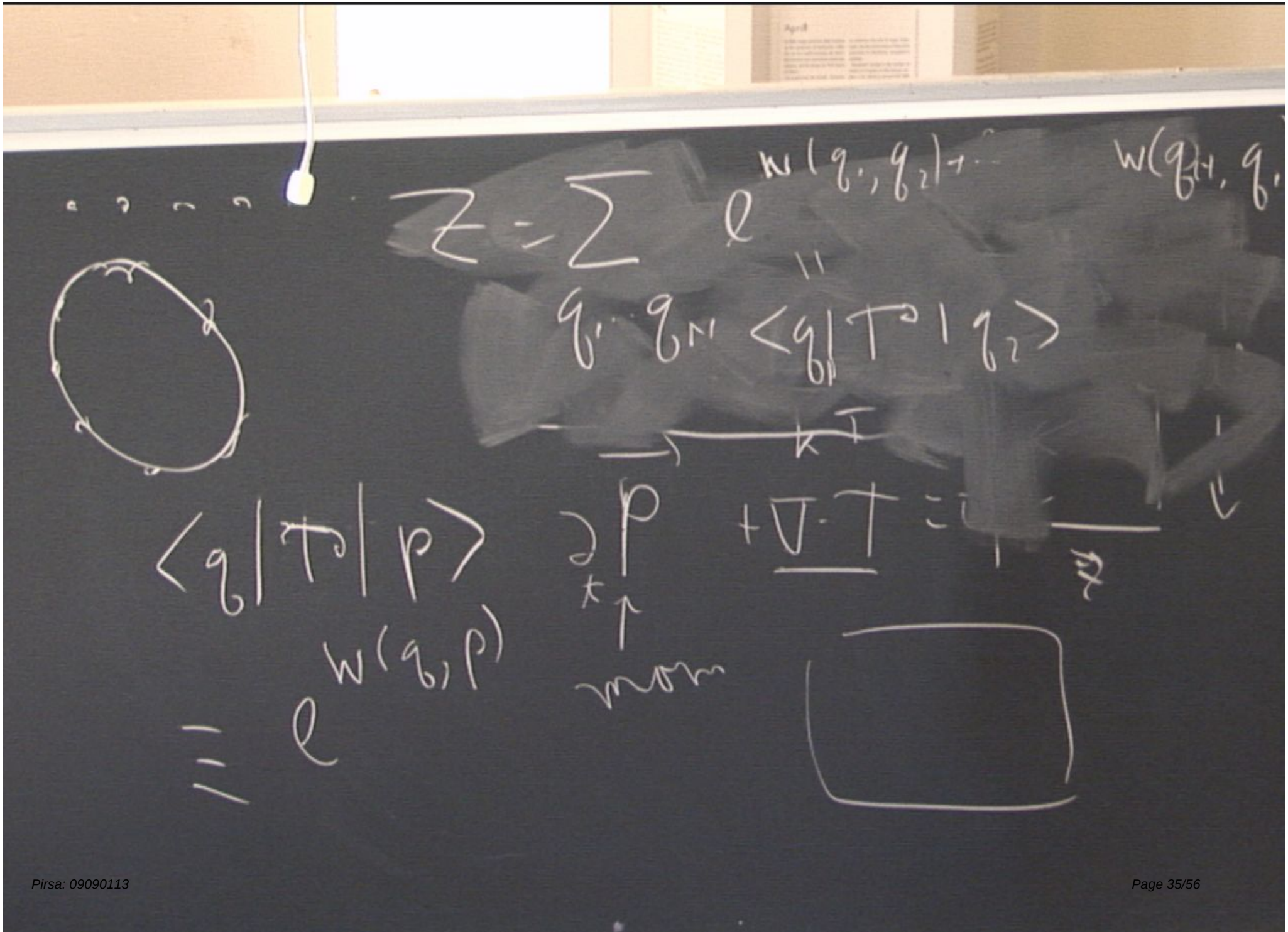
Z = Σ e^{W(q_1, q_2)+...}
W(q_{N+1}, q_1
q_1 ... q_N <q_1| T^n |q_2>
T
<q| T |p>
p
+ ∇·T =
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From Classical to Quantum:

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If you recall the definition for matrix multiplication,

$$< q_1|TS|q_3 >= \sum_{q_2} < q_1|T|q_2 >< q_2|S|q_3 >$$

you will see at once that the partition function is $Z = \sum_{q_1} < q_1|T^N|q_1 >$

so that Z= trace T^N

In order to get something familiar, imagine that T is an exponential of a Hamiltonian, specifically T=exp(−τH)), where H is a Hamiltonian defined in terms of w. In terms of matrix elements

$\langle q|T|p\rangle = exp[w(q,p)] = \langle q|\exp(-\tau H)|p\rangle$

In fact, T is what we called before $T(-i\tau)$. If we write the trace in terms of the eigenvalues, ϵ_α, of H we have

