WIPM Lectures on Models in Statistical Mechanics

Lecture 1: Integrability and Mathematical Techniques

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We shall first review two "integrability" criteria in statistical mechanics:

* One is the star-triangle equation, also known as the Yang-Baxter equation. This leads to Z-invariance and connects with Bethe Ansatz methods.

* The other is a generalization of Gaussian integration to fermionic or bosonic systems. This is used for Ising and Free-Fermion Models.

Remark: We shall not discuss in these lectures:

* Exactly solvable models with long-range interactions of mean-field type.

* Gaussian and spherical models solvable ordinary Gaussian integrals.

Technique 1: Yang–Baxter/Star-Triangle Equation

Yang–Baxter/Star-Triangle Equation History

1899 A.E. Kennelly: Electrical networks

1925 E. Artin: Braid group and knot theory

1926 K. Reidemeister: Reidemeister moves in knot theory

1944 L. Onsager: Critical point of Ising model on triangular lattice

1964 J.B. McGuire: Factorizable S-matrices

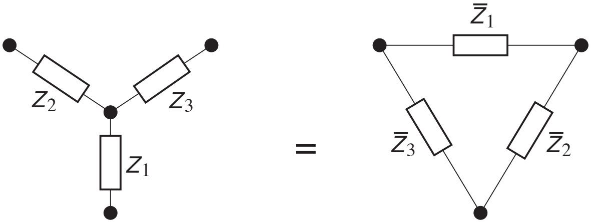
1967 C.N. Yang: Fermions with delta interaction and nested Bethe Ansatz

1971 R.J. Baxter: Eight-vertex model and commuting transfer matrices

1980 R.J. Baxter: Hard hexagon model and other IRF models

Star-Triangle Equation in Electric Networks

In 1899 the Brooklyn engineer A.E. Kennelly published a short paper, entitled *the equivalence of triangles and three-pointed stars in conducting networks* and published in: Electrical World and Engineer **34**, 413–414 (1899).



$$Z_1\overline{Z}_1 = Z_2\overline{Z}_2 = Z_3\overline{Z}_3 = \begin{cases} Z_1Z_2 + Z_2Z_3 + Z_3Z_1 \\ \overline{Z}_1\overline{Z}_2\overline{Z}_3/(\overline{Z}_1 + \overline{Z}_2 + \overline{Z}_3) \end{cases}$$

The *star-triangle transformation* is also known under other names within the electric network theory literature as wye-delta $(\mathrm{Y} - \Delta)$, upsilon-delta $(\Upsilon - \Delta)$, or tau-pi $(\mathrm{T} - \Pi)$ transformation.

As shown in the appendix of arXiv:math-phys/0606053, the solution can be parametrized by 'rapidities' p, q and r and 'normalization' c, for example by studying the $N \to 0$ limit of the critical N-state Potts model:

$$Z_1 = c\tan(p-q), \quad Z_2 = c\cot(p-r), \quad Z_3 = c\tan(q-r),$$
$$\overline{Z}_1 = c\cot(p-q), \quad \overline{Z}_2 = c\tan(p-r), \quad \overline{Z}_3 = c\cot(q-r).$$

The derivation uses Ohm's law ($V = \Delta\Phi = ZI$) and the two laws of Kirchhoff ($\sum I = 0$ at a node and $\sum V = 0$ in a loop). A simple derivation is to first assume that no current is fed into Z_1. Then it is just impedances (or resistors) in series and in parallel:

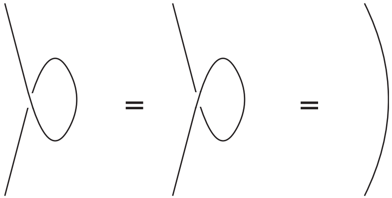
$$Z_2 + Z_3 = \frac{\overline{Z}_1(\overline{Z}_2 + \overline{Z}_3)}{\overline{Z}_1 + (\overline{Z}_2 + \overline{Z}_3)} = \frac{\overline{Z}_1\overline{Z}_2 + \overline{Z}_1\overline{Z}_3}{\overline{Z}_1 + \overline{Z}_2 + \overline{Z}_3}, \quad \text{and similarly}$$

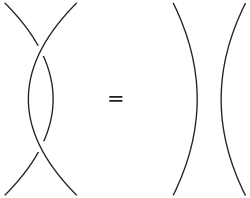
$$Z_1 + Z_2 = \frac{\overline{Z}_1\overline{Z}_3 + \overline{Z}_2\overline{Z}_3}{\overline{Z}_1 + \overline{Z}_2 + \overline{Z}_3}, \quad Z_1 + Z_3 = \frac{\overline{Z}_1\overline{Z}_2 + \overline{Z}_2\overline{Z}_3}{\overline{Z}_1 + \overline{Z}_2 + \overline{Z}_3}.$$

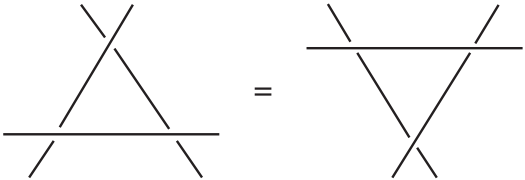
Adding the last two and subtracting the first, we get $Z_1 = \dfrac{\overline{Z}_2\overline{Z}_3}{\overline{Z}_1 + \overline{Z}_2 + \overline{Z}_3}$, etc.

