Chapter 2
Transverse Ising Chain (Pure System)

2.1 Symmetries and the Critical Point

2.1.1 Duality Symmetry of the Transverse Ising Model

Following the duality of the two dimensional Ising model on square lattice [237], one can show [231] the self-duality, and thereby make exact estimate of the critical tunnelling (transverse) field of the one-dimensional spin-1/2 transverse Ising model. Before considering the exact solution of the one dimensional quantum mechanical Hamiltonian, we shall study the duality symmetry hidden in the model, and identify the critical value of the transverse field, for which there exists a second order zero-temperature phase transition from a ferromagnetic phase to a paramagnetic phase.

Let us first consider the quantum Hamiltonian of the transverse Ising chain

$$H = -\sum_i \left[\Gamma S_i^x + J S_i^z S_{i+1}^z\right] = -\sum_i \left[S_i^x + \overline{\lambda} S_i^z S_{i+1}^z\right] \tag{2.1.1}$$

where S^αs are the usual the Pauli spin matrices, $\overline{\lambda} = J/\Gamma$, and the Hamiltonian is scaled with the transverse field ($\Gamma = 1$). The spin operators satisfy the usual commutation relations given by (with $\hbar = 1$)

$$\left[S_i^\alpha, S_j^\beta\right] = 2i\delta_{ij}\epsilon_{\alpha\beta\gamma} S_i^\gamma; \quad \alpha, \beta, \gamma = x, y, z. \tag{2.1.2}$$

It may be noted that the Pauli operators commute on different sites and satisfy the anti-commutation relation

$$\left[S_i^\alpha, S_i^\beta\right]_+ = S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha = 0, \tag{2.1.3}$$

and

$$\left(S_i^\alpha\right)^2 = 1 \tag{2.1.4}$$

on the same site.

To investigate the duality symmetry involved in the model we associate a dual lattice with our original spatial lattice (chain) such that sites in the original chain

S. Suzuki et al., *Quantum Ising Phases and Transitions in Transverse Ising Models*, Lecture Notes in Physics 862, DOI 10.1007/978-3-642-33039-1_2,

are associated with the bonds of the dual chain and vice versa. The operators on the dual lattice are defined as

$$\tau_j^x = S_j^z S_{j+1}^z \quad \text{and} \tag{2.1.5a}$$

$$\tau_j^z = \prod_{k \le j} S_k^x. \tag{2.1.5b}$$

The non-local mapping (2.1.5a), (2.1.5b) represents the "duality" transformation. As mentioned earlier, the new operators are defined on links of the original chain which has one-to-one correspondence with the sites of the "dual" lattice. From (2.1.5a), (2.1.5b) we can easily see that senses whether spins on the original lattice are aligned or not; whereas flips all the spins left to the site i. One can now easily check that the operators τ_i^α's satisfy the same set of commutation relation as the operator i.e., they commute on different sites and anti-commute on the same site

$$\left[\tau_i^x, \tau_i^z\right] = 0 \text{ for } i \neq j \quad \text{and} \quad \left[\tau_i^x, \tau_z\right]_+ = 0. \tag{2.1.6}$$

One can thus readily rewrite the original transverse Ising Hamiltonian in terms of the dual operators τ^α

$$\begin{aligned} H &= -\sum_i \left[\tau_i^z \tau_{i+1}^z + \overline{\lambda}\tau_i^x\right] \\ &= \overline{\lambda}\left[-\sum_i \tau_i^x - (\overline{\lambda})^{-1} \sum_i \tau_i^z \tau_{i+1}^z\right] \end{aligned} \tag{2.1.7}$$

which immediately suggests the (duality) scaling property of the Hamiltonian:

$$H(S; \overline{\lambda}) = \overline{\lambda} H\left(\tau; \overline{\lambda}^{-1}\right). \tag{2.1.8}$$

Since both S and τ operators satisfy the same algebra, the above symmetry implies, for the equivalent classical two dimensional Ising model (where Γ corresponds to inverse temperature), one-to-one correspondence of the high and low temperature phases. Here for the quantum model, it implies that each eigenvalue E of H satisfies the relation,

$$E(\overline{\lambda}) = \overline{\lambda} E(1/\overline{\lambda}). \tag{2.1.9}$$

Equation (2.1.9) has important significance from the point of quantum phase transition in the model. For the quantum phase transition, at the critical point the mass gap (the gap between the ground state and the first excited state of the quantum Hamiltonian) vanishes and the correlation length $\xi(\overline{\lambda})$ (which is the inverse of the mass gap $\Delta(\overline{\lambda})$) diverges. For the present model, if the mass gap vanishes for some nonzero value of then (2.1.9) suggests that it will also have to vanish at. If one assumes that is unique, the self-duality of the model implies that

$$\overline{\lambda}_c = 1, \quad \text{or} \quad \Gamma_c = J \tag{2.1.10}$$

and, as we will show in the next subsection,

$$\xi(\overline{\lambda}) \sim \Delta^{-1} = 2|1 - \overline{\lambda}|^{-1}. \tag{2.1.11}$$

The self-duality of the model thus yields the exact critical value if we assume that the critical value is unique (valid for simple Ising model, but is not true in general).

2.1.2 Perturbative Approach

In this section we shall try to estimate the mass gap associated with the above quantum Hamiltonian (1.2.1) for the transverse Ising chain, using a perturbative approach. We first rewrite the transverse Ising Hamiltonian in the following form

$$H = H_0 + V = \sum_i \left[1 - S_i^x\right] - \overline{\lambda} \sum_i S_i^z S_{i+1}^z, \tag{2.1.12}$$

with

$$H_0 = \sum_i \left[1 - S_i^x\right] \tag{2.1.13a}$$

$$V = -\sum_i S_i^z S_{i+1}^z, \tag{2.1.13b}$$

and write a perturbation series in powers of for any eigenvalue of the total Hamiltonian:

$$E(\overline{\lambda}) = E^{(0)} + \overline{\lambda} E^{(1)} + (\overline{\lambda})^2 E^{(2)} + \cdots. \tag{2.1.14}$$

The Hamiltonian H_0 represents a one dimensional chain of non-interacting spins in a magnetic field, and one can now trivially show that the lowest eigenvalue E_0 of H_0 is zero:

$$H_0|0\rangle = E_0^{(0)}|0\rangle = 0. \tag{2.1.15}$$

The corresponding bare vacuum $|0\rangle$ is given by

$$|0\rangle = \prod_{i=1}^{N} |+\rangle_i \tag{2.1.16}$$

where $|+\rangle_i$ is the eigenstate of the operator S_i^x with eigenvalue $= +1$. Similarly, one can easily see that the first excited state of the Hamiltonian H_0 consists of just one flipped spin $|0\rangle$ at the site i. But it is clearly seen that this state is N-fold degenerate, since the flipped spin can occur on any site of the one-dimensional lattice. Keeping in mind the translational invariance of the model (any eigenstate has to have a definite momentum) we can choose an appropriate linear combination for the first excited state of the Hamiltonian H_0 given by

$$|1\rangle = N^{1/2} \sum_i S_i^z |0\rangle, \tag{2.1.17}$$

the corresponding eigenvalue equation can be written as

$$H_0|1\rangle = E_1^{(0)}|1\rangle = 2|1\rangle. \tag{2.1.18}$$

Hence considering the unperturbed Hamiltonian ($\overline{\lambda} = 0$), we get the mass gap (at the zeroth order) of the system, given by

$$\Delta_0 \equiv E_1^{(0)} - E_0^{(0)} = 2. \tag{2.1.19}$$

We shall now incorporate the effect of V in a perturbative manner. To do this we must recall that the operator acts as a spin-flip operator on state $|0\rangle$ or for that matter, $|1\rangle$. We can thus immediately get for the first order corrections

$$E_0^{(1)} = \langle 0|V|0\rangle = 0, \tag{2.1.20a}$$

$$E_1^{(1)} = \langle 1|V|1\rangle = -2. \tag{2.1.20b}$$

Putting (2.1.20a), (2.1.20b) in the (2.1.14) we get

$$\begin{aligned} \Delta(\overline{\lambda}) \equiv E_1(\overline{\lambda}) - E_0(\overline{\lambda}) &= \left(E_1^{(0)} + \overline{\lambda}E_1^{(1)}\right) - \left(E_0^{(0)} + \overline{\lambda}E_0^{(1)}\right) \\ &= 2(1 - \overline{\lambda}), \end{aligned} \tag{2.1.21}$$

up to first order in $\overline{\lambda}$.

Equation (2.1.21) suggests that as $\overline{\lambda}$ increases from zero, the mass gap decreases and vanishes at the critical value $\overline{\lambda}_c$, which is found to be unity here from the first order perturbation theory. Near the critical point, however, all higher order contributions to the mass gap are expected to become relevant. But Kogut [231], using Raleigh-Schrödinger perturbation theory, estimated the higher order corrections in $\overline{\lambda}$ to the mass gap $\Delta(\overline{\lambda})$ and found that all the higher order contributions vanish identically in $(1 + 1)$-dimension. Note that "+1" in the dimension comes from the imaginary-time Trotter direction. We shall discuss in the next chapter the equivalence between a d-dimensional transverse Ising model and a $(d + 1)$-dimensional Ising model. In dimensions higher than $d = 1$, of course, all the beneficial properties of the perturbation scheme are lost, the perturbation series does not truncate in the first order.

We have just seen that the mass gap of the elementary excitations vanishes as $\overline{\lambda}$ approaches 1 from below. Although this perturbative estimate is valid for $\overline{\lambda} < 1$, one can always extend it for $\overline{\lambda} > 1$ using the duality symmetry of the Hamiltonian. As the mass gap also satisfies the duality condition (cf. (2.1.9))

$$\Delta(\overline{\lambda}) = \overline{\lambda}\Delta\left(\overline{\lambda}^{-1}\right), \tag{2.1.22}$$

we can write the general form for mass gap as

$$\Delta(\overline{\lambda}) = 2|1 - \overline{\lambda}|. \tag{2.1.23}$$

This suggests that the gap vanishes both from below and above the critical point $\overline{\lambda} = \overline{\lambda}_c = 1$. This also gives the estimate of correlation length $\xi(\overline{\lambda}) \sim |\overline{\lambda} - \overline{\lambda}_c|^{-\nu} \sim \Delta^{-1}(\overline{\lambda})$ where ν represents correlation length exponent. From (2.1.23) we get

$$\xi(\overline{\lambda}) = (1/2)|1 - \overline{\lambda}|^{-1}, \tag{2.1.24}$$

giving $\nu = 1$ for the transverse Ising chain.

We now conclude this section with the note that the hidden duality symmetry makes our task simpler in the case of the spin-1/2 transverse Ising system in $1+1$-dimension. Employing duality and perturbation technique we can extract a number of information about the associated quantum phase transition. Unfortunately, this symmetry does not hold for higher dimensional models.

2.2 Eigenvalue Spectrum: Fermionic Representation

The above spin-1/2 transverse Ising chain Hamiltonian can be exactly diagonalised, and the entire eigenvalue spectrum and eigenfunctions can be obtained by employing Jordan-Wigner transformation of the spin operators to spinless fermions [245, 312] (see also [216]).