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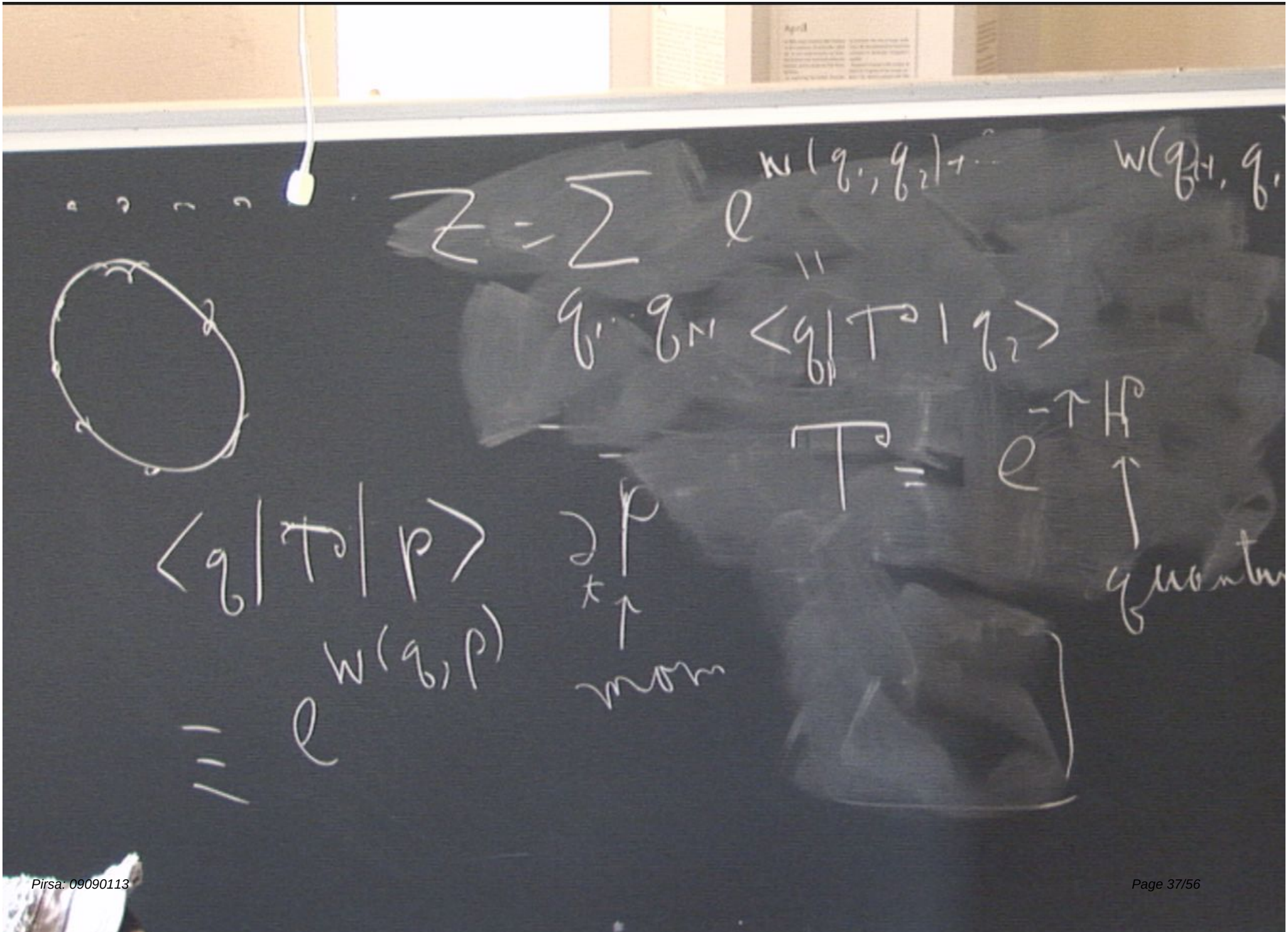
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Summary

$$Z = \mathrm{trace}_{q_1}\mathrm{trace}_{q_2}\ldots\mathrm{trace}_{q_n}\prod_{j=1}^{N}\exp(w(q_j,q_{j+1})) \qquad (4.10)$$

or in a more compact notation

$$Z = \mathrm{Trace}_{\{q\}}\exp[W\{q\}] = \mathrm{trace}\exp[-H\tau N] \qquad \text{iii.4}$$

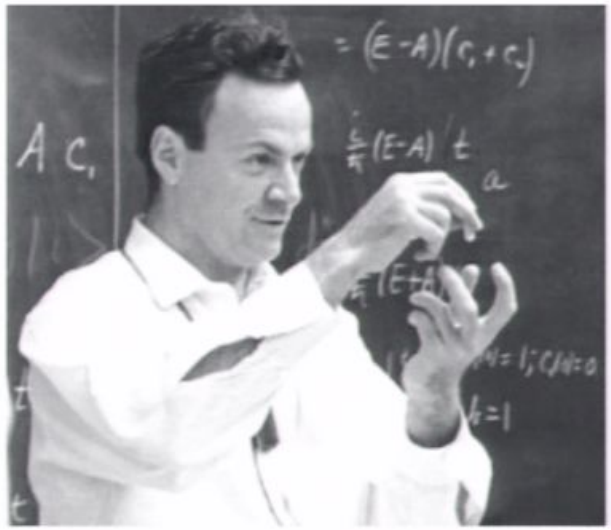
Note that we use the word "trace" to represent both a quantum and a statistical mechanical sum. The trace in equation 4.10 is a statistical sum. The first Trace in equation iii.4 is a statistical mechanical sum, the second is a quantum mechanical trace. We use a capital "T" when we sum over many variables and a lower case one when we sum over only one or a few.

The point of the argument is that they have a direct translation into one another: Every quantum mechanical trace can be converted into a one-dimensional statistical mechanics summation and *vice versa*.

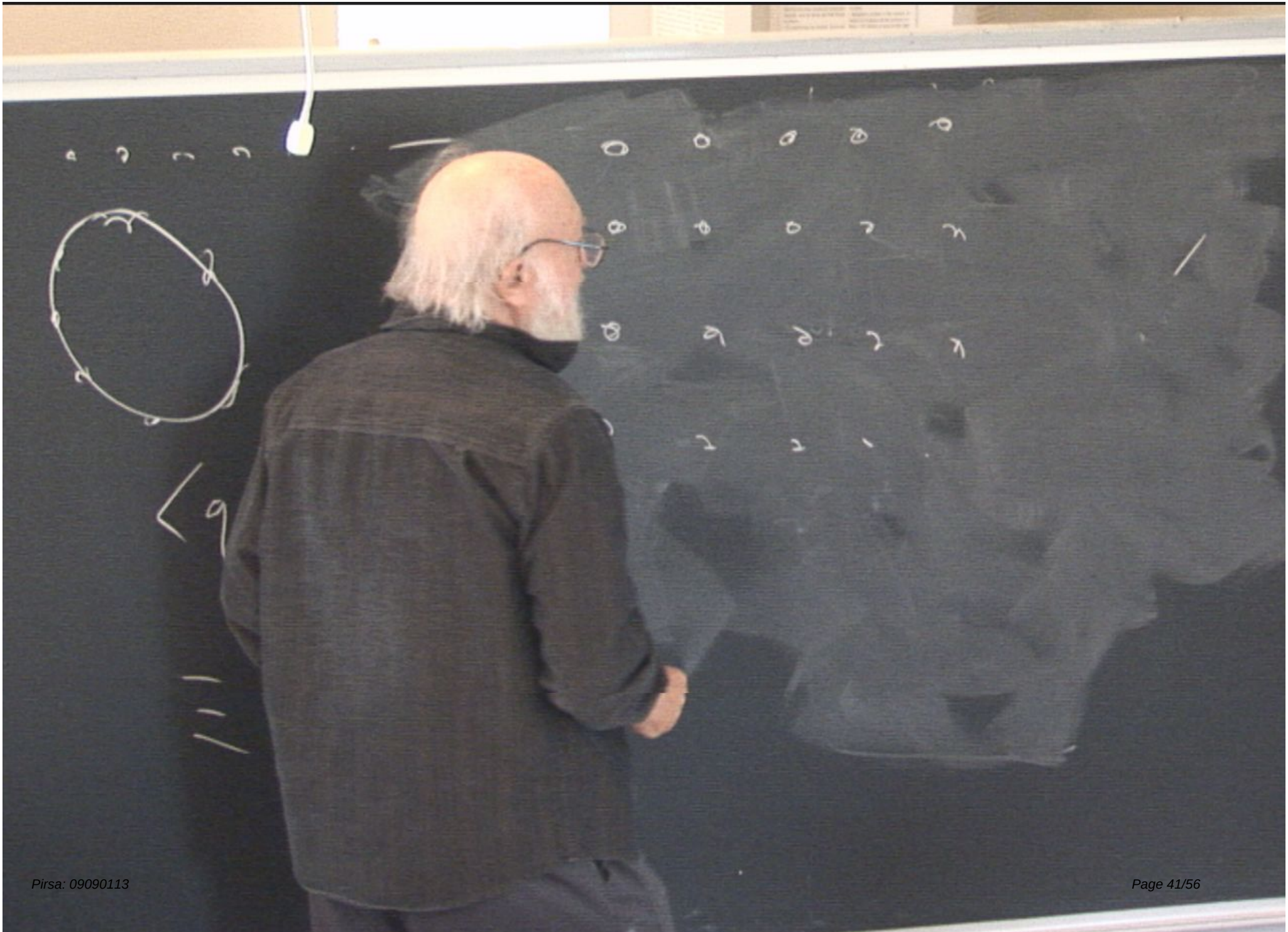
Feynman showed how to convert problem of quantum mechanics into a path integral. We have essentially put his path on a one-dimensional lattice.

