N. Nagaosa

Quantum Field Theory in Strongly Correlated Electronic Systems

强关联电子系统中的量子场论

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Preface

Research on electronic systems in condensed matter physics is at present developing very rapidly, where the main focus is changing from the "single-particle problem" to the "many-particle problem". That is, the main research interest changed from phenomena that can be understood in the single-particle picture, as, for example, in band theory, to phenomena that arise owing to the interaction between many electrons.

As examples of the latter case, we mention superconductivity and magnetism; in both cases the research has a long history. New developments in these fields are the studies on phenomena that are beyond the scope of mean field theories such as BCS theory and mean field theory of the spin density wave – and are related to research on so-called electronic correlation. Electronic correlation effects arise owing to strong quantum as well as thermal fluctuations. When fluctuations are large, the interaction between different degrees of freedom becomes important; for example, the interplay between magnetism and superconductivity in high temperature superconductors.

The best framework to describe strongly interacting degrees of freedom – which is nothing but the "field" itself – is quantum field theory. In this volume, applications of quantum field theory to the problem of strongly correlated electronic systems are presented in a – hopefully – systematic way in order to be understandable to the beginner. Knowledge of the basic topics discussed in *Quantum Field Theory in Condensed Matter Physics*, written by the same author, is presumed.

This volume consists of a series of themes. In the first part, one-dimensional, many-particle quantum systems are discussed. In a single dimension, order cannot emerge owing to strong quantum fluctuations, and therefore, down to zero temperature, a quantum liquid survives. Therefore, the one-dimensional system is a very important toy model for the discussion of electronic correlation, where many ideas and methods can successfully be applied, and where the results are established with the highest accuracy. Discussion of these models determines the basic direction for the whole range of problems related to electronic correlation. In Chap. 1, the XXZ quantum spin chain is discussed in its classical and quantum limits. The most important object here is the kink, which can be described in terms of a fermion that is related to the spins by a non-local phase factor (a Jordan–Wigner transformation).

Here, issues such as a new particle (kink), non-locality and quantum statistics appear for the first time, being important in all problems related to electronic correlation.

In Chap. 2, the quantum field theory of an interacting fermion system, being equivalent to the XXZ spin chain, is discussed. Starting from the fact that the one-dimensional fermion system can be described by the two Fermi points $k_{\mathrm{F}}^{\mathrm{R}}$ and $k_{\mathrm{F}}^{\mathrm{L}}$, the canonical conjugate relation between the density and the current is derived. Using the (bosonic) phase fields θ_+ and θ_- for their description, the fermionic system is finally mapped to the Sine–Gordon system. Kinks (solitons) are the classical solution of the quantum Sine–Gordon system, which correspond to the original fermions. The kink connects the different minima of the sine potential, which has a finite excitation energy in a classical approximation. However, when the quantum fluctuations become large, the sine potential itself is effectively reduced and eventually washed out, and in the excitation spectrum of the kink, the gap disappears. This will be demonstrated in Sect. 2.1 using the renormalization group. When the sine potential can effectively be neglected, the system can simply be described in terms a of Gaussian $(1+1)$-dimensional free bosonic theory. At first sight, the theory looks trivial; however, it contains very fundamental theoretical structures, that is, invariance under conformal (angle conserving) transformations on the complex plane. In Sect. 2.2, the Gaussian theory is discussed using conformal field theory.

In this way, many different theoretical approaches can be used to describe gapless one-dimensional quantum liquids. However, quantum liquids having a gap in the excitation spectrum are also known. The antiferromagnetic Heisenberg model with integer spin S, called the Haldene system, is a representative example. For its analysis we use another method different from bosonization, based on the non-linear sigma model (Sect. 2.3). The advantages of this model are that the meaning of the Berry phase can be seen very clearly, and that it can be generalized to higher dimensions.

Starting from Chap. 3, systems containing both a charge and spin degree of freedom, and higher-dimensional systems are discussed. First, strongly correlated electronic systems are introduced. In Sect. 3.1, many different models are presented, and the idea of deriving effective Hamiltonians by restricting the Hilbert space is introduced. Because these restrictions in the Hilbert space are represented by constraint conditions, strongly correlated electronic systems are often formulated as quantum theory under constraints.

