Windsor Lectures

on

Classical Statistical Mechanics for Quantum Scientists

by

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From Stat Mech in d dimensions to Quantum Theory in d-1

IA The Simplest Problems in State Mech

One spin in a magnetic field:

$H=-\mu B \sigma$

$\text{prob}(\sigma) \sim \exp(-\beta H(\sigma))$

$\text{prob}(\sigma) = \exp(h\sigma)/z \qquad h=B\mu\beta$

$z=2 \cosh h$

$<\sigma> = \sum_{\sigma} [\text{prob}(\sigma) \; \sigma] = \tanh h$

note that we can also calculate this from z as

$= (d/dh) \ln z$

Two Coupled Spins

$z=\sum_{\sigma \sigma'} \exp(K \sigma \sigma') = 4 \cosh K$

$<\sigma \sigma'> = (d/dK) \ln z = \tanh K$

IB. One Dimensional Stat Mech

A simple problem in classical stat mech:
chain of N atoms represented by their spin $\sigma_j = \pm 1$, $j=1,2, \ldots, N$, each coupled to its nearest neighbor with coupling K with periodic boundary conditions. We wish to calculate the partition function written as

$$z = \sum_{\sigma_1 .. \sigma_N} e^{K\sigma_1\sigma_2} e^{K\sigma_2\sigma_3} \ldots . e^{K\sigma_N\sigma_1}$$

After a little thought we see that we can calculate this partition function for any N by replacing the classical problem by a quantum problem formulated in matrix language. Let σ and σ' each take on values ± 1, and write each term in the product as a matrix element

$$e^{K\sigma\sigma'} = (\sigma \,|\, \mathbf{T} \,|\, \sigma') = \begin{bmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{bmatrix}$$

$$z = \sum_{\sigma_1 .. \sigma_N} e^{K\sigma_1\sigma_2} e^{K\sigma_2\sigma_3} \ldots . e^{K\sigma_N\sigma_1}$$

$$= \sum_{\sigma_1 .. \sigma_N} (\sigma_1 \,|\, \mathbf{T} \,|\, \sigma_2)(\sigma_2 \,|\, \mathbf{T} \,|\, \sigma_3)\ldots(\sigma_N \,|\, \mathbf{T} \,|\, \sigma_1)$$

T is called a transfer matrix because it transfers you from one step in the chain to the next.

Properties of Transfer Matrix

We can think that the matrix is labeled by eigenvalues called □ and □ of the standard Pauli spin matrix σ_3-- the quantum representation of a z-direction spin vector. We can analyze this situation using the other Pauli matrices σ_1 and σ_2 which each anti-commute with σ_3 and one another. For example, the matrix T may be written as

$$\mathbf{T} = 1e^{K} + \sigma_1 e^{-K}$$

where σ_1 is a pauli spin matrix and has eigenvalues ± 1. We shall also use the log of T

$$\ln \mathbf{T} = 1\tilde{K}_{\mathbf{o}} + \sigma_1 \tilde{K}$$

where $\tilde{K}$, defined by $\exp(-2\tilde{K})$ =tanh K, is big when K is small and vice versa.

Duality:

Note that

sinh 2K sinh 2 $\tilde{K}$ =1

There is a “dual” connection between K and $\tilde{K}$, i.e. if $\tilde{K}$=F(K) then equally K=F($\tilde{K}$), so that F is its own inverse. Another way of putting this is that F(F(K))=K for all K.

From Sum to Matrix Product

The most important thing about T is that the sum defining the partition function may be written as a trace of a matrix product. Recall from your matrix mechanics that a product is defined by

$$\sum_{\nu} (\mu\,|\,\mathbf{M}\,|\,\nu)(\nu\,|\,\mathbf{N}\,|\,\lambda) = (\mu\,|\,\mathbf{MN}\,|\,\lambda)$$

while the trace of a matrix is $trace\,\mathbf{N} = \sum_{\nu} (\nu\,|\,\mathbf{N}\,|\,\nu)$

Therefore

$$z = \sum_{\sigma_1 .. \sigma_N} e^{K\sigma_1\sigma_2}\, e^{K\sigma_2\sigma_3} \ldots . e^{K\sigma_N\sigma_1}$$

$$= \sum_{\sigma_1 .. \sigma_N} (\sigma_1\,|\,\mathbf{T}\,|\,\sigma_2)(\sigma_2\,|\,\mathbf{T}\,|\,\sigma_3) \ldots (\sigma_N\,|\,\mathbf{T}\,|\,\sigma_1)$$

$$= \sum_{\sigma_1} (\sigma_1\,|\,\mathbf{T}^N\,|\,\sigma_1) = trace\ \ \mathbf{T}^N$$

Thus the partition function is evaluated as a trace of a multiple product of matrices.