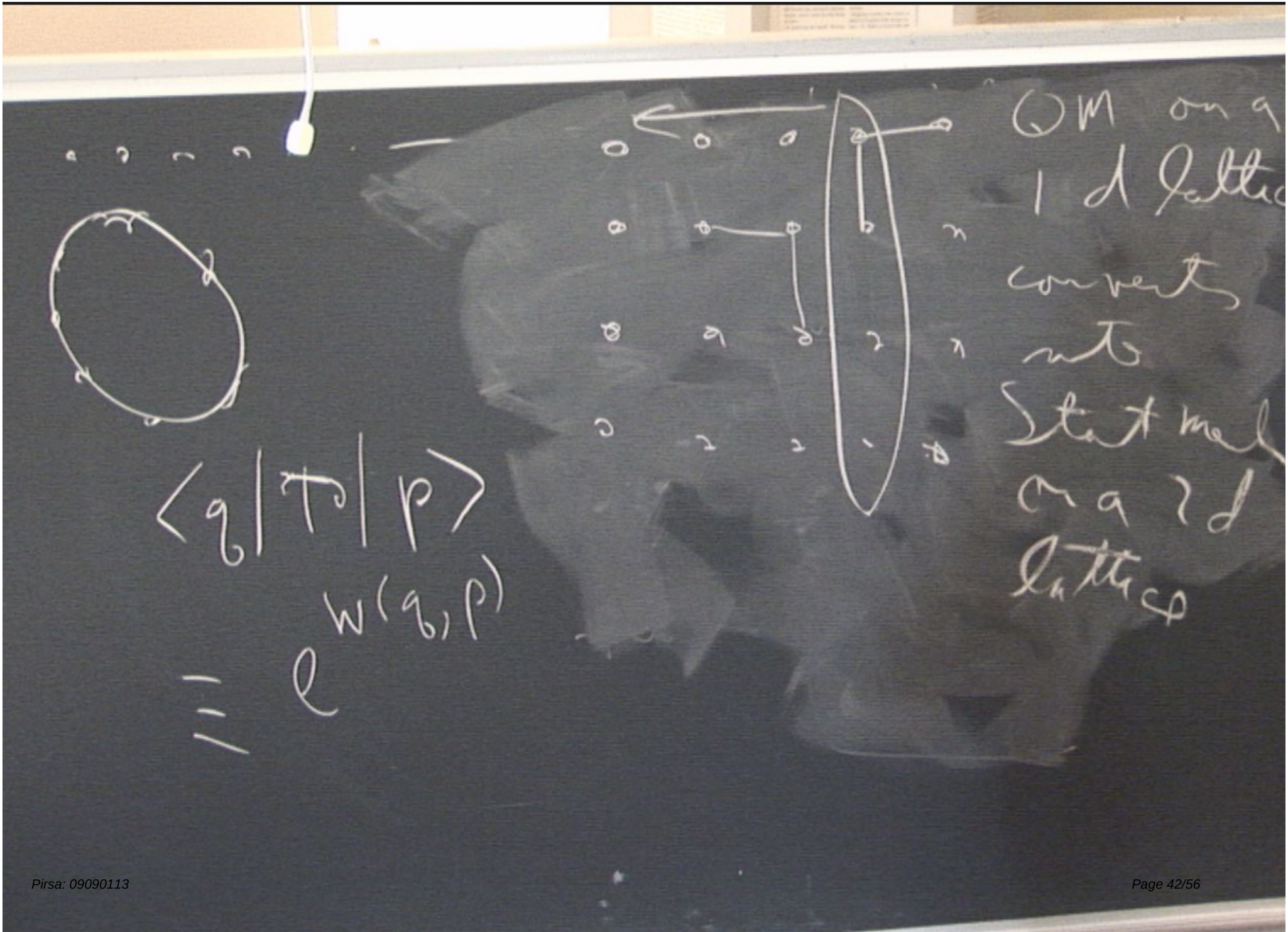
Every quantum mechanical trace can be converted into a one-dimensional statistical mechanics problem and *vice versa*. More generally, d dimensional quantum mechanics converts to d+1 dimensional stat mech. (Here, 0 dimensions of quantum becomes 1 of statistical mechanics).

The basic idea about going up and back between the two disciplines is due to Feynman, and his invention of the path integral. As far as I know, Feynman never quite said the sentence written in blue. The point was pursued and made explicitly by Kenneth Wilson, and used in his invention of the modern renormalization group. I'll come back with more about that later.



Richard Feynman

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Feynman's case: particle mechanics

The simplest and most fundamental problem in quantum theory is a particle in a one-dimensional potential, $H=p^2/(2m) + U(q)$, where p and q obey $[p,q]=-i\hbar$. However, we shall stick with units in which $\hbar=1$.