Spin-charge separation is one of the central issues in strongly correlated electronic systems. This phenomenon appears in the one-dimensional interacting electron system in the most striking way, as described in Sect. 3.2 using a generalization of the bosonization method introduced in Chap. 2. Density and current of spin $\uparrow$ and $\downarrow$ are defined, where the sum and the difference represent the charge and spin degree of freedom, respectively. This spin charge separated one-dimensional quantum liquid – the Tomonaga–Luttinger fluid –

is the representative example of a non-Fermi liquid. Here, the description using bosonization is not principally different from that of the theory of a Fermi liquid; however, because the Fermi surface in a single dimension only consists of two single points, no individual excitation exists, but only collective excitation modes. This is the reason for the non-Fermi-liquid behaviour.

On the other hand, in two and three dimensions, compared with a single dimension, the quantum fluctuations are smaller, and under some circumstances magnetic ordering occurs. For this reason, one crucial degree of freedom for the description of strongly correlated electronic systems is the magnetic moment, and it seems natural to describe the properties of the system by analysing its ordering and fluctuations. Following this outline, in Sects. 3.3 and 3.4, mean field theory and the fluctuations of the magnetic ordering are discussed, respectively. In particular the latter is analysed in terms of both self-consistent renormalization and the quantum renormalization group in order to investigate the singular enhancement of quantum fluctuations in the vicinity of phase transition points at zero temperature – driven by some external parameters like pressure, etc.

Another point of view beside the discussion of magnetic moment and its fluctuations is the discussion of spin singlet formation. One representative example is the magnetic impurities in the metal – the Kondo effect. When only one spin moment exists, magnetic ordering cannot occur. Finally, the localized spin and the spins of conduction electrons of the metal form a singlet and the entropy is quenched. As a result, the system becomes a magnetically inert local Fermi liquid. This state can be analysed in terms of the slave boson method. On the other hand, in the case when the number of channels of conduction electrons is large (the multi-channel Kondo problem), it is known that a local non-Fermi-liquid state can arise also. This state, too, can be described using the slave boson method. By determining a saddle point solution where the bosons do not condensate, it can be shown that the Green's function is characterized by non-trivial critical exponents.

The Kondo model can also be approached using many other theoretical methods. In particular, by partial wave analysis, the incoming wave and the scattered wave can be regarded as one-dimensional in dependence on the polar coordinate r. In such a way, the problem of a localized impurity can be mapped on the problem of an impurity interacting with an electron in one dimension. Here, the framework of the $(1+1)$-dimensional quantum field theory as developed in Chap. 2 can be applied. Furthermore, it can be shown that the impurity problem is equivalent to the effective model developed in Sect. 4.2 using dynamic mean field theory in the limit of large spatial dimension d. With this knowledge, it becomes clear that the problem of electron correlation in $d = 0$ dimensions (local impurity), $d = 1$ and $d = \infty$ are intimately related to each other.

However, this does not mean that all systems with strongly correlating electrons are understood. In particular, it is possible that in the important

dimensions $d = 2$ and $d = 3$ physical phenomena could appear that cannot be explained within this framework. In the theories described above, in every case the degree of freedom on the site – for example, the localized moment or the localized electrons appearing in dynamic mean field theory – has been considered. One might assume that it is a complementary approach to focus on the degree of freedom defined on the link between two sites. The field defined on the link describes the "relation" between the degrees of freedom on each site; mathematically speaking, this is the connection and, in physics, this field is called the gauge field. For example, when the spin moment is considered as the degree of freedom at each site, for a quantum liquid where, owing to quantum fluctuations, the magnetic order has disappeared, we might assume rather that the singlet amplitude defined on the link is a meaningful order parameter. In Chap. 5, theories of strongly correlated electronic systems are developed from this point of view. Explicitly, the quantum anti-ferromagnet (Sect. 5.1), the doped Mott insulator, being deeply related to high temperature superconductivity (Sect. 5.2), and the quantum Hall liquid (Sect. 5.3) are described in terms of gauge theory. In particular, in Sect. 5.3, the use of the Chern–Simons gauge field for the description of non-local quantum statistics is discussed, being the generalization of the Jordan–Wigner transformation of Chap. 1 to the two-dimensional case. In such a way, the book closes with a reprise, and the author hopes that the reader will be able to see the content of this book in a new light from the point of view of gauge theories.