Knot Theory and Braid Group

Reidemeister moves of type I, II, and III to undo a knot (1926):





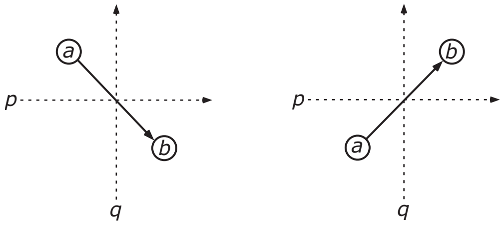


Star-Triangle Equation for Spin Models

Onsager—in his 1944 Ising model paper—made a brief remark on *an obvious star-triangle transformation* relating the model on the honeycomb lattice with the one on the triangular lattice.

Generalizing, we introduce a lattice with spins $a, b, \cdots = 1, \cdots, N$ on the lattice sites and with interactions between spins a and b given in terms of Boltzmann weight factors W_{ab} and $\overline{W}_{ab}$.

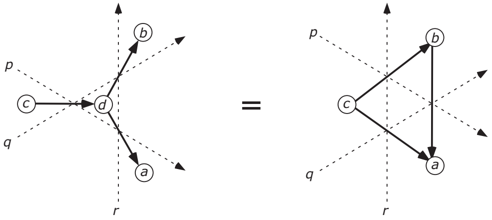
The *integrability* of the model is expressed by the existence of spectral variables (rapidities $p, q, r, \ldots$) that live on oriented lines, drawn dashed here. One can distinguish two kinds of pair interactions depending on the orientations of the spins w.r.t. the *rapidity lines.* Integrability requires that the weights satisfy:



W_{ab} $\overline{W}_{ab}$

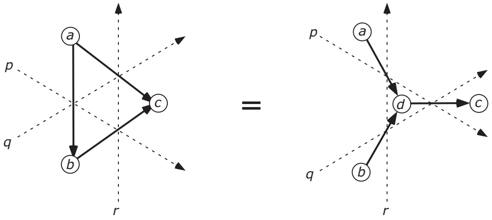
$$\sum_d \overline{W}_{cd}(p,q)\overline{W}_{db}(q,r)W_{da}(p,r)$$

$$= R(p,q,r)\, W_{ba}(p,q)W_{ca}(q,r)\overline{W}_{cb}(p,r)$$

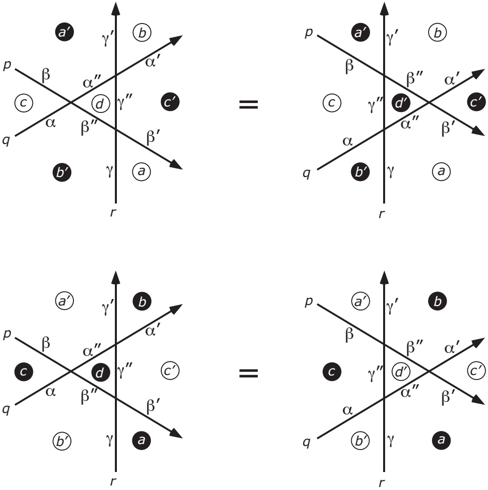


$$\overline{R}(p,q,r)\, W_{ab}(p,q)W_{ac}(q,r)\overline{W}_{bc}(p,r)$$

$$= \sum_d \overline{W}_{dc}(p,q)\overline{W}_{bd}(q,r)W_{ad}(p,r)$$



The two equations differ by the transposition of both spin variables in all six weight factors. In general there are scalar factors $R(p,q,r)$ and $\overline{R}(p,q,r)$, which can often be eliminated by a suitable renormalization of the weights.



Generalizations:

The most general Yang–Baxter Equation has spin variables on the line segments of the rapidity lines and on the faces cut out by them, with faces alternatingly colored black and white.

If the spin variables only on all faces, one has an IRF model.

If the spin variables only live on rapidity lines, one has a vertex model.

JHHP & HAY, *Yang–Baxter Equation*, in *Encyclopedia of Mathematical Physics*, eds. J.-P. Françoise, G.L. Naber and Tsou S.T., Oxford: Elsevier, 2006, Vol. 5, pp. 465–473. See also arXiv:math-ph/0606053.

Partition Function, Free Energy and Correlation Function

The partition function is the sum of the Boltzmann weight over all state variables (spins) σ; the Boltzmann weight is here a product of the weight factors for each vertex ℓ (intersection of a pair of rapidity lines) depending on the spin values $\{\sigma\}_\ell$ around that vertex:

$$Z = \sum_{\text{spins } \{\sigma\}} \mathrm{e}^{-\mathcal{E}(\{\sigma\})/k_{\mathrm{B}}T} = \sum_{\text{spins } \{\sigma\}} \prod_{\text{vertices } \ell} W_\ell(\{\sigma\}_\ell)\,.$$

This provides the normalization for the probability distribution.

The free energy is defined by $F = -k_{\mathrm{B}}T \ln Z$.

The correlation function of n spins $\sigma_1, \sigma_2, \ldots, \sigma_n$ at positions $x_1, x_2, \ldots, x_n$ is

$$\langle \sigma_1 \sigma_2 \cdots \sigma_n \rangle = \frac{1}{Z} \sum_{\text{spins } \{\sigma\}} \prod_{\text{vertices } \ell} W_\ell(\{\sigma\}_\ell)\, \sigma_1 \sigma_2 \cdots \sigma_n\,.$$

Implications of Star-Triangle/Yang–Baxter Equation

- The partition function Z and the free energy are invariant under moving of rapidity lines. Baxter calls this Z-invariance.

- The order parameters (one-point correlation functions) cannot depend on the rapidity variables, as one can move all rapidity lines "to infinity" and move other ones with different values of the rapidity variables in. They can only depend on "moduli"—variables that are common to all rapidity lines.

