April 12, 1979

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Classical magnetism model = Ising model. One has a set I of sites and a state is a way of assigning ± 1 to each site. Thus a state is a function $s : I \to \{\pm 1\}$, $i \mapsto s_i$. The energy of the state is

$$E(s) = \underbrace{\sum h_i s_i}_{\text{from external field. Usually all } h_i = h} + \underbrace{\sum_{i<j} h_{ij} s_i s_j}_{\text{interaction energy } h_{ij}<0 \text{ in ferromagn. case}}$$

and the partition function is

$$Z = \sum_s e^{-\beta E(s)} \qquad \text{where } \beta = \frac{1}{kT}$$

I recall that the state s can be identified with a subset of I and that the partition function is essentially a Lee-Yang polynomial.

Heisenberg ferromagnet model = quantum-mechanical version where state vectors at each site lie in a 2-dimensional spin space with base states $|+\rangle$, $|-\rangle$ for spin up and spin down. The state vectors for the whole magnet lie in the tensor product of these 2-dimensional spin spaces:

$$\mathcal{H} = \bigotimes_I \mathbb{C}^2$$

which has a basis whose elements can be thought of as the classical states. I can also think of $\mathcal{H}$ as an exterior algebra.

The Hamiltonian operator on $\mathcal{H}$ is a sum of two terms like the classical energy. The [redacted] part due to an external magnetic field is the operator

$$H = -\mu \vec{\sigma} \cdot \vec{B}$$
$$= -\mu \left(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z \right)$$

where μ is a positive constant and the $\sigma_x, \sigma_y, \sigma_z$ are the Pauli-spin matrices. Note that

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma_z |+\rangle = |+\rangle \ , \ \sigma_z |-\rangle = -|-\rangle$$

so that if $\vec{B}$ [redacted] $= (0, 0, B_z)$, then
$$H|+\rangle = -\mu |+\rangle$$
$$H|-\rangle = +\mu |-\rangle$$
so that the lower energy occurs with the spins up.

The interaction term [redacted] for the ith and jth site is

$$[redacted] \quad -K \vec{\sigma}_i \cdot \vec{\sigma}_j$$

Now the quantum-mechanical partition function is

$$Z = \operatorname{tr} e^{-\beta H}$$

It would be nice if this turned out to be a determinant.

Suppose $\vec{B} = (0, 0, B_z)$, then

$$\vec{\sigma} \cdot \vec{B} = \sigma_z B_z = B_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

so the external field part of the Hamiltonian

$$-\mu \sum_{i \in I} \vec{\sigma}_i \cdot \vec{B}_i$$

will be diagonal for the given basis for $\mathcal{H}$. So it is clear that we have something like the unperturbed part H_0 of the Hamiltonian.

$$\sigma_i \cdot \sigma_j = 2 P_{ij}^{\text{spin exchange}} - 1$$

Effect on the base states $|\pm\rangle_i \otimes |\pm\rangle_j$ is as follows

$$\begin{array}{llll} P: & |++\rangle & \longmapsto & |++\rangle \\ & |+-\rangle & \longmapsto & |-+\rangle \\ & |-+\rangle & \longmapsto & |+-\rangle \\ & |--\rangle & \longmapsto & |--\rangle \end{array}$$

It would seem then that the Hamiltonian H is a monomial matrix in the given basis for $\mathcal{H}$. Moreover it preserves the total spin grading on $\mathcal{H}$.

[redacted] Obvious question is whether H is a derivation of the exterior algebra structure on $\mathcal{H}$. To see this let us follow Feynman Vol III Ch. [redacted] 15. Suppose $\mathbb{Z}$ is the set of sites, that there is no external field, and that the Hamiltonian is

$$H = \sum_n{}' \left(P_{n,n+1} - 1 \right)$$

where $P_{n,n+1}$ interchanges the spins of the sites $n, n+1$. Let [redacted] the ground state be all spins up, and let e_n be the state with one spin down at position n. Now we are thinking of

$$\mathcal{H} = \bigotimes_n \mathbb{C}^2$$

as an exterior algebra. Let $\theta = P_{n,n+1} - 1$. Then

$$\theta(e_n e_{n+1}) = 0$$

because we interpret $e_n e_{n+1}$ as the state with spins down at $n, n+1$. On the other hand if θ were extended from dimension 1 as a derivation we would have

$$\begin{aligned} \theta(e_n e_{n+1}) &\text{"="} (\theta e_n) e_{n+1} + e_n (\theta e_{n+1}) \\ &= (e_{n+1} - e_n) e_{n+1} + e_n (e_n - e_{n+1}) \\ &= -2 e_n e_{n+1} \end{aligned}$$

So it seems that H is not a derivation for the exterior algebra structure. This seems to be the point of the "independent particle approximation", namely to pretend the Hamiltonian is a derivation, and hence obtain the stationary states as anti-symmetrizations of one-particle states.

April 13, 1979

Gauge theory: Classical one has a principal G-bundle P over X = space-time and the connections A on P are analogous to Feynman classical paths. The variational principle gives Yang-Mills fields; these are analogous to classical trajectories. Supposedly they are solutions of a hyperbolic DE, so are in 1-1 correspondence with Cauchy data at $t=0$.

So let's cut X down to the space hypersurface $t=0$. When one quantizes the different points of X are independent, so the Hilbert space is essentially a tensor product

$$\mathcal{H} = \bigotimes_{x\in X} V_x$$

where the gauge group $\mathcal{G} = \Gamma(\underline{\mathrm{Aut}}(P/X))$ acts via representations of G_x.

So let's consider a discrete model where X is a discrete set I of sites and each i has a symmetry group G_i acting on a Hilbert space V_i. The big state space is

$$\mathcal{H} = \bigotimes_{i\in I} V_i$$

and it is a representation of the gauge group

$$\mathcal{G} = \prod_{i\in I} G_i$$

If each V_i is irreducible under [redacted] G_i, then $\mathcal{H}$ will be an irreducible repn. of $\mathcal{G}$. This connects up nicely with Gelfand looking at irreducible repns. of $\mathcal{G} = C^\infty$ maps $X \to G$. Notice also that the algebra of operators on $\mathcal{H}$ is generated by the gauge symmetries.

Also we see how the center of $\mathcal{G}$

$\mathfrak{z}$ [redacted] $= \prod_{i \in I} Z_i$

gives symmetries commuting with all the relevant operators.

The above is kinematics. We introduce dynamics by [redacted] means of a Hamiltonian operator on $\mathcal{H}$. The program is now as follows. Take a [redacted] model from statistical mechanics, say Heisenberg's magnet, where the Hamiltonian is built out of nearest neighbor interactions, and then see if I can construct a continuous analogue.

April 14, 1979

On Feynman path integrals. Consider motion of a particle on a line with Hamiltonian

$$H = \frac{p^2}{2m} + V(q,t)$$

The Schroedinger equation is

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 + V(x,t)\right]\psi$$

and we are interested in the propagator $U(t,t')$, which has the kernel

$$K(x,t,x';t') = \langle x \,|\, U(t,t') \,|\, x' \rangle$$

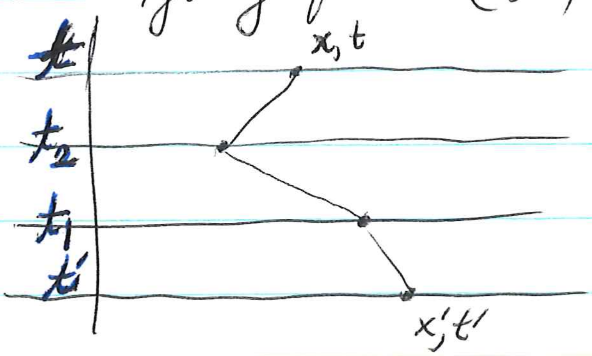
To obtain the propagator as a path integral one subdivides the integral $[t',t]$ into n-equal pieces

$$t' = t_0 < t_1 < \cdots < t_n = t$$

and uses the basic matrix multiplication law

$$K(x,t,x';t') = \iiint K(x,t,x_{n-1},t_{n-1})\,dx_{n-1}\,K(x_{n-1},t_{n-1},x_{n-2},t_{n-2}) \times dx_{n-2} \cdots\cdots dx_1\,K(x_1,t_1,x',t')$$

to express this kernel as an integral over the space of broken paths going from (x',t') to (x,t).