For this, we consider again the Hamiltonian (2.1.1). Using a canonical transformation

$$S^x \to S^z, \qquad S^z \to -S^x,$$

we rewrite the Hamiltonian (2.1.1) as

$$H = -\sum_i S_i^z - \overline{\lambda} \sum_i S_i^x S_{i+1}^x. \tag{2.2.1}$$

We can now express the Hamiltonian H in terms of the raising and lowering operators S_i^+ and S_i^- at every site, where

$$S_i^+ = (1/2)\left[S_i^x + i S_i^y\right]$$
$$S_i^- = (1/2)\left[S_i^x - i S_i^y\right]$$

which satisfy a mixed set of commutation relations, i.e., commute on different sites and satisfy the fermionic anti-commutation relations on the same site:

$$\left[S_i^-, S_j^+\right] = 0, \quad \left[S_i^+, S_j^-\right] = 0; \quad i \neq j$$

and

$$\left[S_i^-, S_i^+\right]_+ = 1$$
$$\left[S_i^-, S_i^-\right]_+ = \left[S_i^+, S_i^+\right]_+ = 0.$$

The last condition implies that if an arbitrary state $|F\rangle$ is not annihilated by , then it is annihilated by $(S_i^+)^2$ (a spin can be flipped only once):

$$S_i^+\left[S_i^+|F\rangle\right] = 0; \qquad \left(S_i^+\right)^2 = 0.$$

The above equation implies that, although the operator S_i^+ creates a bosonic excitation at the site i, it is impossible to have two such excitations at the same site. This is the hard-sphere condition, and the raising and lowering operators should appropriately be treated as hard-core bosons.

The standard procedure to treat one dimensional hard-core bosons is to transform the spin operators into fermions by using the Jordan-Wigner transformation

$$c_1 = S_1^-, \qquad c_i = \prod_{j=1}^{i-1} \exp\left[i\pi S_j^+ S_j^-\right] S_i^- \quad (i = 2, \ldots, N) \tag{2.2.2a}$$

$$c_1^\dagger = S_1^+, \qquad c_i^\dagger = S_i^+ \prod_{j=1}^{i-1} \exp\left[-i\pi S_j^+ S_j^-\right] \quad (i = 2, \ldots, N). \tag{2.2.2b}$$

One can easily check that (see Sect. 2.A.1) the operators c_i and $c_i^\dagger$ are fermionic operators satisfying

$$\left[c_i, c_j^\dagger\right]_+ = \delta_{ij}; \qquad [c_i, c_i]_+ = 0. \tag{2.2.3}$$

Unlike the spin operators, the fermion operators anti-commute even at different sites and this is due to the presence of the non-local factor

$$K_i = \exp\left[i\pi \sum_{j=1}^{i-1} S_j^+ S_j^-\right] \quad (i = 2, \ldots, N), \tag{2.2.4}$$

which is called the disorder or "soliton" term which provides an extra minus sign to convert a commutator to an anti-commutator at different sites. This term is a unitary operator which rotates (up to a phase factor) the spin configuration of all sites left to the i-th site by an angle π about the z-axis. This term is called the disorder term since it cannot have a nonzero expectation value in a state having a long-range order. On the other hand, it may have a nonzero expectation value in a state having no long-range order. We can therefore transform the spin system into a system of spinless fermions with chemical potential zero, defined on a one dimensional lattice.

To write the Hamiltonian (2.2.1), in terms of Jordan-Wigner fermions, we need to worry about the boundary condition. If the spin chain has a periodic boundary condition, i.e.,

$$S_1^\alpha = S_{N+1}^\alpha; \quad \alpha = x, y, z \tag{2.2.5}$$

then we can recast the transverse Ising Hamiltonian in the following form (see Sect. 2.A.1)

$$H = N - 2\sum_i c_i^\dagger c_i - \overline{\lambda} \sum_i \left[c_i^\dagger - c_i\right]\left[c_{i+1}^\dagger + c_{i+1}\right], \tag{2.2.6}$$

where we have neglected the correction term $[(c_1^\dagger + c_1)(c_N^\dagger - c_N)\{\exp(i\pi L) + 1\}]$, where $L = \sum_{i=1}^N c_i^\dagger c_i$, arising from the periodic boundary condition of spins for large systems. One must note here that although the number of fermions $\sum_i c_i^\dagger c_i$ is not a constant of motion, its parity is conserved and hence $\exp(i\pi L)$ is a constant of motion having the value $+1$ or -1. Hence, the fermion problem must have an anti-periodic boundary condition if there is an even number of fermions and periodic boundary condition if there is an odd number of fermions. The correction term

can be neglected for a thermodynamically large system in which case we call it the "c-cyclic" problem (the original problem being the "a-cyclic" one). The above transformed Hamiltonian is already quadratic in the fermion operators and it is obviously diagonalisable. To do so, let us consider fermions in momentum space

$$c_q = (1/N)^{1/2} \sum_{j=1}^{N} c_j \exp(iqR_j) \tag{2.2.7a}$$

$$c_q^\dagger = (1/N)^{1/2} \sum_{j=1}^{N} c_j^\dagger \exp(-iqR_j) \tag{2.2.7b}$$

where the complete set of wavevector is $q = 2\pi m/N$,

$$m = -(N-1)/2, \ldots, -1/2, 1/2, \ldots, (N-1)/2 \quad \text{(for } N \text{ even)}$$

$$m = N/2, \ldots, 0, \ldots, N/2 \quad \text{(for } N \text{ odd)}$$

and the final form of the transverse Ising chain Hamiltonian becomes

$$H = N - 2\sum_q (1 + \overline{\lambda}\cos q) c_q^\dagger c_q - \overline{\lambda} \sum_q \left(\mathrm{e}^{-iq} c_q^\dagger c_{-q}^\dagger - \mathrm{e}^{iq} c_q c_{-q} \right). \tag{2.2.8}$$

To diagonalise the Hamiltonian, we employ the Bogoliubov transformation in which new fermion creation operators $\eta_q^\dagger$ are formed as a linear combination of $c_q^\dagger$ and c_q in order to remove terms in Hamiltonian which do not conserve the particle number.

For this, it is convenient to sum over modes with $q > 0$ and include the others by simply writing them out. Then above Hamiltonian (2.2.8) becomes

$$\begin{aligned} H &= -2\sum_{q>0} (1 + \overline{\lambda}\cos q)\left(c_q^\dagger c_q - c_{-q} c_{-q}^\dagger \right) + 2i\overline{\lambda} \sum_{q>0} \sin q \left(c_q^\dagger c_{-q}^\dagger - c_{-q} c_q \right) \\ &= -2 \begin{pmatrix} c_q^\dagger & c_{-q} \end{pmatrix} \begin{pmatrix} 1 + \overline{\lambda}\cos q & -i\overline{\lambda}\sin q \\ i\overline{\lambda}\sin q & -1 - \overline{\lambda}\cos q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix}, \end{aligned} \tag{2.2.9}$$

where the constant N in (2.2.8) is cancelled by $2\sum_{q>0} 1$. Note that the vacuum of H is not the vacuum of the operator c_q because of the presence of the off-diagonal term $(c_q^\dagger c_{-q}^\dagger + c_q c_{-q})$ in the Hamiltonian. We wish to write the Hamiltonian in the form

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + \text{const}, \tag{2.2.10}$$

so that the single particle excitations are identifiable above the vacuum state $(\eta_q|0\rangle = 0)$. This is achieved by making a canonical transformation from the operators c_q, $c_q^\dagger$ to the operators η_q, $\eta_q^\dagger$ (Bogoliubov transformations)

$$\begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix} = \begin{pmatrix} u_q & iv_q \\ iv_q & u_q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} = \begin{pmatrix} u_q c_q + iv_q c_{-q}^\dagger \\ iv_q c_q + u_q c_{-q}^\dagger \end{pmatrix} \tag{2.2.11}$$

where $q > 0$ everywhere. The functions u_q, v_q are determined by two criteria: (1) These new set of operators η_q, $\eta_q^\dagger$, are fermionic operators. (2) The Hamiltonian (2.2.9) is diagonalised when written in terms of these operators. The choice of the transformation is made in the way such that u_q, v_q are real. The first criterion

$$\left[\eta_{q'}, \eta_q^\dagger\right]_+ = \delta_{q',q}, \qquad [\eta_{q'}, \eta_q]_+ = 0 = \left[\eta_{q'}^\dagger, \eta_q^\dagger\right]_+,$$

leads to the relation

$$u_q^2 + v_q^2 = 1. \tag{2.2.12}$$

Using now the inverse transformation of (2.2.11)

$$\begin{pmatrix} c_q \\ c_{-q}^\dagger \end{pmatrix} = \begin{pmatrix} u_q & -iv_q \\ -iv_q & u_q \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix}, \tag{2.2.13}$$

we can rewrite the Hamiltonian H in terms of the Bogoliubov fermions

$$\begin{aligned} H &= \sum_{q>0} H_q \\ H_q &= -2\begin{pmatrix} \eta_q^\dagger & \eta_{-q} \end{pmatrix} \begin{pmatrix} u_q & iv_q \\ iv_q & u_q \end{pmatrix} \begin{pmatrix} 1+\overline{\lambda}\cos q & -i\overline{\lambda}\sin q \\ i\overline{\lambda}\sin q & -1-\overline{\lambda}\cos q \end{pmatrix} \\ &\quad \times \begin{pmatrix} u_q & -iv_q \\ -iv_q & u_q \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^\dagger \end{pmatrix}. \end{aligned} \tag{2.2.14}$$

To recast the Hamiltonian in the diagonal form we demand that $(u_q, -iv_q)^T$ is an eigenvector of the Hamiltonian matrix

$$\begin{pmatrix} 1+\overline{\lambda}\cos q & -i\overline{\lambda}\sin q \\ i\overline{\lambda}\sin q & -1-\overline{\lambda}\cos q \end{pmatrix} \begin{pmatrix} u_q \\ -iv_q \end{pmatrix} = -\omega_q \begin{pmatrix} u_q \\ -iv_q \end{pmatrix}. \tag{2.2.15}$$

This 2×2 eigenvalue problem is easily solved to yield

$$\omega_q = \left(1 + 2\overline{\lambda}\cos q + \overline{\lambda}^2\right)^{1/2}, \tag{2.2.16}$$

and

$$u_q = \frac{\overline{\lambda}\sin q}{\sqrt{2\omega_q(\omega_q + 1 + \overline{\lambda}\cos q)}}, \quad v_q = \frac{\omega_q + 1 + \overline{\lambda}\cos q}{\sqrt{2\omega_q(\omega_q + 1 + \overline{\lambda}\cos q)}}, \tag{2.2.17}$$

where we have chosen the sign of u_q and v_q such that $u_q > 0$ for $0 < q < \pi$. Having obtained the eigenvalue ω_q, one can write the Hamiltonian in a diagonal form

$$H = 2\sum_{q>0} \omega_q\left(\eta_q^\dagger \eta_q - \eta_{-q}\eta_{-q}^\dagger\right) = 2\sum_q \omega_q \eta_q^\dagger \eta_q + E_0. \tag{2.2.18}$$