We assert, without proof, that the exponential of this operator has the matrix element

$$\langle q|T(-i\tau)|q'\rangle=\langle q|\exp[-\tau H]|q'\rangle = \exp[-m(q-q')^2/(2\tau)-\tau U(q)] \qquad \text{iii.5}$$

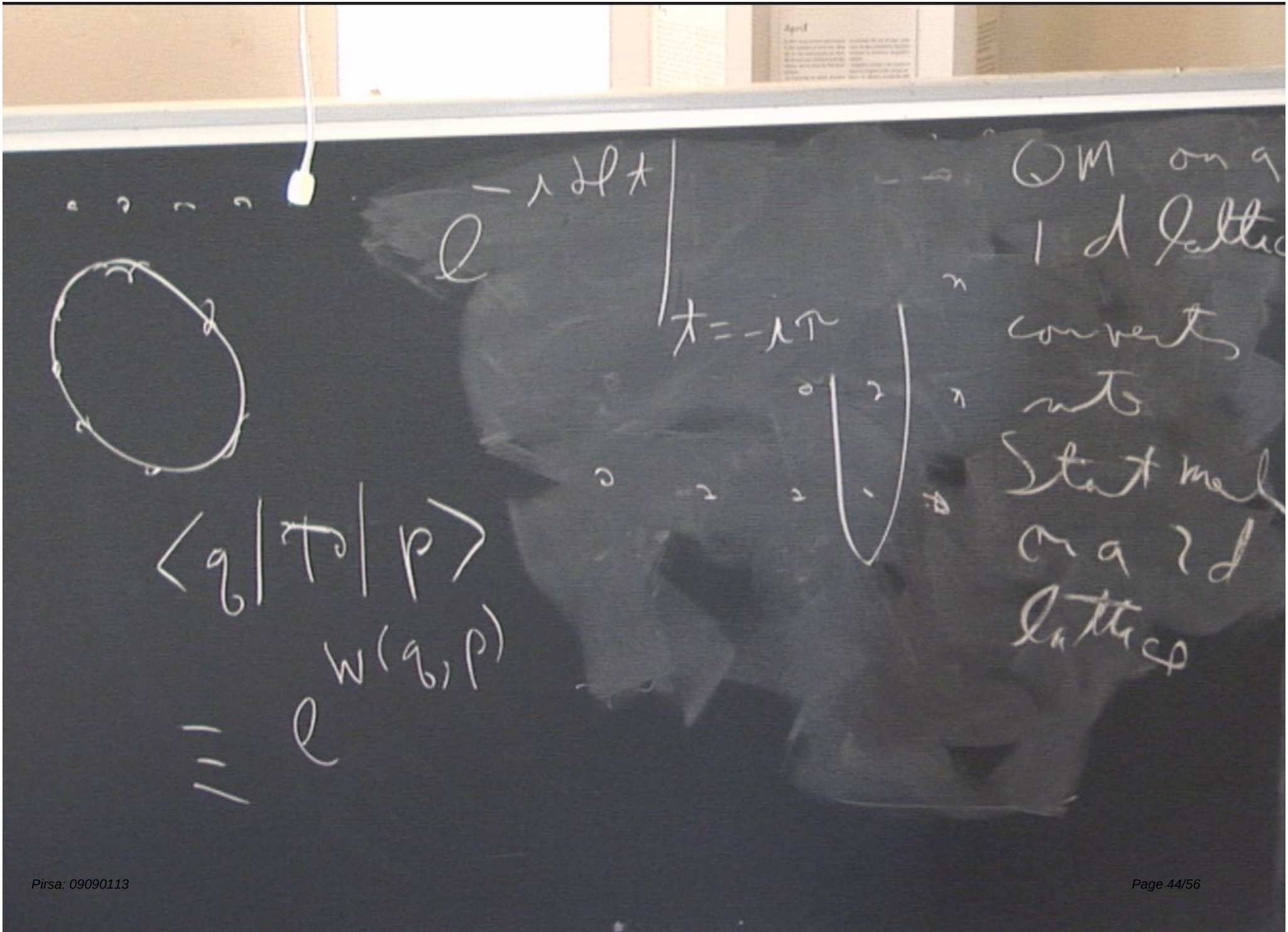
for small values of τ. Because τ is small, q and q′ are necessarily close to one another. For that reason, we can replace U(q) by U(q′) or by [U(q)+ U(q′)]/2 in the analysis that follows. (These choices are close to equivalent, but they are not the same because p and q do not commute.)

Calculate the matrix element of $\exp[-\tau p^2/(2m)]$ between position eigenstates.

Imagine that we wished to know the eigenvalues of the Hamiltonian, *H*. We could, for example, numerically calculate the integral of products of matrix elements as given above. As the number of steps times τ goes to infinity we would pick out the lowest eigenavlue as the leading term in

$$\text{trace}\, T(i\tau)^N = \text{trace}\, e^{-N\tau H} = \sum_\alpha e^{-N\tau\varepsilon_\alpha} \qquad \text{iii.6}$$

This approach provides a powerful method for both numerical and analytic approaches to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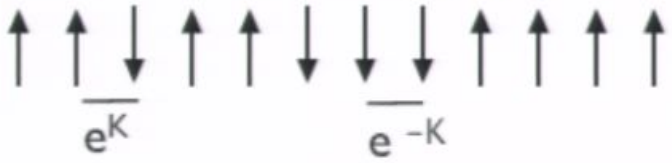
The Ising Linear Chain

We calculate the partition function in the simplest case of this kind. Take an Ising model with spins σ_j at sites $j = 1, 2, \ldots, N$. Take the magnetic field to be zero and arrange the couplings so that immediately neighboring sites (j and $(j+1)$ have a coupling K. The statistical weight for two neighboring sites having spin-values σ and σ' is then defined to be

$$e^{w(\sigma,\sigma')} = e^{K\sigma\sigma'} = (\sigma|\mathcal{T}|\sigma') \qquad (4.17)$$

