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TWO FORMS OF THE PARTITION FUNCTION FOR THE ISING MODEL

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Abstract: Starting with the Fourier representation of the two body potential and by partial integration over certain auxiliary variables, a simple proof is given for the linked cluster expansion of the partition function. The same starting point is also used to derive the functional integration form in both space and momentum variables, leading to the Wilson Hamiltonian.

1. Introduction

Consider the partition function of the Ising model with external fields

$$Z = \mathrm{Tr}\exp\left(\frac{1}{2}\sum_{i,j} V(R_i - R_j)\, s_i\, s_j + \sum_i h_i\, s_i\right).$$

The summation extends over all lattice sites R_i where N spins s_i are located, each spin taking values from $-S$ to $+S$. The potential $V(R_i - R_j)$ between two spins, which already includes the temperature factor $\beta = (k_B T)^{-1}$, depends on the distance between two sites only and takes the value zero at the origin. Therefore $v(k) = v(-k)$, where

$$V(R_n) = \int_{-\infty}^{\infty} v(k)\exp(ikR_n)\,\mathrm{d}k = \int_{q\in BZ} \mathscr{V}(q)\exp(iqR_n)\,\mathrm{d}q$$

and

$\mathscr{V}(q) = \mathscr{V}(q + b) \Rightarrow \sum_b v(q + b)$, where b is a vector of the reciprocal lattice and q runs over vectors in the Brillouin zone. Depending on the explicit form of the potential one or the other integral representation is more appropriate.

Dividing the momentum space of the integral representation into M small cells $\Delta(q_t)$, replacing the integral with a sum and using the identity

$$\exp\left(\frac{1}{2} z^2\right) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \exp\left(-\frac{u^2}{2} + zu\right) du,$$

the following expression for the partition function emerges[1]),

$$Z_M = \mathrm{Tr}\exp\left[\sum_{qt}^{1/2} \Delta(q_t)\, v(q_t) \sum_n e^{iq_t R_n} s_n) (\sum_m e^{-iq_t R_m} s_m) + \sum_i h_i s_i\right],$$

or

$$Z_M = \mathrm{Tr}\exp\{\sum_{qt}^{1/2} \Delta_t v_t [(\sum_n s_n \cos(q_t R_n)^2 + (\sum_n s_n \sin(q_t R_n))^2] + \sum_i h_i s_i\} =$$

$$= \int_{-a}^{\infty} \prod_{t=1}^{M} \left(\frac{1}{2\pi} dx_t\, dy_t\, e^{-\frac{1}{2}(x_t^2 + y_t^2)}\right) \prod_{i=1}^{N} \sum_{S_i = -S}^{S} \exp\{s_i (\sum_{qt}^{1/2} (2\Delta_t v_t)^{\frac{1}{2}} \cdot$$

$$\cdot (x_t \cos q_t R_i) + y_t \sin(q_t R_i)) + h_i)\}.$$

Hence,

$$Z_M = \int_{-\infty}^{\infty} \prod_{t=1}^{M} \left(\frac{1}{2\pi} dx_t\, dy_t\, e^{-\frac{1}{2}(x_t^2 + y_t^2)}\right) \prod_{i=1}^{N} \frac{\mathrm{sh}\left(S + \frac{1}{2}\right)(F_i + h_i)}{\mathrm{sh}\frac{1}{2}(F_i + h_i)}, \tag{1}$$

where

$$F_i = \sum_{qt}^{1/2} (2\Delta_t v_t)^{\frac{1}{2}} (x_t \cos(q_t R_i) + y_t \sin(q_t R_i)). \tag{2}$$

The sign $\sum_{qt}^{1/2}$ means that we sum only over one half of the integration space, the other half being accounted for through the factor 2 on behalf of the inversion symmetry of the potential $v(q)$; Δ_t and v_t stand for $\Delta(q_t)$ and $v(q_t)$, respectively.