Calculation of Partition Function

Since we know the eigenvalues of T we know the trace is the sum of those eigenvalues to the Nth power, and hence we know the partition function.

$$z = trace\ \mathbf{T}^N = trace(1e^K + \square_1 e^{-K})^N$$

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

We have gone from 1 dimensional statistical mechanics to ordinary (zero dimensional) quantum theory).

As N goes to infinity, the first term dominates
As K goes to infinity, the terms become equal. There is a nonuniform passage to the limit, characteristic of a phase transition...here at K=∞.

Averages

The calculation of averages uses the relative weights found in the formula for the partition function:

$$Z = \sum_{\sigma_1 .. \sigma_N} e^{K\sigma_1\sigma_2} e^{K\sigma_2\sigma_3} \ldots . e^{K\sigma_N\sigma_1}$$

Thus the average of the product of the 2nd spin times the Nth. spin is defined to be

$$Z < \sigma_2 \sigma_N >$$

$$= \sum_{\sigma_1 .. \sigma_N} e^{K\sigma_1\sigma_2} \sigma_2 e^{K\sigma_2\sigma_3} \ldots \sigma_N e^{K\sigma_N\sigma_1}$$

$$= \sum_{\sigma_1 .. \sigma_N} (\sigma_1 | \mathbf{T} | \sigma_2) \sigma_2 (\sigma_2 | \mathbf{T} | \sigma_3) \ldots \sigma_N (\sigma_N | \mathbf{T} | \sigma_1)$$

$$= trace\ (\mathbf{T}\, \sigma_3\, \mathbf{T}^{N-2}\, \sigma_3\, \mathbf{T})$$

$$= trace\ (\sigma_3 \mathbf{T}^2 \sigma_3 \mathbf{T}^{N-2})$$

The last line is obtained using the cyclic invariance of the trace.

Note how the placement of the Pauli matrix describes its j-value. Thus T serves as a space displacement operator analogous to exp.(i H/$\hbar$) of quantum theory, which does a time displacement.

Evaluation of Correlation Function

Now we invoke a couple of quantum tricks to do this trace. If N is very large T^N is proportional to a projection operator onto the "ground state" of T, i.e. the one with largest eigenvalue, which we write as $|0><0|$. The bra and the ket here are each eigenstates of σ_1 with σ_1 equal to +1. If the eigenvalue is T_0 the result is

$$<\sigma_2 \sigma_N> = (0|\sigma_3 (\mathbf{T}/\mathbf{T}_0)^2 \sigma_3|0)$$

Similarly if the two spins are separated by k units (with 0<k<<N) we find for large N

$$<\sigma_j \sigma_{j+k}> = (0|\sigma_3 (\mathbf{T}/\mathbf{T}_0)^k \sigma_3|0)$$

Now σ_3 σ_3 flips the eigenvalue of T:

$\sigma_3|0> = |1>$,

where $|1>$ is the excited state of the transfer matrix. That has an eigenvalue given by

$(T_1/T_0)' = \exp(-2\tilde{K})$ so that

$$<\sigma_j \sigma_{j+k}> = \exp(-2k\tilde{K})$$

Correlation length

This exponentially decaying result can also be written in terms of the distance r between the two spins. If a_0 is the distance between nearest neighbors, $r=ka_0$. The correlation function then falls off with a characteristic distance $\xi = a_0(2\tilde{K})$, called the correlation length. The resulting resulting form for the correlation function is

$$<\sigma_j \sigma_{j+k}> = \exp(-r/\xi)$$

In our later work, we shall have lots of use for the correlation length. Here we should notice that at the phase transition, at K equal to infinity, the correlation length also goes to infinity.

In the 1930's Yakuza recognized the importance of exponential decay in particles physics. For slow-moving particles the probability of finding the particle virtually produced away from a source dies exponentially with decay constant

$$\kappa = \xi^{-1} = m$$

Here we denote the decay constant by kappa while in the context it is the particle mass, m.

Two Dimensional Problem in Stat Mech.

Consider a problem in two dimensional stat mech., with sites labeled by j and k, and with periodic boundary conditions in which j=N+1 is the same as j=1 and k=M+1 means the same as k=1. The summation problem is

$$z = \sum_{\sigma' s} \exp(W)$$

$$W = \sum_{j,k} (K_x \sigma_{j,k} \sigma_{j+1,k} + K_y \sigma_{j,k} \sigma_{j,k+1})$$

By precisely the same trick as before, we reduce the summation problem to a trace over M different variables representing the spins on the different rows of the lattice. The trace has the form

$$z = trace\ (\mathbf{T}_x \ \ \mathbf{T}_y)^N$$

$$\mathbf{T}_y = \exp(\sum_k K_y \sigma_3^k \sigma_3^{k+1})$$

$$\mathbf{T}_x = \exp(\sum_k (K_0 + \tilde{K}_x \sigma_1^k))$$

where the σ's are Pauli matrices which commute for different values of the y-index, k.