Then one takes the limit as $n \to \infty$ and gets an expression [redacted] for K ~~as~~ a "sum" over all paths from (x', t') to (x, t). The only problem is to compute the amplitude that goes with a given path $x(t)$. [redacted]

To do this one could hope by a kind of "Duhamel's principle" that [redacted] over each infinitesimal time interval $t, t+dt$ we can separate the effect of the potential and kinetic energies. If there is no kinetic term we have

$$i\hbar \frac{\partial \psi}{\partial t} = V(q,t)\psi$$

and
$$U(t,t') = \text{mult. by } e^{-\frac{i}{\hbar}\int_t^{t'} V(q,\hat{t})\,d\hat{t}}$$

If there is no potential term we have

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

which [redacted] becomes a heat equation, [redacted] if we put $\tau = it$

$$\frac{\partial \psi}{\partial \tau} = \frac{\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

$$\psi(x,\tau) = \int \frac{d\xi}{2\pi} e^{-i\xi x}\hat{\psi}(\xi,\tau)$$

$$\frac{\partial \hat{\psi}}{\partial \tau} = -\frac{\hbar}{2m}\xi^2\hat{\psi} \qquad \hat{\psi} = e^{-\frac{\hbar}{2m}\xi^2\tau}\hat{\psi}_0$$

Put $a = \frac{\hbar\tau}{m}$
$$\int \frac{d\xi}{2\pi} e^{-i\xi x - \frac{a}{2}\xi^2} = e^{-\frac{x^2}{2a}}\int e^{-\frac{a}{2}\xi^2}\frac{d\xi}{2\pi}$$

$$\frac{a}{2}\left(\xi^2 + 2i\xi\frac{x}{a} + \left(i\frac{x}{a}\right)^2\right) + \frac{x^2}{2a} \qquad = e^{-\frac{x^2}{2a}}\frac{1}{2\pi}\sqrt{\frac{2}{a}}\sqrt{\pi}$$

$$= \frac{1}{\sqrt{2\pi a}}e^{-x^2/2a}$$

Therefore we get the kernel

$$K(x,t,x',t') = \frac{1}{\sqrt{2\pi \frac{\hbar}{m} i(t-t')}} e^{-\frac{(x-x')^2}{2(\hbar/m)i(t-t')}}$$

$$= \frac{1}{\sqrt{2\pi \frac{\hbar}{m} i(t-t')}} e^{\underbrace{\frac{i}{\hbar}\frac{m}{2}\left(\frac{x-x'}{t-t'}\right)^2 (t-t')}_{\text{integral of K.E. } \frac{m}{2}v^2 \text{ over the straight line path from } (x',t') \text{ to } (x,t).}}$$

So therefore it seems clear that the amplitude factor belonging to a classical path is

$$e^{\frac{i}{\hbar}\int_{t'}^{t} L\,dt}$$

April 15, 1979

Path integrals from Abers-Lee. Use P, Q to denote operators, p, q to denote numbers. Fourier transform formulas are

$$\psi(q) = \int \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}pq} \hat{\psi}(p)$$

so that $\frac{\hbar}{i}\frac{\partial}{\partial q}$ corresponds to multiplying by p. In Dirac's notation

$$\psi(q) = \langle q|\psi\rangle \qquad \langle q'|q\rangle = \delta(q'-q).$$

$$\hat{\psi}(p) = \langle p|\psi\rangle = \int dq\, e^{-\frac{i}{\hbar}pq} \underbrace{\psi(q)}_{\langle q|\psi\rangle}$$

hence

$$\boxed{\langle p|q\rangle = e^{-\frac{i}{\hbar}pq}}$$

and so

$$\delta(q-q') = \int \frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}p(q-q')} = \int \langle q|p\rangle \frac{dp}{2\pi\hbar} \langle p|q'\rangle$$

So we have

$$\langle q|q'\rangle = \delta(q-q') \qquad \text{orthonormality}$$

$$\int |q\rangle\, dq \,\langle q| = Id \qquad \text{completeness}$$

$$\langle p|p'\rangle = \int \langle p|q\rangle\, dq\, \langle q|p'\rangle = \int dq\, e^{\frac{i}{\hbar}q(p'-p)} = 2\pi\hbar\,\delta(p-p')$$

$$\int |p\rangle \frac{dp}{2\pi\hbar} \langle p| = Id.$$

Notice also that $\hbar$ is measured in erg sec $= gm \frac{cm^2}{sec^2} sec = gr \frac{cm^2}{sec}$, pq is meas. in $gr \frac{cm}{sec} cm$, hence $pq/\hbar$ is dimensionless.

Now let us return to computing

$$K(q,t,q',t') = \langle q|U(t,t')|q'\rangle$$

by subdividing t',t into $t' = t_0 < t_1 < \cdots < t_n = t$. For a small time interval $t, t+dt$ we make the approximation

$$U(t+dt,t) = I - \frac{i}{\hbar}H(t)\,dt$$

$$\cancel{\langle q|U(t+dt,t)|q'\rangle = \delta(q-q') - \frac{i}{\hbar}\langle q|H(t)|q'\rangle\, dt}$$

and compute $H(t)$ as a Fourier integral operator:

$$\langle q|H|q'\rangle = \int \frac{dp}{2\pi\hbar}\, e^{i/\hbar\, pq}\, H(p,q')\, e^{-i/\hbar\, pq'}$$

$$= \int \langle q|p\rangle \frac{dp}{2\pi\hbar} \langle p|H|q'\rangle$$

Thus

$$\langle q|U(t+dt,t)|q'\rangle = \int \frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}p(q-q')} \underbrace{\left\{1 - \frac{i}{\hbar}H(p,q')dt\right\}}_{= e^{-\frac{i}{\hbar}H(p,q')dt}}$$

so

$$\langle q|U(t+dt,t)|q'\rangle = \int \frac{dp}{2\pi\hbar}\, e^{\frac{i}{\hbar}\left(p(q-q') - H(p,q')dt\right)}$$

This seems to be an exact formula provided H as an operator is taken to be the [redacted] pseudo-differential operator with symbol $H(p,q)$.

Now the idea is to use the above [redacted] formula as an approximation for the left side when $dt = \Delta t$. So if t', t is subdivided into n parts

$$t' = t_0 < t_1 < \cdots < t_n = t$$

we have integration variables $q_j = q(t_j)$ $\quad j = 1, \dots, n-1$

and p_j = momentum variable belonging to (t_{j-1}, t_j) for $j = 0, \dots, n$. So the approximate formula for the propagator is

$$\langle q|U(t,t')|q'\rangle = \int\!\!\cdots\!\!\int \prod_{j=1}^{n-1} dq_j \prod_{j=1}^{n} \frac{dp_j}{2\pi\hbar}\, e^{\frac{i}{\hbar}\left\{\sum_{j=1}^{n} p_j(q_j - q_{j-1}) - \sum_{j=1}^{n} H(p_j, q_{j-1})\Delta t\right\}}$$

and in the limit as $n \to \infty$ it becomes

$$\boxed{\langle q|U(t,t')|q'\rangle = \int\limits_{\{\text{paths going from }(q',t')\text{ to }(q,t)\}} \left[\frac{dq\,dp}{2\pi\hbar}\right] e^{\frac{i}{\hbar}\int_{t'}^{t}(p\dot{q}-H(p,q))d\tau}}$$

where in some sense

$$\left[\frac{dq\,dp}{2\pi\hbar}\right] = \prod_{\tau\in(t',t)} \frac{dq(\tau)\,dp(\tau)}{2\pi\hbar}$$

The first question to ask is, assuming there is no problem with the integral's existence, does the integral automatically interpret a function $H(p,q)$ as an operator in an unambiguous way. Probably not, because of the usual quantization ambiguity.

[redacted] The physicists now assume that there is a way of defining the Hamiltonian operator $H(P,Q)$ so that the above formula holds. This means that one has, at least on the heuristic level, a definite quantization process.

Let's use the above to compute vacuum expectation values. Start with a time-independent Hamiltonian H_0, say for the oscillator

$$H_0 = \frac{1}{2}(p^2+\omega^2 q^2),$$

which has a definite [redacted] ground state $|0\rangle$ and perturb it by adding a source term:

$$H_J = H_0 - J(t)q$$

where $J(t)$ has compact support. The path integral gives us an expression in terms of Lagrangian.

$$\cancel{\langle q|U(t,t')|q'\rangle_J}$$

Let's first do the p-integrations when

$$H(p,q) = \frac{p^2}{2} + V(q)$$

We need to evaluate

$$\int \frac{dp}{2\pi\hbar}\, e^{\underbrace{\frac{i}{\hbar}\left(p\dot{q} - \frac{p^2}{2}\right)dt}_{-\frac{i\,dt}{2\hbar}\left(p^2 - 2p\dot{q} + \dot{q}^2\right) + \frac{i\,dt}{2\hbar}\dot{q}^2}}$$

$$= e^{\frac{i}{\hbar}\frac{\dot{q}^2}{2}dt}\,\frac{1}{2\pi\hbar}\sqrt{\frac{\pi}{\frac{i\,dt}{2\hbar}}} = \frac{1}{\sqrt{2\pi\hbar i\,dt}}\, e^{\frac{i}{\hbar}\frac{\dot{q}^2}{2}dt}.$$

So

$$\int\left[\frac{dp\,dq}{2\pi\hbar}\right] e^{\frac{i}{\hbar}\int_{t'}^{t}\left[p\dot{q} - H(p,q)\right]d\tau} = \int\left[\frac{dq}{\sqrt{2\pi\hbar i\,dt}}\right] e^{\frac{i}{\hbar}\int_{t'}^{t}\underbrace{\left[\frac{\dot{q}^2}{2} - V(q)\right]}_{L(q,\dot{q})}d\tau}$$

This refers to subdivision size. (denoted ϵ by A. Lee)

Put $\hbar = 1$ to simplify

$$\langle q|U(t,t')|q'\rangle = \int\left[\frac{dq}{\sqrt{2\pi i\varepsilon}}\right] e^{i\int_{t'}^{t} L\,d\tau}$$