The zero-point (ground-state) energy of the spinless fermion system is given by

$$E_0 = -\sum_q \omega_q. \tag{2.2.19}$$

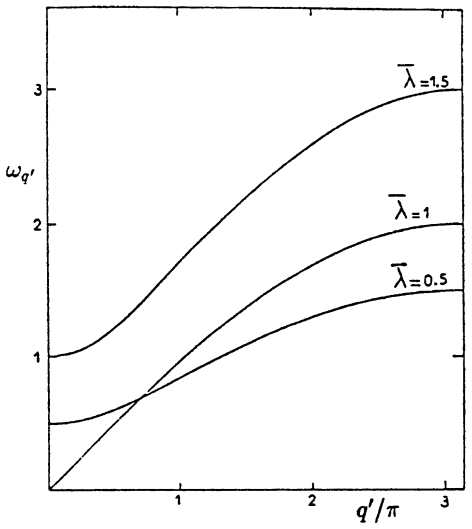

Fig. 2.1 Elementary excitation energy as a function of q'/π for different $\overline{\lambda}$ [312]

The Bogoliubov fermion operators are written as the linear combination of the original Jordan-Wigner fermions

$$\eta_q = \sum_i \left[\left(\frac{\phi_{qi} + \psi_{qi}}{2} \right) c_i + \left(\frac{\phi_{qi} - \psi_{qi}}{2} \right) c_i^\dagger \right], \tag{2.2.20}$$

where for $\overline{\lambda} \neq 1$ the normal modes [245, 312] are given by

$$\phi_{q,j} = \left(\frac{2}{N} \right)^{1/2} \sin(qR_j); \quad q > 0 \tag{2.2.21a}$$

$$= \left(\frac{2}{N} \right)^{1/2} \cos(qR_j); \quad q \leq 0 \tag{2.2.21b}$$

$$\psi_{qj} = -\omega_q^{-1} \left[(1 + \overline{\lambda} \cos q)\phi_{qj} + (\overline{\lambda} \sin q)\phi_{-qj} \right]. \tag{2.2.21c}$$

For $\overline{\lambda} = 1$ and $m = -1/2$ (i.e., $q = -\pi$),

$$\omega_q = 0, \qquad \phi_{qj} = N^{-1/2}, \qquad \psi_{qj} = \pm N^{-1/2}. \tag{2.2.22}$$

One can thus transform the spin Hamiltonian into a non-interacting set of fermions obeying the dispersion relation given by (2.2.16).

The energy of the elementary excitations as a function of wave vector $q' = \pi - q$ for different values of $\overline{\lambda}$ is shown in Fig. 2.1. There is an energy gap in the excitation spectrum of the system which goes to zero at $q' = 0$ for $\overline{\lambda} \equiv \overline{\lambda}_c = 1$ as

$$\Delta(\overline{\lambda}) \equiv E_1 - E_0 = 2|1 - \overline{\lambda}|, \tag{2.2.23}$$

indicating the divergence of the correlation length and a quantum phase transition at $\overline{\lambda} = \overline{\lambda}_c = 1$ from an ordered state ($\langle S^x \rangle = 1$) to a disordered state ($\langle S^x \rangle = 0$). One should mention at this point that the critical value of the transverse (tunnelling) field,

obtained from the exact solution of the one-dimensional chain, is $\Gamma_c = J$, whereas the mean field theory employed by Brout et al. (see Sect. 1.2), overestimates for the one-dimensional nearest neighbour chain and yields $\Gamma_c = 2J$.

At this point we remark on the simplification resulting from the consideration of the "c-cyclic" problem rather than the "a-cyclic" problem. The Hamiltonian for the "a-cyclic" problem is complicated by the presence of the term

$$\left[\left(c_1^\dagger + c_1\right)\left(c_N^\dagger - c_N\right)\right]\left[\exp(i\pi L) + 1\right].$$

As mentioned earlier, that although L is not a constant of motion, $\exp(i\pi L)$ is. Now in the ground state of the "c-cyclic" problem, in all states with even number of excitations, the number of fermions is odd (the q's are assumed to be occupied symmetrically around $q = 0$, except that $q = \pi$ but not $q = -\pi$ is occupied). Therefore, the additional term gives zero acting on such states and they remain eigenstates of the "a-cyclic" problem. States with odd number of excitation, on the other hand, have L even, giving an additional term in the Hamiltonian. This has the effect of making changes of the order of $1/N$ in the q's, ϕ_q's etc., which one can ignore for a thermodynamically large system. Strictly speaking the elementary excitations are not independent in the "a-cyclic" problems [245].

One must note that the above method of diagonalising a spin Hamiltonian in terms of free fermions is exact only in the case of pure transverse Ising chain in absence of any longitudinal field. One cannot generalise it to higher dimensional systems. For spin chains incorporating frustrations the resulting fermions are interacting (see Chap. 4) and hence can not be diagonalised exactly. For random interaction and transverse field Ising chain (see Chap. 5), one can map the problem to free fermion problem but as both J_i's and Γ_i's are random one has to adopt numerical diagonalisation technique.

2.2.1 The Ground State Energy, Correlations and Exponents

The ground state energy of the fermion system, given by the expression (2.2.19), can be reduced to the elliptic integral of second kind

$$-\frac{E_0}{NJ} = \frac{2}{\pi}(1+\overline{\lambda})E\left(\frac{\pi}{2},\theta\right); \quad \theta^2 = \frac{4\overline{\lambda}}{(1+i\overline{\lambda})^2}. \tag{2.2.24}$$

The ground state energy decreases monotonically with the transverse field and is non-analytic at the point $\overline{\lambda} = 1$ (see Fig. 2.2).

Defining the divergence of correlation length ($\xi(\overline{\lambda}) = \Delta^{-1}$) in the neighbourhood of the critical point $\overline{\lambda}_c = 1$ as $\xi(\overline{\lambda}) \sim (\overline{\lambda}_c - \overline{\lambda})^{-\nu}$, one can readily obtain from (2.2.23) the value of exponent $\nu = 1$. If one defines the variation of the energy gap as $\Delta(\overline{\lambda}) \sim (\overline{\lambda}_c - \overline{\lambda})^s$, the same equation yields $s = 1$. To evaluate the other exponents of the transition one has to calculate magnetisations and the different correlation functions using "Wick's Theorem" to evaluate the vacuum expectation value of many fermion operators [312]. The longitudinal magnetisation $\langle S^x \rangle$ (the order parameter

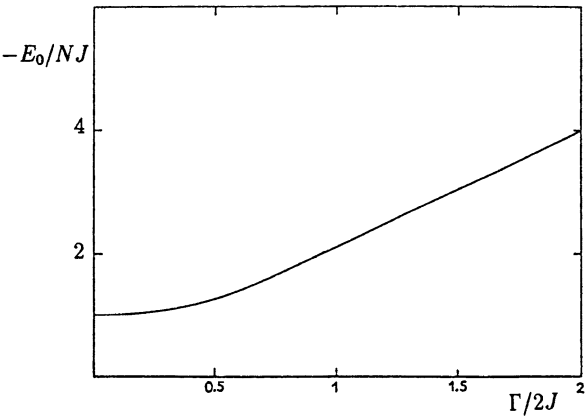

Fig. 2.2 Ground state energy as a function of $\Gamma/2J$ [312]

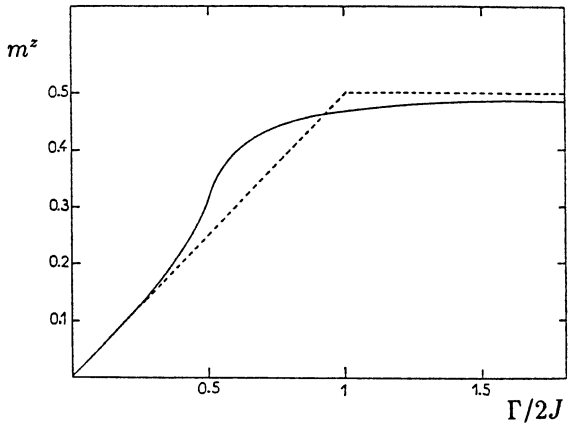

Fig. 2.3 Variation of the transverse magnetisation $m^z = \langle S^z \rangle$ with $\Gamma/2J$. *Dashed curve* is the mean field result [312]

in the present problem) cannot be evaluated directly because of the up-down symmetry of the Hamiltonian unless one applies a symmetry breaking longitudinal field. The transverse magnetisation can be written as [312] (see Sect. 2.A.3)

$$\begin{aligned} m^z = G_0 &= \langle \psi_0 | S_i^z | \psi_0 \rangle \\ &= \frac{1}{\pi} \int_0^\pi dq\, \omega_q^{-1} + \frac{1}{\pi} \int_0^\pi dq\, \omega_q^{-1} \cos q, \end{aligned} \tag{2.2.25}$$

which gives an elliptic integral of the first kind, and is non-analytic at $\overline{\lambda} = \overline{\lambda}_c = 1$. (Fig. 2.3).

The correlation functions given in Sect. 2.A.3 depend only on G_r. As a function of $\overline{\lambda}$, G_r is non-analytic for $\overline{\lambda} = 1$ and so are the correlation functions. The critical case $\overline{\lambda} = 1$ can be studied more easily because of the simple form of G_r (see Sect. 2.A.3). We get the correlation functions given as [265, 312]

$$C_r^z = \langle\psi_0|S_i^z S_{i+r}^z|\psi_0\rangle = \frac{4}{\pi^2}\frac{1}{4r^2-1}$$
$$C_r^x = \langle\psi_0|S_i^x S_{i+r}^x|\psi_0\rangle = \left(\frac{2}{\pi}\right)^r 2^{2r(r-1)}\frac{H(r)^4}{H(2r)}$$

where $H(r) = 1^{r-1}2^{r-1}\cdots(r-1)$. C_r^y and C_r^z behave in the analogous way and all the correlations at $\overline{\lambda} = 1$ go to zero as $r \to \infty$.

The spin-spin correlation in the longitudinal direction C_r^x vanishes for large r ($\lim_{r\to\infty} C_r^x = 0$) when $\overline{\lambda} \leq 1$, indicating the absence of any long-range correlation in the disordered phase. For $\overline{\lambda} > 1$ [265, 312]

$$\lim_{r\to\infty} C_r^x = \left(1 - \overline{\lambda}^{-2}\right)^{1/4}, \tag{2.2.26}$$

and hence the longitudinal magnetisation (as $r \to \infty$) can be written as

$$m^x = \langle\psi_0|S_i^x|\psi_0\rangle = 0; \quad \overline{\lambda} \leq 1, \tag{2.2.27a}$$
$$= \left(1 - \overline{\lambda}^{-2}\right)^{1/8} \quad \overline{\lambda} > 1. \tag{2.2.27b}$$

Equation (2.2.27b) gives the value of the magnetisation exponent $\beta = 1/8$. All the other exponents can be obtained in a similar fashion and it is readily observed that the value of these exponents are identically same with the exponents associated with the thermal phase transition in classical two-dimensional Ising model. One should mention that these correlation functions can be derived alternatively using "bosonisation" technique [367].

