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1

The chain of spin-1/2 atoms

1.1 Model for a one-dimensional metal

In a famous contribution to the theory of metals published in 1931, Bethe studies one of the simplest quantum models one can imagine for N mutually interacting atoms: a linear chain of two-level atoms interacting with their nearest neighbours, constituting a one-dimensional crystal. If the interaction between two neighbouring atoms is represented graphically by a link, the chain obviously realizes the simplest connected configuration. In order to avoid edge effects, one considers a closed or cyclic chain. The problem of the open chain will be treated in Chapter 5.

The levels of each atom are those of the two-spin states of a spin-1/2 electron outside a completely filled electronic level. In the absence of interactions between atoms, in other words for a sufficiently large value of the lattice spacing, the degeneracy of the 2^N levels is complete. Bethe considers calculating the states and energies of the atomic chain to first order in the electronic interaction, in the framework of the theory of Slater. In a first approximation, the Coulomb forces and eventually also the spin-dependent magnetic forces have the following consequences:

(a) they separate the average value of the energy of each pair of neighbouring atoms into parallel $\uparrow\uparrow$ and antiparallel $\uparrow\downarrow$ states;
(b) they exchange the spin states of electrons localized on neighbouring atoms.

The non-vanishing elements of the energy matrix are thus intuitively defined. More rigorously, if one first neglects the magnetic moments coming from spin, degenerate perturbation theory gives the Hamiltonian (Heisenberg, 1928; Dirac, 1967)

$$H = -J \sum_{n=1}^{N} P_{n,n+1} \tag{1.1}$$

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in which P_{12}, P_{23}, ... are operators exchanging the orbital states, and J represents Slater's exchange integral. In view of Pauli's principle, H in the basis of completely antisymmetric states is equivalent to the so-called isotropic spin Hamiltonian

$$H = \frac{J}{2} \sum_n \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} \tag{1.2}$$

since one has, in this basis, the representation

$$P_{12} = -\frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2).$$

The spin vector of the index n atom of the chain is $\vec{S}_n = \frac{1}{2}\vec{\sigma}_n$, where $\sigma^{x,y,z}$ are the spin-1/2 Pauli matrices. For the closed chain, sites $N + n$ and n are identified: $\vec{S}_{N+1} \equiv \vec{S}_1$.

If one must take into account average magnetic forces between electrons along a certain anisotropy direction, one considers the so-called Heisenberg–Ising Hamiltonian depending on a parameter Δ; this anisotropy parameter takes the value 1 for the isotropic case in which only exchange interactions occur

$$H_\Delta = 2J \sum_{n=1}^{N} S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta \left(S_n^z S_{n+1}^z - \frac{1}{4} \right). \tag{1.3}$$

A constant has been added to ensure that the ferromagnetic reference state $|S^z = \frac{1}{2}N\rangle$ has zero energy. The H_Δ Hamiltonian commutes with the total spin projection on the anisotropy axis $S^z = \sum_n S_n^z$. For the case $\Delta = 1$, isotropy implies $[H, \vec{S}] = 0$.

More generally, one considers the three-parameter Hamiltonian defining the XYZ model (Bonner, 1968; Sutherland, 1970; Baxter, 1971b)

$$H_{\Delta,\Gamma} = 2 \sum_n J_x S_n^x S_{n+1}^x + J_y S_n^y S_{n+1}^y + J_z S_n^z S_{n+1}^z \tag{1.4}$$

depending on two anisotropy parameters Δ and Γ such that

$$J_x : J_y : J_z = 1 - \Gamma : 1 + \Gamma : \Delta. \tag{1.5}$$

Its spectrum will be determined in Chapter 8 following Baxter's method.

Concerning the physics of the magnetic chain and a list of useful references, the reader can consult the article of Bonner and Fisher (1964) and Bonner's thesis (1968); for the classical (non-quantum) chain, see the article of Fogedby (1980).

