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Theoretical Tools for Spin Models in Magnetic Systems

Antonio Sergio Teixeira Pires

Appendix A

Group theory

A group G is a set of elements $g_1, g_2, ...,$ and a rule for combining (multiplying) any two elements to form a 'product', subject to the following properties:

- 1. The product $g_i g_i$ of any two group elements must be a group element.
- 2. Group multiplication is associative: $(g_ig_i)g_k = g_i(g_ig_k)$.
- 3. There is a unique group element $g_I = I$, called the *identity*, such that
- $Ig_I = g_I I = g_I$ for all $g_i \in G$. 4. Each element has a unique inverse; that is, for each g_i there is a unique group element g_i^{-1} such that $g_i g_i^{-1} = g_i^{-1} g_i = I$.

A *finite group* is a group with a finite number of elements. If $g_i g_j = g_j g_i$ for every pair of elements in the group, it is called an Abelian group.

The group \mathbb{Z}_2 is a group with two elements *e* and *x* such that ex = xe = x and $e^2 = x^2 = e$. An example is the multiplicative group comprising 1 and -1. This group is used in the study of the Ising model.

A representation of a group is a set of square nonsingular matrices (one matrix for each group element), which multiply just like the group elements, and therefore, also constitute a group.

We will be interested in groups with an infinite number of elements, whose elements may be labeled by real parameters, which vary continuously. One example is the group of rotation in three dimensions.

A generating set of a group is a subset such that every element of the group can be expressed as a combination (under the group operations) of finitely many elements of the subset and their inverses.

The group of all unitary $N \times N$ matrices is designed by U(N). In the case, N = 1the group U(1) consists of all complex numbers with absolute value 1. The group of all unitary $N \times N$ matrices with determinant 1 is called SU(N). The group operation is the standard matrices multiplication. A unitary $N \times N$ matrix with determinant 1 has $N^2 - 1$ independent elements, so the group SU(N) has $N^2 - 1$ generators.

It is well known that a spinor wave function for the spin $\frac{1}{2}$ particles is described by state vectors in a complex two-dimensional space, and rotation in this space is described by the SU(2) matrices. The generators can be taken as the 3 Pauli matrices. Representations of the SU(2) group by higher-order matrices describe higher values of spins. We show below representations for spins 1, $\frac{3}{2}$ and 2. Note that the 3×3 matrices for spin-1 do not form a SU(3) group.

In the following, we show some representations for the group SU(2): For $S = \frac{1}{2}$

$$S^{x} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^{y} = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^{z} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For S = 1

$$S^{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^{y} = \frac{1}{\sqrt{2i}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad S^{z} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

For S = 3/2

$$S^{x} = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \qquad S^{y} = \frac{1}{2i} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{pmatrix},$$
$$S^{z} = \begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}.$$

For S = 2

The group SU(3) has eight generators that are taken as the Gell-Mann matrices. Now, when expressing all three spin matrices and all five quadrupolar operators in terms of the basis (6.19), we find that the spin matrices become equal to the three imaginary Gell-Mann matrices. In contrast, the five quadrupolar operators equal the remaining five real Gell-Mann matrices.

The *symplectic* group of $2N \times 2N$ matrices Sp(N) is the set of unitary matrices U, which satisfy the condition $U^{t}\mathfrak{T}U = \mathfrak{T}$ where

$$\mathfrak{T} = \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & & \\ & \bullet & & \\ & & \bullet & \\ & & & 0 & 1 \\ & & & -1 & 0 \end{pmatrix}.$$

A.1 Gauge theory

Wen [1] defines a gauge theory as a theory where we use more than one label to label the same quantum state. The idea is a generalization from electromagnetism, where a gauge change in the potential vector does not change the electromagnetic fields. A global U(1) transformation is given by $\phi \rightarrow e^{i\alpha}\phi$, where α is a constant. If $\alpha(\vec{r}, t)$ we say that we have a local U(1) transformation. A U(1) gauge theory is a theory invariant under a U(1) transformation.