April 16, 1979

Consider motion [redacted] on the line

$$i \frac{\partial \psi}{\partial t} = H_0 \psi$$

where, to fix the ideas, we have the oscillator

$$H_0 = \tfrac{1}{2}\left(P^2 + \omega^2 Q^2\right).$$

Let ϕ_n be [redacted] an orthonormal basis of eigenvectors for H_0:

$$H_0 \phi_n = E_n \phi_n$$

with $\phi_0 = |0\rangle$ the ground state. It seems that in [redacted] quantum field theory, the relevant quantities are the "expectation values of products of Heisenberg ops":

$$\langle 0 | Q(t_1) \cdots Q(t_n) | 0 \rangle = \langle 0 | U_0(0,t_1) Q \, U_0(t_1,t_2) Q \cdots Q \, U_0(t_n, 0) | 0 \rangle$$

and where the interesting case is where $t_1 > t_2 > \cdots > t_n$, so $Q(t_1) \cdots Q(t_n)$ is time-ordered. In order to obtain these time-ordered-product-expectation-values, Schwinger introduced a "source" term: ~~[illegible]~~

$$H = H_0 - J(t) Q$$

where $J(t)$ has compact support. The effect of this perturbation is

$$U(t,t') = U_0(t,t') + \int_{t'}^{t} dt_1 \, U_0(t,t_1) \frac{-1}{i} J(t_1) Q \, U_0(t_1,t')$$

$$+ \int_{t'}^{t} dt_1 \int_{t'}^{t_2} dt_2 \; U_0(t,t_1) \frac{-1}{i} J(t_1) Q \, U_0(t_1,t_2) \frac{-1}{i} J(t_2) Q \, U_0(t_2,t') + \cdots .$$

[redacted] In terms of the scattering operator

$$S = U_0(0,t)\,U(t,t')\,U_0(t',0) \qquad t' \ll 0 \text{ [redacted] } \ll t$$

$$S = I + \frac{1}{i}\int_{t'}^{t} J(t_1)\,dt_1 \underbrace{U_0(0,t_1)\,Q\,U_0(t_1,0)}_{Q(t_1)}$$

$$+ \left(\frac{1}{i}\right)^2 \int_{t'}^{t}\int_{t'}^{t_1} J(t_1)J(t_2)\,dt_1 dt_2 \quad Q(t_1)Q(t_2) + \cdots$$

Thus

$$\langle 0|S|0\rangle = 1 + \frac{1}{i}\int_{t'}^{t} dt_1\, J(t_1) \text{ [redacted] } \langle 0|Q(t_1)|0\rangle$$

$$+ \left(\frac{1}{i}\right)^2 \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2\, J(t_1)J(t_2)\langle 0|Q(t_1)Q(t_2)|0\rangle.$$

$$+ \cdots\cdots$$

Therefore

$$\frac{1}{i}\langle 0|Q(t_1)|0\rangle = \frac{\delta}{\delta J(t_1)}\langle 0|S|0\rangle$$

$$\left(\frac{1}{i}\right)^2 \langle 0|Q(t_1)Q(t_2)|0\rangle = \frac{\delta^2}{\delta J(t_1)\,\delta J(t_2)}\langle 0|S|0\rangle \qquad \text{for } t_1 > t_2$$

hence we see that time-ordered-product-expection-values can be obtained by taking the functional derivatives of $\langle 0|S|0\rangle$ with respect to the external source function J.

Now I should work out the [redacted] example of the simple harmonic oscillator with sources. We did this earlier essentially.

$$\langle 0|S|0\rangle = \frac{\langle 0|U(t_f,t_i)|0\rangle}{\langle 0|U_0(t_f,t_i)|0\rangle}$$

$$\delta \ln \langle 0|S|0\rangle = \frac{\langle 0|\delta U(t_f,t_i)|0\rangle}{\langle 0|U(t_f,t_i)|0\rangle}$$

$$= \int_{t_i}^{t_f} dt_1 \; i\delta J(t_1) \underbrace{\frac{\langle 0|U(t_f,t_1)\,Q\,U(t_1,t_i)|0\rangle}{\langle 0|U(t_f,t_i)|0\rangle}}_{\langle Q(t_1)\rangle}$$

Because the Hamiltonian is quadratic, we know that $q(t) = \langle Q(t)\rangle$ satisfies the classical equations of motion

$$\frac{d^2}{dt^2} q = -\omega^2 q + J$$

$$H = \tfrac{1}{2}(p^2 + \omega^2 q^2) - Jq$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -\omega^2 q + J$$

and we recall the boundary conditions are such that

$$q(t) = \int_{-\infty}^{\infty} G_0(t,t')\,J(t')\,dt' \qquad G_0(t,t') = \frac{e^{-i\omega|t-t'|}}{-2i\omega}$$

so

$$\delta \ln \langle 0|S|0\rangle = \int_{-\infty}^{\infty} dt_1 \; i\,\delta J(t_1) \int_{-\infty}^{\infty} G_0(t_1,t_2)\,J(t_2)\,dt_2$$

$$= i \iint_{-\infty}^{\infty} dt_1\,dt_2 \;\; \delta J(t_1)\, \underbrace{G_0(t_1,t_2)}_{\text{symmetric}}\, J(t_2)$$

Integrating with boundary condition $\langle 0|S|0\rangle = 1$ when $J=0$ we get

$$\boxed{\langle 0|S|0\rangle = e^{\frac{1}{2} i \iint_{-\infty}^{\infty} dt_1\,dt_2\; J(t_1)\,G_0(t_1,t_2)\,J(t_2)}}$$

Imaginary time [redacted] or Euclidean formalism.

The idea here perhaps is that

$$U_0(t,t') = e^{-iH_0(t-t')}$$

has an analytic continuation to the LHP as a function of $t-t'$. Consequently

$$U(T,T') = U_0(T,t_f)\,U(t_f,t_i)\,U_0(t_i,T')$$

[redacted] for $T > t_f$ and $T' < t_i$ extends to the LHP in T and UHP in T'.

So one ~~looks~~ at the heat equation

$$\frac{\partial\psi}{\partial\tau} = -H_0\psi$$

which can be solved for increasing τ:

$$U_0(\tau,\tau') = e^{-H_0(\tau-\tau')}$$

$$= \sum_{n\geq 0} e^{-E_n(\tau-\tau')}\,|\phi_n\rangle\langle\phi_n|$$

This makes sense for $\tau \geq \tau'$. Assume $E_0 = 0$, so that

$$U_0(\tau-\tau') \longrightarrow |\phi_0\rangle\langle\phi_0| \quad \text{as } \tau-\tau' \to +\infty.$$

So the next thing is to add a source term

$$\frac{\partial\psi}{\partial\tau} = (-H_0 + JQ)\psi$$

with J of compact support. [redacted] Suppose you solve to get

$\mathcal{U}(\tau,\tau')$:

$$\frac{\partial}{\partial\tau}\left(e^{\tau H_0}\psi\right) = e^{\tau H_0}\left(\frac{\partial}{\partial\tau} + H_0\right)\psi = e^{\tau H_0} J Q \psi$$

$$\left[e^{\tau H_0}\psi\right]_{\tau'}^{\tau} = \int_{\tau'}^{\tau} e^{\tau_1 H_0} J(\tau_1) Q \psi(\tau_1)\, d\tau_1$$

$$\psi(\tau) = e^{-H_0(\tau-\tau')}\psi(\tau') + \int_{\tau'}^{\tau} e^{-H_0(\tau-\tau_1)} J(\tau_1) Q \psi(\tau_1)\, d\tau_1$$

$$\therefore \quad \mathcal{U}(\tau,\tau') = \mathcal{U}_0(\tau,\tau') + \int_{\tau'}^{\tau} d\tau_1\, \mathcal{U}_0(\tau,\tau_1) J(\tau_1) Q\, \mathcal{U}(\tau_1,\tau')$$

so iterating

$$\mathcal{U}(\tau,\tau') = \mathcal{U}_0(\tau,\tau') + \int_{\tau'}^{\tau} d\tau_1\, \mathcal{U}_0(\tau,\tau_1) J(\tau_1) Q\, \mathcal{U}_0(\tau_1,\tau')$$

$$+ \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau_1} d\tau_2\, \mathcal{U}_0(\tau,\tau_1) J(\tau_1) Q\, \mathcal{U}_0(\tau_1,\tau_2) J(\tau_2) Q\, \mathcal{U}_0(\tau_2,\tau')$$

$$+ \cdots\cdots .$$

So having normalized H_0 so that $E_0 = 0$, everything decays away from the ground state. The quantity of interest is

$$\langle 0 | \mathcal{U}(\tau_f,\tau_i) | 0 \rangle$$

which is independent of τ_f, τ_i for $\tau_f \gg 0$, $\tau_i \ll 0$. This obviously gets calculated in the same way, except the Green's function will be nicer.