linear chain

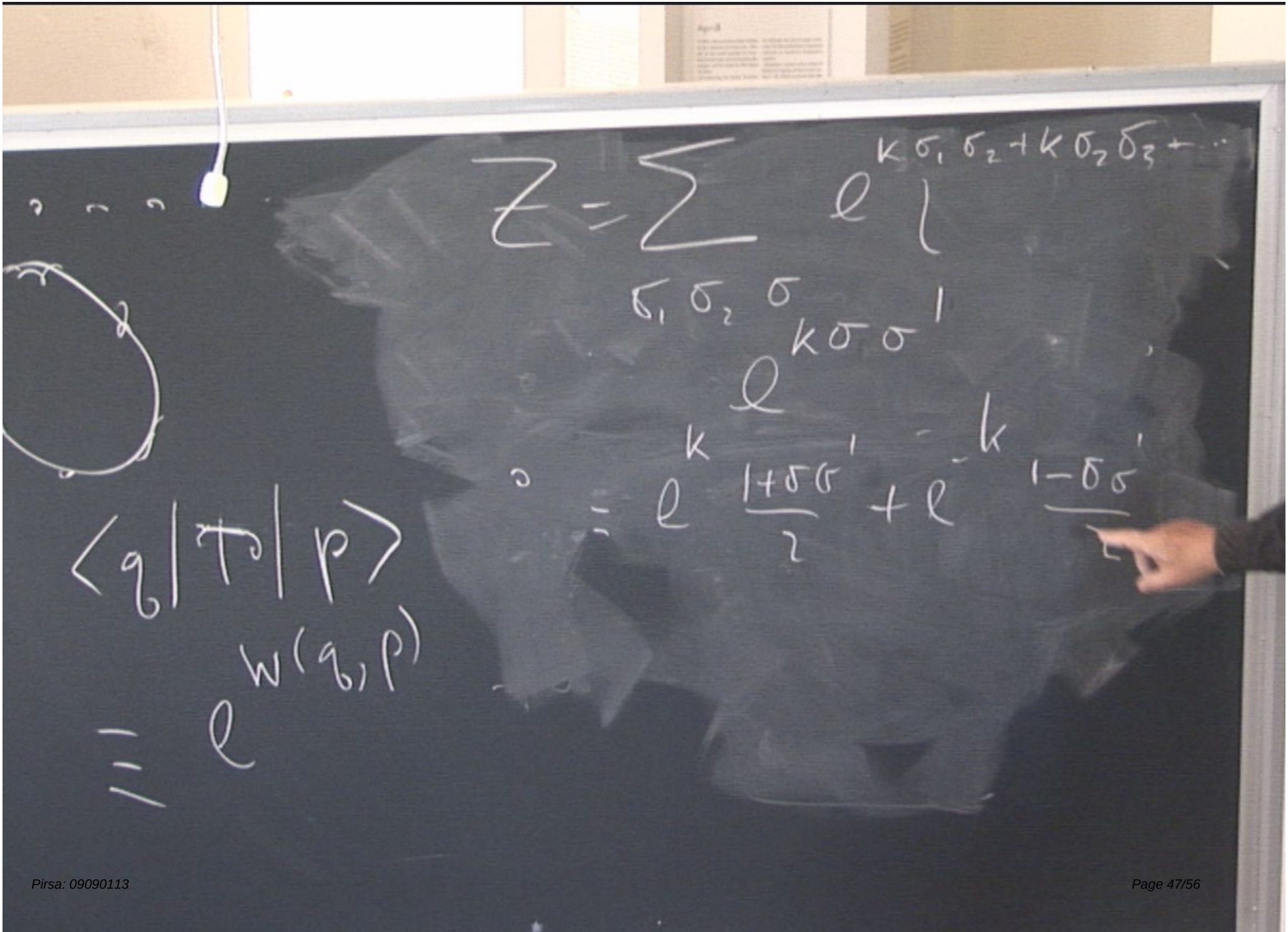


This kind of two by two system is generally analyzed in terms of the Pauli matrices which are the four basic matrices that we can use to span this two by two space. They are

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (4.18)$$

In going up and back between the notation of equations (4.17) and (4.18) we have to think a little. In (4.17), we interpret σ and σ' as eigenvalues of the matrix τ_3. Any two by two matrix, M, can be written in terms of the eigenstates corresponding to these eigenvalues:

$$M = \begin{pmatrix} (-1|M|-1) & (-1|M|1) \end{pmatrix}$$


$Z = \sum_{\sigma_1 \sigma_2 \sigma} e^{k\sigma_1\sigma_2 + k\sigma_2\sigma_3 + \cdots}$
$e^{k\sigma\sigma'}$
$= e^{k\frac{1+\sigma\sigma'}{2}} + e^{-k\frac{1-\sigma\sigma'}{2}}$
$\langle q|T|p\rangle$
$= e^{W(q,p)}$

The transfer Matrix

A useful form for these Pauli matrices is

$$(\sigma|\mathbf{1}|\sigma') = \delta_{\sigma,\sigma'} \qquad (\sigma|\tau_1|\sigma') = \delta_{\sigma,-\sigma'} \qquad (4.19b)$$
$$(\sigma|\tau_2|\sigma') = i\sigma\delta_{\sigma,-\sigma'} \qquad (\sigma|\tau_3|\sigma') = \sigma\delta_{\sigma,\sigma'}$$

these matrices have a very direct physical meaning.
The matrix τ_3 is diagonal in the σ-representation and represents the spin. Conversely, τ_1 has only off-diagonal elements. It is an operator whose effect is to change the σ-value.

The matrix element of the transfer matrix, *T*, is equal to e^K when $\sigma = \sigma'$ and equal to e^{-K} otherwise. In symbols,

$$(\sigma|T|\sigma') = \frac{1+\sigma\sigma'}{2}e^K + \frac{1-\sigma\sigma'}{2}e^{-K} \qquad (4.20)$$
$$= e^K \mathbf{1} + e^{-K}\boldsymbol{\tau_1}$$

Here the matrices in **bold** are the ones defined in eq. 4.19b. We can also write the result as an exponential, $T=\exp(-H)$ where