Reference

[1] Wen X 2004 Quantum Field Theory of Many-Body Systems (Oxford: Oxford University Press)

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Appendix B

Green function in magnetic models

In this appendix, I present the method of perturbation theory for the Green function in a way that is more adequate to be used to treat magnetic models. In general, as we saw in chapter 4, the interacting Hamiltonian is of the form

$$H_{I} = \frac{1}{2} \sum_{q,l,m,n} A(l, q, m, n) a_{l}^{\dagger} a_{q}^{\dagger} a_{m} a_{n},$$
(B.1)

where l, q, m, n here are momentum variables. As we saw in chapter 8, the first term in equation (8.37) is the Green function for noninteracting particles (here magnons). The second term is given by

$$\delta G^{(1)}(k_2, k_1, t_2 - t_1) = -\frac{1}{2} \sum_{q,l,m,n} A(q, l, m, n) \int_{-\infty}^{\infty} dt_1' \langle 0 | T\{a_l^{\dagger}(t_1') a_q^{\dagger}(t_1') a_m(t_1') a_{k_2}(t_2) a_{k_1}^{\dagger}(t_1)\} | 0 \rangle.$$
(B.2)

We see that the first two terms in the integrand in the above equation vanish, i.e.,

$$\langle 0|Ta_{l}^{\dagger}(t_{1}')a_{q}^{\dagger}(t_{1}')|0\rangle \langle 0|Ta_{m}(t_{1}')a_{n}(t_{1}')|0\rangle \langle 0|Ta_{k_{2}}(t_{2})a_{k_{1}}^{\dagger}(t_{1})|0\rangle = 0 \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{m}(t_{1}')|0\rangle \langle 0|Ta_{n}(t_{1}')a_{k_{2}}(t_{2})|0\rangle \langle 0|Ta_{q}^{\dagger}(t_{1}')a_{k_{1}}^{\dagger}(t_{1})|0\rangle = 0.$$
(B.3)

The non-null terms are

$$\langle 0|Ta_{l}^{\dagger}(t_{1}')a_{m}(t_{1}')|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{n}(t_{1}')|0\rangle\langle 0|Ta_{k_{2}}(t_{2})a_{k_{1}}^{\dagger}(t_{1})|0\rangle \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{n}(t_{1}')|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{m}(t_{1}')|0\rangle\langle 0|Ta_{k_{2}}(t_{2})a_{k_{1}}^{\dagger}(t_{1})|0\rangle \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{k_{2}}(t_{2})|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{m}(t_{1}')|0\rangle\langle 0|Ta_{n}(t_{1}')a_{k_{1}}^{\dagger}(t_{1})|0\rangle \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{m}(t_{1}')|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{k_{2}}(t_{2})|0\rangle\langle 0|Ta_{n}(t_{1}')a_{k_{1}}^{\dagger}(t_{1})|0\rangle \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{n}(t_{1}')|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{k_{2}}(t_{2})|0\rangle\langle 0|Ta_{m}(t_{1}')a_{k_{1}}^{\dagger}(t_{1})|0\rangle \langle 0|Ta_{l}^{\dagger}(t_{1}')a_{k_{2}}(t_{2})|0\rangle\langle 0|Ta_{q}^{\dagger}(t_{1}')a_{n}(t_{1}')|0\rangle\langle 0|Ta_{m}(t_{1}')a_{k_{1}}^{\dagger}(t_{1})|0\rangle .$$

B-1

Using Wick's theorem, we write:

$$\delta G^{(1)}(k_2, k_1, t_2 - t_1) = \frac{i}{2} \sum_{q,l,m,n} A(q, l, m, n) \int_{-\infty}^{\infty} dt_1' \Big\{ G^{(0)}(m, l, t_1' - t_1') G^{(0)}(n, q, t_1' - t_1') G^{(0)}(k_2, k_1, t_2 - t_1) + G^{(0)}(n, l, t_1' - t_1') G^{(0)}(m, q, t_1' - t_1') G^{(0)}(k_2, k_1, t_2 - t_1) + G^{(0)}(k_2, l, t_2 - t_1') G^{(0)}(m, q, t_1' - t_1') G^{(0)}(n, k, t_1' - t_1) + G^{(0)}(m, l, t_1' - t_1') G^{(0)}(k_2, q, t_2 - t_1') G^{(0)}(n, k_1, t_1' - t_1) + G^{(0)}(n, l, t_1' - t_1') G^{(0)}(k_2, q, t_2 - t_1') G^{(0)}(m, k_1, t_1' - t_1) + G^{(0)}(k_2, l, t_2 - t_1') G^{(0)}(n, q, t_1' - t_1') G^{(0)}(m, k_1, t_1' - t_1) \Big\}.$$
(B.5)

Using the following relation for noninteracting particles

$$G^{(0)}(k, q, t) = G^{(0)}(k, t)\delta_{kq},$$
(B.6)

we can write:

First term:
$$G^{(0)}(m, 0)G^{(0)}(n, 0)G^{(0)}(k_1, t_2 - t_1)\delta_{lm}\delta_{nq}\delta_{k_1k_2}$$