So let's work things through for a system of oscillators

$$H = \frac{1}{2}\left(\sum_j p_j^2 + q_j (\omega^2)_{jk} q_k\right) - \sum_j J_j q_j$$

$$H = \frac{1}{2}(p\cdot p + q\cdot\omega^2 q) - J\cdot q$$

We will work with the heat equation this time, so that

$$\frac{\partial}{\partial\tau}\mathcal{U}(\tau,\tau') = -H\,\mathcal{U}(\tau,\tau') = (-H_0 + J\cdot Q)\,\mathcal{U}(\tau,\tau')$$

As usual

$$\delta\mathcal{U}(\tau,\tau') = \int_{\tau'}^{\tau} d\tau_1\ \mathcal{U}(\tau,\tau_1)\,J(\tau_1)\,Q\,\mathcal{U}(\tau_1,\tau')$$

so

$$\frac{\delta\langle 0|\mathcal{U}(\tau,\tau')|0\rangle}{\langle 0|\mathcal{U}(\tau,\tau')|0\rangle} = \int_{\tau'}^{\tau} d\tau_1\ J(\tau_1)\ \underbrace{\frac{\langle 0|\mathcal{U}(\tau,\tau_1)\,Q\,\mathcal{U}(\tau_1,\tau')|0\rangle}{\langle 0|\mathcal{U}(\tau,\tau')|0\rangle}}_{\langle Q(\tau_1)\rangle}$$

Take $\tau = \tau_f \gg 0$, $\tau' = \tau_i \ll 0$ and then $\langle Q(\tau)\rangle$ is well-defined. Clearly

$$\frac{\partial}{\partial\tau}\ \mathcal{U}(\tau_f,\tau)\,Q\,\mathcal{U}(\tau,\tau_i) = \mathcal{U}(\tau_f,\tau)\left[HQ - QH\right]\mathcal{U}(\tau,\tau_i)$$

So

$$\frac{\partial^2}{\partial\tau^2}\langle Q(\tau)\rangle = \langle [H,[H,Q]]\,(\tau)\rangle$$

and this will be missing i^2 from previous formulas, so we get

$$\frac{\partial^2}{\partial\tau^2}\langle Q(\tau)\rangle = -\left[-\omega^2\langle Q(\tau)\rangle + J\right]$$

The boundary conditions ought to work out as before, so

$$\langle Q(\tau)\rangle = -\int_{-\infty}^{\infty} G_0(\tau,\tau')\,J(\tau')\,d\tau'$$

where $\quad G_0 \equiv$ Green's function for $\left(\frac{d^2}{d\tau^2} - \omega^2\right)$

$$= \frac{e^{-\omega|\tau|}}{-2\omega}$$

So it appears that in the imaginary time situation we get the "scattering"

$$\frac{\langle 0 | U(t_f, t_i) | 0 \rangle}{\langle 0 | U_0(t_f, t_i) | 0 \rangle} = \exp\left\{ -\frac{1}{2} \iint J(\tau_1) G_0(\tau_1, \tau_2) J(\tau_2)\, d\tau_1 d\tau_2 \right\}$$

April 17, 1979

Is there an interesting discrete analogue of quantum mechanical motion on the line? Let q range over $\mathbb{Z}$, so that the wave function $\psi(q)$ is a sequence. The Hamiltonian H is to be something like a Jacobi matrix. ~~In the Heisenberg magnet model $\psi(q)$ ranges over a 2-dim'l spin space. The Hamiltonian connects nearest neighbors and it is translation invariant with respect to $\mathbb{Z}$.~~ Is there a discrete analogue of the harmonic oscillator?

April 19, 1979

Fran Dubin – Solvable models in algebraic statistical mechanics: Chapter on the BCS model for superconductivity.

Recall that spin space is $\mathbb{C}^2$ with the Pauli spin matrices acting on it

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

These matrices generate the Lie algebra for $SU(2)$ which is the group of symmetries of spin-spaces. $\mathbb{C}^2$ has the basis $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ [redacted] which one calls "spin up" (in the z axis-direction) and "spin down". Actually it seems that the lines in spin space form a 2-sphere which on can think of as the possible axes for a rotating top.

Put $V = \mathbb{C}^2$ with $SU(2)$ acting. Now one wants to consider n-spinning gadgets which are distinguishable, so one has the Hilbert space

$$\mathcal{H}_n = \bigotimes_{i=1}^{n} V \ .$$ [redacted]

[redacted] The algebra of operators (dynamical variables) on $\mathcal{H}_n$ is generated by the Pauli matrices in each factor of the product. This algebra is

$$\text{End}(\mathcal{H}_n) = \bigotimes \underbrace{\text{End}(V)}$$

2×2 matrices [redacted]; Natural basis $\sigma_z, \sigma_x, \sigma_y, I$.

One of the basic things to notice is that there is an obvious embedding

$$\mathrm{End}(\mathcal{H}_n) \hookrightarrow \text{[redacted]}\ \mathrm{End}(\mathcal{H}_m)$$

corresponding to an embedding $[1, \dots, n] \hookrightarrow [1, \dots, m]$, but the same is not true of $\mathcal{H}_n$, unless one picks a ground state. Therefore in the limit one gets an algebra $\mathfrak{a}$ of dynamical variables in an obvious way. Then you want to construct a state on $\mathfrak{a}$, usually a Gibbs state, and take the Hilbert space associated by the Gelfand-Neumark-Segal construction.

In the BCS model the Hamiltonian on $\mathcal{H}_n$ is given by an element of the universal enveloping algebra of $SU(2)$:

$$H = \varepsilon n - \varepsilon L^{(3)} - \frac{2g}{n} L^+ L^-$$

where
$$L^{(3)} = 2 \cdot \text{effect of } \sigma_z \text{[redacted]}$$
$$L^{\pm} = 2 \cdot \text{effect of } \sigma_x \pm i \sigma_y = \begin{pmatrix} 0 & \left\{ \begin{smallmatrix} 2 \\ 0 \end{smallmatrix} \right\} \\ \left\{ \begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \right\} & 0 \end{pmatrix}$$

The problem is to compute the Gibbs state.

The first point is to use the action of Σ_n which commutes with the $SU(2)$-action. The idea is that $\mathrm{End}(\mathcal{H}_n)$ is generated by the spin operators:

$$\text{[redacted]} \quad \sigma_{\substack{x \\ y \\ z}} \text{ on [redacted] } i\text{th copy of } V$$

and that the Gibbs state is invariant under Σ_n.

Review of statistical mechanics. Let $(M, d\mu, H)$ be a classical mechanical system. Form an ensemble of N independent identical systems; you get $(M^N, d\mu^N, H_N = \sum_{i=1}^{N} H pr_i)$. Place some small interaction between these systems, so there is a means for energy to move between the individual systems. The ergodic hypothesis tells us that the time average of any dynamical variable (= function on M^N) over a trajectory is its average over the hypersurface $H_N^{-1}(E)$ with respect the natural volume; where E is the energy of the trajectory:

$$\lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} F(\vec{x}(t))\,dt = \frac{\int_{M^N} F\,\delta(H_N - E)\,d\mu^N}{\int_{M^N} \delta(H_N - E)\,d\mu^N}$$

What I am especially interested in is an F of the form

$$F(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

i.e. the average of some one-particle dynamical variable. The above average is

$$\int_{M^N} f pr_1\,\delta(H_N - E)\,d\mu^N \Big/ \int_{M^N} \delta(H_N - E)\,d\mu^N$$

We want to let $N\to\infty$, $E\to\infty$ in such a way that this converges. Note the numerator can be written

$$\int_{M^N} f\,pr_1\, \delta(H_N - E)\, d\mu^N = \int_M f(x_1)\,d\mu \int_{M^{N-1}} \delta(H_{N-1} + H(x_1) - E)\, d\mu^{N-1}$$

so if I put $\theta(N,E) = \int_{M^N} \delta(H_N - E)\, d\mu^N$ I am trying to get a measure [redacted] $\rho(x_1)\,d\mu$ where

$$\rho(x_{\text{[redacted]}}) = \lim \frac{\theta(N-1, E - H(x))}{\theta(N,E)}$$

So I need an asymptotic formula [redacted] for $\theta(N,E)$. Use Laplace transform:

$$\int_0^\infty e^{-sE}\,\theta(N,E)\,dE = \int_0^\infty e^{-sE} \int_{M^N} \delta(H_N - E)\, d\mu^N$$

$$= \int_{M^N} e^{-sH_N}\, d\mu^N = \left(\int_M e^{-sH}\, d\mu\right)^N$$

Put $Z(s) = \int_M e^{-sH}\, d\mu$. This is the partition fn. One has by Laplace inversion

$$\theta(N,E) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{sE}\, Z(s)^N\, ds$$

Put $E = N\varepsilon$, so that ε is the average energy per "particle". Apply steepest descent to

$\theta(N, N\varepsilon) =$ [redacted] $\frac{1}{2\pi i} \int$ [redacted] $\left(e^{s\varepsilon} Z(s)\right)^N ds$

Critical points are given by

$$0 = \frac{d}{ds}\left(e^{s\varepsilon} Z(s)\right) = \varepsilon e^{s\varepsilon} Z(s) + e^{s\varepsilon} Z'(s)$$

$$\varepsilon = -\frac{Z'(s)}{Z(s)} = -\frac{d}{ds}\log Z(s)$$

or

$$\boxed{\varepsilon = \frac{\int H e^{-sH}\,d\mu}{\int e^{-sH}\,d\mu} = -\frac{d}{ds}\log Z(s)}$$