2. *Perturbational expansion*

In order to carry out the perturbational expansion of the partition function in (1), let us introduce the polar coordinates r_t, φ_t through

$$x_t = r_t \cos \varphi_t,$$

$$y_t = r_t \sin \varphi_t.$$

Hence,

$$Z_M = \int_0^\infty \int_0^{2\pi} D_M \exp\left(-\frac{1}{2}\sum_{t=1}^{M} r_t^2\right) Z^0, \tag{3}$$

where

$$D_M = \prod_{t=1}^{M}\left(\frac{1}{2\pi} r_t \, dr_t \, d\varphi_t\right), \quad Z^0 = \prod_{i=1}^{N} Z^1 (F_i + h_i)$$

and

$$Z_1(x) = \frac{\mathrm{sh}\left(S + \frac{1}{2}\right) x}{\mathrm{sh}\frac{x}{2}},$$

$$F_i = \sum_{q_t}^{1/2} (2\Delta_t v_t)^{\frac{1}{2}} r_t \cos (q_t R_i - \varphi_t).$$

The expression in (3) can be evaluated by successive partial integration over the polar coordinates. Suppose that we start with the radial coordinate r_M

$$Z_M = \int_0^\infty \int_0^{2\pi} D_{M-1} \exp\left(-\frac{1}{2}\sum_t r_t^2\right) \prod_{i=1}^{N} Z_1 (F_i + h_i) \,|\, r_M = 0 +$$

$$+ (2\Delta_M v_M)^{\frac{1}{2}} \int_0^\infty \int_0^{2\pi} D_{M-1} \int_0^\infty \int_0^{2\pi} dr_M \frac{d\varphi_M}{2\pi} \exp\left(-\frac{1}{2}\sum_t r_t^2\right) \sum_{n=1}^{N} \frac{\partial Z^0}{\partial h_n} \cdot$$

$$\cdot \cos (q_M R_M - \varphi_M).$$

Another partial integration over the angle φ_M in the second term yields

$$Z_M = Z_{M-1} + 2\Delta_M v_M \int_0^\infty \int_0^{2\pi} D_M \exp\left(-\frac{1}{2}\sum_t r_t^2\right) \sum_{n,m} \frac{\partial^2 Z^0}{\partial h_n \, \partial h_m}$$

$$\cdot \sin (q_M R_n - \varphi_M) \sin (q_M R_m - \varphi_M).$$

Repeating the partial integration in both terms one has to keep only those contributions which are nonzero in the limit as $\Delta_t \to 0$. This is the case with the terms which are multiplied by Δ_t because of the additional summation in the q_t variables. The same is true for terms which contain the factor Δ_t, Δ_t since they are included into a double sum over q-space. Such a term appears for example after another partial integration of the second term in (4), yielding a contribution

$$(2\Delta_M v_M)(2\Delta_t v_t) \sum_{l,m,n,p} \frac{\partial^4 Z^0}{\partial h_l \, \partial h_m \, \partial h_n \, \partial h_p} \sin(q_M R_l - \varphi_M) \cdot$$

$$\cdot \sin(q_M R_m - \varphi_M) \sin(q_t R_n - \varphi_t) \sin(q_t R_p - \varphi_t). \tag{5}$$

After setting to zero all of the functions F_i which appear in Z^0 of Equs. (4) and (5), integrating over the polar coordinates and performing the corresponding integrations in the q-space one arrives at the first three terms of the perturbational expansion

$$Z = Z^0 \Big|_{F=0} + \sum_{q_t}^{1/2} \Delta_t v_t \sum_{m,n} \frac{\partial^2 Z^0}{\partial h_m \, \partial h_n} \cos(q_t (R_m - R_n)) \Big|_{F=0} +$$

$$+ \frac{1}{2!} \sum_{l,m,n,p} \sum_{q_t}^{1/2} \Delta_t v_t \cos(q_t (R - R_m)) \sum_{q_{t'}}^{1/2} \Delta_{t'} v_{t'} \cdot$$

$$\cdot \cos(q_{t'} (R_n - R_p)) \frac{\partial^4 Z^0}{\partial h_l \, \partial h_m \, \partial h_n \, \partial h_p} \Big|_{F=0} + \ldots =$$

$$= Z^0 \Big|_{F=0} + \frac{1}{2} \sum_{m,n} V(R_m - R_n) \frac{\partial^2 Z^0}{\partial h_m \, \partial h_n} \Big|_{F=0} +$$

$$+ \frac{1}{2!} \left(\frac{1}{2} \sum_{l,m} V(R - R_m) \frac{\partial^2}{\partial h_l \, \partial h_m} \right) \left(\frac{1}{2} \sum_{n,p} V(R_n - Rp) \frac{\partial^2}{\partial h_n \, \partial h_p} \right) Z^0 \Big|_{F=0} + \ldots . \tag{6}$$

