Advanced Statistical Mechanics

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Week 2

4 Quantum and Statistical Mechanics

A convenient way to describe a quantum particle is by Feynman path integral. It allows to calculate the Green's functions of the Schrödinger equation. The Green's function $G(x_f, x_i; t_f, t_i)$ is defined as a probability amplitude of a particle to hop from the point x_i at a time t_i to the point x_f at a time t_f. In other words, it is a wave function $\psi(x,t)$ of a particle at a point x_2 and time t_f whose wave function at time t_i was $\psi(x, t_i) = \delta(x - x_i)$. It can be expressed in terms of

$$G(x_f, x_i; t_f, t_i) = \sum_n \exp\left(-iE_n\left(t_f - t_i\right)\right)\psi_n(x_f)\psi_n^*(x_i). \tag{4.1}$$

Here ψ_n are the eigenfunctions of the Hamiltonian. A retarded Green's function is supplemented by the boundary condition $G = 0$ for $t_f < t_i$, and, by definition, $G(x_f, x_i; t, t) = \delta(x_f - x_i)$. Retarded Green's function satisfies the Schrödinger equation

$$i\frac{\partial G}{\partial t} = H(x_f)G + i\delta(t_f - t_i)\delta(x_f - x_i) \tag{4.2}$$

It follows from this definition that, if a particle's wave function is $\psi_i(x)$ at time $t = t_i$, its wave function at $t = t_f$ is

$$\psi_f(x) = \int dy\ G(x, y; t_f, t_i)\psi_i(y). \tag{4.3}$$

A formal way to write down G is

$$G = \left\langle\, x_f \left|\exp\left(-i\left(t_f - t_i\right)H\right)\right| x_i \,\right\rangle. \tag{4.4}$$

Although this expression is useless for direct calculations, it will be useful for making contact with the formalism later.

Feynman gave a beautiful expression of the Green's function in terms of a path integral:

$$G(x_f, x_i, t_f, t_i) = \int_{x(t_i)=x_1}^{x(t_f)=x_2} \mathcal{D}x(t)\ \exp\left(iS\right), \tag{4.5}$$

where S is the classical action calculated along the trajectory $x(t)$,

$$S = \int_{t=t_i}^{t=t_f} dt\ \mathcal{L}, \tag{4.6}$$

where $\mathcal{L}$ is the Lagrange function,

$$\mathcal{L} = \frac{1}{2}\dot{x}^2 - U(x). \tag{4.7}$$

This expression can be understood in the following way. If $t_f - t_i = \epsilon$ is very small, then

$$G(x,y;\epsilon) = \int \frac{dp}{2\pi}\, e^{i\left[p(x-y)-\epsilon\frac{p^2}{2m}-\epsilon V(y)\right]} \tag{4.8}$$

This can be checked by expanding in powers of ϵ and then comparing with (4.2). Doing the p integral gives

$$G(x,y;\epsilon) = \sqrt{\frac{m}{2\pi i\epsilon}}\, e^{i\left[\frac{(x-y)^2}{\epsilon}-\epsilon V(y)\right]} \tag{4.9}$$

It is clear that, for example,

$$G(x,y;2\epsilon) = \int dz\; G(x,z;\epsilon)G(z,y;\epsilon) \tag{4.10}$$

Now if $t_f - t_i = n\epsilon$ and $x = x_n$, $y = x_0$.

$$G(x,y;n\epsilon) = \int \prod_{i=1}^{n-1} dx_i \left(\frac{m}{2\pi i\epsilon}\right)^{\frac{n-1}{2}} e^{i\sum_{i=0}^{n-1}\left[\frac{(x_{i+1}-x_i)^2}{\epsilon}-\epsilon V(x_i)\right]}. \tag{4.11}$$

The expression in the exponential becomes the action in the continuum limit, while the whole expression becomes the Feynman path integral.

In a very formal way, consider motion in the imaginary time t. If t is imaginary, it makes sense to introduce the variable $\tau = -it$, which is real. The trajectory is now $x(\tau)$ and the Feynman path integral becomes

$$G(x_2,x_1;\tau_f,0) = \int_{x(0)=x_1}^{x(\tau_f)=x_2} \mathcal{D}x(\tau)\exp\left(-\int_{\tau=0}^{\tau=\tau_f} d\tau\mathcal{L}(\tau)\right), \tag{4.12}$$

where the imaginary time lagrange function

$$\mathcal{L} = \frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 + U(x). \tag{4.13}$$

This imaginary time Green's function can be expressed in the following way

$$G(x_f,x_i;\tau,0) = \sum_n \exp\left(-E_n\tau\right)\psi_n(x_f)\psi_n^*(x_i). \tag{4.14}$$

and its solves the imaginary time Shrödinger equation

$$\frac{\partial G}{\partial\tau} = -H(x_f)G + \delta(t_f - t_i)\delta(x_f - x_i). \tag{4.15}$$

Knowing the imaginary time Green's functions it is possible to find real Green's functions by analytic continuation. Therefore, imaginary time formalism is equivalent to the real time formalism.