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Tokyo, January 1999 *Naoto Nagaosa*

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1. The One-Dimensional Quantum Spin Chain

Among many-body quantum systems, the one-dimensional occupies a special position. Owing to strong quantum fluctuations, the system is a quantum liquid, and down to zero temperature, no ordered state emerges. In this chapter, the one-dimensional quantum spin system will be discussed, being the introduction to the theory of strongly correlated systems.

1.1 The $S = 1/2$ XXZ Spin Chain

First, we consider the following Hamiltonian:

$$H = J_\perp \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + J_z \sum_i S_i^z S_{i+1}^z \,. \tag{1.1.1}$$

Here, $\boldsymbol{S}_i$ is the spin $S = 1/2$ operator. Expressing the $\uparrow$ spin state as $[1,0]^t$ and the $\downarrow$ state as $[0,1]^t$, and using the Pauli matrices $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma^y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \qquad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

the spin operator is given by $\boldsymbol{S}_i = (\hbar/2)\boldsymbol{\sigma}_i$. The spin operator satisfies

$$\left[S_i^\alpha, S_j^\beta\right] = \mathrm{i}\hbar\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_i^\gamma \,. \tag{1.1.2}$$

$\varepsilon_{\alpha\beta\gamma}$ is the total antisymmetric tensor with $\varepsilon_{xyz} = 1$. In what follows, we usually set $\hbar = 1$. $J_\perp$ as well as J_z are the nearest-neighbour exchange interactions; and for the case $J_\perp = J_z$, the Hamiltonian is called the Heisenberg model.

From the commutation relation (1.1.2), it is clear that the unitary operator

$$U_i(\boldsymbol{n}, \theta) = \mathrm{e}^{\mathrm{i}\theta \boldsymbol{n}\cdot\boldsymbol{S}_i} \tag{1.1.3}$$

rotates the spin. Here, $\boldsymbol{n}$ is the unit vector, and θ is the rotation angle. For example, the case where $\boldsymbol{n} = \boldsymbol{e}_z = (0,0,1)$,

$$U_i(\boldsymbol{e}_z, \theta) S_i^\alpha U_i^\dagger(\boldsymbol{e}_z, \theta) = \tilde{S}_i^\alpha(\theta) \,, \tag{1.1.4}$$

leads to

$$\frac{\mathrm{d}\tilde{S}_i^x(\theta)}{\mathrm{d}\theta} = U_i \cdot \mathrm{i}\,[S_i^z, S_i^x]\,U_i^\dagger = -\tilde{S}_i^y(\theta)\,, \tag{1.1.5a}$$

$$\frac{\mathrm{d}\tilde{S}_i^y(\theta)}{\mathrm{d}\theta} = \tilde{S}_i^x(\theta)\,, \tag{1.1.5b}$$

$$\frac{\mathrm{d}\tilde{S}_i^z(\theta)}{\mathrm{d}\theta} = 0\,. \tag{1.1.5c}$$

The solution is then given by

$$\tilde{S}_i^x(\theta) = S_i^x \cos\theta - S_i^y \sin\theta\,, \tag{1.1.6a}$$

$$\tilde{S}_i^y(\theta) = S_i^x \sin\theta + S_i^y \cos\theta\,, \tag{1.1.6b}$$

$$\tilde{S}_i^z(\theta) = S_i^z\,. \tag{1.1.6c}$$

Obviously, this describes a rotation around the z-axis. Next, constructing the unitary operator $T = \prod_{n:\mathrm{odd}} U_n(\boldsymbol{e}_z, \pi)$ from U_i, because of

$$TS_i^xT^\dagger = (-1)^i S_i^x\,, \tag{1.1.7a}$$

$$TS_i^yT^\dagger = (-1)^i S_i^y\,, \tag{1.1.7b}$$

$$TS_i^zT^\dagger = S_i^z\,. \tag{1.1.7c}$$

the transformation $THT^\dagger$ of (1.1.1) interchanges $J_\perp \to -J_\perp, J_z \to J_z$. We conclude that the sign of $J_\perp$ is not essential.