- Pair correlation functions can only depend on rapidity variables of rapidity lines crossing between the two spins under consideration and the moduli.

- Integrable quantum chain hamiltonians can be found to be logarithmic derivatives of commuting transfer matrices of two-dimensional classical spin models.

Technique 2: Fermionic/Bosonic Gaussian Integration

Ising/Free-Fermion Family of Models

There are two main approaches to such classical 2-dimensional models:

2D: Treat both directions equivalently. One translates the problem into a loop model, or a dimer problem, or an integral over Grassmann (anticommuting) variables, or some other related representation. One usually ends up with Pfaffians.

1D: Building up the two-dimensional model one row (or one column) at a time, using a transfer matrix method. Then, in the simplest case of a uniform lattice model with periodic boundary conditions, $Z = \mathrm{Tr}\, \mathsf{T}^N$, with T the transfer matrix.

This approach usually ends up using Clifford algebra, or equivalently fermion creation and annihilation operators, followed by diagonalizing the transfer matrix or applying a Wick theorem leading to Pfaffians.

We shall use this method as quantum spin chain Hamiltonians may can often be derived directly from the transfer matrix. We then have one approach for the classical 2D and quantum 1D cases.

Quadratic Identity for Gaussian Integrals

The second integrability principle is a generalization of Gaussian integration. One can double the space and then employ rotational symmetry as in:

$$I \equiv \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \mathrm{d}x, \quad I_{2n} \equiv \int_{-\infty}^{\infty} x^{2n} \mathrm{e}^{-x^2} \mathrm{d}x \qquad \Longrightarrow$$

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-(x^2+y^2)} \mathrm{d}x \, \mathrm{d}y = \int_0^{2\pi} \int_0^{\infty} \mathrm{e}^{-r^2} r \mathrm{d}r \, \mathrm{d}\theta = \pi \,,$$

$$\begin{aligned} I \, I_{2n} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^{2n} \mathrm{e}^{-(x^2+y^2)} \mathrm{d}x \, \mathrm{d}y \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x \cos\theta + y \sin\theta)^{2n} \mathrm{e}^{-(x^2+y^2)} \mathrm{d}x \, \mathrm{d}y \,. \end{aligned}$$

Maclaurin at order θ^2 then gives

$$0 = -\frac{1}{2} \, 2n \, I \, I_{2n} + \frac{2n(2n-1)}{2} \, I_2 \, I_{2n-2} \qquad \Longrightarrow \qquad I \, I_{2n} = (2n-1) \, I_2 \, I_{2n-2} \,.$$

Generalizations of the Wick Theorem

(Details on following pages)

Applying this idea to bosonic or fermionic quantum systems, one can derive generalizations of the Wick theorem as Ward identities under rotations in the doubled space, e.g.

$$\begin{aligned}
&\mathrm{Tr}(Q_1Q_2Q_3Q_4)\,\mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2\Gamma_3Q_3\Gamma_4Q_4)\\
&\quad= \mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2Q_3Q_4)\,\mathrm{Tr}(Q_1Q_2\Gamma_3Q_3\Gamma_4Q_4)\\
&\qquad\pm \mathrm{Tr}(\Gamma_1Q_1Q_2\Gamma_3Q_3Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2Q_3\Gamma_4Q_4)\\
&\qquad+ \mathrm{Tr}(\Gamma_1Q_1Q_2Q_3\Gamma_4Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2\Gamma_3Q_3Q_4)
\end{aligned}$$

with $+$ for bosons and $-$ for fermions. The Γ's are linear combinations of creation and annihilation operators. The Q's are products of factors that are either exponentials of quadratic forms or linear expressions.

More general, using traces with $2n$ Γ's, $(n = 2, 3, \ldots)$, one gets recurrence relations determining Hafnians or Pfaffians.

JHHP, Phys. Lett. A **79** (1980) 1–5, JHHP et al., Physica A **123** (1984) 1–49.

Let us do the fermionic case only here and begin with the Pauli matrices:

$$\sigma^x \equiv \sigma^1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y \equiv \sigma^2 \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma^z \equiv \sigma^3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$\mathrm{i} \equiv \sqrt{-1}$. These matrices anticommute and are both unitary and hermitian:

$$\sigma^k \sigma^l = -\sigma^l \sigma^k, \text{ for } k \neq l, \qquad \sigma^k = (\sigma^k)^\dagger = (\sigma^k)^{-1}, \qquad (\sigma^k)^2 = \mathbf{1} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

These Pauli matrices act on a two-dimensional space with basis vectors

$$|+\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

One may say, we have a spin-$\frac{1}{2}$ object on the given site.

(Many of you may also remember $\sigma^k \sigma^l = \delta_{kl} \mathbf{1} + \mathrm{i}\, \varepsilon_{klm} \sigma^m$ with $k, l = 1, 2, 3$, with $\sum_{m=1}^{3}$ implied by the Einstein summation convention, with Kronecker delta $\delta_{kl} = 1$ if $k = l$, but $= 0$ if $k \neq l$, and with the completely antisymmetric Levi-Civita symbol ε_{klm}, $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$, $\varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1$ and $\varepsilon_{klm} = 0$ otherwise by antisymmetry if two or three subscripts are equal.)