Following the development in the study of quantum computation and quantum information, the quantum entanglement has drawn increasing attention [295]. In the context of the statistical physics, the behaviour of the entanglement near a quantum critical point has been often discussed. It has been known in general that the entanglement increases when the system approaches the quantum phase transition.

The entanglement is basically measured by the entanglement entropy. To define the entanglement entropy, one considers a partition of a system into subsystems A and B. Let $\rho_A = \mathrm{Tr}_B(\rho)$ be the density matrix of the subsystem A, which is given by the trace of the density matrix of the whole system ρ with respect to the subsystem B. The entanglement entropy between A and B is defined by the von Neumann entropy of ρ_A as $S(\rho_A) = \mathrm{Tr}_A(-\rho_A \log \rho_A)$. One can readily see that the entanglement entropy vanishes if the subsystem A is decoupled from B such that $\rho = \rho_A \rho_B$ and the rank of ρ_A is 1, whereas it has the maximum when all the eigenvalues of ρ_A are equivalent. Let us now consider an infinite transverse Ising chain and focus on a subsystem of size l. The entanglement entropy S_l of this block is obtained by considering the matrix [12, 410]

$$\Lambda = \begin{pmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{l-1} \\ \Pi_{-1} & \Pi_0 & \cdots & \Pi_{l-2} \\ \vdots & \vdots & \ddots & \vdots \\ \Pi_{-l+1} & \Pi_{-l+2} & \cdots & \Pi_0 \end{pmatrix}, \tag{2.2.28}$$

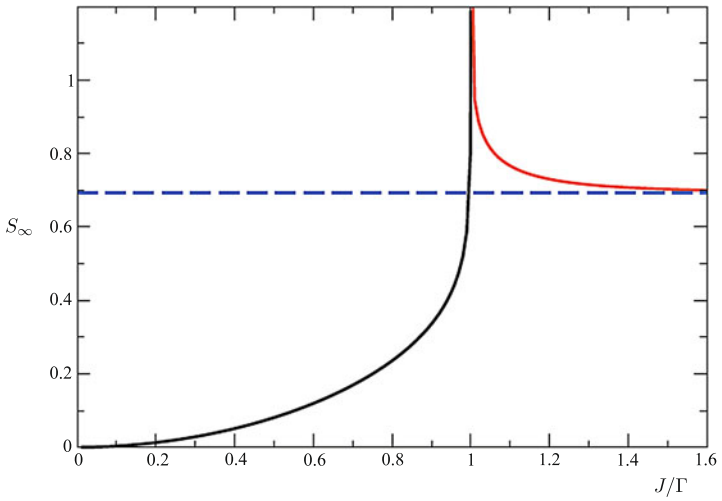

Fig. 2.4 Entanglement entropy $S_{l=\infty}$ versus J/Γ. $S_{l=\infty}$ has a singularity at $\Gamma = J$, namely, at $\overline{\lambda} = 1$. Note that $S_\infty = \log 2$ when $\Gamma = 0$. This comes from doubly degenerated ground states of the Ising chain. (After Calabrese and Cardy [54])

with

$$\Pi_n = \begin{pmatrix} 0 & g_n \\ -g_n & 0 \end{pmatrix}; \quad g_n = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-in\phi} \frac{e^{-i\phi} - \overline{\lambda}}{|e^{-i\phi} - \overline{\lambda}|}.$$

Letting λ_n's denote positive eigenvalues of the matrix (2.2.28) and defining $h(x) = -x\log(x) - (1-x)\log(1-x)$, S_l is given by

$$S_l = \sum_{n=1}^{l} h\left(\frac{1+\lambda_n}{2}\right). \tag{2.2.29}$$

The behaviour of (2.2.29) has been studied numerically [410] and analytically [54, 200, 310]. Figure 2.4 shows $\overline{\lambda}$ dependence of $S_{l=\infty}$ [54]. As shown in this figure, the entanglement entropy $S_{l=\infty}$ diverges at the critical point $\overline{\lambda} = 1$. Focusing on the critical point, S_l scales as $S_l \sim \frac{1}{6}\log l$ [410]. This logarithmic scaling of the entanglement entropy is universal in one-dimensional quantum critical systems. It has been known from the conformal field theory that, in general, the entanglement entropy of a one-dimensional quantum critical system with the central charge c behaves as $S_l \sim \frac{c}{3}\log l$ [54, 176]. The prefactor $\frac{1}{6}$ in S_l of the transverse Ising chain $\overline{\lambda} = 1$ is consistent with $c = \frac{1}{2}$ of the same system.

Another measure of the entanglement is the concurrence [425]. We consider a density matrix with respect to sites i and $i+r$, $\rho_{i,r} = \mathrm{Tr}'(\rho)$, where Tr' stands for the partial trace with respect to the degree of freedom on sites except i and $i+r$. We define the time-reversal of $\rho_{i,r}$ as $\tilde{\rho}_{i,r} = (S_i^y S_{i+r}^y)\rho_{i,r}^*(S_i^y S_{i+r}^y)$, where $\rho_{i,r}^*$ is the complex conjugate of $\rho_{i,r}$. Let λ_k $(k = 1, \ldots, 4)$ be the eigenvalues of $\rho_{i,r}\tilde{\rho}_{i,r}$. Note that λ_k is a non-negative number. We fix k such that $\lambda_1 \geq \cdots \geq \lambda_4$. Then

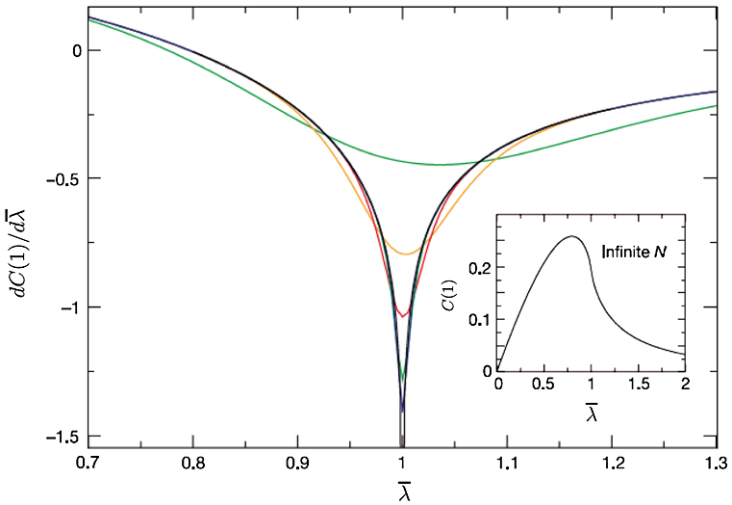

Fig. 2.5 Nearest neighbour concurrence versus $\overline{\lambda} = J/\Gamma$. The main panel shows the first derivative $dC(1)/d\overline{\lambda}$ for several sizes, while the *inset* shows $C(1)$ of the infinite size system. The dip of $dC(1)/d\overline{\lambda}$ at the critical point $\overline{\lambda} = 1$ becomes deeper with increasing size. In the infinite size system, $dC(1)d\overline{\lambda}$ behaves as $(8/3\pi^2)\ln|\overline{\lambda} - 1| + \text{const}$ and diverges at $\overline{\lambda} = 1$. (After Osterloh et al. [303])

the concurrence is defined by $C(r) = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}$. It has been shown that this quantity gives the so-called entanglement of formation, which is an elementary measure of the entanglement, and thus can be regarded itself as an entanglement measure [425]. The concurrence in the transverse Ising chain has been studied in Refs. [303, 392]. It has been shown that $C(r)$ vanishes for $r \geq 3$ even at the critical point $\overline{\lambda} = 1$. Confining our attention to the concurrence between the nearest neighbour $C(1)$, it has a peak near the critical point and is a smooth function of $\overline{\lambda}$. The singularity at the critical point is clearer in the first derivative of $C(1)$. Osterloh et al. [303] have shown that, as $\overline{\lambda}$ approaches its critical point $\overline{\lambda}_c = 1$, $dC(1)/d\overline{\lambda}$ behaves as $dC(1)/d\overline{\lambda} = (8/3\pi^2)\ln|\overline{\lambda} - 1| + \text{const}$ in the infinite size system. Figure 2.5 shows $C(1)$ and $dC(1)/d\overline{\lambda}$ as functions of $\overline{\lambda}$ [303].

2.3 Diagonalisation Techniques for Finite Transverse Ising Chain

Although, as discussed in the previous section, the spin-1/2 transverse Ising chain (and its classical analogue i.e., classical Ising system on a square lattice) is exactly solvable, the subtlety for the condition of exact solubility is very unique. With slightest change in the conditions (like presence of next nearest neighbour interaction or disorder, or in higher dimensions etc.), the above tricks fail and one requires accurate approximate methods. One such method, which can be (and has been) utilised

to extract accurate information in such cases (see Chaps. 4 and 6), is exact diagonalisation of finite-size quantum systems and employment of finite size scaling. In order to test the accuracy of such methods, we can employ it here for a spin-1/2 transverse Ising chain (where we can compare with the exact results).

2.3.1 Finite-Size Scaling

The idea of finite-size scaling was introduced by Fisher and Barber [143] to explain the effect of the thermodynamic singularities on finite size variations. Let $\psi(\lambda)$ be some quantity which diverges in the thermodynamic limit at a critical value (λ_c)

$$\psi(\lambda) \sim A|\Delta|^{-\psi}; \qquad \Delta\lambda = \frac{(\lambda - \lambda_c)}{\lambda_c} \to 0, \tag{2.3.1}$$

where the correlation length $\xi \sim |\Delta\lambda|^{-\nu}$ also diverges with the correlation length exponent λ. For a finite system of linear dimension L, the behaviour of $\psi(\lambda, L)$ is given by the finite size scaling ansatz

$$\psi(\lambda, L) = L^{\psi/L} f\big(L/\xi(\lambda)\big) \tag{2.3.2}$$

where the scaling function $f(x)$ is asymptotically defined with a power law: $f(x) \sim x^{-\psi/\nu}$, as $x \to \infty$. One thus recovers (2.3.1) from (2.3.2) when $L \to \infty$.

The above ansatz (2.3.2) is helpful in the following ways: (1) If the critical point λ_c is exactly known, then the finite size variation there is precisely given by

$$\psi(\lambda_c, L) = L^{\psi/\nu}. \tag{2.3.3}$$

Using thus the data of finite systems one can estimate the exponent relations for the transition in infinite system. (2) If the critical point for the infinite system is not exactly known, then $\psi(\lambda, L)$ is evaluated at the effective $\lambda_c(L)$ (at which the effective order parameter vanishes). This $\lambda_c(L)$ approaches the true critical value as $L \to \infty$. Since the effective $\lambda_c(L)$ is the point where $\xi(\lambda_c(L)) \sim L$, one immediately gets

$$\lambda_c(L) = \lambda_c + AL^{-1/\nu} \tag{2.3.4}$$

(where A is a constant) and can extract the value of ν.