On the other hand, the sign of J_z plays an essential role for the quantum system. This is owing to the fact that, different from (1.1.7), the commutation relation (1.1.2) of the spin components is changed for $\boldsymbol{S}_i \to -\boldsymbol{S}_i$. First, we construct with S^x and S^y:

$$S^\pm = S^x \pm \mathrm{i}S^y\,. \tag{1.1.8}$$

Because of

$$S^+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad S^- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

S^+ is the operator that flips the spin $\uparrow$ state to $\downarrow$, and S^- flips $\downarrow$ to $\uparrow$. Using these operators, the Hamiltonian (1.1.1) can be re-expressed as

$$H = \frac{J_\perp}{2} \sum_i \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + J_z \sum_i S_i^z S_{i+1}^z\,. \tag{1.1.9}$$

Now, regarding S_i^z as a 'coordinate', $S_i^\pm$ displace this coordinate as if it were the 'momentum'. In this interpretation, the unitary operator U_i (1.1.3) corresponds to the linear transformation operator $U = e^{\mathrm{i}\alpha p}$ (x: coordinate; p: momentum; α: constant). Then, the term proportional to $J_\perp$ in (1.1.9) represents the 'kinetic energy' causing the quantum fluctuations of S_i^z, and

the term proportional to J_z represents the 'potential energy' that causes the ordering of S_i^z. The competition between these two tendencies is the physics that is contained in (1.1.1) as well as in (1.1.9).

We first consider the classical limit $J_\perp = 0$. This is the so-called Ising-model; and the spins align at zero temperature depending on the sign of J_z ferromagnetic ally ($J_z < 0$), or anti-ferromagnetically ($J_z > 0$). Notice that the ground state is two-fold degenerate because the Hamiltonian is invariant under the transformation $S_z^i \to -S_z^i$, performed at all sites i. Calling these two ground states A and B and assuming that the system at the right-hand side is in state A, and at the left-hand side in state B, then somewhere there must exist a boundary between region A and region B. This boundary is called a kink or soliton. Because at finite temperature this excitation occurs with a finite density, the spin correlation function $F(r) = \langle S_i^z S_{i+r}^z \rangle$ will decay exponentially with a correlation length ξ.

Let us determine this explicitly. We align N spins from $i = 1$ to $i = N$ with free ends. In the thermodynamic limit $N \to \infty$, we can ignore the influence of the boundary. We first assume that the spin S_1^z at the left side is fixed to, say, $1/2$. Then, instead of S_2^z, it is possible to consider $L_{12} \equiv S_1^z S_2^z$ as variable. In the same manner, instead of S_3^z, defining $L_{23} \equiv S_2^z S_3^z$ and so on, the statistical mechanics can be formulated in terms of $L_{i,i+1}$ instead of S_i^z. The correlation between S_i^z and S_{i+1}^z, being defined on the site, is expressed by $L_{i,i+1}$, being defined on the link. In the parallel or anti-parallel case, the obtained value is $\pm 1/4$, respectively. Now, we write $L_{i+1/2}$ instead of $L_{i,i+1}$. Then, the Ising model can be expressed as

$$H = J_z \sum_{i=1}^{N-1} L_{i+1/2}\,, \tag{1.1.10}$$

which is the independent sum of the energy at every link. The free energy of every site can be calculated easily:

$$\begin{aligned} f &= -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N} \ln Z = -\frac{1}{\beta} \ln \sum_{L=\pm 1/4} \mathrm{e}^{-\beta J_z L} \\ &= -\frac{1}{\beta} \ln \left(2 \cosh \frac{\beta J_z}{4} \right) . \end{aligned} \tag{1.1.11}$$

Next, based on the above discussion, we calculate $F(r) = \langle S_i^z S_{i+r}^z \rangle$. First, we observe that $S_i^z S_{i+r}^z$ is 'non-local' when expressed in terms of $L_{j+1/2}$. That is,

$$4 S_i^z S_{i+r}^z = (4L_{i+1/2})(4L_{i+3/2}) \ldots (4L_{i+r-1/2}) \tag{1.1.12}$$

can be expressed as the product of r terms in L connecting the sites i and $i + r$. With (1.1.10), from this fact we obtain

$$4F(r) = \prod_{j=1}^{r} \left[\frac{\sum_{L=\pm 1/4} 4L\, \mathrm{e}^{-\beta J_z L}}{\sum_{L=\pm 1/4} \mathrm{e}^{-\beta J_z L}} \right]$$
$$= \left[\tanh\left(\frac{-\beta J_z}{4} \right) \right]^r$$
$$= (-\operatorname{sgn} J_z)^r \exp\left[r \ln \tanh\left(\frac{\beta |J_z|}{4} \right) \right] . \qquad (1.1.13)$$