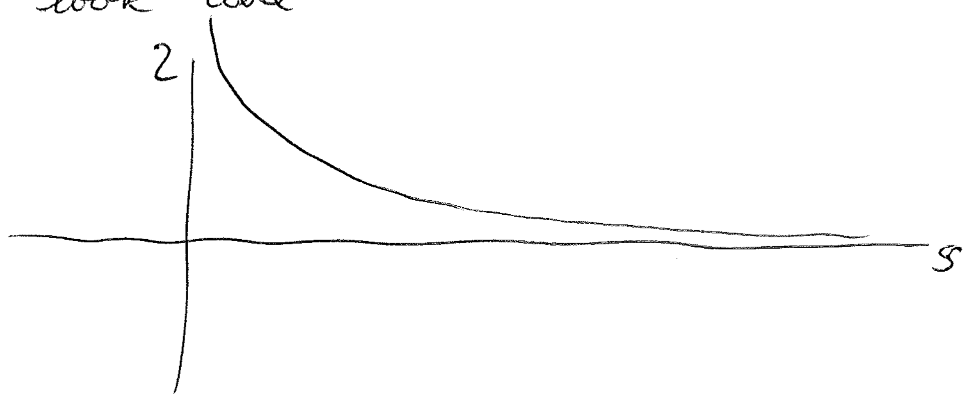
Now

$$\left(-\frac{Z'}{Z}\right)' = \frac{-ZZ'' + Z'^2}{Z^2} = \frac{\left(\int H\,d\nu\right)^2 - \left(\int d\nu\right)\left(\int H^2 d\nu\right)}{Z^2} < 0$$

where $d\nu = e^{-sH}d\mu$, because

$$0 \leq \int (xH+1)^2 d\nu = x^2 \underbrace{\int H^2 d\nu}_{a} + 2x \underbrace{\int H\,d\nu}_{b} + \underbrace{\int d\nu}_{c}$$

for all x, hence $b^2 - ac < 0$. Thus $\log Z(s)$ is concave upward, or $\frac{Z'}{Z}$ is increasing; as $Z(s) \to +\infty$ as $s \to 0^+$, $Z(s) \to 0$ as $s \to +\infty$, one expects $Z(s)$ to look like



so $\frac{Z'}{Z} \to -\infty$ as $s \to 0$. Actually from

$$-\frac{Z'}{Z} = \frac{\int H e^{-sH}\,d\mu}{\int e^{-sH}\,d\mu}$$

it is more or less clear that as s goes from 0 to ∞, this expression decreases from $+\infty$ to 0, because you are taking the average value of the energy H with respect to a weighting which favors lower energies as s increases.

In any case, let us assume that for each ε, the is a unique pos. real s satisfying the preceding boxed formula. Denote this quantity β:

$$\varepsilon = \frac{\int H e^{-\beta H} d\mu}{\int e^{-\beta H} d\mu}$$

So then using steepest descent, we get

$$\Theta(N, N\varepsilon) \approx \left(e^{\beta\varepsilon} Z(\beta)\right)^N \cdot \text{ some Gaussian integral}$$

Rather than worry about the details, we use

$$\frac{\Theta(N-1, N\varepsilon - H(x))}{\Theta(N, N\varepsilon)} = \frac{\int e^{s(N\varepsilon - H(x))} Z(s)^{N-1} ds}{\int e^{sN\varepsilon} Z(s)^N ds}$$

$$= \frac{\int e^{s\varepsilon - sH(x)} \left(e^{s\varepsilon} Z(s)\right)^{N-1} ds}{\int e^{s\varepsilon} Z(s) \left(e^{s\varepsilon} Z(s)\right)^{N-1} ds}$$

$$\longrightarrow \frac{e^{\beta(\varepsilon - H(x))}}{e^{\beta\varepsilon} Z(\beta)} = \frac{e^{-\beta H(x)}}{Z(\beta)}$$

Therefore we get the Maxwell-Bolzman distribution on the phase space M.

<u>Example</u>: $H = \frac{1}{2}(p^2+q^2)$

$$Z(s) = \int_{\mathbb{R}^2} e^{-sH}\,d\mu = \int_{\mathbb{R}^2} e^{-\frac{s}{2}(p^2+q^2)}\,dp\,dq$$

$$= \frac{2\pi}{s}\int_0^\infty e^{-\frac{s}{2}r^2}\,s\,r\,dr = \frac{2\pi}{s}$$

$$\varepsilon = -\frac{d}{ds}\log Z(s) = \frac{1}{s} \quad \Rightarrow \beta = \frac{1}{\varepsilon}$$

So in the case of the oscillator $\beta = \frac{1}{\varepsilon}$ where $\varepsilon =$ average energy of a particle. Thus the basic measure corresponding to an ensemble of oscillators with average energy ε is

$$\frac{1}{2\pi\varepsilon}\, e^{-\frac{1}{2\varepsilon}(p^2+q^2)}\,dp\,dq$$

Do same derivation but for a quantum [redacted] situation. Instead of points of phase space M describing states, we use vectors in a Hilbert space [redacted] V acted on by a Hamiltonian operator H. A dynamical variable **is** an operator A on V, and the "value" of A when the system has the state vector ψ is

$$\frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle} = \operatorname{trace}(A \circ \text{proj on } \mathbb{C}\psi).$$

If the system has a definite energy E, then $H\psi = E\psi$. Let ψ_n be an orthonormal basis of eigenvectors for H

$$H\psi_n = E_n \psi_m$$

Then the "value" of A when the system has energy E is

$$\frac{\sum_{E_n = E} \langle \psi_n | A | \psi_n \rangle}{\sum_{E_n = E} 1} = \frac{\operatorname{tr}(A \circ \text{proj on } E\text{-th eigenspace})}{\operatorname{tr}(E\text{-th eigenspace})}$$

This is the quantum analogue of $\int_{H^{-1}(E)} f \, d\mu \Big/ \int_{H^{-1}(E)} d\mu$ which is the same as the time average of f under the ergodic hypotheses.

Now form an ensemble of N identical systems. The Hilbert space is

$$V_N = \bigotimes_{i=1}^{N} V.$$

What I want to is to take a "dynamical variable" A on the system and extend it as a "derivation" on V_N:

$$A_N = \sum_{i=1}^{N} 1 \otimes \cdots \otimes \underset{\substack{\uparrow \\ i\text{th position}}}{A} \otimes \cdots \otimes 1$$

and then take the average value of $\frac{1}{N} A_N$ knowing the ensemble has total energy E. The hope is that as $N \to \infty$, $E \to \infty$ suitably, there is a state on the system, the so-called Gibbs state, [redacted] whose A-value is the limiting value for the ensemble.

There are complications due to the discrete energy levels, so we have to proceed carefully to see how the limiting process works. By symmetry

$$(*) \qquad tr\left(\frac{1}{N}A_N \circ P_{H_N^{-1}(E)}\right) = tr\left((A \otimes 1^{\otimes N-1}) \circ P_{H_N^{-1}(E)}\right).$$

Use the orthonormal basis for $V^{\otimes N}$ given by

$$\psi_{n_1} \otimes \cdots\cdots \otimes \psi_{n_N}$$

which diagonalizes H_N. [redacted] This is an eigenvector for H_N with eigenvalue $E_{n_1} + \cdots + E_{n_N}$. The trace $(*)$ [redacted] computed via this orthonormal basis [redacted] is

$$\sum_{E_{n_1}+\cdots+E_{n_N}=E} \langle \psi_{n_1} | A | \psi_{n_1} \rangle = \sum_n \langle \psi_n | A | \psi_n \rangle \, \Theta(N-1, E-E_n)$$

where

$$\Theta(N,E) = [redacted] \; tr\left(P_{H_N^{-1}(E)}\right)$$
$$= \sum_{E_{n_1}+\cdots+E_{n_N}=E} 1$$

$\Theta(N,E)$ can as before be understood via its Laplace transform. (It seems that the discrete energy levels have to give rise to δ-fns, so it might [redacted] be better to write

$$\Theta(N,E) = \sum_{n_1,\dots,n_N} \delta\left(E - (E_{n_1} + \cdots + E_{n_N})\right) \qquad .)$$

The Laplace transform is

$$\sum_{n_1,\dots,n_N} e^{-s(E_{n_1}+\dots+E_{n_N})} = tr\left(e^{-sH_N}\right) = \left(tr\, e^{-sH}\right)^N$$

This time the partition function is

$$Z(s) = tr\left(e^{-sH}\right)$$

and so as before

$$\theta(N,E) = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} e^{sE}\left(Z(s)\right)^N ds$$

At this point it is clear that if we estimate

$$\frac{\theta(N-1, N\varepsilon - E_n)}{\theta(N, N\varepsilon)}$$

as we did before using steepest descent, we get the Maxwell-Bolzman distribution:

$$\frac{e^{-\beta E_n}}{Z(\beta)}$$

and hence our average A-value is

$$\sum_n \langle \psi_n | A | \psi_n \rangle \frac{e^{-\beta E_n}}{Z(\beta)} = \frac{tr\left(Ae^{-\beta H}\right)}{tr\left(e^{-\beta H}\right)}$$

which gives the Gibbs state on the system.

The meaning of the above calculation is not as clear as one would like, especially replacing the discrete energy levels by smeared out ones. But maybe its the same thing as approximating the binomial distribution by the normal distribution.