It is evident that the general expansion series can be expressed in the form

$$Z = \sum_{p=0}^{\infty} \frac{1}{p!} \left(\frac{1}{2} \sum_{m,n} V(R_m - R_n) \frac{\partial^2}{\partial h_m \, \partial h_n} \right)^p Z^0 \Big|_{F=0} , \tag{7}$$

or, equivalently

$$Z = \exp\left(\frac{1}{2} \sum_{m,n} V(R_m - R_n) \frac{\partial^2}{\partial h_m \, \partial h_n} \right) Z^0 \Big|_{F=0} , \tag{7a}$$

which is identical in form to the Hori formula in field theory, and from which the standard diagrammatic expansion of the partition function in terms of the semi--invariants could be derived. This follows from the observation, that after associating p different bonds with the p factors $V(R)$ of perturbational expansion (7), one can find the contribution of a particular disconnected graph by counting the number of ways how to construct topologically equivalent graphs from p bonds. If a given disconnected graph consists of $n_1, n_2, \ldots, n_p$ different connected graphs $G_1, G_2, \ldots, G_P$ having $p_1, p_2, \ldots, p_P$ bonds, it is evident that this number equals

$$p! \prod_{i=1}^{P} (n_i!(p_i!)^{n_i})^{-1} (p_i! g_i^{-1})^{n_i},$$

where g_i stands for the number of permutations of p_i different bonds which transform a graph G_i into itself. This is equivalent to the rule that lnZ should be written as a sum of contributions of all linked graphs, each being multiplied by a factor g_i^{-1} [2].

3. *Partition function as a functional integral*

The form in (1) is also very suitable for expressing the partition function in terms of a functional integral. In this case it is convenient to introduce a normalization factor

$$\mathcal{N} = \int_{-\infty}^{\infty} \prod_t^{1/2} (\mathrm{d}x_t \, \mathrm{d}y_t) \exp\left(\frac{1}{2} \sum_t (x_t^2 + y_t^2)\right)$$

instead of the factor $(2\pi)^M$ in the denominator of (1), what allows a very simple change of integration variables.

As a first step let us rescale the variables x_t, y_t to

$(\Delta_t)^{-\frac{1}{2}} x_t, (\Delta_t)^{-\frac{1}{2}} y_t$ and formally take the limit $\Delta_t \to 0$

$$Z = \frac{1}{\mathcal{N}} \int_{-\infty}^{\infty} \prod_q^{1/2} \mathrm{d}[x(q)] \, \mathrm{d}[y(q)] \exp\left(-\frac{1}{2} \int^{1/2} \mathrm{d}q \, (x^2(q) + y^2(q)) + \right.$$

$$\left. + \sum_i \ln Z_1 (F_i + h_i)\right), \tag{8}$$

with

$$F_i = \int^{1/2} (2 v(q))^{\frac{1}{2}} (x(q) \cos(q R_i) + y(q) \sin(q R_i)) \, \mathrm{d}q.$$