Writing the absolute value of the left-hand side of (1.1.13) as $\mathrm{e}^{-r/\xi}$, the correlation length ξ is determined to be

$$\xi = -\frac{1}{\ln \tanh\left(\frac{\beta |J_z|}{4} \right)} . \qquad (1.1.14)$$

Furthermore, at low temperature $\beta |J_z| \gg 1$, in the limit where a small number of kinks are thermally excited, equation (1.1.14) becomes

$$\xi^{-1} = 2\, \mathrm{e}^{-\beta |J_z|/2} . \qquad (1.1.15)$$

Recalling that the creation energy for a kink is given by $\Delta E = |J_z|/2$, the right-hand side corresponds to the number of kinks, and ξ can be interpreted as the mean distance between two kinks. That is, the long-range order $F(r) = \frac{1}{4}(-\operatorname{sgn} J_z)^r$ at $T = 0\,\mathrm{K}$ is destroyed owing to kink excitation. Notice that a kink comes up as a change in sign of $L_{i+1/2}$.

The classical statistical mechanics described above almost did not depend on the sign of J_z. The only dependence emerges in $(-\operatorname{sgn} J_z)^r$ in (1.1.13), and, indeed, J_z changes to $-J_z$ when in the Hamiltonian all S_i^z are altered to $-S_i^z$. When proceeding to quantum mechanics, this is no longer correct. This is owing to the following reason. The term proportional to $J_\perp$ in (1.1.9) causing the quantum mechanical motion expresses the simultaneous flip of two neighbouring spins. It can be expressed as a product of S^+ and S^-, therefore when one S^z is growing, the other must diminish, and the sum $S_i^z + S_{i+1}^z$ is conserved. This simultaneous spin flip is the change between $|S_i^z = 1/2, S_{i+1}^z = -1/2\rangle$ and $|S_i^z = -1/2, S_{i+1}^z = 1/2\rangle$. For parallel spins, this change cannot occur. In a more mathematical language, let us define the total spin operator:

$$\boldsymbol{S}_{\mathrm{tot}} = \sum_i \boldsymbol{S}_i . \qquad (1.1.16)$$

Then, $S_{\mathrm{tot}}^2 = \boldsymbol{S}_{\mathrm{tot}} \cdot \boldsymbol{S}_{\mathrm{tot}}$, and S_{tot}^z commute with the Hamiltonian (1.1.9):

$$[S_{\mathrm{tot}}^2, H] = [S_{\mathrm{tot}}^z, H] = 0 . \qquad (1.1.17)$$

That is, the quantum system can be decomposed into eigenstates of S_{tot}^2 and S_{tot}^z. In the case when $J_z < 0$ of the ferromagnetic interaction, it is clear

that the classical ground states $|\{S_i^z = 1/2\}\rangle$ and $|\{S_i^z = -1/2\}\rangle$ are also the eigenstates of the Hamilton operator H. On the other hand, the classical ground state in the anti-ferromagnetic case (the so-called Néel state) is not an eigenstate of the Hamiltonian. This becomes clear by constructing the staggered magnetization

$$S_{\text{staggered}} = \sum_i (-1)^i S_i \,. \tag{1.1.18}$$

The Néel state is an eigenstate of $S^z_{\text{staggered}}$. However, $[S^z_{\text{staggered}}, H]$ is different from zero. That is, for $S^z_{\text{staggered}}$ there must exist a zero point quantum fluctuation. The physical picture for this zero point fluctuation is just the resonance between the states $|S_i^z = 1/2, S_{i+1}^z = -1/2\rangle$ and $|S_i^z = -1/2, S_{i+1}^z = 1/2\rangle$ that has been mentioned before. Considering for simplicity only two spins, S_i and S_{i+1}, setting $J_\perp > 0$, owing to this resonance the ground state becomes a linear combination of two states

$$|\text{singlet}\rangle = \frac{1}{\sqrt{2}} \left(\left| \frac{1}{2}, -\frac{1}{2} \right\rangle - \left| -\frac{1}{2}, \frac{1}{2} \right\rangle \right) . \tag{1.1.19}$$

This is the spin singlet wave function. That is, the quantum fluctuation of S_i^z leads to the singlet formation. Equation (1.1.9) can be interpreted as competition between the tendency of $J_\perp$ to create singlet states leading to the emergence of a quantum liquid, and the tendency of J_z to order the spins.