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1.2 Bethe's method

1.2.1 Equation for the amplitudes

The method invented by Bethe for the diagonalization of H (1.2) is also simply applicable to H_Δ (1.3) (Orbach, 1958). The important distinguishing feature with respect to the three-parameter Hamiltonian (1.4) is the conservation of the magnetic component S^z. An eigenstate $|M\rangle$ of H_Δ belonging to spin $S^z = \frac{N}{2} - M$, where M is the spin deviation with respect to the ferromagnetic state $|S^z = \frac{N}{2}\rangle$, is a superposition of states of basis

$$|n_1 n_2 \dots n_M\rangle = S^-_{n_1} S^-_{n_2} \dots S^-_{n_M} |0\rangle \tag{1.6}$$

characterized by a sequence of integer coordinates of atoms with magnetic component $-\frac{1}{2}$ (denoted $\downarrow$) along the chain. One has

$$|M\rangle = \sum_{\{n\}} a(n_1 n_2 \dots n_M) |n_1 n_2 \dots n_M\rangle. \tag{1.7}$$

The sum goes over the C_M^N sets $\{n\}$ of M increasing integers varying from 1 to N

$$1 \le n_1 < n_2 < \dots < n_M \le N. \tag{1.8}$$

A typical configuration of the chain is represented in Figure 1.1. It can also be characterized by the coordinates of the antiparallel links, alternating the two types $-\bullet- \equiv \uparrow\downarrow$ and $-\bullet- \equiv \downarrow\uparrow$.

The off-diagonal elements of H_Δ

$$\langle\{n'\}| \sum_n S^+_n S^-_{n+1} + S^-_n S^+_{n+1} |\{n\}\rangle \tag{1.9}$$

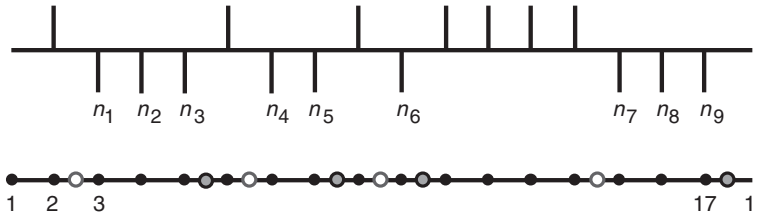

Figure 1.1 The figure represents the base state $|n_1 n_2 \dots n_9\rangle$ for $N = 17$, $M = 9$. The transitions operated by the non-diagonal part of H_Δ number 8, which exactly equals the number of antiparallel links; $3 \to 2$, $5 \to 6$, $7 \to 6$, $8 \to 9$, $10 \to 9$ and $11, 15 \to 14$, $17 \to 18 \equiv 1$.

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lead to the transitions

$$|n_1 n_2 \dots n_M\rangle \to |n'_1 n'_2 \dots n'_M\rangle \tag{1.10}$$

in which configurations $\{n'\}$ are obtained from $\{n\}$ by the exchange of a single pair of antiparallel neighbours

$$n'_1 = n_1, \quad n'_2 = n_2, \quad \dots, \quad n'_\alpha = n_\alpha \pm 1, \quad \dots, \quad n'_M = n_M \tag{1.11}$$

provided that the set $\{n'\}$ thus defined is an admissible configuration with respect to (1.8). In order to make inequalities (1.11) valid on the whole defining interval of the n_α coordinates, this interval shall however be extended beyond N by identifying sites n and $N + n$. The periodicity condition on the amplitudes is thus

$$a(n_1 n_2 \dots n_M) \equiv a(n_2 n_3 \dots n_M, n_1 + N). \tag{1.12}$$

These have been defined up to now only for sets of increasing integers with $n_M - n_1 < N$.

The diagonal elements of H_Δ are

$$\begin{aligned} &2\Delta \langle\{n\}| \sum_m \left(S^z_m S^z_{m+1} - \frac{1}{4} \right) |\{n\}\rangle \\ &\quad = -\Delta \times \text{number of antiparallel links } \uparrow\downarrow \text{ or } \downarrow\uparrow \\ &\quad = -\Delta \times \text{number of allowed transitions } |\{n\}\rangle \to |\{n'\}\rangle. \end{aligned} \tag{1.13}$$

The equation for the amplitudes $a(\{n\})$ and the energy levels $2JE$ of Hamiltonian H_Δ is thus

$$\sum_{\{n'\}} (a(\{n'\}) - \Delta a(\{n\})) = 2Ea(\{n\}) \tag{1.14}$$

in which the sum is over all allowed transitions defined by (1.11).