Dual Couplings

$$-\mathcal{H} = \tilde{K}_0 \mathbf{1} + \tilde{K}\tau_1 \qquad (4.22)$$

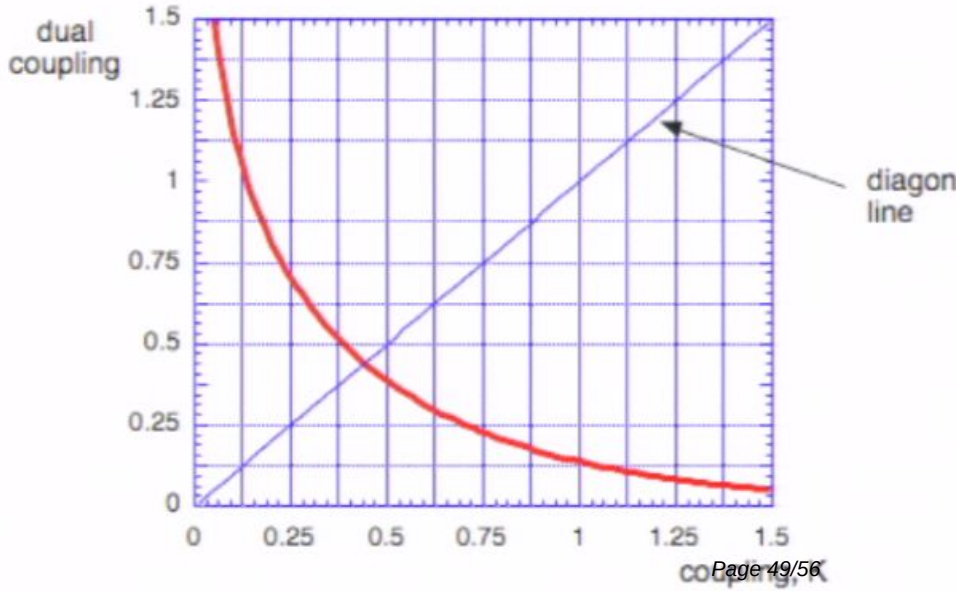
The quantity $\tilde{K}$ is said to be the dual of K. For a simpler notation, we call this function by another name so that the dual of K is $D(K)$ This name implies in part that the function $D(K)$ has the property that if it is applied twice that you get precisely the same thing once more:

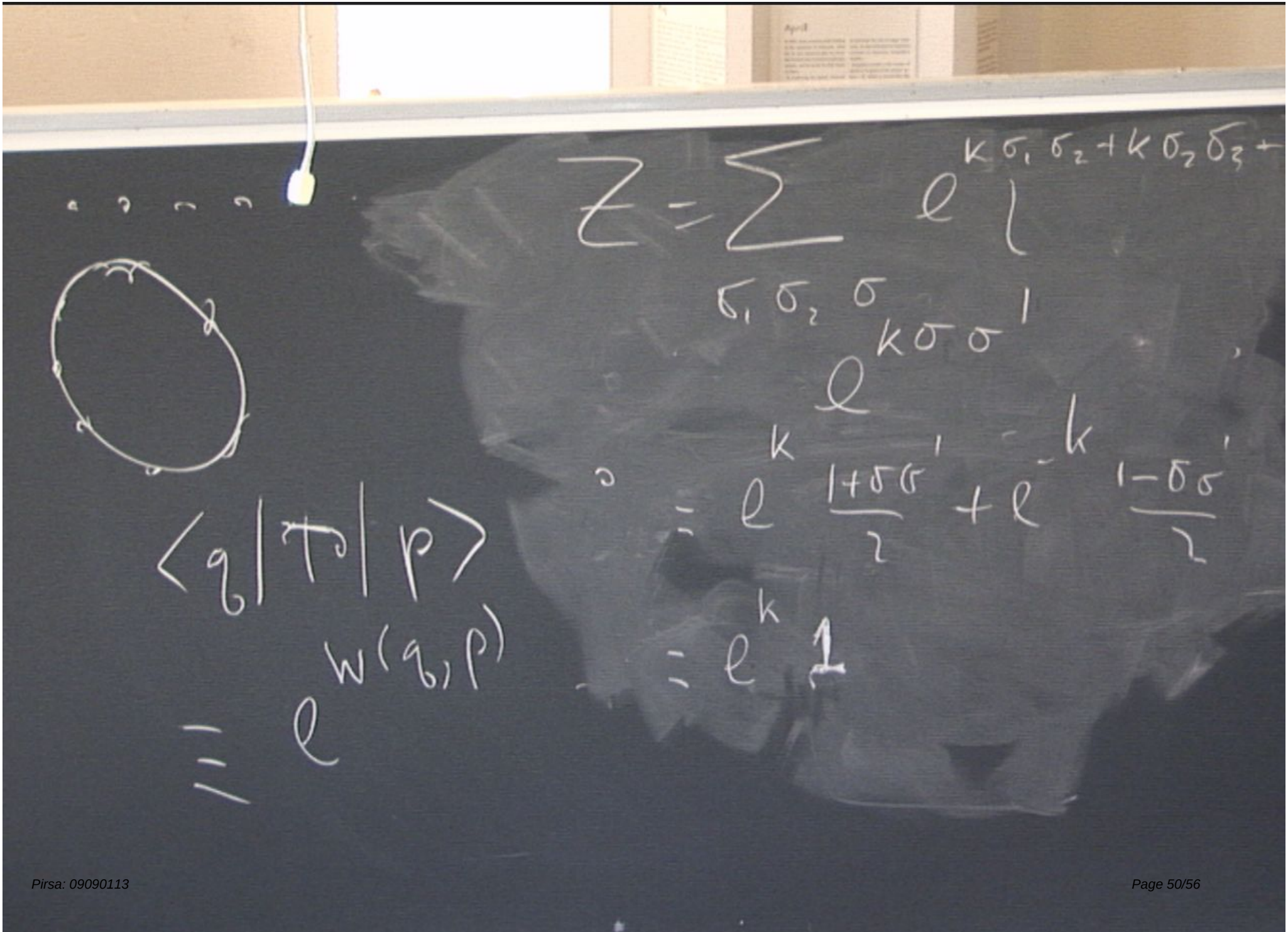
$D(D(K))=K$ or $D^{-1}(K)=D(K)$

How would I find the function D(K)?

$\tilde{K}= D(K)=[\ln (\tanh K)]/2$ $\tilde{K}_0= [\ln(\sinh 2K)]/2$

This function has the property that when K is strong its dual is weak and *vice versa*. This property has proven to be very important in both statistical physics and particle physics. Often we know both a basic model and its dual. Often models are hard to solve in strong coupling. But the dual models have weak coupling when the basic model has strong coupling. So then we get an indirect solution of the basic model.