Example: $H = \frac{1}{2}(P^2+Q^2)$. The eigenvalues are $n+\frac{1}{2}$, $n \geq 0$, so

$$Z(s) = \operatorname{tr}\left(e^{-sH}\right) = \sum_{n=0}^{\infty} e^{-s(n+\frac{1}{2})}$$

$$= \frac{e^{-\frac{1}{2}s}}{1-e^{-s}} = \frac{1}{e^{s/2}-e^{-s/2}}$$

$$-\frac{Z'(s)}{Z(s)} = \frac{1}{2}\,\frac{e^{s/2}+e^{-s/2}}{e^{s/2}-e^{-s/2}} = \frac{1}{2}\coth(s) = \varepsilon$$

$$e^{s/2}+e^{-s/2} = 2\varepsilon\left(e^{s/2}-e^{-s/2}\right)$$

$$e^{s}(1-2\varepsilon) = -1-2\varepsilon$$

$$e^{\beta} = \frac{2\varepsilon+1}{2\varepsilon-1}$$

$$\beta = \log\left(\frac{2\varepsilon+1}{2\varepsilon-1}\right) = \log\left(\frac{1+\frac{1}{2\varepsilon}}{1-\frac{1}{2\varepsilon}}\right) = \frac{1}{\varepsilon}+O\left(\frac{1}{\varepsilon^2}\right)$$

So what's important for statistical mechanics is the operator

$$\frac{e^{-\beta H}}{\operatorname{tr}(e^{-\beta H})}$$

which I think is called the density matrix, because when you take its trace with A you get the expected value for A. One can use path integrals to compute the operator $e^{-\beta H}$.

Let's review the derivation

$$\frac{\partial \psi}{\partial \tau} = - H\psi$$

$$U(\tau+d\tau, \tau) = I - H\psi\, d\tau \qquad \text{to first order}$$

$$\langle q | U(\tau+d\tau, \tau) | q' \rangle = \int \frac{dp}{2\pi} e^{ip(q-q')}(1 - H(p,q)\,d\tau)$$

$$= \int \frac{dp}{2\pi} e^{ip(q-q') - H(p,q)\,d\tau} \qquad \text{to first order}$$

This leads to $\qquad 0 < \tau_1 < \cdots < \tau_n = \tau$

$$\langle q | e^{-\tau H} | q' \rangle = \lim \int \prod_{j=1}^{n} \frac{dp_j}{2\pi} \prod_{j=1}^{n-1} dq_j \; e^{\sum_{j=1}^{n} ip_j(q_j - q_{j-1}) - H(p_j, q_{j-1})\,d\tau}$$

$$= \int\limits_{\substack{q(\tau)=q \\ q(0)=q'}} \left[\frac{dp\,dq}{2\pi}\right] e^{\int_0^\tau (ip\,dq - H(p,q)\,d\tau)}$$

If $H(p,q) = \frac{p^2}{2} + V(q)$, then we do out the p integrations

$$\int \frac{dp}{2\pi} e^{\left(2ip\frac{dq}{d\tau} - \frac{p^2}{2}\right)\frac{d\tau}{2} + \left[\left(i\frac{dq}{d\tau}\right)^2 + \left(i\frac{dq}{d\tau}\right)^2\right]\frac{d\tau}{2}}$$

$$= e^{-\frac{1}{2}\left(\frac{dq}{d\tau}\right)^2 d\tau} \underbrace{\int \frac{e^{-p^2\frac{d\tau}{2}}}{2\pi}\,d\tau}_{\frac{1}{2\pi}\sqrt{\frac{2}{d\tau}}\sqrt{\pi}} = \frac{1}{\sqrt{2\pi\,d\tau}} e^{-\frac{1}{2}\dot{q}^2 d\tau}$$

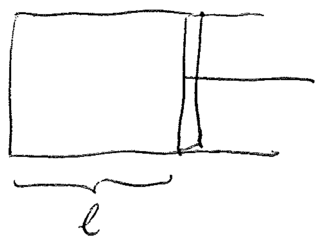
So

$$\langle q | e^{-\tau H} | q' \rangle = \int\limits_{\substack{\text{paths } q:[0,\tau]\to\mathbb{R} \\ \text{start } q',\ \text{end } q}} \left[\frac{dq}{\sqrt{2\pi\,d\tau}}\right] e^{\int_0^\tau -\left(\frac{1}{2}\dot{q}^2 + V(q)\right) d\tau}$$

April 22, 1979

Above I considered a system of a large number of identical particles, and understood somewhat why it leads to the Maxwell-Bolzman-Gibbs distribution. The next goal is to understand a little of thermodynamics, especially the role of the partition function.

The simplest model is an ideal gas in a cylinder



A = area of piston
P = pressure $= F/A$
$V = A\ell$

Suppose we have a molecule with x component of velocity $\pm v_x$ and mass m. Each time it hits the piston it transfer momentum $2mv_x$ to the piston. It take $2\ell/v_x$ secs between hits, so the momentum/sec it gives the piston is

$$2mv_x \, v_x/2\ell = \frac{mv_x^2}{\ell}$$

Total force on piston is

number of molecules

$$\sum_{i=1}^{N} \frac{m\left(v_x(\text{ith part.})\right)^2}{\ell} = PA$$

Thus

$$PV = Nm\langle v_x^2\rangle \qquad \langle\ \rangle \text{ denotes average}$$

$$= \frac{1}{3}Nm\langle v^2\rangle = \frac{2}{3}N\langle \underset{\text{of a molecule}}{\text{Kin. Energy}}\rangle$$

or $\quad PV = \frac{2}{3} \cdot \text{total Kin. Energy}$

Suppose the gas expands or contracts adiabatically. The work done is PdV and this must come out of the Kin. En. of gas.

$$-d(\text{Kin En}) = d\left(\tfrac{3}{2} PV\right) = PdV$$

$$\tfrac{3}{2} dP \cdot V + \tfrac{3}{2} P \cdot dV = -PdV$$

$$\frac{dP}{P} + \frac{5}{3}\frac{dV}{V} = 0$$

or

$$\boxed{PV^{5/3} = \text{Const} \qquad \text{adiabatic}}$$

Now what I want to do is to replace the gas in a cylinder whose volume can be changed, by a large collection of harmonic oscillators with the same spring constant ω^2 and then I want to change ω slowly. The idea is that then I ought to get an analogue of the pressure, by calculating the change in energy.

So I want to look at a single oscillator

$$\ddot{q} = -\omega^2 q$$

where $\omega = \omega(t)$ starts out at ω_i for $t \ll 0$ and ends at ω_f for $t \gg 0$. Assume that ω changes very slowly, and see if we can compute the change in the oscillators energy. But this is like a scattering problem

$$e^{-i\omega_i t} \longleftrightarrow A e^{i\omega_f t} + B e^{-i\omega_f t}$$

conjugate $$e^{-i\omega_i t} \longleftrightarrow \bar{B} e^{i\omega_f t} + \bar{A} e^{-i\omega_f t}$$

Now use the Wronskian is constant

$$\begin{vmatrix} 1 & 1 \\ -i\omega_i & i\omega_i \end{vmatrix} = \begin{vmatrix} \bar{B}+\bar{A} & A+B \\ (\bar{B}-\bar{A})i\omega_f & (A-B)i\omega_f \end{vmatrix}$$

$$2i\omega_i = \left[(\bar{B}+\bar{A})(A-B) + (-\bar{B}+\bar{A})(A+B)\right] \text{[redacted]} i\omega_f$$

$$\frac{\omega_i}{\omega_f} = \text{[redacted]}\left(|A|^2 - |B|^2\right)$$

The idea should be that if $\omega(t)$ varies slowly then the B coefficient is negligible. In any case we can find the energy of the real part

$$y = \mathrm{Re}\left(e^{i\omega_i t}\right) = \cos\omega_i t$$

$$E_i \text{[redacted]} = \tfrac{1}{2}\left(y'^2 + \omega_i^2 y^2\right) = \tfrac{1}{2}\left(\omega^2\sin^2\omega t + \omega^2\cos^2\omega t\right) = \tfrac{1}{2}\omega_i^2$$

$$y = \mathrm{Re}\left(Ae^{i\omega_f t} + Be^{-i\omega_f t}\right) = \mathrm{Re}\left(Ae^{i\omega t} + \bar{B}e^{i\omega t}\right)$$

$$= |A+\bar{B}|\cos\left(\omega_f t + \varphi\right)$$

$$E_f = |A+\bar{B}|^2 \tfrac{1}{2}\omega_f^2$$

In general shifting the phase of the initial vibration will change $A+\bar{B}$ to $\zeta A + \bar{\zeta}\bar{B}$. So if the B coefficient is negligible, then

$$\frac{E_f}{E_i} \approx \frac{|A \text{[redacted]}|^2\omega_f^2}{\omega_i^2} = \frac{\omega_f^2}{\omega_i^2}\,\text{[redacted]}\,\frac{\omega_i}{\omega_f} = \text{[redacted]}\,\frac{\omega_f}{\omega_i}$$

April 23, 1979

Thus if ω is increased to $\omega + d\omega$ we have

$$\frac{E + dE}{E} = \frac{\omega + d\omega}{\omega} \qquad \text{or} \qquad \frac{dE}{E} = \frac{d\omega}{\omega}$$

and hence the energy changes proportionally to ω.