Next we want L independent copies, with one for each 'site' j:

$$\sigma_j^x := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \overbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}^{j\text{-th}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\sigma_j^y := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\sigma_j^z := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

This has been achieved using the Kronecker product, for example,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} p & q \\ r & s \end{pmatrix} = \begin{pmatrix} a\begin{pmatrix} p & q \\ r & s \end{pmatrix} & b\begin{pmatrix} p & q \\ r & s \end{pmatrix} \\ c\begin{pmatrix} p & q \\ r & s \end{pmatrix} & d\begin{pmatrix} p & q \\ r & s \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ap & aq & bp & bq \\ ar & as & br & bs \\ cp & cq & dp & dq \\ cr & cs & dr & ds \end{pmatrix},$$

with the property $(\mathsf{A} \otimes \mathsf{B})(\mathsf{C} \otimes \mathsf{D}) = \mathsf{AC} \otimes \mathsf{BD}$. For repeated Kronecker products, $\mathsf{A} \otimes \mathsf{B} \otimes \mathsf{C} \otimes \cdots \otimes \mathsf{Z}$, one uses the obvious generalization of the example.

We still have not represented any fermion operators, as the operators defined commute if they act on different sites, but anticommute on the same site.

$$[\sigma_j^k, \sigma_{j'}^l] = 2\,\mathrm{i}\,\varepsilon_{klm}\sigma_j^m\,\delta_{j,j'} = 0, \text{ if } j \neq j', \qquad \{\sigma_j^k, \sigma_j^l\} = 2\delta_{kl}\mathbf{1},$$

with $\mathbf{1}$ the 2^L-dimensional identity matrix and with the standard notations,

$$\begin{cases} [\,\mathsf{A},\mathsf{B}\,] \equiv [\mathsf{A},\mathsf{B}]_- \equiv \mathsf{AB}-\mathsf{BA}, & \text{for the commutator,} \\ \{\mathsf{A},\mathsf{B}\} \equiv [\mathsf{A},\mathsf{B}]_+ \equiv \mathsf{AB}+\mathsf{BA}, & \text{for the anticommutator.} \end{cases}$$

Such mixed commutation rules are very unpleasant in further calculations, but fortunately Jordan and Wigner [Z. Phys. **47**, 631 (1928)] have shown that we can choose commutation or anticommutation at will for operators on different positions. Also, much credit has to go to Brauer and Weyl [Am. J. Math. **57**, 425 (1935)] and Bruria Kaufman [Phys. Rev. **76**, 1232 (1949)].

$\Longrightarrow$ We can change to fermion operators by the Jordan–Wigner transformation:

We define the Jordan–Wigner transform by

$$\Gamma_{2j-1} = \left[\prod_{k=1}^{j-1}(-\sigma_k^z)\right]\sigma_j^x, \qquad \Gamma_{2j} = \left[\prod_{k=1}^{j-1}(-\sigma_k^z)\right]\sigma_j^y,$$

and its inverse is given by

$$\sigma_j^x = \left[\prod_{k=1}^{j-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2j-1}, \quad \sigma_j^y = \left[\prod_{k=1}^{j-1}(\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right]\Gamma_{2j}, \quad \sigma_j^z = -\mathrm{i}\,\Gamma_{2j-1}\Gamma_{2j}.$$

One can easily check that these Γ operators are hermitian and unitary and (as good fermion operators) they anticommute,

$$\{\Gamma_p, \Gamma_q\} = 2\delta_{pq}\mathbf{1}.$$

They are generators of a Clifford algebra. From them we can get fermion creation and annihilation operators,

$$a_j^\dagger = \frac{1}{2}(\Gamma_{2j-1} + \mathrm{i}\,\Gamma_{2j}), \qquad a_j = \frac{1}{2}(\Gamma_{2j-1} - \mathrm{i}\,\Gamma_{2j}),$$

with anticommutation relations $\{a_p, a_q\} = 0, \quad \{a_p^\dagger, a_q^\dagger\} = 0, \quad \{a_p, a_q^\dagger\} = \delta_{pq}.$

One can make other rather arbitrary linear combinations of the Γ-matrices with modified anticommutation relations $\{\gamma_p, \gamma_q\} = g_{pq}\mathbf{1}$, where g_{pq} are elements of a $2L$-by-$2L$ symmetric matrix. One choice is $\gamma_p = \Gamma_p/\sqrt{2}$, so that $g_{pq} = \delta_{pq}\mathbf{1}$, as is done in some of my papers, another we just saw is $\gamma_{2j-1} = a_j^\dagger$, $\gamma_{2j} = a_j$.

To derive the general Wick theorem, we need to double the number of fermion operators using Jordan–Wigner again:

$$\Gamma_p^x = \Gamma_p \otimes \mathbf{1}, \qquad \Gamma_p^y = \left[\prod_{k=1}^{L} (\mathrm{i}\,\Gamma_{2k-1}\Gamma_{2k})\right] \otimes \Gamma_p, \qquad (p = 1, \cdots, 2L),$$

so that, writing $\mathbf{1}$ also for $\mathbf{1} \otimes \mathbf{1}$,

$$\{\Gamma_p^i, \Gamma_q^j\} = 2\delta_{ij}\delta_{pq}\mathbf{1}, \qquad i, j = x \text{ or } y, \quad p, q = 1, \cdots, 2L.$$

We also must find a generalization of rotations in the x-y plane. We note that both the trace and the fermion anticommutation relations are invariant under similarity transform,

$$\mathrm{Tr}\,\mathsf{SAS}^{-1} = \mathrm{Tr}\,\mathsf{A}, \qquad \{\mathsf{S}\Gamma_p^i\mathsf{S}^{-1}, \mathsf{S}\Gamma_q^j\mathsf{S}^{-1}\} = \mathsf{S}\{\Gamma_p^i, \Gamma_q^j\}\mathsf{S}^{-1} = 2\delta_{ij}\delta_{pq}\mathbf{1}.$$