1.2.2 Decoupling of the eigenvalue equation

Let us start with the elementary case of one downturned spin $M = 1$ leading to a difference equation

$$a(n+1) + a(n-1) - 2\Delta a(n) = 2Ea(n) \tag{1.15}$$

with solution

$$a(n) = e^{ikn}, \qquad E = \cos k - \Delta, \tag{1.16}$$

where the wavenumber k is quantized by the periodicity condition (1.12)

$$e^{ikN} = 1 \quad \Leftrightarrow \quad kN = 2\pi\lambda, \qquad \lambda = 0, 1, 2, \dots, N-1. \tag{1.17}$$

Going to the $M = 2$ case, Bethe obtains a solution defined by two momenta k_1 and k_2:

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$$a(n_1 n_2) = e^{\frac{i}{2}\psi_{12}+ik_1n_1+ik_2n_2} + e^{-\frac{i}{2}\psi_{12}+ik_2n_1+ik_1n_2}. \tag{1.18}$$

The remarkable fact in this spin wave scattering is that the wavefunction $a(n_1n_2)$ coincides with its asymptotic expression which, in one dimension, only contains two elastic terms, the direct and exchange terms. This result generalizes, using appropriate phase shifts, when superimposing M spin waves with distinct momenta forming a set $\{k\} \equiv \{k_1 k_2 \dots k_M\}$.

The success of this scheme formally comes from decoupling the system (1.14), which is achieved as follows.

(a) The definition of the $a(\{n\})$ is extended to values of n such that equality is allowed:

$$n_1 \leq n_2 \leq n_3 \leq \dots \leq n_M. \tag{1.19}$$

(b) One assumes that equations (1.14) are still verified if the sum is no longer constrained to the allowed configurations (distinct n_α) only, but is freely extended to all transitions (1.11). One thus obtains second-order difference equations with constant coefficients

$$\sum_{\alpha=1}^{M} (a(n_1 \dots n_\alpha + 1 \dots n_M) + a(n_1 \dots n_\alpha - 1 \dots n_M) \\ -2\Delta a(n_1 \dots n_\alpha \dots n_M)) = 2Ea(n_1 n_2 \dots n_M). \tag{1.20}$$

(c) Since equalities (1.14) and (1.20) are by hypothesis simultaneously verified, the terms of the left-hand side of (1.20) which do not appear in (1.14) have a vanishing total contribution. These terms come from two possible sources
- $n'_\alpha = n_{\alpha+1} = n_\alpha + 1$,
- $n'_\beta = n_{\beta-1} = n_\beta - 1$,

for certain values of the α and β indices.

Let us examine the two terms associated with two neighbouring down spins $\downarrow$ on sites n_α and $n_{\alpha+1} = n_\alpha + 1$. A first forbidden term in (1.14) comes from $n'_\alpha = n_\alpha + 1$, since n'_α coincides with $n_{\alpha+1} = n'_{\alpha+1}$, i.e.

$$a(\dots n_\alpha + 1, n_\alpha + 1, \dots) - \Delta a(\dots n_\alpha, n_\alpha + 1, \dots).$$

A second term in (1.14) comes from $n'_{\alpha+1} = n_{\alpha+1} - 1 = n_\alpha$, i.e.

$$a(\dots n_\alpha, n_\alpha, \dots) - \Delta a(\dots n_\alpha, n_\alpha + 1, \dots).$$

Collecting the two forbidden terms associated with the neighbouring pair $(n_\alpha, n_\alpha + 1)$, equations (1.14) and (1.20) will be identical provided one can impose the constraints

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$$a(\ldots n_\alpha+1, n_\alpha+1, \ldots)+a(\ldots n_\alpha, n_\alpha, \ldots)$$
$$-2\Delta a(\ldots n_\alpha, n_\alpha+1, \ldots)=0, \tag{1.21}$$

which must be verified for all values of coordinates subject to conditions (1.19).