Another way to check this is to average over a cycle to compute the dE corresponding to an infinitesimal $d\omega$. Let us take $q(t) = a \sin(\omega t + \theta)$. Its potential energy is $\frac{1}{2}\omega^2 q^2$ and this is the only thing that changes as we increase ω. We assume the $d\omega$ take place over a long time period so that the energy increase is dE $d(\frac{1}{2}\omega^2 q^2) = \omega\, d\omega\, q^2$ averaged over the possible values of q. This gives

$$dE = \omega d\omega \langle q^2 \rangle = \omega\, d\omega \frac{a^2}{2} = \frac{d\omega}{\omega} \frac{a^2\omega^2}{2}$$

But the total energy for $q(t) = a\sin(\omega t + \theta)$ is

$$\frac{1}{2}\left[(a\omega \cos)^2 + \omega^2 (a \sin)^2\right) = \frac{a^2\omega^2}{2}$$

Thus again we get

$$dE = \frac{d\omega}{\omega} E .$$

Now the reason I made this calculation is because I want to think of ω as being like the volume of a gas, so I want to understand the energy increase produced by an adiabatic change in ω. So let us suppose we have a "gas" made of N independent oscillators as above. Let U be the total energy $$U = \sum_{i=1}^{N}{}' \frac{1}{2} a_i^2 \omega^2$$

where a_i is the amplitude of the i-th particle.

Go back to a single particle with

$$E = \frac{1}{2} a^2 \omega^2$$

$$dE = a\,da\,\omega^2 + a^2 \omega\, d\omega = \frac{d\omega}{\omega} E = d\omega \frac{1}{2} a^2 \omega$$

$$\frac{da}{a} + \frac{1}{2}\frac{d\omega}{\omega} = 0$$

$$a^2 \omega = \text{const.}$$

Thus $a^2 = \frac{\text{const}}{\omega}$, so the amplitude decreases with ω, but the energy increases linearly wrt. ω.

So now suppose the system is in equilibrium which means the particles are distributed at any instant like

$$\frac{e^{-\frac{\beta}{2}(p^2+\omega^2 q^2)}\,dp\,dq}{\int e^{-\beta/2 (p^2+\omega^2 q^2)}\,dp\,dq}$$

The denominator is

$$Z(\beta) = \int e^{-\beta/2 (p^2+\cancel{\omega^2} q^2)} \frac{dp\,dq}{\beta\,\omega} = \frac{2\pi}{\beta\omega}$$

The average potential energy / molecule is

$$\frac{\int \frac{1}{2} \cancel{\omega^2} q^2\, e^{-\frac{\beta}{2}(p^2+\cancel{\omega^2} q^2)}\, dp \frac{dq}{\omega}}{Z(\beta)} = \frac{\frac{1}{2}\int \frac{1}{2}(p^2+q^2)\, e^{-\frac{\beta}{2}(p^2+q^2)}\, dp\,dq}{\omega Z(\beta)}$$

$$= \frac{1}{2} \frac{\int \frac{1}{2}(p^2+\omega^2 q^2)\, e^{-\frac{\beta}{2}(p^2+\omega^2 q^2)}\, dp\, dq}{Z(\beta)}$$

$$= \frac{1}{2}(-)\frac{\partial}{\partial \beta} \log Z(\beta) = \frac{1}{2}\frac{1}{\beta} = \frac{1}{2} kT$$

So as one knows from equipartition the average kinetic or [redacted] potential energy / molecule is $\frac{1}{2} kT$. Thus the total energy is

$$U = NkT$$

[redacted] So now let's use analogy with ideal gas:

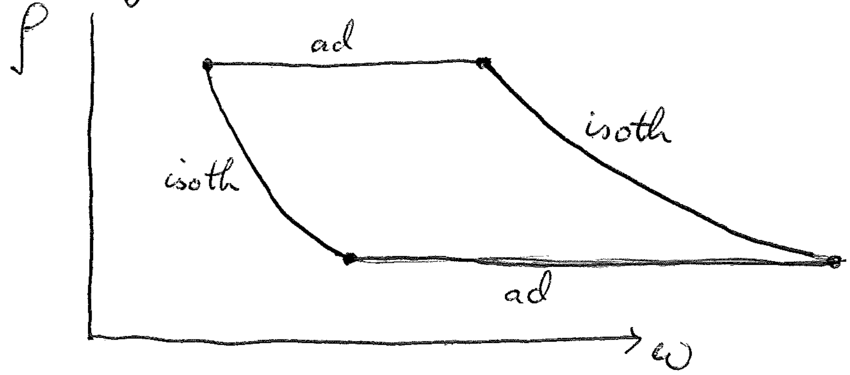
Ideal gas		Oscillator gas
$U = 3N\frac{1}{2}kT$	equipart.	$U = NkT$
$PV = \frac{2}{3}U$	mechanics	
(These imply $PV = NkT$)		
$-PdV = dU$	adiabatic change	$dU = \frac{U}{\omega} d\omega$

We are missing an analogue of the pressure. Let's define the pressure ρ to be

$$\rho = +\frac{U}{\omega}$$

so that we have $dU = \rho\, d\omega$ for adiabatic change. Because [redacted] we have seen that U/ω is constant for adiabatic change, adiabatic is the same as constant pressure; [redacted]

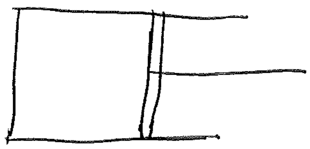
Also since $U = NkT$, isothermal is the same as $\rho\omega =$ constant, as for the ideal gas. So a Carnot cycle looks as follows



The only difference is that increasing ω is like decreasing the volume, but this is confusing.

April 24, 1979

Thermodynamics: Let's consider an ideal gas engine

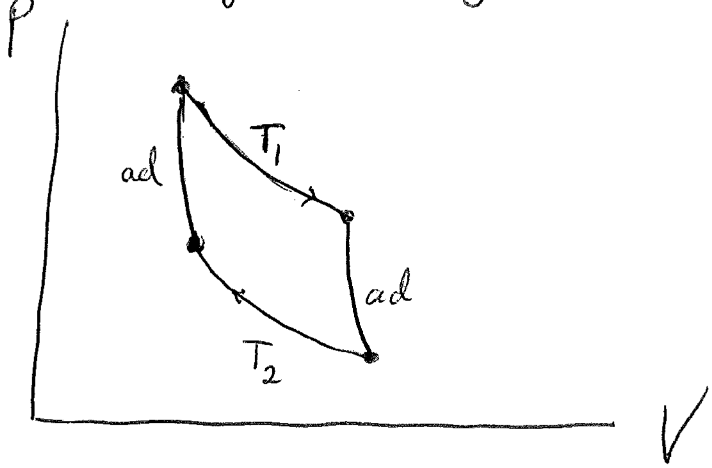


Let U be the internal energy of the gas. If the system makes a small change, the work done by the gas is PdV, so the first law of thermo. (conservation of energy) says

$$dU = -PdV + dQ$$

where dQ is the heat that has to be added.

Run this engine along a Carnot cycle



Q_1 = heat added at temp T_1

Q_2 = heat removed at temp T_2

This means the engine is operated reversibly, i.e. slow enough to be in equilibrium.

The 2nd law of thermo implies that two reversible engines operating between the same temperatures have the same efficiency. (In fact the efficiency of a reversible engine > any irreversibly engine). The efficiency is $\dfrac{Q_1 - Q_2}{Q_1}$

One can use this result to define an absolute temperature scale, namely

$$\frac{Q_1 - Q_2}{Q_1} = \frac{T_1 - T_2}{T_1} \qquad \text{or} \qquad \frac{Q_2}{Q_1} = \frac{T_2}{T_1}.$$

[redacted] (The second law says you can't get useful work from heat energy at a fixed temperature, so if you have a reversible engine with efficiency e operating between T_1, T_2 and another (possibly irreversible) with efficiency e', then by running the former backward connected to the latter:

$$\underset{\substack{\text{heat in}\\ \text{at } T_2}}{Q_2} + \underset{\substack{\text{mech}\\ \text{work}}}{W} = \underset{\substack{\text{heat}\\ \text{out at}\\ T_1}}{Q_1} \mapsto = \underset{\substack{\text{heat}\\ \text{in 'engine}\\ \text{at } T_1}}{Q_1'} = \underset{\substack{\text{heat out}\\ \text{'engine}\\ \text{at } T_2}}{Q_2'} + \underset{\substack{\text{mech}\\ \text{work}}}{W'}$$

[redacted] 2nd law $\Rightarrow$ $W \geq W'$ [redacted]

$$\Rightarrow \quad e = \frac{W}{Q_1} \geq \frac{W'}{Q_1'} = e'.)$$

So now return to Carnot cycle. Since $dQ = 0$ [redacted] for an adiabatic change one has

$$\oint \frac{dQ}{T} = \frac{Q_1}{T_1} - \frac{Q_2}{T_2} = 0$$

[redacted] Since any closed curve in the PV plane can be broken into little Carnot cycles, one sees that upon operating the engine reversibly along any closed
(means under equilibrium conditions)

curve we get

$$\oint \frac{dQ}{T} = 0 \qquad \text{so}$$

$$\frac{dQ}{T} = \frac{dU + PdV}{T} \qquad \text{is an exact differential}$$

The entropy is defined up to an additive constant by

$$dS = \frac{dQ}{T} = \frac{dU + PdV}{T}$$

For an ideal monatomic gas we have

$$PV = NkT \qquad U = \frac{3}{2}NkT = \frac{3}{2}PV$$

$$dU = \frac{3}{2}PdV + \frac{3}{2}dP\,V$$

$$dQ = dU + PdV = \frac{5}{2}PdV + \frac{3}{2}VdP$$

$$dS = \frac{dQ}{T} = \frac{\frac{5}{2}PdV + \frac{3}{2}V\,dP}{PV/Nk} = Nk\left\{\frac{5}{2}\frac{dV}{V} + \frac{3}{2}\frac{dP}{P}\right\}$$

$$S = \frac{3}{2}Nk \log\left(PV^{5/3}\right) + C.$$

For an oscillator gas we found

$$\rho\omega = U = NkT$$

$$dU = \rho\, d\omega \qquad \text{for adiabatic change}$$

$$\therefore\ d\rho = 0 \qquad \text{for} \quad \text{"} \quad \text{"}$$

First law:
$$dU = \rho\, d\omega + dQ$$

so

$$dS = \frac{dQ}{T} = \frac{dU - p\,dw}{T} = \frac{w\,d\rho}{\rho w / Nk} = Nk\,\frac{d\rho}{\rho}$$

So

$$S = Nk \log(\rho) + \text{const.}$$

Program: So far [redacted] I have been looking at ideal non-interacting systems, whose behavior is understood using law of large numbers, and which [redacted] leads to the Maxwell-Bolzman distribution. The next thing is to incorporate some interaction. What I want to do is to take a finite system and let the size go to infinity, and see if there is a definite limit. Philosophy is that of the law of large numbers.