Let us try

$$\mathsf{S} = \exp\left[\frac{1}{2}\theta\sum_{q=1}^{2L}\Gamma_q^x\Gamma_q^y\right] = \prod_{q=1}^{2L} \mathrm{e}^{\frac{1}{2}\theta\Gamma_q^x\Gamma_q^y}.$$

Then

$$\mathsf{S}\Gamma_p^x\mathsf{S}^{-1} = \mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^x\,\mathrm{e}^{-\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y} = \mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^x = \mathrm{e}^{\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^x,$$

$$\mathsf{S}\Gamma_p^y\mathsf{S}^{-1} = \mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^y\,\mathrm{e}^{-\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y} = \mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\mathrm{e}^{\frac{1}{2}\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^y = \mathrm{e}^{\theta\Gamma_p^x\Gamma_p^y}\,\Gamma_p^y,$$

so that, as $(\Gamma_p^x\Gamma_p^y)^2 = -(\Gamma_p^x)^2(\Gamma_p^y)^2 = -\mathbf{1}$,

$$\mathsf{S}\Gamma_p^x\mathsf{S}^{-1} = (\mathbf{1}\cos\theta + \Gamma_p^x\Gamma_p^y\sin\theta)\Gamma_p^x = \Gamma_p^x\cos\theta - \Gamma_p^y\sin\theta,$$

$$\mathsf{S}\Gamma_p^y\mathsf{S}^{-1} = (\mathbf{1}\cos\theta + \Gamma_p^x\Gamma_p^y\sin\theta)\Gamma_p^y = \Gamma_p^x\sin\theta + \Gamma_p^y\cos\theta,$$

representing a rotation over θ in the x-y plane:

$$\mathsf{S}\begin{pmatrix}\Gamma^x_p\\ \Gamma^y_p\end{pmatrix}\mathsf{S}^{-1}=\begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\Gamma^x_p\\ \Gamma^y_p\end{pmatrix},$$

from which one easily finds

$$\mathsf{S}(\Gamma^x_p\Gamma^x_q+\Gamma^y_p\Gamma^y_q)\mathsf{S}^{-1}=\Gamma^x_p\Gamma^x_q+\Gamma^y_p\Gamma^y_q,\qquad \mathsf{S}\,\Gamma^x_p\Gamma^y_p\,\mathsf{S}^{-1}=\Gamma^x_p\Gamma^y_p,$$

which classically corresponds to the rotational invariance of the inner product and the invariance of the cross product under rotations with axis perpendicular to the plane of the two vectors.

More generally,

$$\exp\left[\sum_{p=1}^{2L}\sum_{q=1}^{2L}A_{pq}(\Gamma^x_p\Gamma^x_q+\Gamma^y_p\Gamma^y_q)\right]=\exp\left[\sum_{p=1}^{2L}\sum_{q=1}^{2L}A_{pq}\Gamma^x_p\Gamma^x_q\right]\exp\left[\sum_{p=1}^{2L}\sum_{q=1}^{2L}A_{pq}\Gamma^y_p\Gamma^y_q\right]$$

$$\text{and}\qquad \left(\sum_{p=1}^{2L}\lambda_p\Gamma^x_p\right)\left(\sum_{p=1}^{2L}\lambda_p\Gamma^y_p\right)$$

are also invariant.

We are now in a position to derive a general Wick theorem for

$$\operatorname{Tr}\prod_{k=1}^{2s} Q_k \Gamma_{p_k}, \quad Q_k \equiv \prod_{\nu=1}^{r_k}\left[\exp\left(\sum_{p=1}^{2L}\sum_{q=1}^{2L} A_{pq}^{(k\nu)}\Gamma_p\Gamma_q\right)\prod_{\mu=1}^{S_{k\nu}}\left(\sum_{q=1}^{2L}\lambda_q^{(k\nu\mu)}\Gamma_q\right)\right],$$

with $\sum_k \sum_\nu S_{k\nu} = \text{even}$, so that the trace does not automatically vanish because it would change sign under $\Gamma_p \to -\Gamma_p$ for all $p = 1, \ldots, 2L$. When $S_{k\nu} = 0$, the corresponding product over μ equals 1. ($\Gamma_p\Gamma_q = \exp(\frac{1}{2}\pi\Gamma_p\Gamma_q)$ is also Gaussian.) Next we introduce Q_k^x to be Q_k with all Γ_p replaced by Γ_p^x and Q_k^y with each Γ_p replaced by Γ_p^y. It is easily checked that $Q_k^x Q_k^y$ is invariant under the rotations. Also, the space on which the Γ_p act is 2^L-dimensional, whereas the space on which the Γ_p^x and Γ_p^y act is 2^{2L}-dimensional. So,

$$\operatorname{Tr}\prod_{k=1}^{2s} Q_k^x \Gamma_{p_k}^x = 2^L \operatorname{Tr}\prod_{k=1}^{2s} Q_k \Gamma_{p_k}, \quad \operatorname{Tr}\prod_{k=1}^{2s} Q_k^y = 2^L \operatorname{Tr}\prod_{k=1}^{2s} Q_k,$$

and

$$\operatorname{Tr}\prod_{k=1}^{2s} Q_k^x Q_k^y \Gamma_{p_k}^x = \pm \operatorname{Tr}\left[\prod_{k=1}^{2s} Q_k^x \Gamma_{p_k}^x \prod_{k=1}^{2s} Q_k^y\right] = \pm\left(\operatorname{Tr}\prod_{k=1}^{2s} Q_k \Gamma_{p_k}\right)\left(\operatorname{Tr}\prod_{k=1}^{2s} Q_k\right).$$