1.2.3 The Bethe wavefunction

The difference equation (1.20) is separable in each coordinate and admits factorized solutions $\exp(ik_1n_1+ik_2n_2+\ldots+ik_Mn_M)$ associated with a set $\{k\}$. The corresponding energy is thus

$$E=\sum_{\alpha=1}^{M}(\cos k_\alpha-\Delta). \tag{1.22}$$

Bethe attempts to fulfil the complementary constraints (1.21) by expressing the amplitude as a sum over the $M!$ identical energy waves obtained by permuting the momenta in set $\{k\}$. Bethe's sum (or Bethe's Ansatz) is the following:

$$a(n_1\ldots n_M)=\sum_{P\in\pi_M}A(P)\exp\left(i\sum_{\alpha=1}^{M}k_{P\alpha}n_\alpha\right). \tag{1.23}$$

The $A(P)$ coefficients are to be determined from (1.21), which is written as

$$\sum_P A(P)\left\{e^{i(k_{P\alpha}+k_{P(\alpha+1)})}-2\Delta e^{ik_{P(\alpha+1)}}+1\right\}\times e^{ik_{P1}n_1+\ldots+i(k_{P\alpha}+k_{P(\alpha+1)})n_\alpha+\ldots}=0 \tag{1.24}$$

and must be verified for all $\{n\}$ and each α such that $n_{\alpha+1}=n_\alpha+1$. In the sum, one can then associate terms $A(P)\ldots$ and $A(PP_{\alpha,\alpha+1})\ldots$ which have the same $\{n\}$ dependence, and sum over the subset $P/P_{\alpha,\alpha+1}$ of permutations of π_M, where $P_{\alpha,\alpha+1}\equiv(\alpha,\alpha+1)$ represents the permutation of two neighbours α and $\alpha+1$. To simplify the notation, take $(\alpha,\alpha+1)=(34)$. It is sufficient to have the following relations for $A(P)$:

$$A(P)(e^{i(k_{P3}+k_{P4})}-2\Delta e^{ik_{P4}}+1)+A(PP_{34})(e^{i(k_{P4}+k_{P3})}-2\Delta e^{ik_{P3}}+1)=0. \tag{1.25}$$

Defining the antisymmetric phases $\psi_{\alpha\beta}=-\psi_{\beta\alpha}$ by the relation

$$e^{i\psi_{\alpha\beta}}=-\frac{e^{i(k_\alpha+k_\beta)}-2\Delta e^{ik_\alpha}+1}{e^{i(k_\alpha+k_\beta)}-2\Delta e^{ik_\beta}+1}, \tag{1.26}$$

condition (1.25) is written as

$$A(PP_{\alpha,\alpha+1})=A(P)e^{-i\psi_{P\alpha,P(\alpha+1)}},\ \forall P \text{ and } \alpha. \tag{1.27}$$

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The unique solution up to a trivial factor is

$$A(P) = \exp\left(\frac{i}{2}\sum_{\alpha<\beta}\psi_{P\alpha,P\beta}\right). \tag{1.28}$$

Note that the relation between the phases and momenta can be written

$$\cot\frac{\psi_{\alpha\beta}}{2} = \Delta\frac{\sin(k_\alpha - k_\beta)/2}{\cos(k_\alpha + k_\beta)/2 - \Delta\cos(k_\alpha - k_\beta)/2}. \tag{1.29}$$

1.2.4 Periodicity conditions

If we were dealing with an infinite one-dimensional crystal, we would choose the momenta $\{k\}$ arbitrarily (real, modulo 2π), the phases would be determined by (1.20), and we would have thus constructed a continuous set of eigenstates of the infinite chain. However, in view of the thermodynamic limit and in order to address the questions of classification and completeness, it is necessary to consider a finite system; thus, the idea of treating the periodic chain. It so happens that periodicity conditions (1.12) are compatible with the structure (1.23) of the Bethe sum. These conditions are written as

$$A(P) = A(PC)e^{ik_{P1}N}, \tag{1.30}$$

in which C designates the cyclic permutation $C\alpha = \alpha + 1$, or $C = (1, 2, \ldots, M)$. With the help of (1.28), we have

$$\begin{aligned} A(PC) &= \exp\left(\frac{i}{2}\sum_{1\le\alpha<\beta\le M}\psi_{P(\alpha+1),P(\beta+1)} + \frac{i}{2}\sum_{1\le\alpha<M}\psi_{P(\alpha+1),P1}\right) \\ &= \exp\left(\frac{i}{2}\sum_{1\le\alpha<\beta<M}\psi_{P\alpha,P\beta} + i\sum_{1<\alpha\le M}\psi_{P\alpha,P1}\right). \end{aligned}$$