Second term: $G^{(0)}(n, 0)G^{(0)}(m, 0)G^{(0)}(k_1, t_2 - t_1)\delta_{nl}\delta_{mq}\delta_{k_1k_2}$
Third term: $G^{(0)}(k_2, t_2 - t_1')G^{(0)}(m, 0)G^{(0)}(k_1, t_1' - t_1)\delta_{k_2l}\delta_{mq}\delta_{nk_1}$
Fourth term: $G^{(0)}(k_2, t_2 - t_1')G^{(0)}(m, 0)G^{(0)}(k_1, t_1' - t_1)\delta_{nk_1}\delta_{ml}\delta_{k_2q}$
Fifth term: $G^{(0)}(k_2, t_2 - t_1')G^{(0)}(n, 0)G^{(0)}(k_1, t_1' - t_1)\delta_{k_2q}\delta_{nl}\delta_{mk_1}$
Sixth term: $G^{(0)}(k_2, t_2 - t_1')G^{(0)}(n, 0)G^{(0)}(k_1, t_1' - t_1)\delta_{k_1}\delta_{nq}\delta_{mk_1}$.
(B.7)

The first and second terms are represented by disconnected diagrams and we neglect them. In general, the Hamiltonian imposes restrictions in the momentum l, q, m, n such that there is momentum conservation in each vertex. These restrictions appear as δ functions in the factor A(l,q,m,n). For instance, we could have a term such as

$$H_{I} = \frac{1}{2} \sum_{kqm} A(k-q, q, m, k-m) a_{q} a_{k-q} a_{m}^{\dagger} a_{k-m}^{\dagger}.$$
 (B.8)

In the third term of (B.7) we have $k_2 = k - q$, m = q, $k - m = k_1$ and so $k_2 = k_1$. Each term from the third to the sixth contributes to the same factor

$$\delta G^{(1)}(k_2, t_2 - t_1) = 2i \sum_q A(q) \int_{-\infty}^{\infty} dt_1' G^{(0)}(k_2, t_2 - t_1') G^{(0)}(q, 0) G^{(0)}(k_2, t_1' - t_1), \quad (B.9)$$

where, for simplicity, I have written the A term as A(q). Introducing the Fourier transform

$$G^{(0)}(k, t_1 - t_2) = \int \frac{d\omega}{2\pi} G^{(0)}(k, \omega) e^{i\omega(t_1 - t_2)},$$
(B.10)

we can write

$$\delta G^{(1)}(k_2, k_1, t_2 - t_1) = 2\delta_{k_2k_1} i \sum_q \int \frac{d\omega}{2\pi} e^{i\omega(t_2 - t_1)} G^{(0)}(k_2, \omega) G^{(0)}(q, t = 0) G^{(0)}(k_2, \omega)$$
(B.11)

or

$$\delta G^{(1)}(k_2, k_1, t_2 - t_1) = 2\delta_{k_2k_1} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega(t_2 - t_1)} \delta G^{(1)}(k_2, \omega), \tag{B.12}$$

where

$$\delta G^{(1)}(k,\,\omega) = i \sum_{q} A(q) G^{(0)}(k,\,\omega) G^{(0)}(q,\,t=0) G^{(0)}(k,\,\omega). \tag{B.13}$$

Note that

$$\lim_{t \to 0^{-}} G(0)(q, t) = \lim_{t \to 0^{-}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G^{(0)}(q, \omega) e^{-i\omega t}.$$
 (B.14)

Then we can write (B.13) as

$$\delta G^{(1)}(k,\,\omega) = [G^{(0)}(k,\,\omega)]^2 i \sum_q A(q) G^0(k,\,t=0). \tag{B.15}$$

For the second-order term, we have

$$\delta G^{(2)}(k_{2}, k_{1}, t_{2} - t_{1}) = \frac{i}{2!} \int dt'_{1} dt'_{2} \langle 0 | T \left\{ \sum_{kqm} A(k, q, m) a_{q}(t'_{1}) a_{k-q}(t'_{1}) a^{\dagger}_{m}(t'_{1}) a^{\dagger}_{k-m}(t'_{1}) \right.$$

$$\left. \sum_{ijl} A(i, j, l) a_{j}(t'_{2}) a_{i-j}(t'_{2}) a^{\dagger}_{l}(t'_{2}) a^{\dagger}_{i-l}(t'_{2}) a_{k_{2}}(t_{2}) a^{\dagger}_{k_{1}}(t_{1}) \right\} | 0 \rangle.$$
(B.16)