Until now we did not specify if the Fourier transform of the potential $v(q)$ or $\mathscr{V}(q)$ is either positive or negative. One should therefore allow for the possibility that the functions F_i contain both real and imaginary parts, $F_i = F_i' + i F_{i'}'$, whereas in the evaluation of the partition function only the real part of Z^0 appears, the contribution of the imaginary part being zero after integration. With this in mind the variables $x(q)$ and $y(q)$ could be rescaled with a factor $(|v(q)|)^2$. Introducing the complex functions $\sigma(q)$,

$$\sigma(q) = x(q) - iy(q), \quad \sigma(-q) = \sigma^{\star}(q),$$

expression (8) can be written in the form of a functional integral

$$Z = \frac{1}{\mathscr{N}} \int \left| \mathscr{D}[\sigma(q)] \right| \exp\left(- \frac{1}{2} \int \mathrm{d}q \, | v^{-1}(q) | \sigma(q) \sigma(-q) \right) \mathrm{Re} \prod_i Z_1 (F_i + h_i), \tag{9}$$

$$F_i = \int_{v(q)>0} \mathrm{d}q \, \mathrm{e}^{-iqR_i} \sigma(q) + \int_{v(q)>0} \mathrm{d}q \, \mathrm{e}^{-iqR_i} \sigma(q), \tag{9a}$$

$$\mathscr{N} = \int_{-\infty}^{\infty} \mathscr{D}[\sigma(q)] \exp\left(- \frac{1}{2} \int \mathrm{d}q \, | v^{-1}(q) | \sigma(q) \sigma(-q) \right). \tag{9b}$$

The functional integration runs over complex functions $\sigma(q)$, defined on that part of the momentum space over which the potential $V(R)$ is represented.

It is easy to change (9) — (9b) into expressions defined on the configuration space

$$\sigma(r) = \int \mathrm{d}q \mathrm{e}^{-iqr} \sigma(q), \qquad \sigma(q) = (2\pi)^{-d} \int \mathrm{d}r \mathrm{e}^{iqr} \sigma(r) \tag{10}$$

or

$$\sigma_i = \int_{q \in BZ} \mathrm{d}q \mathrm{e}^{-iqR_i} \sigma(q), \quad \sigma(q) = (2\pi)^{-d} \sum_{R_i} \mathrm{e}^{iqR_i} \sigma_i. \tag{11}$$

These functions are all real. In the case that the momentum integration in (10) extends only over the first Brillouin zone, the functions $\sigma(r)$ are specified as functions whose Fourier transform is zero outside the Brillouin zone. On using (10), the (9) — (9b) change into

$$Z = \frac{1}{\mathscr{N}} \int \mathscr{D}[\sigma(r)] \exp\left(- \frac{1}{2} (2\pi^{-}d \int \mathrm{d}r \, \mathrm{d}r' \, \sigma(r) \mathscr{K}(r - r') \sigma(r_j) \right) \cdot$$

$$\cdot \mathscr{R}e \prod_i Z_1 (F_i + h_i), \tag{12}$$

where

$$\mathcal{K}(r - r') = (2\pi)^{-d})\int dq\, e^{iq(r-r')}\,(r \,|\, v^{-1}(q)\,|, \tag{12a}$$

and

$$F_l = \int dr\,\sigma(r)\,((2\pi)^{-d} \int_{v(q)>0} dq e^{-iqR_l} + i\,(2\pi)^{-d} \int_{v(q)<0} dq e^{-iqR_l})\, e^{iqr}. \tag{12b}$$

In a special case, when the potential is short ranged and positive definite ($v(q) \sim a + bq^2$), the form (12) reduces after expansion in $\sigma(q)$ or $\sigma(r)$ to the Wilson model Hamiltonian. This has been already observed by Hubbard[3], taking different steps. The substitution (11) takes (9) into the standard functional form which was the starting point of Hubbard's work. One should also observe that the continuous limit, when the lattice spacing is going to zero, $S = 12$, and after expanding to second order in $\sigma(r)$, the expression (12) becomes identical to the partition function for the classical van der Waals gas[4)].

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DVE OBLIKI FAZNE VSOTE ISINGOVEGA MODELA

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Vsebina

S pomočjo Fourierove predstavitve dvodelčnega potenciala je v prispevku podan enostaven dokaz razvoja fazne vsote Isingovega modela v povezane gruče. Isto reprezentacijo je mogoče uporabiti tudi za izpeljavo fazne vsote kot funkcionalnega integrala. V primeru sil kratkega dosega sledi Wilsonov modelni hamiltonian.