For a quantum phase transition, the inverse of the mass gap of the quantum Hamiltonian gives the correlation length. At the transition point, the mass gap $\Delta(\lambda)$ vanishes inversely as the correlation length and for finite sizes the mass gap variation is given by

$$\Delta(\lambda, L) \sim L^{-1} g\big(\Delta\lambda L^{1/\mu}\big),$$

where $g(x) \sim x^{\nu}$ as $x \to 0$. Hence at the critical point

$$L\Delta(\lambda_c, L) = (L+1)\Delta(\lambda_c, L+1). \tag{2.3.5}$$

Using the above relation one can estimate the critical point for an infinite system from the mass gap obtained from the diagonalisation of finite systems. It has been analytically established by Hamer and Barber [167] that finite size scaling is exact for the mass gap of the transverse Ising chain in the limit $L \to \infty$ and $\lambda \to 1$ with $(1 - \lambda)L$ of the order of unity.

2.3.2 The Diagonalisation Techniques

One considers here a system of finite size N and diagonalises $2N \times 2N$ dimensional Hamiltonian matrix. Here, the observation of the symmetries of H_N can help in reducing the size of the matrix. Also the interest in some very specific states (like the ground state and the low lying excited states) may not need the search in the entire Hilbert space and one can restrict to very specific subspace. Let us now consider here a spin-$1/2$ transverse Ising system on an open chain of N spins

$$H_N = -\sum_{i=1}^{N-1} S_i^z S_{i+1}^z - \lambda \sum_{i=1}^{N} S_i^x. \tag{2.3.6}$$

The above Hamiltonian has discrete spin-flip symmetry. We choose a set of basis vectors in which is diagonal. We can write the 2^N basis vectors, spanning the Hilbert space associated with the Hamiltonian, in the form $|\epsilon_1, \ldots, \epsilon_p, \ldots, \epsilon_N\rangle$ where ϵ_p is given by

$$S_p^x |\epsilon_1, \ldots, \epsilon_p, \ldots, \epsilon_N\rangle = \epsilon_p |\epsilon_1, \ldots, \epsilon_p, \ldots, \epsilon_N\rangle. \tag{2.3.7}$$

Clearly, ϵ_p can take two values $+1$ and -1. We can now easily check that the Hamiltonian H_N acting on a basis vector does not change the parity of total number of $(+)$ and $(-)$ spins. Hence, we can divide the entire 2^N-dimensional Hilbert space into two 2^{N-1}-dimensional subspaces: one having basis vectors with even number of up spins and the other with basis vectors with odd number of up spins. At this point one can separately diagonalise the Hamiltonian in two subspaces and reduce a 2^N-dimensional problem into two 2^{N-1} problems. In the present case, the ground state of the Hamiltonian in the first subspace gives the ground state in the entire space whereas the ground state in the second subspace gives the first excited state; the difference of the two gives us the required mass gap of the quantum Hamiltonian.

2.3.2.1 Strong Coupling Eigenstate Method

The idea of strong coupling eigenstate method was introduced by Hamer and Barber [167] to estimate approximately (in a very small subspace) the mass gap of a quantum Hamiltonian, for a finite size N. We rewrite the quantum Hamiltonian in the form

$$\begin{aligned} H_N &= H_0 + V \\ V &= -\sum_{i=1}^{N-1} S_i^z S_{i+1}^z \\ H_0 &= -\lambda \sum_{i=1}^{N} S_i^x. \end{aligned} \tag{2.3.8}$$

The essential idea is to generate a set of (strong coupling) eigenstate of H_0 by the successive application of the operator V to an unperturbed eigenstate of H_0. The

advantage of using this scheme is that the number of strongly coupled eigenstates is much smaller than the total number of basis vectors, and hence the effective Hamiltonian matrix is of much reduced dimension.

Let us consider, for example, a lattice of 5 spins with periodic boundary condition. The ground state of the Hamiltonian H_0 is

$$S_i^x|0\rangle = 1|0\rangle, \quad i = 1, 2, \ldots, 5.$$

Using the notation introduced in the previous section we can write the ground state in the form

$$|0\rangle = |+++++\rangle.$$

Applying the operator V on the ground state we get a state

$$|1\rangle = (1/5)^{1/2}\big(|--+++\rangle + |+--++\rangle + |++--+\rangle + |+++--\rangle + |-++++-\rangle\big). \tag{2.3.9}$$

Considering the translational invariance of the model we simply write the state $|1\rangle = |{-}{-}\rangle$. Applying V on this state $|1\rangle$ gives

$$V|{-}{-}\rangle = 2\big(|-+-++\rangle + |----+\rangle + 5|0\rangle\big).$$

We call these states $|-+-++\rangle = |2\rangle$ and $|----+\rangle = |3\rangle$. Application of V on this states does not generate any new state. We have thus effectively generated a complete set of strongly coupled eigenstates of the operator H_0. In the present case the series terminates because the unperturbed Hamiltonian has a finite number of states, whereas in the case of Hamiltonians with continuous symmetry the series does not terminate but converges very rapidly. Using the above four basis vectors we can write the Hamiltonian in the truncated 4-dimensional Hilbert space and now diagonalisation is much easier. To evaluate the first excited one has to repeat the same procedure starting from the state with a single spin flipped. This method gives the exact value of the mass gap for transverse Ising system and is also effective for estimating the phase diagram of other quantum Hamiltonians.

We now give some typical numerical results. The variation of the mass gap $\Delta(\lambda, L)$ with λ of the transverse Ising chain (of size $3 < L < 50$) is shown below (Fig. 2.6). As the size of the system increases, the curve approaches the exact variation of mass gap with λ for an infinite chain ($\Delta(\lambda) \sim |1 - \lambda|$), but for a finite chain the mass gap vanishes only in the limit of asymptotic value of λ, indicating the absence of phase transition in a finite size system. To estimate numerically the critical coupling of an infinite system, using finite size results, one has to consider the "scaled mass gap ratio" R_L given by

$$R_L = \frac{L\Delta(\lambda, L)}{(L-1)\Delta(\lambda, L-1)} \tag{2.3.10}$$

and calculate the effective critical coupling $\lambda_c(L)$ from the equation $R_L(\lambda_c) = 1$. For example, in the case of transverse Ising system, one gets, with $L = 9$, the value of effective critical coupling $\lambda_c(L = 9) = 0.9985$ [143, 167] which converges to the

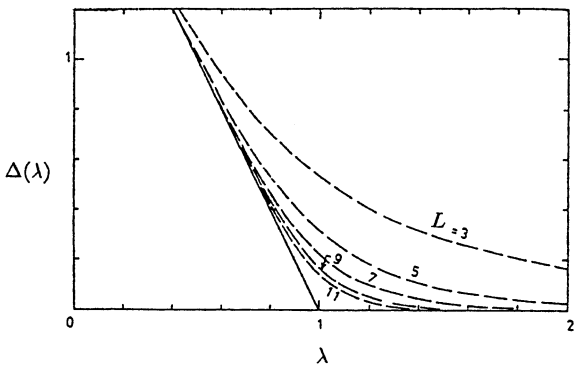

Fig. 2.6 The mass gap $\Delta(\lambda)$ plotted against λ for various chain size L. The *full curve* denotes the exact result [167]

critical value ($\lambda_c = 1$) for an infinite system, as L increases. One can thus extrapolate finite size results to make a very good approximate (exact, for a transverse Ising chain) estimation for the infinite system results.

Using the extrapolated value of critical coupling for an infinite system, as obtained above, we can estimate the value of the correlation length exponent ν using the scaling relation (2.3.4). For a transverse Ising system, using $L = 9$, one gets $\nu = 0.995$, which again extrapolates to the exact value ($\nu = 1$) in the infinite chain limit. To calculate the susceptibility exponent γ one applies a magnetic field h in the longitudinal direction and the zero field susceptibility $\chi = -(\partial^2 E_0/\partial h^2)_{h=0}$ shows a peak for a finite system at the point $\lambda_c(L)$. This peak becomes sharper in the limit of large L (Fig. 2.7), and from the slope of the logarithmic plot of the above curve one can estimate the value of γ for a finite system: for transverse Ising chain of size $L = 9$, $\gamma = 1.758$. One can also use (2.3.3), with the extrapolated approximate value of the coupling constant to estimate the value of γ for an infinite system. The approximate value of γ, thus obtained, is 1.75 ± 0.005, compared to the exact value 1.75. These demonstrate the strength of diagonalisation technique, when implemented along with finite size scaling. This diagonalisation technique has also been applied to other quantum systems with appreciable amount of success [143].

2.4 Real-Space Renormalisation

Real-space renormalisation group (RSRG) techniques have been frequently used to study the phase transition in classical systems. These techniques have also been extended to study quantum systems at $T = 0$ [113, 208] (see also Ref. [209]), where one develops various schemes for generating (rescaling) the ground state and the low-lying excited states of the quantum Hamiltonians at various levels of scaling. In this section, we shall discuss block renormalisation group method, introduced by Drell et al. [113] and extended by Jullien et al. [208], to the problem of the spin-1/2 transverse Ising chain.

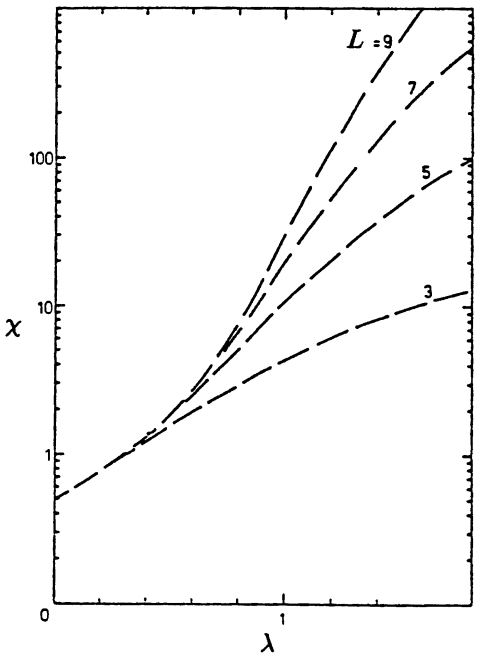

Fig. 2.7 A semi-logarithmic plot of the finite lattice susceptibility against λ [167]

2.4.1 Block Renormalisation Group Method

We shall illustrate the essential idea of the block RSRG method by applying the above to the spin-1/2 transverse Ising Hamiltonian (2.1.1) on an open chain. The idea is to generate an iterative procedure which yields for the Hamiltonian (2.1.1) in the nth iteration

$$H^{(n)} = -\sum_i \left(J^{(n)} S_i^{z(n)} S_{i+1}^{z(n)} + \Gamma^{(n)} S_i^{x(n)} \right) + c^{(n)} \sum_i I_i^{(n)} \tag{2.4.1}$$

where $I_i^{(n)}$ is the 2×2 identity matrix.

To generate an iterative scheme as shown in (2.4.1), the starting point is to divide the entire one dimensional chain of N sites into N/b blocks each having b spins (i.e., changing the length scale of the problem by a factor b) and rewrite the Hamiltonian (2.1.1) as $H = H_B + H_{IB}$ where H_B is the intra-block part and H_{IB} is the inter-block part of the Hamiltonian

$$H_B = \sum_{p=1}^{N/b} H_p, \qquad H_{IB} = \sum_{p=1}^{N/b-1} H_{p,p+1} \tag{2.4.2}$$

with

$$H_p = -\sum_{i=1}^{b-1} J S_{i,p}^z S_{i+1,p}^z + \Gamma \sum_{i=1}^{b} S_{i,p}^x \tag{2.4.3a}$$

$$H_{p,p+1} = -J S_{n,p}^z S_{1,p+1}^z, \tag{2.4.3b}$$

where indices i, p refers to the ith spin in the pth block.