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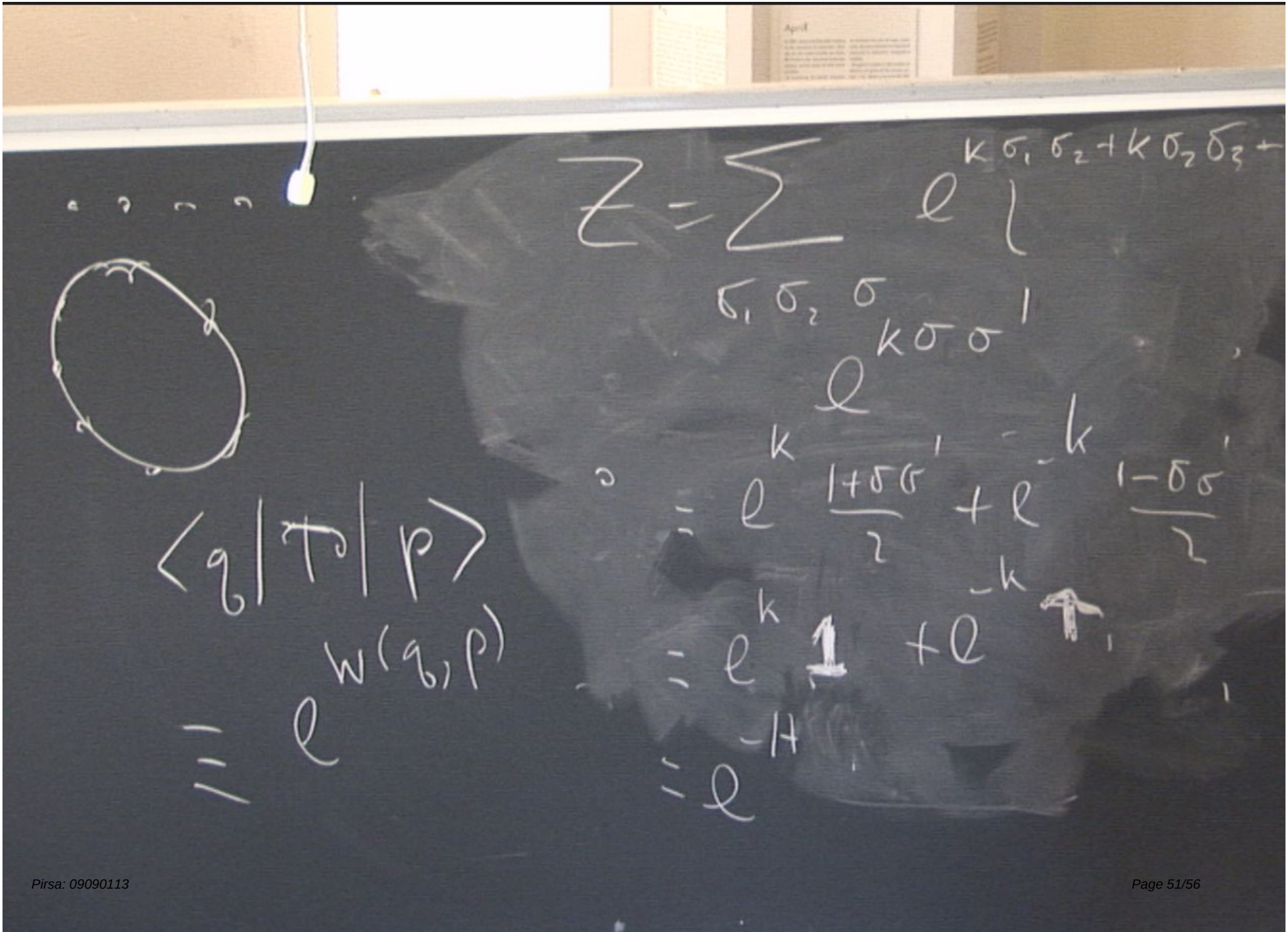
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$\langle \sigma | T | \sigma' \rangle$
$= e^{W(\sigma,\sigma')}$
$= e^{K} \mathbf{1} + e^{-K} T$
$= e^{-H}$

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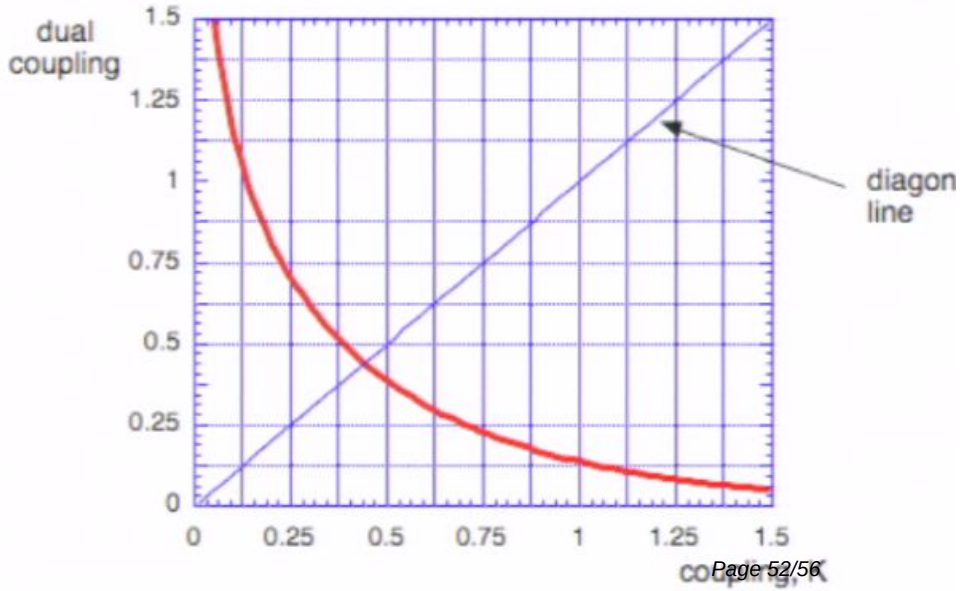