We note that this expression looks very much like a partition function of a one dimensional object whose length is τ_f and whose energy is

$$E = \int dx \, \left[\frac{1}{2}\dot{x}^2 + U(x) \right]. \tag{4.16}$$

$$Z = \int \mathcal{D}x \; e^{-E}. \tag{4.17}$$

This provides the first example of equivalence between quantum and statistical mechanics. In general, quantum field theory in d dimensional space and 1 time is equivalent to the statistical mechanics in the $d+1$ dimensional space.

5 1D Ising Model

The 1D Ising model is model of a 1D magnet. Its partition function is

$$Z = \sum_{\sigma_i = \pm 1} e^{-\frac{H}{T}} \tag{5.18}$$

where

$$H = -J \sum_{i=0}^{N-1} \sigma_i \sigma_{i+1} \tag{5.19}$$

We denote $\beta = \frac{J}{T}$ from now on. N is the length of the chain.

Although the energy factor prefers all the spin to look up, the entropy factor destroys that. Indeed, if n is the number of kinks, the partition function can be rewritten as

$$Z = \sum_n 2 \frac{N!}{n!(N-n)!} e^{-2\beta n}. \tag{5.20}$$

Let's find the typical value of n. It's the value where the term to be summed is the biggest. Taking a derivative of a log (using the Stirling formula $\frac{d}{dn} \log n! \approx \log n$) we get

$$\frac{\partial}{\partial n} \log \left(\frac{N!}{n!(N-n)!} e^{-2\beta n} \right) = \log \left(\frac{N-n}{n} \right) - 2\beta = 0, \tag{5.21}$$

or

$$n_{\text{typ}} = N \left(\exp(2\beta) + 1 \right)^{-1}. \tag{5.22}$$

Therefore a typical distance between kinks is $N/n \propto \exp(2\beta)$. It can be large at large β, yet for large enough chains it is always much smaller than the length of the chain. We deduce that the 1D Ising chain is not ordered at any temperature, even though it has a tendency towards order as the temperature is lowered.

Introduce the transfer matrix

$$T = \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix} \tag{5.23}$$

The Ising partition function can be rewritten as

$$Z_{\sigma_0 \sigma_N} = T^N \tag{5.24}$$

Now

$$T = \sqrt{2 \sinh{(2\beta)}}\; e^{\gamma \tau_1}, \tag{5.25}$$

where τ_1 is the first Pauli matrix and $\sinh\gamma = \exp(-\beta)/\sqrt{2\sinh{(2\beta)}}$. At large β, $\gamma \propto \exp{(-2\beta)}$. Therefore,

$$Z = a^N \exp{(-NH)}\,, \tag{5.26}$$

where

$$H = -\gamma\tau_1,\; a = \sqrt{2\sinh{(2\beta)}}. \tag{5.27}$$

We can think of H as the Hamiltonian and (5.26) as equivalent to (4.4). We reduced statistical mechanics of one dimensional object (Ising chain) to a quantum mechanics problem.

Diagonalizing the Hamiltonian, we find two energy levels $E_0 = -\gamma$ and $E_1 = \gamma$. Correspondingly, there are two eigenstates,

$$\psi_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix},\; \psi_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{5.28}$$

Therefore,

$$Z_{\sigma_N \sigma_0}/a^N = \exp{(-NE_0)}\, \psi^0_{\sigma_N}\psi^0_{\sigma_0} + \exp{(-NE_1)}\, \psi^1_{\sigma_0}\psi^1_{\sigma_0} \tag{5.29}$$

For large N only the ground state survives,

$$Z_{\sigma_N \sigma_0}/a^N = \exp{(-NE_0)}\, \psi^0_{\sigma_N}\psi^0_{\sigma_0}. \tag{5.30}$$

As a result,

$$Z_{11}/a^N = Z_{01}/a^N = \exp{(-NE_0)}\,. \tag{5.31}$$

In other words, the sign of the last Ising variable does not depend on the sign of the first, as long as N is sufficiently large. N at which this happens can be estimated as

$$\exp{[-N(E_1 - E_0)]} \ll 1,\; N \gg \frac{1}{E_1 - E_0} \tag{5.32}$$

$\xi = (E_1 - E_0)^{-1}$ is called the correlation length. We showed that the correlation length is the inverse of the excitation gap of the spectrum.

A correlation function is defined as

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z} \sum_{\sigma_k = \pm 1} \sigma_i \sigma_j \; e^{\beta \sum_k \sigma_k \sigma_{k+1}}. \tag{5.33}$$

We could write it with the help of $Z_{\sigma_i \sigma_j}$ introduced above

$$\langle \sigma_i \sigma_j \rangle = \mathrm{Tr} \; \left[e^{-(N-i)H} \tau_3 e^{-(i-j)H} \tau_3 e^{-jH} \right]. \tag{5.34}$$

From what has been discussed above, it is clear that

$$\langle \sigma_i \sigma_j \rangle \propto \exp \left(- \frac{|i-j|}{\xi} \right). \tag{5.35}$$

The quantum mechanical analog of this is to introduce the "time" dependent spin operator

$$\tau(i) = e^{Hi} \tau_3 e^{-Hi}. \tag{5.36}$$

Then the correlation function becomes

$$\langle \tau(i) \; \tau(j) \rangle \tag{5.37}$$

Finally, $\langle \; \rangle$ is understood depending on the boundary conditions. If it is a sum over boundary spins independently, this is going to be the ground state. If the boundary conditions are periodic, this could mean trace.