Using Wick's theorem, let us consider the term

$$\frac{(-1)}{2!} \sum_{kqm} \sum_{ijl} A(k, q, m) A(i, j, l) \int dt_1' dt_2' G^{(0)}(q, k_1, t_1' - t_1) G^{(0)}(k_2, l, t_2 - t_2')$$

$$G^{(0)}(k - q, i - l, t_1' - t_2') G^{(0)}(j, m, t_2' - t_1') G^{(0)}(i - j, k - m, t_2' - t_1').$$
(B.17)

We have $q = k_1$, $l = k_2$, k-q = i-l, j = m, i - j = k - m, which gives i = k and $k_2 = k_1$. Hence, we can write

$$\frac{(-1)}{2!} \sum_{k,m} A(k, k_1, m) A(k, m, k_2) \int dt_1' dt_2' G^{(0)}(k_1, t_1' - t_1) G^{(0)}(k_2, t_2 - t_2')$$

$$G^{(0)}(k - k_1, t_1' - t_2') G^{(0)}(m, t_2' - t_1') G^{(0)}(k - m, t_2' - t_1').$$
(B.18)

Using equation (B.9) we can write the above expressions as

$$\frac{(-1)}{2!} \sum_{k,m} A(k, k_1, m) A(k, m, k_2) \frac{1}{(2\pi)^5}
\int dt_1' dt_2' \left\{ \int d\omega_1 d\omega_2 d\omega_3 d\omega_4 d\omega_5 G^{(0)}(k_1, \omega_1) G^{(0)}(k_1, \omega_2)
G^{(0)}(k - k_1, \omega_3) G^{(0)}(m, \omega_4) G^{(0)}(k - m, \omega_5) e^{i\omega_1(t_1^{'} - t_1)} e^{i\omega_2(t_2^{'} - t_2)} e^{i\omega_3(t_1^{'} - t_2^{'})} e^{i\omega_4(t_2^{'} - t_1^{'})} e^{i\omega_5(t_2^{'} - t_1^{'})} \right\}.$$
(B.19)

We have the following results

$$\int dt_1' e^{it_1'(\omega_1 + \omega_3 - \omega_4 - \omega_5)} \rightarrow \omega_1 + \omega_3 = \omega_4 + \omega_5$$

$$\int dt_2' e^{it_2'(-\omega_2 - \omega_3 + \omega_4 + \omega_5)} \rightarrow \omega_2 + \omega_3 = \omega_4 + \omega_5,$$
(B.20)

which lead to $\omega_1 = \omega_2$. Equation (B.19) can then be written as

$$\frac{(-1)}{2!} \sum_{k,m} A(k, k_1, m) A(k, m, k_2) \frac{1}{(2\pi)^3} \int d\omega_1 d\omega_3 d\omega_4 G^{(0)}(k_1, \omega_1) G^{(0)}(k_1, \omega_1) G^{(0)}(k - k_1, \omega_3) G^{(0)}(m, \omega_4) G^{(0)}(k - m, \omega_1 + \omega_3 - \omega_4) e^{i\omega_1(t_2 - t_1)}.$$
(B.21)

Let $\omega_3 = \omega' - \omega_1 \rightarrow \omega_5 = \omega' - \omega_4$. Using this result in equation (B.20) we write

$$\frac{1}{2\pi} \int d\omega_1 e^{i\omega_1(t_2-t_1)} \Biggl\{ \frac{(-1)}{2!} \sum_{k,m} A(k, k_1, m) A(k, m, k_2) \frac{1}{(2\pi)^2} [G^{(0)}(k_1, \omega_1)]^2 \\ \int d\omega_4 d\omega' G^{(0)}(k - k_1, \omega' - \omega_1) G^{(0)}(m, \omega_4) G^{(0)}(k - m, \omega' - \omega_4) \Biggr\}.$$
(B.22)

The Fourier transform is given by

$$\delta \tilde{G}^{(2)}(k_1, t_2 - t_1) = \frac{1}{2\pi} \int d\omega_1 \delta \tilde{G}^{(2)}(k_1, \omega_1).$$
(B.23)

As we saw in section (8.4), we can cancel the term 1/m!. We also have two diagrams equivalent to (B.23). Hence, we can write the final result as

$$\delta G^{(2)}(k,\,\omega) = -2\sum_{q,m} A(q,\,k,\,m)A(q,\,m,\,k)[G^{(0)}(k,\,\omega)]^2$$

$$\frac{1}{(2\pi)^2} \int d\omega' d\omega'' G^{(0)}(q-k,\,\omega'-\omega)G^{(0)}(m,\,\omega'')G^{(0)}(q-m,\,\omega'-\omega'').$$
(B.24)