So consider an Ising model — states are $s : I \to \{\pm 1\}$, energy is

$$H(s) = -B \sum s_i - \sum J_{ij} s_i s_j$$

where B is the external magnetic field. Note that $B > 0$ makes the spins tend to align "up", i.e. $s_i = +1$ has lower energy. Similarly $J_{ij} > 0$ describes the ferromagnetic situation.

The quantity of interest will be the total magnetization at a given temperature. This is

$$\left\langle \sum s_i \right\rangle = \frac{\sum_s \left(\sum s_i\right) e^{-\beta H(s)}}{\sum_s e^{-\beta H(s)}}$$

$$= \frac{1}{\beta} \frac{\partial}{\partial B} \log Z \text{[redacted]} (\beta, \text{[redacted]} B, N)$$

Let's begin with the case of no interaction: $J_{ij}=0$.
Then

$$Z_N = (Z_1)^N$$

where

$$Z_1 = e^{\beta B} + e^{-\beta B} = 2\cosh(\beta B).$$

Now what?

It will be necessary to review the law of large numbers for Bernoulli trials. Suppose $p+q=1$ with $0<p<1$, and we make N independent trials and keep track of the number of heads, obtaining the prob. measure

$$d\mu_N = \sum_{k=0}^{N} \binom{N}{k} p^k q^{N-k} \delta(x-k)$$

with char. function

$$\int e^{itx}\, d\mu_N = \sum_{k=0}^{N} \binom{N}{k} p^k q^{N-k} (e^{it})^k = (pe^{it}+q)^N$$

The expected number of heads is

$$\int x\, d\mu_N = \frac{1}{i}\frac{d}{dt}(pe^{it}+q)^N \Big|_{t=0}$$
$$= N(pe^{it}+q)^{N-1} pe^{it}\Big|_{t=0} = Np$$

and so we center at the expectation

$$d\mu_N^c = \sum_{k=0}^{N} \binom{N}{k} p^k q^{N-k} \delta(x+Np-k)$$

$$\int e^{itx}\, d\mu_N^c = (pe^{it}+q)^N e^{-iNpt}$$
$$= (pe^{iqt}+qe^{-ipt})^N$$

Suppose we are interested in the limiting distribution for the average number of heads $\frac{1}{N}\sum s_i$. This gives the measure

$$d\mu_N' = \sum_{k=0}^{N} \binom{N}{k} p^k q^{N-k}\, \delta\left(x-\frac{k}{N}\right)$$

$$\int e^{itx}\, d\mu_N' = \left(pe^{it/N}+q\right)^N$$

As $N \longrightarrow \infty$
$$\left(pe^{it/N}+q\right)^N = \left(p\left(1+\frac{it}{N}+\cdots\right)+q\right)^N$$
$$\simeq \left(1+it\frac{p}{N}\right)^N \longrightarrow e^{itp}$$

and so
$$d\mu_N' \longrightarrow \delta(x-p).$$ law of large numbers.

On the other hand if we are interested in

$$\frac{1}{\sqrt{N}}\left(\sum s_i - Np\right)$$

we get
$$d\mu_N'' = \sum_{k=0}^{N} \binom{N}{k} p^k q^{N-k}\, \delta\left(x-\frac{k}{\sqrt{N}}+\sqrt{N}p\right)$$

$$\int e^{itx}\, d\mu_N'' = \sum_0^N \binom{N}{k} p^k q^{N-k}\, e^{it\frac{k}{\sqrt{N}}-i\sqrt{N}pt}$$
$$= \left(pe^{it/\sqrt{N}}+q\right)^N \left(e^{-ip\frac{t}{\sqrt{N}}}\right)^N$$
$$= \left(pe^{iq/\sqrt{N}t}+qe^{-ip/\sqrt{N}t}\right)^N$$

$$\approx \left(p - \frac{pq^2}{2N}t^2 + q - \frac{qp^2}{2N}t^2\right)^N = \left(1 - \frac{pq}{N}\frac{t^2}{2}\right)^N$$

$$\longrightarrow e^{-\frac{pq}{2}t^2}$$

Thus $x = \frac{1}{N}\sum s_i$ is distributed like $\delta(x-p)$

$y = \frac{1}{\sqrt{N}}\left(\sum s_i - Np\right)$ ———— a normal distribution.

Now let's look at the Ising model again

$$H(s) = -B\sum s_i - \sum_{i<j} J_{ij} s_i s_j$$

with no interaction first: $J_{ij} = 0$. Then

$$Z_1(\beta) = e^{\beta B} + e^{-\beta B}$$

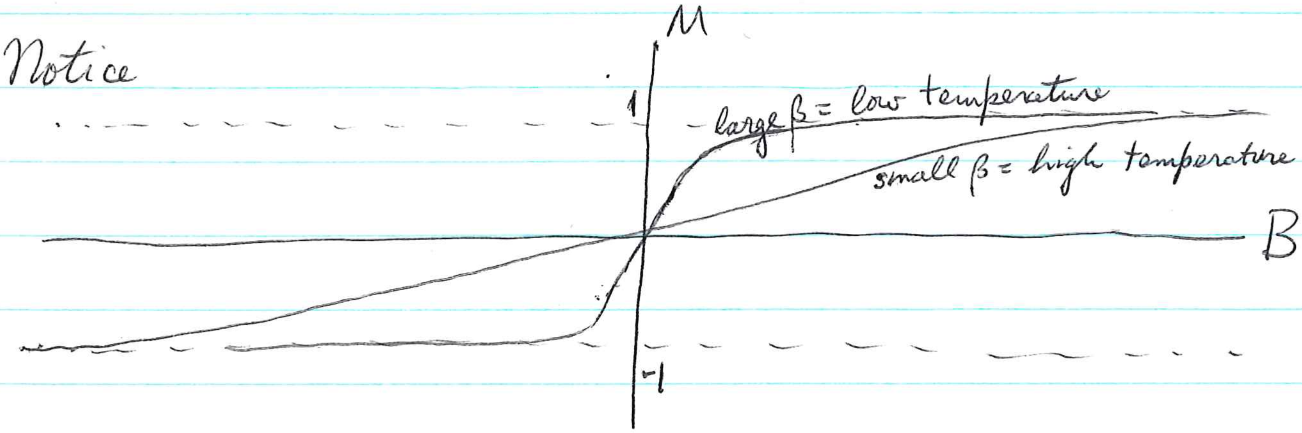
so we have N independent coin tosses with

[redacted] $$p = \frac{e^{\beta B}}{e^{\beta B} + e^{-\beta B}}$$

The [redacted] magnetization per site is

$$M = \langle s_i \rangle = p - q = \frac{e^{\beta B} - e^{-\beta B}}{e^{\beta B} + e^{-\beta B}} = \tanh(\beta B)$$

Notice



Notice the magnetization $M = M(B,T)$ is intuitively a random quantity – you should think of the actual spins flipping back and forth randomly, but with the probabilities given by MB. Consequently the actual magnetization at any instant is also changing, however with N very large we know the average magnetization per site is distributed close to $\delta(M - \tanh \beta B)$, so therefore you see a fixed M in practice. [This is the argument [redacted] using the ergodic hypothesis – one supposes the actual trajectory fills up phase space in such a way that macroscopic [redacted] time averages correspond to phase space averages at that [redacted] energy.)

[redacted] In this example there doesn't seem to be any immediate reason to bring in the normal distribution, that is, the deviation [redacted] of the actual distribution of $\frac{1}{N}(\sum s_i)$ [redacted] from the δ function peaking at $\tanh(\beta B)$.

Next we want to consider some interaction. First suppose that all $J_{ij} = J$, so that

$$H(s) = -B\sum s_i - \sum_{i<j} J s_i s_j$$

Then this is a function of $\sum s_i$

$$\left(\sum s_i\right)^2 = \sum s_i + 2\sum_{i<j} s_i s_j$$

so

$$H(s) = -B\sum s_i - \frac{J}{2}\left[\left(\sum s_i\right)^2 - \sum s_i\right]$$

$$= -\left(B - \frac{J}{2}\right)\sum s_i - \frac{J}{2}\left(\sum s_i\right)^2$$