But by rotational invariance,

$$\operatorname{Tr} \prod_{k=1}^{2s} Q_k^x Q_k^y \Gamma_{p_k}^x = \operatorname{Tr} \prod_{k=1}^{2s} Q_k^x Q_k^y (\Gamma_{p_k}^x \cos\theta - \Gamma_{p_k}^y \sin\theta).$$

Taking the second derivative in θ at $\theta = 0$, we get

$$\begin{aligned} 0 &= -2s \operatorname{Tr} \prod_{k=1}^{2s} Q_k^x Q_k^y \Gamma_{p_k}^x \\ &- 2 \sum\sum_{1 \leqslant k < l \leqslant 2s} \operatorname{Tr} \Big[\prod_{i<k} Q_i^x Q_i^y \Gamma_{p_i}^x \Big] Q_k^x Q_k^y \Gamma_{p_k}^y \Big[\prod_{k<i<l} Q_i^x Q_i^y \Gamma_{p_i}^x \Big] Q_l^x Q_l^y \Gamma_{p_l}^y \Big[\prod_{i>l} Q_i^x Q_i^y \Gamma_{p_i}^x \Big]. \end{aligned}$$

We can now move all the y-operators to the right of the x-operators in each trace and then factor the traces as products of traces over x-space or y-space.

The factors $\prod_j (\mathrm{i}\Gamma_{2j-1}\Gamma_{2j-1}) \otimes \mathbf{1}$ introduced by the Jordan–Wigner trick in the y-operators commute through and cancel out completely, as $\sum_k \sum_\nu S_{k\nu} =$ even.

Therefore, keeping track of minus signs from anticommutations,

$$
\begin{aligned}
&\left[\mathrm{Tr}\prod_{k=1}^{2s} Q_k\Gamma_p\right]\left[\mathrm{Tr}\prod_{k=1}^{2s} Q_k\right] \\
&\quad = \frac{1}{s}\sum\sum_{1\leqslant k<l\leqslant 2s}(-1)^{k+l-1}\left[\mathrm{Tr}\Big(\prod_{i<k}Q_i\Gamma_{p_i}\Big)Q_k\Big(\prod_{k<i<l}Q_i\Gamma_{p_i}\Big)Q_l\Big(\prod_{i>l}Q_i\Gamma_{p_i}\Big)\right] \\
&\qquad \times\left[\mathrm{Tr}\Big(\prod_{i<k}Q_i\Big)Q_k\Gamma_{p_k}\Big(\prod_{k<i<l}Q_i\Big)Q_l\Gamma_{p_l}\Big(\prod_{i>l}Q_i\Big)\right], \quad s=1,2,\cdots.
\end{aligned}
$$

For $s=1$ this is trivially satisfied. For $s=2$ we obtain the earlier announced

$$
\begin{aligned}
&\mathrm{Tr}(Q_1Q_2Q_3Q_4)\,\mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2\Gamma_3Q_3\Gamma_4Q_4) \\
&\quad = \mathrm{Tr}(\Gamma_1Q_1\Gamma_2Q_2Q_3Q_4)\,\mathrm{Tr}(Q_1Q_2\Gamma_3Q_3\Gamma_4Q_4) \\
&\qquad - \mathrm{Tr}(\Gamma_1Q_1Q_2\Gamma_3Q_3Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2Q_3\Gamma_4Q_4) \\
&\qquad + \mathrm{Tr}(\Gamma_1Q_1Q_2Q_3\Gamma_4Q_4)\,\mathrm{Tr}(Q_1\Gamma_2Q_2\Gamma_3Q_3Q_4),
\end{aligned}
$$

with $\Gamma_1,\Gamma_2,\Gamma_3,\Gamma_4$ any four linear combinations of the fermion operators Γ_p. For $s>2$ we recognize the recurrence relation for a Pfaffian, as we shall discuss next.

Pfaffians

Start with the determinant of an antisymmetric 4-by-4 matrix:

$$\begin{vmatrix} 0 & X_{12} & X_{13} & X_{14} \\ -X_{12} & 0 & X_{23} & X_{24} \\ -X_{13} & -X_{23} & 0 & X_{34} \\ -X_{14} & -X_{24} & -X_{34} & 0 \end{vmatrix} = (X_{12}X_{34} - X_{13}X_{24} + X_{14}X_{23})^2.$$

It factors as a complete square and the repeated factor can be denoted by the Pfaffian of the triangular array

$$\begin{vmatrix} X_{12} & X_{13} & X_{14} \\ & X_{23} & X_{24} \\ & & X_{34} \end{vmatrix} = X_{12}X_{34} - X_{13}X_{24} + X_{14}X_{23}\,,$$

which has the same structure as the result for $s = 2$ that we just derived. That more generally the determinant of an even-size antisymmetric matrix is the square of a Pfaffian was first shown by A. Cayley [J. reine angew. Math. **38**, 93–96 (1849)]:

$$\det \mathsf{A} = (\mathrm{Pf}\,\mathsf{A})^2, \quad \text{if } \mathsf{A}^{\mathrm{T}} = -\mathsf{A},$$

while $\det \mathsf{A} = 0$ and $\mathrm{Pf}\,\mathsf{A}$ is not defined for odd-size A.

Let A be a $2s$-by-$2s$ antisymmetric matrix, $\mathsf{A}^{\mathrm{T}} = -\mathsf{A}$. Then its determinant is defined as

$$\det \mathsf{A} \equiv \sum_{\mathrm{P}} (-1)^{\mathrm{P}} \prod_{i=1}^{2s} A_{i,\mathrm{P}i},$$

where the sum is over all permutations P of $\{1, 2, \cdots, 2s\}$, so that $i \to \mathrm{P}i$, and $(-1)^{\mathrm{P}}$ is the sign of the permutation, that is $+1$ if P can be written as an even product of pair interchanges and -1 if that requires an odd product.