The next task is to diagonalise the Block Hamiltonian H_p using the same tricks as discussed in Sect. 2.3.2. Using the same notations we can write the eigenvectors corresponding to the ground state energy E_0 and first excited state energy E_1 as

$$|0\rangle = \sum^{+} \lambda^{+}_{\epsilon_1,\ldots,\epsilon_b} |\epsilon_1, \epsilon_2, \ldots, \epsilon_b\rangle \tag{2.4.4a}$$

$$|1\rangle = \sum^{-} \lambda^{-}_{\epsilon_1,\ldots,\epsilon_b} |\epsilon_1, \epsilon_2, \ldots, \epsilon_b\rangle \tag{2.4.4b}$$

where $\sum^{+}(\sum^{-})$ is summation restricted to the Hilbert space consisting of the basis vectors with even (odd) number of down spins.

To perform the renormalisation procedure we just retain the ground state and the first excited state of the block Hamiltonian and introduce a new set of spin operator $S_p^{\alpha(1)}$ associated with each block p, such that the eigenstates of $S_p^{x(1)}$ are precisely the states $|0\rangle$ and $|1\rangle$. Thus, we can rewrite the block Hamiltonian in a renormalised form (in the first iteration) in terms of the new block spins,

$$H_p^{(1)} = -\Gamma^{(1)} S_p^{x(1)} + c^{(1)} I_p^{(1)}, \tag{2.4.5}$$

where

$$\Gamma^{(1)} = (1/2)(E_1 - E_0), \qquad c^{(1)} = (1/2)(E_1 + E_0). \tag{2.4.6}$$

To rewrite the renormalised form of the total Hamiltonian, we include the interblock part of the Hamiltonian in a perturbative way. To the zeroth order $H^{(1)} = H_p^{(1)}$. To the first order in perturbation, obtained by taking the matrix element of old spin operators $S_{i,p}^z$ between the new block states $|0\rangle$ and $|1\rangle$, $H_{p,p+1}$ takes the form

$$H_{p,p+1}^{(1)} = -J^{(1)} \sum_p S_p^{z(1)} S_{p+1}^{z(1)}$$

where

$$J^{(1)} = \left(\sum^{+} \lambda^{+}_{\epsilon_1,\ldots,\epsilon_p,\ldots,\epsilon_b} \lambda^{-}_{\epsilon_{-1},\ldots,\epsilon_p,\ldots,\epsilon_b} \right)^2 J \equiv \left(\eta_1^{(0)}\right)^2 J. \tag{2.4.7}$$

Equations (2.4.6) and (2.4.7) constitute the recursion relation of J and Γ in the first iteration. Thus one obtains for $(n+1)$th iteration

$$\Gamma(n+1) = \frac{1}{2}\left(E_1^{(n)} - E_0^{(n)}\right) \tag{2.4.8a}$$

$$J(n+1) = \left(\eta_1^{(n)}\right)^2 J^{(n)} \tag{2.4.8b}$$

$$c(n+1) = bc^{(n)} + \frac{1}{2}\left(E_1^{(n+1)} + E_0^{(n+1)}\right). \tag{2.4.8c}$$

The above recursion relations along with the initial conditions

$$J(0) = J, \qquad \Gamma(0) = \Gamma \quad \text{and} \quad c(0) = 0,$$

define a renormalisation group transformation, which can be readily exploited to estimate the critical point and exponents for the Hamiltonian (2.1.1).

We now apply the scheme to the transverse Ising chain, using block size $b = 2$ [183, 184, 208]. Let us start from the canonically transformed Hamiltonian (2.2.1)

$$H = -\Gamma \sum_i S_i^z - J \sum_i S_i^x S_{i+1}^x \tag{2.4.9}$$

and write in the form of (2.4.2) with N sites of the chain divided into $N/2$ blocks ($b = 2$), and

$$H_p = -\Gamma\left(S_{1,p}^x + S_{2,p}^x\right) - J S_{1,p}^x S_{2,p}^x$$

and

$$H_{p,p+1} = -J S_{2,p}^x S_{1,p+1}^x.$$

The block Hamiltonian H_p can be diagonalised exactly, with the eigenstates given by

$$|0\rangle = \frac{1}{(1+a^2)^{1/2}}\left(|{+}{+}\rangle + a|{-}{-}\rangle\right)$$

$$|1\rangle = \frac{1}{\sqrt{2}}\left(|{+}{-}\rangle + |{-}{+}\rangle\right)$$

$$|2\rangle = \frac{1}{\sqrt{2}}\left(|{+}{-}\rangle - |{-}{+}\rangle\right)$$

$$|3\rangle = \frac{1}{(1+a^2)^{1/2}}\left(a|{+}{+}\rangle - |{-}{-}\rangle\right)$$

where $a = (1/J)[(4\Gamma^2 + J^2)^{1/2} - 2\Gamma]$, and the respective eigenenergies given by E_0, E_1, $-E_1$ and $-E_0$, where

$$E_0 = -\sqrt{4\Gamma^2 + J^2} \quad \text{and} \quad E_1 = -J. \tag{2.4.10}$$

Retaining now the two lowest energy states $|0\rangle$ and $|1\rangle$ and treating them as the renormalised block spin state $S^{z(1)}$, the inter-block interaction can be written as

$$-J^{(1)} S_p^{x(1)} S_{p+1}^{x(1)}$$

where

$$J^{(1)} = J\frac{(1+a)^2}{2(1+a^2)}. \tag{2.4.11a}$$

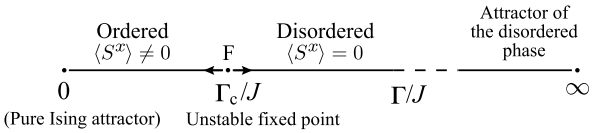

Fig. 2.8 Schematic phase diagram for renormalisation group flow for transverse Ising chain

This is because, $\langle 0|S^x|1\rangle = (1+a)/[2(1+a^2)]^{1/2}$. Since $2\Gamma^{(1)}$ equals the energy difference of states $|0\rangle$ and $|1\rangle$, we get

$$\Gamma^{(1)} = \frac{E_1 - E_0}{2} = \frac{\sqrt{4\Gamma^2 + J^2} - J}{2} \tag{2.4.11b}$$

$$c^{(1)} = \frac{E_1 + E_0}{2} = \frac{\sqrt{4\Gamma^2 + J^2} + J}{2}, \tag{2.4.11c}$$

with the last term as the additive constant appearing due to renormalisation (see (2.4.1)).

One can now write the recursion relation for the variable $\lambda = \gamma/J$ as

$$\lambda^{(1)} = \frac{[\sqrt{4\lambda^2 + 1} - 1](1 + a^2)}{(1+a)^2} \tag{2.4.12}$$

where $a = \sqrt{4\lambda^2 + 1} - 2\lambda$. Solving numerically (2.4.12) for the fixed point λ^*, one gets (apart from the trivial fixed points at $\lambda^* = 0$ or ∞) $\lambda^* = 1.277$, and linearising the recursion relation (2.4.12) in the neighbourhood of the fixed point, one gets

$$\lambda' - \lambda = \Omega\big(\lambda - \lambda^*\big), \tag{2.4.13}$$

which gives the correlation length exponent $\lambda = \ln \Omega / \ln 2 \simeq 1.47$ (with $b = 2$ here), compared to the exact value $\lambda^* = \lambda_c = 1$ and $\nu = 1$. Also, writing $J^{(1)}/J = \Gamma(1)/\Gamma \sim b^{-z}$ near the fixed point, one gets $z = 0.55$, compared to the exact value $z = 1$. It may be noted here if the mass gap $\Delta(\lambda) \sim |\lambda - \lambda_c|^s$, then $s = \nu z$. The results improve considerably with larger block size [183, 184, 208].

The schematic flow diagram of transverse Ising chain, as obtained from the above block real-space renormalisation group technique, is as shown in Fig. 2.8. The information we derive is the following:

(1) There exists an unstable (critical) fixed point in the one parameter space $\gamma/J = \lambda$ at a point λ_c. If one starts from a point $\lambda \geq \lambda_c$, the system is iterated towards the trivial fixed point at $\lambda = \infty$ (the disordered phase), whereas if started from a point $\lambda \leq (\gamma/J)_c$ the system is iterated towards the point $\lambda = 0$ (classical Ising phase).
(2) The value of λ_c approaches the exact value ($\lambda_c = 1$) as one considers larger and larger block size.
(3) Ground state energy per site is given by

$$(E_0/N)_{N\to\infty} = \lim_{n\to\infty} \big(c^{(n)}/b^{(n)}\big). \tag{2.4.14}$$

The second derivative of E_0 with respect to Γ, $-\partial^2(E_0/N)/\partial\Gamma^2$, shows a non-analytic behaviour at the point λ_c (Fig. 2.9). This singular behaviour approaches the exact behaviour as larger block size is considered.

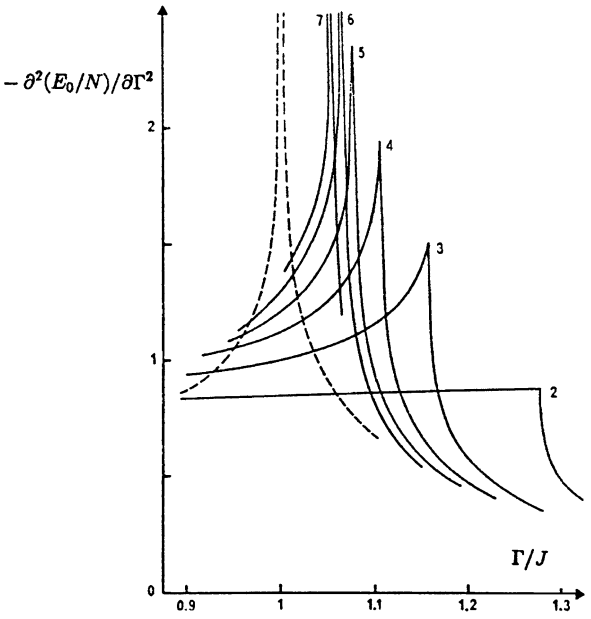

Fig. 2.9 Variation of specific heat ($=-\partial^2(E_0/N)/\partial\Gamma^2$) for different b. The exact result is represented by the *dashed line* [208]

As mentioned before, the values of these exponents, thus obtained, can be made more accurate by using larger block [208]. Hirsch and Mazenko [175], obtained better results for the mass gap and the critical exponents considering the next order in perturbation. Better results can also be derived by increasing the number of energy states of the block Hamiltonian, retained in each iteration [207].

We shall conclude this section with the note that, although we have restricted our discussion to the transverse Ising chain, this model has also been applied to interacting fermions, spin-1/2 XY and Heisenberg Chain, XY chain in 2 and 3 dimension [208] etc. One should note that the block renormalisation group technique has been extended to study quantum spin systems at finite temperature [377]. Recently transverse Ising system has also been studied using density matrix renormalisation group techniques [114].