Relation (1.30) is thus written as

$$e^{ik_{P1}N + i\sum_{1<\alpha\le M}\psi_{P\alpha,P1}} = 1, \qquad \forall P. \tag{1.31}$$

There must thus be a set of integers λ_α such that

$$Nk_\alpha = 2\pi\lambda_\alpha + \sum_\beta \psi_{\alpha,\beta}, \qquad \alpha = 1, 2, \ldots, M, \tag{1.32}$$

with $\psi_{\alpha,\alpha} = 0$ by convention.[1]

[1] Note that this entails that $\psi_{\alpha,\beta}$ is discontinuous at $k_\alpha - k_\beta = 0$. See the paragraph preceding equation (1.59).

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These are the coupled equations used to determine the admissible sets of momenta $\{k\}$, and consequently the energies and amplitudes. We note that this is a high-degree algebraic system in the e^{ik} variables. The complexity of system (1.32) renders the problems of existence and classification particularly acute, and these will be treated in Section 1.5 (see Yang and Yang, 1966a–d).

1.3 Parameters and quantum numbers

1.3.1 Orbach's parametrization

Before defining the sets $\{\lambda\}$ and classifying the solutions, it is necessary to fix the branches of k and ψ. We shall take

$$0 \leq \Re k_\alpha \leq 2\pi, \qquad -\pi \leq \Re \psi_{\alpha,\beta} \leq \pi. \tag{1.33}$$

In contrast, relation (1.29) between the momenta and the phases can be parametrized in a way which is useful for our further purposes; we take

$$\cot \frac{\psi_{\alpha,\beta}}{2} = \Delta \frac{\cot \frac{k_\alpha}{2} - \cot \frac{k_\beta}{2}}{\cot \frac{k_\alpha}{2} \cot \frac{k_\beta}{2} (\Delta - 1) + (\Delta + 1)} \tag{1.34}$$

which leads us to distinguishing the regions $|\Delta| \gtrless 1$.

(a) $\Delta > 1$.
We take

$$\Delta = \cosh \Phi, \qquad 0 < \Phi < \infty \tag{1.35}$$

and we have, as a function of parameters φ_α,

$$\begin{cases} \cot \dfrac{k_\alpha}{2} = \coth \dfrac{\Phi}{2} \tan \dfrac{\varphi_\alpha}{2} & \text{or} \quad e^{ik_\alpha} = \dfrac{e^{i\varphi_\alpha} - e^{\Phi}}{e^{i\varphi_\alpha + \Phi} - 1}, \\ \cot \dfrac{\psi_{\alpha,\beta}}{2} = \coth \Phi \tan \dfrac{\varphi_\alpha - \varphi_\beta}{2}, & -\pi < \Re \varphi_\alpha < \pi. \end{cases} \tag{1.36}$$

(b) $-1 < \Delta < 1$.
We take

$$\Delta = \cos \Theta, \qquad 0 < \Theta < \pi \tag{1.37}$$

and we obtain, in terms of the parameters θ_α,

$$\begin{cases} \cot \dfrac{k_\alpha}{2} = \cot \dfrac{\Theta}{2} \tanh \dfrac{\theta_\alpha}{2}, \\ \cot \dfrac{\psi_{\alpha,\beta}}{2} = \cot \Theta \tanh \dfrac{\theta_\alpha - \theta_\beta}{2}. \end{cases} \tag{1.38}$$

One must take note that the real domain of k is covered by the θ domain

$$-\infty < \Re \theta_\alpha < +\infty, \qquad \Im \theta_\alpha = 0 \text{ or } \pi.$$

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(c) The boundary case $\Delta = 1$ is obtained from either side by taking

$$x_\alpha = \lim_{\Phi\to 0} \frac{\varphi_\alpha}{\Phi} = \lim_{\Theta\to 0} \frac{\theta_\alpha}{\Theta},$$
$$\cot\frac{k_\alpha}{2} = x_\alpha, \qquad \cot\frac{\psi_{\alpha,\beta}}{2} = \frac{1}{2}(x_\alpha - x_\beta). \tag{1.39}$$

(d) Finally, the region $\Delta < -1$ is brought back to the study of the region $\Delta > 1$ by virtue of a proposition demonstrated in the following subsection, see (1.42).