Above, considerations concerning the ground state have been done. Next, we consider the first excited state based on the Néel ground state of the classical system. This is the domain wall as shown in Fig. 1.1. In what follows, we think about the Ising limit $J_z \gg J_\perp > 0$, where mixing between states with different numbers of domain walls can be ignored. First, we consider the state containing one domain wall. Calling Ψ_n the wave function of the state where a domain wall is present between site n and $n+1$, we obtain

$$(H - E_{\text{Néel}})\Psi_n = \frac{J_z}{2}\Psi_n + \frac{J_\perp}{2}(\Psi_{n+2} + \Psi_{n-2}) \,. \tag{1.1.20}$$

Constructing a plane wave state of a domain wall

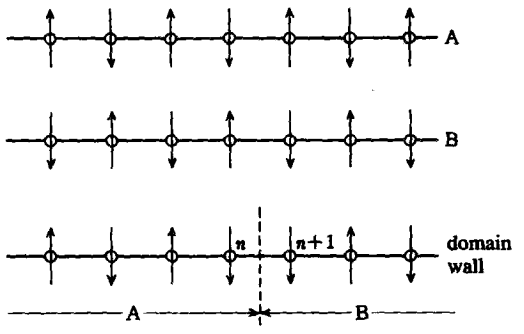

Fig. 1.1. The two degenerate classical Néel ground states A and B and the domain wall

$$\Psi(k) = \frac{1}{\sqrt{N}} \sum_n \mathrm{e}^{\mathrm{i}kn} \Psi_n \,, \tag{1.1.21}$$

we obtain

$$(H - E_{\text{Néel}})\Psi(k) = \left(\frac{J_z}{2} + J_\perp \cos 2k \right) \Psi(k) \,. \tag{1.1.22}$$

Therefore, the excitation energy is given by

$$\varepsilon_{\text{DW}}(k) = \frac{J_z}{2} + J_\perp \cos 2k \,. \tag{1.1.23}$$

When one domain wall is present (in general, an odd number), the sign of the staggered magnetization of the configuration at the boundaries $n = -\infty$ and $n = +\infty$ changes. Therefore, no long-range order is present in the Ising model at finite temperature as discussed above. Here, because we consider excited states at zero temperature, we set the staggered magnetization at $n = \pm\infty$ to be equal, corresponding to periodic boundary condition. Then, at least two domain walls have to be created. Calling the momenta k_1 and k_2, respectively, the total momentum q and the excitation energy ΔE are given by

$$\begin{aligned} q &= k_1 + k_2 \\ \Delta E &= \varepsilon_{\text{DW}}(k_1) + \varepsilon_{\text{DW}}(k_2) \,. \end{aligned} \tag{1.1.24}$$

The possible values for ΔE for every q are given by the oblique region in Fig. 1.2. In particular, the lower boundary is given by

$$\Delta E_{\text{LB}} = J_z - 2J_\perp |\cos q| \,. \tag{1.1.25}$$

We conclude that the excitation spectrum does not consist of isolated spin wave states, but is the continuum, reflecting the fact that the elementary excitations are kinks (domain walls).

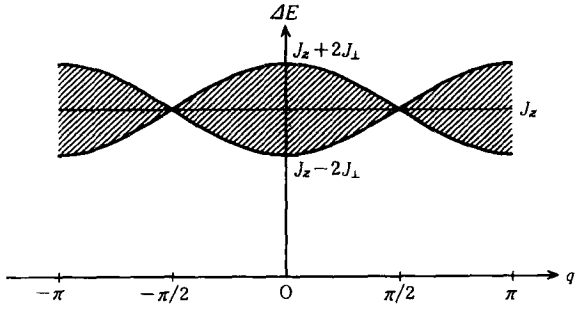

Fig. 1.2. The energy of the domain wall pair

1.2 The Jordan–Wigner Transformation and the Quantum Kink

In the previous section, the one-dimensional Ising model has been discussed as an example to demonstrate the importance of the kink. In this chapter, the quantum mechanics of the kink will be discussed in more detail. Starting with the conclusion, we note that the kink can be described in terms of fermions obtained by the following so-called Jordan–Wigner transformation