2.5 Finite Temperature Behaviour of the Transverse Ising Chain

In this section, we shall discuss the finite temperature behaviour of the spin-1/2 transverse Ising chain. Using the dispersion relation of the elementary excitations (2.2.16), one can readily write out the free energy of the system

$$F=-Nk_BT\left[\ln 2+\int_0^{\pi}dq\,\ln\cosh\left(\frac{1}{2}\beta\omega_q\right)\right];\quad \beta=\frac{1}{k_BT},\qquad(2.5.1)$$

from which all the thermodynamic quantities can be obtained. The free energy does not show any singularity at any finite temperature. Since the model is one-dimensional, even when the transverse field is absent, the long range order and the

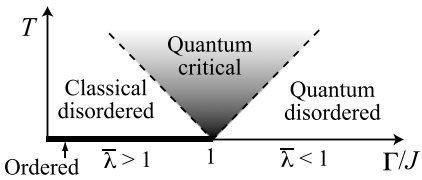

Fig. 2.10 Schematic phase diagram of the transverse Ising chain. The finite temperature phase is divided into three phases. *Dashed lines* stand for crossovers. (After Sachdev [339])

correlations of the system are destroyed with the introduction of infinitesimal thermal fluctuations ($T_c = 0$). Hence, there is no finite temperature transition for the one-dimensional model.

In spite of the absence of the long range order, the finite temperature phase diagram is divided into three phases by crossover lines $T \sim \Delta(\overline{\lambda}) = 2|1 - \overline{\lambda}|$. For $T < \Delta(\overline{\lambda})$ with $\overline{\lambda} < 1$ and with $\overline{\lambda} > 1$ one has the classical disordered phase and the quantum disordered phase respectively. There exists a quantum critical phase between these phases where $T > \Delta(\overline{\lambda})$. This picture is corroborated by analysis of finite temperature correlation functions [338, 339] (see Sect. 2.A.3). We show the schematic phase diagram in Fig. 2.10. In the classical disordered phase, the thermal fluctuation destroys the long-range order as the classical Ising chain at finite temperature is. On the other hand, the quantum fluctuation is responsible for the quantum disordered state. In the quantum critical region, the system is governed by the quantum criticality. It is remarkable that a nature of quantum criticality may be observed even at finite temperatures in the quantum critical region.

2.6 Experimental Studies of the Transverse Ising Chain

In realisation of a transverse Ising chain, we are restricted by dimensionality and the Ising anisotropy. $CoNb_2O_6$ has been perhaps the best candidate so far that provides us with a quasi-one-dimensional spin system with strong Ising anisotropy. Coldea et al. [81] performed neutron scattering experiments for this material in the presence of a transverse field and obtained distinct excitation spectra. Due to an interchain coupling, each Ising-spin chain in this material undergoes a ferromagnetic transition with a critical temperature $T = 2.95$ K. At sufficiently low fields and low temperature (i.e., $\overline{\lambda} > 1$ and $T \ll \Delta(\overline{\lambda})$), the elementary excitations from the ordered ground state is a kink and anti-kink. They form a continuum in the excitation spectrum. On the other hand, when the transverse field is sufficiently high ($\overline{\lambda} < 1$ and $T \ll \Delta(\overline{\lambda})$), the excitation consists of a flip of a single spin from the ground state polarised along the transverse axis. This excitation is signified by a single branch in the excitation spectrum. The results of experiment [81] clearly show the change of excitation spectrum between two regimes (Fig. 2.11). In addition to this observation, Coldea et al. detected a nature of quantum criticality, which is described as follows, in this material. The present system is represented effectively by an Ising chain with a weak longitudinal mean field induced by interchain couplings. This model in the presence of the transverse field cannot be mapped to a free fermion model (see Sect. 2.2).

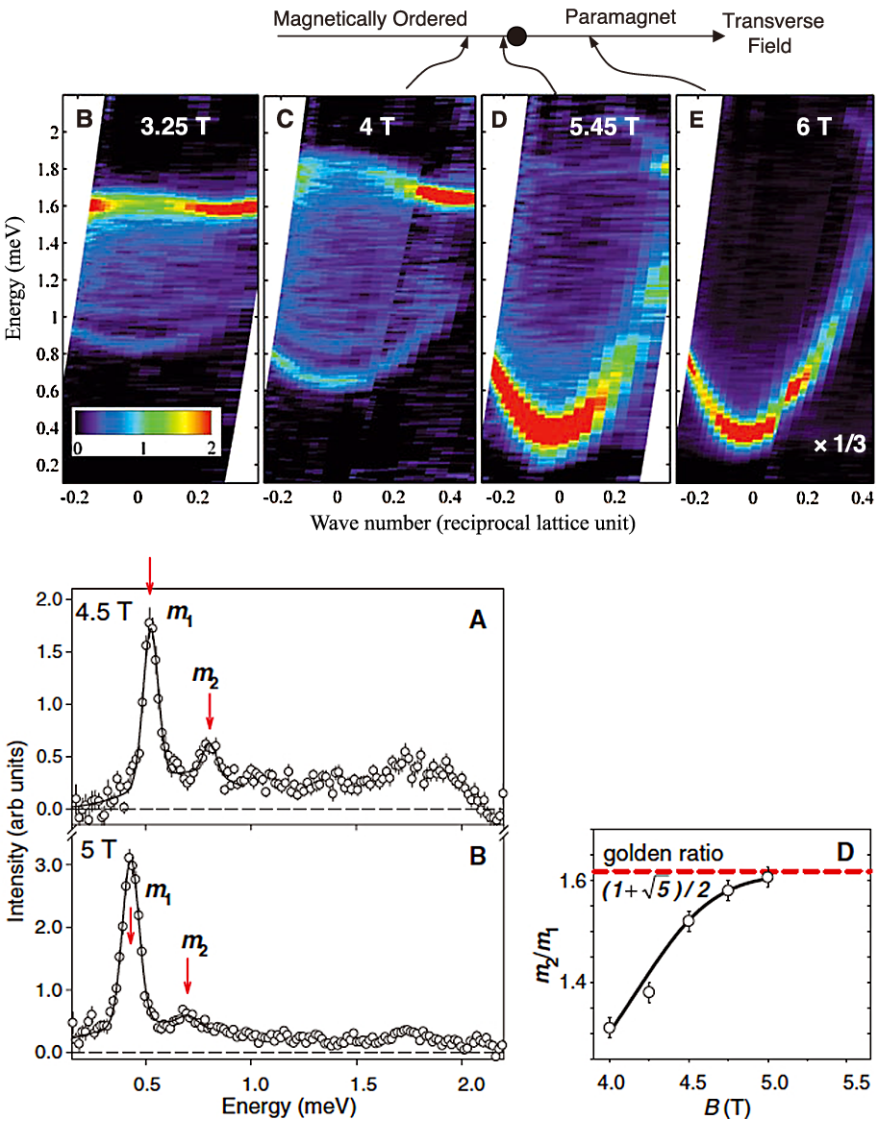

Fig. 2.11 (*upper panels*) Excitation spectra of a quasi-one-dimensional transverse Ising chain observed in $CoNb_2O_6$ by neutron scattering. The *left two panels* **B** and **C** show spectra in the low field regime, where one finds a continuum formed by scattering states of kink-antikink pair. In the *rightmost panel* **E**, the spectrum consists of a single branch which is attributed to the excitation by a single-spin flip from the polarised ground state along the transverse axis. The *panel* **D** is the result near the quantum critical point. (*lower panels*) **A** and **B** show spectral intensities below and near the critical field respectively. m_1 and m_2 denotes the lowest and the second lowest excitation energies. **D** is a plot of the ratio m_1/m_2 as a function of the transverse field. One finds that the ratio approaches the golden ratio with increasing the field toward to the critical value. (After Coldea et al. [81])

However, at the critical transverse field, the system is described by an integrable field theory [289]. Zamolodchikov [442] showed that the system possesses the E_8 symmetry of the exceptional Lie group and eight elementary excitations with different masses should exist. Coldea et al. [81] confirmed that the ratio of the lowest two excitation energies approaches the golden ratio $(1+\sqrt{5})/2$ as one shifts the transverse field to the critical point (Fig. 2.11). The golden ratio is nothing but what Zamolodchikov predicted. This experimental result reveals that the transverse Ising chain is not only a mathematical model but a realisable system which contains essences of quantum critical phenomena.

Appendix 2.A

2.A.1 Jordan-Wigner Fermions

To check that the operators c_i and $c_i^\dagger$ satisfy fermionic anti-commutation relations

$$\left[c_i, c_i^\dagger\right]_+ = \delta_{ik}, \qquad [c_i, c_k]_+ = 0 \quad \text{and} \quad \left[c_i^\dagger, c_k^\dagger\right]_+ = 0, \tag{2.A.1}$$

one uses the simple relations obeyed by Pauli spin operators

$$S_i^- S_i^+ = \frac{1}{2}\left(1 - S_i^z\right); \quad S_i^+ S_i^- = \frac{1}{2}\left(1 + S_i^z\right); \quad \exp\left(\frac{i\pi}{2} S_i^z\right) = i S_i^z. \tag{2.A.2}$$

So that, the Jordan-Wigner transformation (2.2.2a), (2.2.2b) can be rewritten as

$$c_i = \prod_{j=1}^{i-1}\left[-S_j^z\right] S_i^- \tag{2.A.3a}$$

$$c_i^\dagger = S_i^+ \prod_{j=1}^{i-1}\left[-S_j^z\right]. \tag{2.A.3b}$$

Using (2.A.3a) and (2.A.3b), one can immediately check that

$$c_i c_i^\dagger + c_i^\dagger c_i = S_i^- S_i^+ + S_i^+ S_i^- = 1. \tag{2.A.4}$$

To prove $[c_i, c_k^\dagger]_+ = 0$, for $k \neq i$, without loss of generality we assume $k < i$. Now

$$c_k c_i^\dagger + c_i^\dagger c_k = S_k^- \prod_{j=k}^{i-1}\left[-S_j^z\right] S_i^+ + S_i^+ \prod_{j=k}^{i-1}\left[-S_j^z\right] S_k^-. \tag{2.A.5}$$

If one now uses the fact

$$S_m^- S_m^z = -S_m^z S_m^-$$

the right hand side of (2.A.5) vanishes identically. Similarly, one can derive the other anti-commutation relations.