The Pfaffian of A is defined as

$$\mathrm{Pf}\,\mathsf{A} \equiv \frac{1}{2^s s!} \sum_{\mathrm{P}} (-1)^{\mathrm{P}} \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)} = {\sum_{\mathrm{P}}}' (-1)^{\mathrm{P}} \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)},$$

where the second sum with prime is restricted to ordered permutations:

$$\mathrm{P}(2i-1) < \mathrm{P}(2i) \quad \text{and} \quad \mathrm{P}(2i-1) < \mathrm{P}(2i+1) \quad \text{for } {\sum_{\mathrm{P}}}'.$$

There are $s!$ ways to permute the pairs and 2^s ways to change the order within the pairs. Thus the Pfaffian has $(2s)!/(2^s s!) = (2s-1)!! \equiv (2s-1)(2s-3)\cdots 3\cdot 1$ terms.

Remark: For the bosonic case we have to replace $(-1)^{\mathrm{P}}$ by $+1$ and define the permanent and Hafnian of symmetric matrix A with zero diagonal:

$$\mathrm{per}\,\mathsf{A} \equiv \sum_{\mathrm{P}} \prod_{i=1}^{2s} A_{i,\mathrm{P}i}\,, \qquad \mathrm{Hf}\,\mathsf{A} \equiv \sum_{\mathrm{P}}{}' \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)}.$$

For $s=2$ we have

$$\mathrm{per}\begin{pmatrix} 0 & X_{12} & X_{13} & X_{14} \\ X_{12} & 0 & X_{23} & X_{24} \\ X_{13} & X_{23} & 0 & X_{34} \\ X_{14} & X_{24} & X_{34} & 0 \end{pmatrix} = (X_{12}X_{34} + X_{13}X_{24} + X_{14}X_{23})^2,$$

$$\mathrm{Hf}\left\{\begin{matrix} X_{12} & X_{13} & X_{14} \\ & X_{23} & X_{24} \\ & & X_{34} \end{matrix}\right\} = X_{12}X_{34} + X_{13}X_{24} + X_{14}X_{23}\,,$$

but this does not generalize, as $\mathrm{per}\,\mathsf{A} \neq (\mathrm{Hf}\,\mathsf{A})^2$ for $s > 2$.

Properties of Pfaffians

So far we have encountered

$$\boxed{\det \mathsf{A} = (\mathrm{Pf}\,\mathsf{A})^2 \quad \text{for antisymmetric } \mathsf{A}},$$

which we shall not prove here.*

Also, from the definitions we immediately have the antisymmetry properties

$$\det(\{A_{\mathrm{P}i,j}\}) = \det(\{A_{i,\mathrm{P}i}\}) = (-1)^{\mathrm{P}} \det \mathsf{A}, \qquad \mathrm{Pf}(\{A_{\mathrm{P}i,\mathrm{P}j}\}) = (-1)^{\mathrm{P}} \mathrm{Pf}\,\mathsf{A}.$$

Another identity we need is a recurrence relation for expanding the Pfaffian.

---

* A modern English version of Cayley's proof can be found in chapter 7 of the book 'Algebraic Combinatorics' by C.D. Godsil (Chapman and Hall, New York, 1993). A very different proof is given in section 2 of chapter IV of 'The Two Dimensional Ising Model' by B.M. McCoy and T.T. Wu (Harvard Univ. Press, Cambridge, Mass., 1973).

Remember:

$$\mathsf{Pf\,A} = \sum_{\substack{\mathrm{P} \\ \mathrm{P}(2i-1)<\mathrm{P}(2i) \\ \mathrm{P}(2i-1)<\mathrm{P}(2i+1)}}{}' (-1)^{\mathrm{P}} \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)}.$$

From the conditions we know $\mathrm{P}1 = 1$ and $\mathrm{P}2 = j$, with $2 \leqslant j \leqslant 2s$. To move j to position 2 it has to interchange position with $j-1, j-2, \cdots, 3$ in that order, which takes $j-2$ interchanges that together make up permutation P_j. Permutation P can be seen as the product $\mathrm{P}'\mathrm{P}_j$, with the permutation P' ordering the $2s-2$ indices that remain after taking out 1 and j. It follows that

$$\mathsf{Pf\,A} = \sum_{j=2}^{2s} (-1)^j A_{1j} \sum_{\mathrm{P}'}{}' (-1)^{\mathrm{P}'} \prod_{i=1}^{s-1} A_{\mathrm{P}'k_{2i-1},\mathrm{P}'k_{2i}}\,, \qquad (-1)^{\mathrm{P}} = (-1)^{j-2}(-1)^{\mathrm{P}'}.$$

with $[k_1, k_2, \cdots, k_{2s-2}] = [2, 3, \cdots, j-1, j+1, \cdots, 2s]$. Note that the restricted sum over P' is the Pfaffian of triangular array (taking only the part above the principal diagonal from the corresponding antisymmetric matrix, so that column 1 of the triangular array is the second column of the matrix) $\mathsf{A}[1, j]$ obtained after deleting all rows and columns with indices 1 and/or j from A.