$$S_i^+ = S_i^x + \mathrm{i}S_i^y = f_i^\dagger K(i) = K(i) f_i^\dagger \,, \tag{1.2.1a}$$

$$S_i^- = S_i^x - \mathrm{i}S_i^y = K(i) f_i = f_i K(i) \,, \tag{1.2.1b}$$

$$S_i^z = f_i^\dagger f_i - \tfrac{1}{2} \,. \tag{1.2.1c}$$

Here, $K(i)$ is a non-local operator, defined by

$$K(i) = \exp\left[\mathrm{i}\pi \sum_{j=1}^{i-1} f_j^\dagger f_j\right] = \exp\left[\mathrm{i}\pi \sum_{j=1}^{i-1} \left(S_j^z + \frac{1}{2}\right)\right] \,. \tag{1.2.2}$$

$K(i) = K(i)^\dagger$, and $[K(i), K(j)] = 0$. Furthermore, for $i \leq j$, $K(i)$ and $\boldsymbol{S}_j$ also commute. From (1.2.1) we conclude:

$$\begin{aligned} f_i^\dagger &= S_i^+ K(i) \,, \\ f_i &= S_i^- K(i) \,. \end{aligned} \tag{1.2.3}$$

From these equations, the anti-commutation relation of fermions can be deduced.

We first examine the meaning of $K(i)$. Using the unitary operator U_i introduced in (1.1.3), we can write

$$K(i) = \left[\prod_{j=1}^{i-1} U_j(\boldsymbol{e}_z, \pi)\right] \mathrm{e}^{\frac{\mathrm{i}\pi}{2}(i-1)} \,. \tag{1.2.4}$$

We conclude that $K(i)$ rotates all spins from $j = 1$ to $i - 1$ by π around the z axis; that is, this operator shifts S^x and S^y to $-S^x$ and $-S^y$. $K(i)$ is a non-local spin rotating operator, and therefore creates a kink. Now, for $i < j$ we consider

$$f_i f_j = S_i^- K(i) S_j^- K(j) \,. \tag{1.2.5}$$

From the above considerations, we obtain

$$K^\dagger(j) S_i^- K(j) = -S_i^- \tag{1.2.6}$$

that is, $K(j)$ and S_i^- do anti-commute (for $j > i$). Finally, the right-hand side of (1.2.5) becomes

$$S_i^- K(i) S_j^- K(j) = S_i^- S_j^- K(i)K(j) = S_j^- S_i^- K(i)K(j)$$
$$= -S_j^- K(j) S_i^- K(i) = -f_j f_i \tag{1.2.7}$$

and therefore

$$\{f_i, f_j\}_+ = 0 \tag{1.2.8}$$

holds. In the same manner, for $i < j$, because of

$$f_i f_j^\dagger + f_j^\dagger f_i = S_i^- K(i) S_j^+ K(j) + S_j^+ K(j) S_i^- K(i)$$
$$= S_i^- S_j^+ K(i)K(j) - S_j^+ S_i^- K(j)K(i)$$
$$= \left[S_i^-, S_j^+\right] K(i)K(j) = 0\,,$$

we obtain

$$\left\{f_i, f_j^+\right\} = \delta_{ij}\,. \tag{1.2.9}$$

In this manner, the non-local spin rotating operator (in the xy-plane) translates the commutation relation of the spin operators at different sites into the anti-commutation relation of fermion operators. As follows from (1.2.1c), at one site, the two possible states $S_i^z = \pm 1/2$ correspond to fermion number $n_i = f_i^\dagger f_i = 1, 0$, respectively. We see how the Pauli principle naturally describes the limited possibilities for the allowed spin states. That these fermions correspond to kinks can be seen by considering, for example, the state $|F\rangle$ where all spins are in the state $S_i^x = +1/2$. Acting with $f_n^\dagger$, we obtain the state $f_n^\dagger|F\rangle$ with $S_i^x = -\frac{1}{2}$ $(1 \le i < n)$, $S_n^x = +\frac{1}{2}$, $S_i^z = +\frac{1}{2}$ $(i > n)$.