Proposition: The H_Δ and $H_{-\Delta}$ Hamiltonians are equivalent.

To close this subsection, let us write down the form that the coupled equations (1.31) take in terms of the φ or θ parameters:

$$\left(\frac{\sin\frac{1}{2}(\varphi_\alpha + i\Phi)}{\sin\frac{1}{2}(\varphi_\alpha - i\Phi)}\right)^N = \prod_{\beta\neq\alpha} \frac{\sin\frac{1}{2}(\varphi_\alpha - \varphi_\beta + 2i\Phi)}{\sin\frac{1}{2}(\varphi_\alpha - \varphi_\beta - 2i\Phi)}. \tag{1.40}$$

Let us also mention the expression for the energy levels:

$$E = -\sum_\alpha \frac{\sin^2\Theta}{\cosh\theta_\alpha - \cos\Theta} \quad \text{or} \quad -\sum_\alpha \frac{\sinh^2\Phi}{\cosh\Theta - \cos\varphi_\alpha}, \tag{1.41}$$

depending on the case. We go from one to the other by the continuations $\varphi = i\theta$, $\Phi = i\Theta$.

1.3.2 Quantum numbers

We first have the following symmetry in the Δ parameter, allowing us to restrict our study to the domain $\Delta > 0$:

$$U H_\Delta U^{-1} = -H_{-\Delta}, \tag{1.42}$$

with the S^z-conserving unitary operator

$$U = \exp\left(i\pi \sum_{n=1}^N n S_n^z\right). \tag{1.43}$$

The spectra of H_Δ and $H_{-\Delta}$ are thus inverted with respect to each other.

Besides the S^z magnetic component, the total momentum K is another conserved quantum number of the periodic chain. The one-site translation operator $T = e^{iK}$ commutes with H by virtue of the property

$$T^{-1}\vec{S}_n T = \vec{S}_{n+1}. \tag{1.44}$$

T is thus the circular site permutation operator along the chain; it admits the classical representation

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$$T = \operatorname*{Tr}_{\tau} P_{01} P_{02} \dots P_{0N} \equiv C^{-1} \tag{1.45}$$

$$C : \alpha \to \alpha + 1$$

with

$$P_{0n} = \frac{1}{2}(1 + \vec{\tau} \cdot \vec{\sigma}_n). \tag{1.46}$$

We deduce from (1.23)

$$T|M\rangle = e^{i(k_1 + \dots + k_M)}|M\rangle. \tag{1.47}$$

In other words

$$K = \sum_{\alpha=1}^{M} k_\alpha = \frac{2\pi}{N} \sum_{\alpha} \lambda_\alpha. \tag{1.48}$$

The U transformation commutes with K if M is even, but shifts K by π if M is odd, N being assumed even.

1.3.3 Total spin

For the value $\Delta = 1$, there exists an additional absolute quantum number which is the total spin S such that $\vec{S}^2 = S(S+1)$.

> **Proposition:** If the numbers k_α solving (1.32) for $\Delta = 1$ are all different from zero (modulo 2π), then the eigenstate $|M\rangle$ belongs to the sector with total spin $S = S^z = \frac{N}{2} - M$.

Proof:

$$|M\rangle = \sum_{\{n\}} a(n_1 \dots n_M) S^-_{n_1} \dots S^-_{n_M}|0\rangle. \tag{1.49}$$

The condition $S^+|M\rangle = 0$ which characterizes the $S = S^z$ state is

$$\sum_{n=1}^{n_2-1} a(n n_2 \dots n_M) + \sum_{n=n_2+1}^{n_3-1} a(n_2 n n_3 \dots n_M) + \dots$$
$$+ \sum_{n=n_M+1}^{N} a(n_2 n_3 \dots n_M n) = 0. \tag{1.50}$$

Let us substitute in the first term of (1.50) the expressions for the amplitudes (1.23), perform the sums over n under the hypothesis $z_j = e^{ik_j} \neq 1$, and regroup terms of the same nature to obtain

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