Therefore,

$$\boxed{\mathsf{Pf\,A} = \sum_{j=2}^{2s} (-1)^j A_{1j}\, \mathsf{Pf\,A}[1,j]}.$$

More generally, we may want to choose $\mathrm{P}1 = l$ and $\mathrm{P}2 = m > l$ in

$$\mathsf{Pf\,A} = \sum_{\substack{\mathrm{P} \\ \mathrm{P}(2i-1)<\mathrm{P}(2i) \\ \mathrm{P}(2i-1)<\mathrm{P}(2i+1)}}{}' (-1)^{\mathrm{P}} \prod_{i=1}^{s} A_{\mathrm{P}(2i-1),\mathrm{P}(2i)}.$$

To move l up to position 1 and m to position 2 takes $(l-1)+(m-2)$ pair interchanges. Thus we find

$$\boxed{\mathsf{Pf\,A} = \frac{1}{s} \sum\sum_{1\leqslant l<m\leqslant 2s} (-1)^{l+m-1} A_{lm}\, \mathsf{Pf\,A}[l,m]},$$

with triangular array $\mathsf{A}[l,m]$ obtained by deleting rows and columns l and m from A. The factor $1/s$ is needed, as the double sum has $\frac{1}{2}(2s)(2s-1) = s(2s-1)$ terms, where as the above sum over j has $2s-1$ terms. All three expressions here for $\mathsf{Pf\,A}$ are fully antisymmetric and have $(2s-1)!!$ terms when worked out.

Now rewrite our recurrence

$$\left[\mathrm{Tr}\prod_{k=1}^{2s} Q_k\Gamma_p\right]\left[\mathrm{Tr}\prod_{k=1}^{2s} Q_k\right]$$

$$= \frac{1}{s}\sum\sum_{1\leqslant k<l\leqslant 2s}(-1)^{k+l-1}\left[\mathrm{Tr}\left(\prod_{i<k} Q_i\Gamma_{p_i}\right)Q_k\left(\prod_{k<i<l} Q_i\Gamma_{p_i}\right)Q_l\left(\prod_{i>l} Q_i\Gamma_{p_i}\right)\right]$$
$$\times\left[\mathrm{Tr}\left(\prod_{i<k} Q_i\right)Q_k\Gamma_{p_k}\left(\prod_{k<i<l} Q_i\right)Q_l\Gamma_{p_l}\left(\prod_{i>l} Q_i\right)\right], \quad s = 1, 2, \cdots.$$

as

$$\left\langle\prod_{k=1}^{2s} Q_k\Gamma_p\right\rangle = \frac{1}{s}\sum\sum_{1\leqslant k<l\leqslant 2s}(-1)^{k+l-1}\left\langle\left(\prod_{i<k} Q_i\Gamma_{p_i}\right)Q_k\left(\prod_{k<i<l} Q_i\Gamma_{p_i}\right)Q_l\left(\prod_{i>l} Q_i\Gamma_{p_i}\right)\right\rangle$$
$$\times\left\langle\left(\prod_{i<k} Q_i\right)Q_k\Gamma_{p_k}\left(\prod_{k<i<l} Q_i\right)Q_l\Gamma_{p_l}\left(\prod_{i>l} Q_i\right)\right\rangle, \quad s = 1, 2, \cdots,$$

using the definition

$$\langle O\rangle \equiv \frac{\mathrm{Tr}\, O}{\mathrm{Tr}\prod_{k=1}^{2s} Q_k}.$$

This has exactly the form of the last recurrence relation for Pfaffians. Therefore, defining the triangular array A by

$$A_{kl} = \left\langle \left(\prod_{i<k} Q_i \right) Q_k \Gamma_{p_k} \left(\prod_{k<i<l} Q_i \right) Q_l \Gamma_{p_l} \left(\prod_{i>l} Q_i \right) \right\rangle \qquad \text{for } 1 \leqslant k < l \leqslant 2s,$$

we have proved

$$\left\langle \prod_{k=1}^{2s} Q_k \Gamma_p \right\rangle = \mathrm{Pf}\, \mathsf{A}\,,$$

or

$$\boxed{\frac{\mathrm{Tr} \prod_{k=1}^{2s} Q_k \Gamma_{p_k}}{\mathrm{Tr} \prod_{k=1}^{2s} Q_k} = \mathop{\mathrm{Pf}}_{1 \leqslant k < l \leqslant 2s} \left\{ \frac{\mathrm{Tr} \left(\prod_{i<k} Q_i \right) Q_k \Gamma_{p_k} \left(\prod_{k<i<l} Q_i \right) Q_l \Gamma_{p_l} \left(\prod_{i>l} Q_i \right)}{\mathrm{Tr} \prod_{k=1}^{2s} Q_k} \right\}},$$

which is our general Wick theorem [Physica A **123**, 1–49 (1984), see section 3], generalizing various thermodynamic Wick theorems.

Remark: Compound Pfaffians

If we introduce the notation

$$\mathrm{Pf}(\mathsf{S}) \equiv \mathop{\mathrm{Pf}}_{\substack{\{i,j\}\subset \mathsf{S} \\ i<j}} (\{A_{ij}\}),$$

with S an index set and A a triangular array, then the general Wick theorem can be seen to be equivalent with

$$\boxed{\frac{\mathrm{Pf}(S_1 \cup S_2)}{\mathrm{Pf}(S_2)} = \mathop{\mathrm{Pf}}_{\{i,j\}\subset S_1} \left(\left\{ \frac{\mathrm{Pf}(\{i,j\} \cup S_2)}{\mathrm{Pf}(S_2)} \right\} \right)}.$$

This is a compound Pfaffian theorem : A Pfaffian of Pfaffians is a Pfaffian.

Though not widely known, this version is particularly useful in approaches to Ising-class models when one does not use operator techniques.