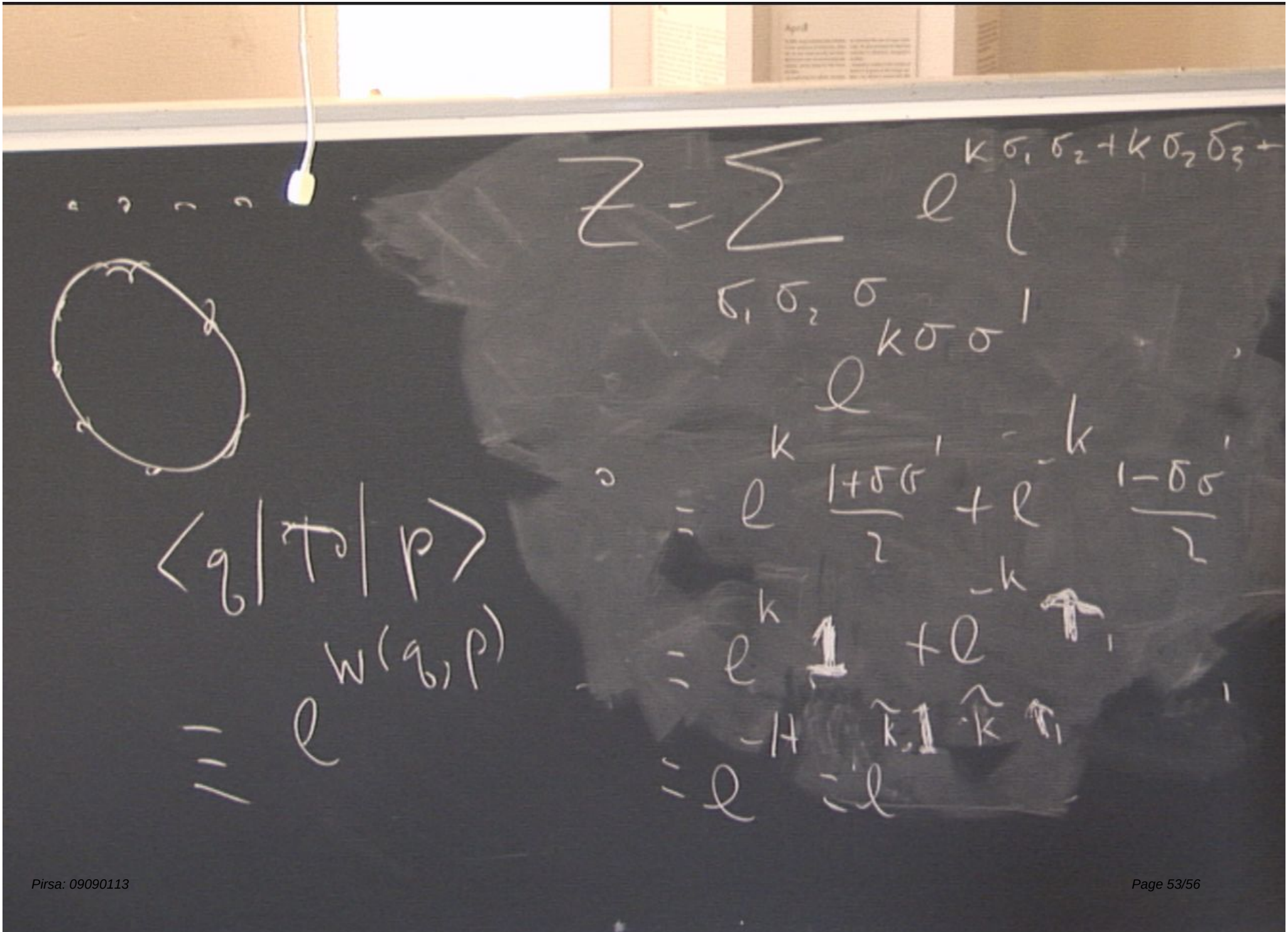
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$= e^{W(q,p)}$
$= e^{K} \mathbb{1} + e^{-K} T_1$
$= e^{-H}$
$\tilde{K}, \mathbb{1}, \hat{K}, T_1$
$= e^{-\tilde{K}} e^{-\hat{K}} e^{-T_1}$

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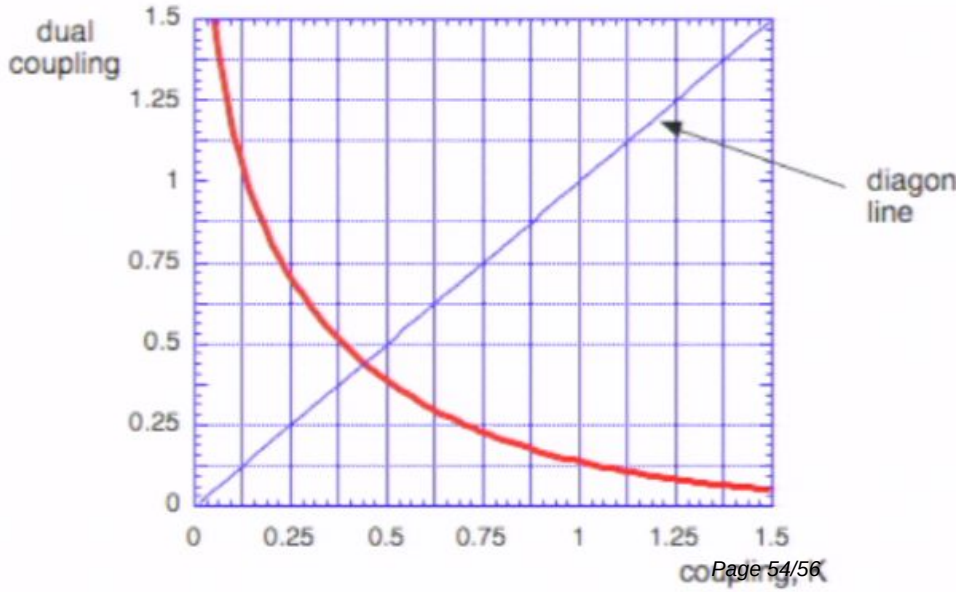

Solution of the one-dimensional Ising model

From equation 4.20, we find that the partition function of the one-dimensional Ising model is

$$Z = \text{ trace } (e^K \mathbf{1} + e^{-K} \tau_1)^N$$

But the trace is a sum over eigenvalues and the eigenvalues of τ_1 are plus or minus one. Thus, the answer is:

$$Z = (2 \cosh K)^N + (2 \sinh K)^N \qquad (4.25)$$

If N is very large, the first term is much larger than the second and thus in this limit of large system size:

$$-\beta F = \ln Z = N \ln(2 \cosh K) \qquad (4.26)$$

What quantum mechanics problem have we solved?

More about quantum from the Long Chain

We should be able to say more about quantum problems based upon the analysis of the long chain. For example let us imagine that we wish to calculate the average of some quantum operator, $X(q)$, which happens to be diagonal in the q-representation. The text book goes through a long song and dance to prove a rather obvious result. You have seen that the trace in equation 4.10 pushes us into a sum over energy states, and if N is very large that sum reduces to a projection onto the ground state of the system. Specifically,

$$Z = \mathrm{trace}_{q_1} \mathrm{trace}_{q_2} \ldots \mathrm{trace}_{q_n} \prod_{j=1}^{N} \exp(w(q_j, q_{j+1})) \qquad (4.10)$$

becomes $Z=\exp(-\tau\epsilon_0)$

So if we insert an X, for any any operator X, in that sum the result should give what happens to that X in the ground state, specifically

$$(1/Z)\ \mathrm{Trace}_{\{q\}}\ \exp[W\{q\}]\ X = \langle 0|\ X(q)\ |0\rangle$$

In this way, we can use statistical mechanics to calculate the average of any operator in the ground state. If we do not take N to infinity, we can do the corresponding calculation to calculate the average of any operator at a inverse temperature ($\beta-$ value) equal to N τ.

By playing with the times in an appropriate fashion, we can even calculate time-dependent correlation functions in the ground state or in a finite-temperature state.