The Jordan–Wigner transformation works well because although (1.2.1) is non-local, the Hamiltonian (1.1.1) [(1.1.9)] can be expressed with these fermions in a local manner. First, we consider the term proportional to $J_\perp$:

$$S_i^+ S_{i+1}^- = f_i^+ K(i)K(i+1) f_{i+1}$$
$$= f_i^+ \exp\left[\mathrm{i}\pi f_i^\dagger f_i\right] f_{i+1} = f_i^+ f_{i+1}\,. \tag{1.2.10}$$

Here, we used the fact that in the state multiplied with $\exp[\mathrm{i}\pi f_i^\dagger f_i]$, owing to $f_i^\dagger$, at the ith site no more fermion can be present. Also, the term proportional to J_z can be expressed locally using (1.2.1c), leading finally to

$$H = -\frac{J_\perp}{2} \sum_{i=1}^{N} \left(f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i\right) + J_z \sum_{i=1}^{N} \left(f_i^\dagger f_i - \frac{1}{2}\right)\left(f_{i+1}^\dagger f_{i+1} - \frac{1}{2}\right). \tag{1.2.11}$$

As mentioned in Sect. 1.1, the sign of $J_\perp$ can be chosen freely, therefore we can put a minus sign before $J_\perp > 0$. We obtained the spinless fermion model with nearest site interaction J_z.

At this point, we discuss the periodic boundary conditions. Considering a ring and setting

$$\boldsymbol{S}_{N+1} = \boldsymbol{S}_1\,, \tag{1.2.12}$$

the term $i = N$ proportional to $J_\perp$ in (1.2.11) becomes

$$\frac{J_\perp}{2}\left(S_N^+ S_1^- + S_N^- S_1^+\right) . \tag{1.2.13}$$

Here, we obtain

$$S_N^+ S_1^- = K(N) f_N^\dagger f_1 = -K f_N^\dagger f_1 . \tag{1.2.14}$$

The factor K can be expressed as

$$K = \exp\left[\mathrm{i}\pi \sum_{i=1}^{N} f_i^\dagger f_i\right] = (-1)^M \tag{1.2.15}$$

using the total number $M = \sum_{i=1}^{N} f_i^\dagger f_i$ of fermions. The minus sign on the right-hand side of (1.2.14) arises because in $K(N)$, $f_N^\dagger f_N$ is not contained. Defining

$$f_{N+1} = -f_1 \qquad (M : \text{even}) \tag{1.2.16a}$$

$$f_{N+1} = f_1 \qquad (M : \text{odd}) \tag{1.2.16b}$$

then (1.2.11) is valid as it stands.

As was mentioned in the previous section, (1.2.11) expresses competition between the formation of a spin singlet state and magnetic ordering, that is, competition between the kinetic energy of the fermions, i.e. itineracy, and the formation of density waves owing to the particle interaction. One remarkable feature of (1.2.11) is that in the case $J_z = 0$ (XY model); that is, in the quantum limit, the model becomes a free fermion theory that can be solved exactly. This limit is the opposite to the Ising limit that has been mentioned in the previous section. Introducing the Fourier transformations

$$f_n = \frac{1}{\sqrt{N}} \sum_k f_k \, \mathrm{e}^{\mathrm{i}kn} , \tag{1.2.17a}$$

$$f_n^\dagger = \frac{1}{\sqrt{N}} \sum_k f_k^\dagger \, \mathrm{e}^{-\mathrm{i}kn} , \tag{1.2.17b}$$

we obtain from (1.2.11)

$$H_{XY} = \sum_k \varepsilon(k) \cdot f_k^\dagger f_k \qquad (\varepsilon(k) = -J_\perp \cos k) . \tag{1.2.18}$$

The energy dispersion is shown in Fig. 1.3.

Owing to (1.2.1c), the relationship between the fermion number M and S_{tot}^z is $S_{\mathrm{tot}}^z = M - N/2$. The Hilbertspace $S_{\mathrm{tot}}^z = 0$ corresponds to the half-filled case $M = N/2$. In this case, the ground state is given by the state where the fermions occupy all states up to the Fermi energy $E_\mathrm{F} = 0$. Excited states can be expressed as particle–hole creation. When N is even, the ground state is a singlet $S_{\mathrm{tot}} = 0$, and the excited states start with $S_{\mathrm{tot}} = 0$ or $S_{\mathrm{tot}} = 1$.