Nature of the Stat Mech. Problem

The next step is to see the large N and M limit of the problem we have just defined. In this limit there are two possibilities: either T_x dominates or T_y does. In the latter case the couplings in the y direction are strong while the "quantum" coefficient, $\tilde{K}$, in the x direction is weak. The effect of the strong coupling in T_y is that the system is pushed into a state in which the y-direction-neighboring σ_3 are likely to have the same value. Thus, the spins in the rows line up. The weak σ_1 coupling in T_x means that whatever happens in one column is faithfully translated to the next. The net effect is that correlations among the spins are transmitted through the entire system. If the constants, K_x and K_y, are weak then the system is pushed into eigenstates of all the σ_1^k's equal to +1 and as a result there is no long-range ordering of the σ_3^k's. Thus the system displays two different phases, one in which the K's are strong and the ground state includes many lined-up spins, and the other in which the K's are weak, and the eigenstates of the first Pauli matrices dominate the behavior.

The Phase Transition

The two phases just described are distinct, because the neighboring spin alignment produces a doubly degenerate state, one for spin up and the other for spin down, while the dominance of σ_1^k's produces a single state. Since the structure of the commutation relations among the $\sigma_3^k\sigma_3^{k+1}$'s and the σ_1^k's is symmetrical between the two kinds of operators, an important change must occur when the coefficients become equal. Indeed it is true that the system is in its ordered phase for $K_y > \tilde{K}_x$. If the sign of the inequality is reversed, the system is in its disordered phase, while if $K_y = \tilde{K}_x$ the system is its critical phase.

The relation between the "ordering term" involving the third Pauli matrices and the "disorder term" involving the first Pauli matrix reflects a symmetry between the ordered and disordered phases of the two dimensional Ising model. This relation is a more sophisticated kind of dual symmetry, like the relation between K and $\tilde{K}$. You recall this is a situation in which the symmetry operation is its own inverse, so that two symmetry operations take one back to the starting point.

Duality Demonstrated

To see this duality it is useful to notice the relationship between the two kinds of terms in the transfer matrix $u_k = \sigma_3^k \sigma_3^{k+1}$ and $v_j = \sigma_1^j$. In quantum theory, commutation relations fully determine the possibly values of the operators. For u and v the relations are:

1. All u's commute with each other
2. All v's commute with each other
3. $u_k^2 = v_j^2 = 1$ and
4. $u_k v_j = - v_j u_k$ for j =k or k+1

   $u_k v_j = v_j u_k$ otherwise

Therefore interchange of u's and v's gives us an equivalent problem.... one in which the roles of K and $\tilde{K}$ are interchanges.... while two such transforms take one back to the beginning.

Using this logic Kramers and Wannier proposed that the 2d Ising model had its critical point where

$K_y = \tilde{K}_x$. This is the right answer.

Hamiltonian Formulation

One particularly interesting case occurs when K_y and $\tilde{K}_x$ are both small. This situation can bring us to any one of the three phases since the x-coupling must be large and balanced by a weak y-coupling. The two exponents can be combined

$$z = trace\ (\mathbf{T}_x\ \ \mathbf{T}_y)^N$$

$$\mathbf{T}_y = \exp(\sum_k K_y \sigma_3^k \sigma_3^{k+1})$$

$$\mathbf{T}_x = \exp(\sum_k (K_0 + \tilde{K}_x \sigma_1^k))$$

$$z = trace\ \ \exp(-N\mathbf{H})$$

$$-H = \sum_k (K_y \sigma_3^k \sigma_3^{k+1} + K_0 + \tilde{K}_x \sigma_1^k)$$

Our statistical mechanics problem has now reduced itself to finding the properties of the Hamiltonian for a one-dimensional system. This is quite non-trivial. It has been carried out by Onsager and by Onsager and Kauffman. I shall not carry on only a little bit further here.

Method of Solution

There are of whole collection of one dimensional quantum problems which have very elegant solutions that can be constructed via using an ansatz for the ground state of a type first proposed by Bethe. (Recall that the N goes to infinity limit is a ground state calculation.) The two dimensional Ising model falls into this class, but it is even simpler. It can be reduced to a non-interaction fermion problem.

One can form fermion creation and annihilation operators by using a string of σ's all multiplied together, as $\mu_k = \sigma_1^1 \sigma_1^2 \sigma_1^3 \ldots \sigma_1^{k-1} \sigma_1^k$

Now construct

$$b_+^k = i\,\mu_k \sigma_3^k / \sqrt{2}$$
$$b_-^k = \mu_k \sigma_3^{k+1} / \sqrt{2}$$

Note that all the b_+'s anti-commute with b_-'s except that for the case in which the two b's have identical indices their anti-commutator is unity. Hence they have exactly the same commutation properties as fermion creation and annihilation operators. Since the exponents in the transfer matrices are bilinear in these fermion operators the commutation of transfer matrices and fermion operators can be calculated. Onsager and Kaufmann did this to obtain all the properties of the 2d Ising model.