To express the spin Hamiltonian in terms of the fermion operators, we use the relation, which can be checked using (2.A.3a) and (2.A.3b). Now from (2.A.2), we get

$$S_i^z = 2S_i^+ S_i^- - 1 = 2c_i^\dagger c_i - 1, \tag{2.A.6}$$

which can be easily derived using (2.A.3a), (2.A.3b). The coupling term

$$S_i^x S_{i+1}^x = \left[S_i^+ + S_i^-\right]\left[S_{i+1}^+ + S_{i+1}^-\right] \tag{2.A.7}$$

is now to be rewritten in terms of fermions. Consider the product

$$c_i^\dagger c_{i+1} = S_i^+\left[-S_i^z\right]S_{i+1}^- \quad \left(\text{from (2.A.3a), (2.A.3b)}\right). \tag{2.A.8}$$

But $S_i^+ S_i^z = -S_i^+$, so we get

$$c_i^\dagger c_{i+1} = S_i^+ S_{i+1}^-. \tag{2.A.9a}$$

Similarly one can derive the following relations

$$c_i c_{i+1}^\dagger = -S_i^- S_{i+1}^+, \tag{2.A.9b}$$

$$c_i^\dagger c_{i+1}^\dagger = S_i^+ S_{i+1}^+, \tag{2.A.9c}$$

$$c_i c_{i+1} = -S_i^- S_{i+1}^-. \tag{2.A.9d}$$

The coupling term can be written in terms of fermion operators which are also only coupled to nearest neighbours. This result is a consequence of the Ising character $S_i^2 = +1$ of the original degrees of freedom. Collecting all the terms in (2.A.5) and (2.A.9a), (2.A.9b), (2.A.9c), (2.A.9d), one can arrive at the Hamiltonian (2.2.6). One should note here that if the original spin Hamiltonian incorporates next-nearest neighbour interaction, the resulting fermion Hamiltonian includes four-fermion term.

2.A.2 *To Diagonalise a General Hamiltonian Quadratic in Fermions*

We wish to diagonalise a general quadratic Hamiltonian of the form

$$H = \sum_{ij} c_i^\dagger A_{ij} c_j + \frac{1}{2}\sum_{ij} c_i^\dagger B_{ij} c_j^\dagger + h.c. \tag{2.A.10}$$

where c_i and $c_i^\dagger$ are fermion annihilation and creation operators respectively. For system size N, A and B are both $N \times N$ matrices. Hermiticity of H demands A to be a Hermitian matrix and anti-commutation of fermion operators demands B to be antisymmetric. Both can be chosen to be real.

Equation (2.A.10) is most effectively diagonalised by Bogoliubov transformation employed for fermion operators by Lieb et al. [245]. In particular, the technique is directly applicable for quite general nearest neighbour interactions, including for

example quasiperiodic and random ones [77]. One wants to rewrite the Hamiltonian in a diagonal form using variables η_q and $\eta_q^\dagger$ as

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + \text{const}, \tag{2.A.11}$$

ω_q are one fermion energies. One makes a linear transformation of the form [245]

$$\eta_q = \sum_i \left(g_{qi} c_i + h_{qi} c_i^\dagger\right) \tag{2.A.12a}$$

$$\eta_q^\dagger = \sum_i \left(g_{qi} c_i^\dagger + h_{qi} c_i\right) \tag{2.A.12b}$$

where g_{qi} and h_{qi} can be chosen to be real. For η_q's to satisfy fermionic anti-commutation relations we require

$$\sum_i (g_{qi} g_{q'i} + h_{qi} h_{q'i}) = \delta_{qq'} \tag{2.A.13a}$$

$$\sum_i (g_{qi} h_{q'i} - g_{q'i} h_{qi}) = 0. \tag{2.A.13b}$$

If (2.A.11) holds, then we must have

$$[\eta_q, H]_+ - \omega_q \eta_q = 0. \tag{2.A.14}$$

Using (2.A.12a), (2.A.12b) in (2.A.14) one finds

$$\omega_q g_{qi} = \sum_j (g_{qj} A_{ji} - h_{qj} B_{ji}) \tag{2.A.15a}$$

$$\omega_q h_{qi} = \sum_j (g_{qj} B_{ji} - h_{qj} A_{ji}). \tag{2.A.15b}$$

The above coupled equations can be written in the following form

$$\Phi_q (A - B) = \omega_q \Psi_q \tag{2.A.16a}$$

$$\Psi_q (A + B) = \omega_q \Phi_q \tag{2.A.16b}$$

where the components of the $2N$ vectors Φ and Ψ are obtained from the matrices g and h as

$$(\Phi_q)_i = g_{qi} + h_{qi} \tag{2.A.17a}$$

$$(\Psi_q)_i = g_{qi} - h_{qi}. \tag{2.A.17b}$$

One fermion energies ω_q are obtained from the eigenvalues of a $N \times N$ matrix

$$(A + B)(A - B)\Phi_q = \omega_q^2 \Phi_q \tag{2.A.18a}$$

$$\Psi_q (A + B)(A - B) = \omega_q^2 \Psi_q. \tag{2.A.18b}$$

For $\omega_q \neq 0$, either (2.A.18a) or (2.A.18b) is solved for Φ_q or Ψ_q and the other vector is obtained from (2.A.17a) or (2.A.17b). For $\omega_q = 0$ these vectors are determined

by (2.A.18a), (2.A.18b) or more simply by (2.A.17a), (2.A.17b), their relative sign being arbitrary.

The achievement of the method is obvious. The problem of diagonalising a $2N \times 2N$ matrix has been reduced to the eigenvalue problem of a $N \times N$ matrix [77, 245]. Even when the eigenvalues of $M = (A+B)(A-B) = (A-B)(A+B)^T$ cannot be found analytically, numerical studies can be made for large systems, for example, in one dimensional nearest-neighbour model with random transverse field (see Sect. 5.3). The price to pay is that one only obtains the one particle energies directly. Multiparticle states have to be built up by linear superposition of the one particle ones. Since A is symmetric and B is antisymmetric both $(A-B)(A+B)$ and $(A+B)(A-B)$ are symmetric and at least positive semi-definite. Thus all the λ_q's are real and all the Φ_q's and Ψ_q's can be chosen to be real as well as orthogonal. If Φ_q's are normalised, Ψ_q's are automatically normalised. To evaluate the constant in (2.A.11) we use the trace invariance of the Hamiltonian under the canonical transformation to the variables η. From (2.A.10)

$$\mathrm{Tr}H = 2^{N-1}\sum_i A_{ii}\,.$$

Again

$$\mathrm{Tr}H = 2^{N-1}\sum_q \omega_q + 2^N \times \text{const},$$

from (2.A.11). The constant is thus

$$\frac{1}{2}\left[\sum_i A_{ii} - \sum_q \omega_q\right]. \tag{2.A.19}$$

The complete diagonalised form of the Hamiltonian (2.A.10) is therefore written as

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + \frac{1}{2}\left(\sum_i A_{ii} - \sum_q \omega_q\right). \tag{2.A.20}$$

We illustrate the above diagonalisation procedure using the example of the one dimensional anisotropic XY chain in a transverse field described by the Hamiltonian (see Sect. 10.1.2)

$$H = -\frac{J}{2}\sum_i \left[(1+\gamma)S_i^x S_{i+1}^x + (1-\gamma)S_i^y S_{i+1}^y\right] - \Gamma\sum_i S_i^z \tag{2.A.21}$$

where γ is the measure of anisotropy. $\gamma = 0$ corresponds to the isotropic XY chain in a transverse field, $\gamma = 1$ corresponds to the transverse Ising chain. The Hamiltonian (2.A.21) is written in terms of Jordan-Wigner fermions as

$$H = -2\left(\sum_i \left(c_i^\dagger c_i - \frac{1}{2}\right) + \frac{1}{2}\overline{\lambda}\sum_{i=1}^{N}\left(c_i^\dagger c_{i+1} + c_i c_{i+1}^\dagger + \gamma c_i^\dagger c_i^\dagger + \gamma c_i c_{i+1}\right)\right), \tag{2.A.22}$$

where $\overline{\lambda} = J/\Gamma$. Equation (2.A.22) can be put in the general form

$$H = \left(\sum_{ij} c_i^\dagger A_{ij} c_j + \frac{1}{2} \sum_{ij} \left(c_i^\dagger B_{ij} c_j^\dagger + h.c. \right) \right) + N, \tag{2.A.23}$$

where

$$A_{ii} = -1, \quad A_{i\,i+1} = -\frac{1}{2}\gamma\overline{\lambda} = A_{i+1\,i}, \quad B_{i\,i+1} = -\frac{1}{2}\gamma\overline{\lambda}, \quad B_{i+1\,i} = \frac{1}{2}\gamma\overline{\lambda}. \tag{2.A.24}$$

The eigenvalue problem (2.A.18a), (2.A.18b) is solved considering an ansatz wave function $\exp(i\boldsymbol{q} \cdot \boldsymbol{R}_j)$ and the excitation spectrum is given as

$$\omega_q = \sqrt{(\gamma\overline{\lambda})^2 \sin^2 q + (1 - \overline{\lambda}\cos q)^2}, \tag{2.A.25}$$

so that the diagonalised form of the Hamiltonian (with $\sum_i A_{ii} = -N$) is given by

$$H = 2\sum_q \sqrt{(\gamma\overline{\lambda}\sin q)^2 + (1 - \overline{\lambda}\cos q)^2}\,\eta_q^\dagger \eta_q - \sum_q \omega_q \tag{2.A.26}$$

which reduces to the transverse Ising Hamiltonian (2.2.18) for $\gamma = 1$.

2.A.3 Calculation of Correlation Functions

Longitudinal spin-spin correlation function is defined as

$$\begin{aligned} C_{ij}^x &= \langle\psi_0|S_i^x S_j^x|\psi_0\rangle \\ &= \langle\psi_0|\left(S_i^+ + S_i^-\right)\left(S_j^+ + S_j^-\right)|\psi_0\rangle. \end{aligned} \tag{2.A.27}$$

In terms of Jordan-Wigner fermions (with $j > i$)

$$C_{ij}^x = \langle\psi_0|\left(c_i^\dagger + c_i\right)\exp\left(-i\pi\sum_{i=0}^{j-1} c_l^\dagger c_l\right)\left(c_j^\dagger + c_j\right)|\psi_0\rangle \tag{2.A.28}$$

where the averages are calculated over the ground state. One can now verify using a representation in which $c_l^\dagger c_l$ is diagonal, that

$$\begin{aligned} \exp\left[-i\pi c_l^\dagger c_l\right] &= -\left(c_l^\dagger - c_l\right)\left(c_l^\dagger + c_l\right) \\ &= \left(c_l^\dagger + c_l\right)\left(c_l^\dagger - c_l\right). \end{aligned}$$

Defining $A_l = c_l^\dagger + c_l$ and $B_l = c_l^\dagger - c_l$ and noting that $A_l^2 = 1$, we have

$$C_{ij}^x = \langle\psi_0|B_i(A_{i+1}B_{i+1}\cdots A_{j-1}B_{j-1})A_j|\psi_0\rangle. \tag{2.A.29}$$

The complicated expression can be simplified using Wick's theorem, and following relations

$$\langle\psi_0|A_i A_j|\psi_0\rangle = \langle\psi_0|\left(\delta_{ij} - c_j^\dagger c_i + c_i^\dagger c_j\right)|\psi_0\rangle = \delta_{ij}, \tag{2.A.30}$$

and

$$\langle\psi_0|B_i B_j|\psi_0\rangle = -\delta_{ij}. \tag{2.A.31}$$

Only nonzero contractions are $\langle A_j B_i\rangle$ and $\langle B_i A_j\rangle$, since $\langle A_i A_j\rangle$ and $\langle B_i B_j\rangle$ never occur. Defining $\langle B_i A_{i+r}\rangle = -\langle A_{i+r} B_i\rangle = G_{i\,i+r} = G_r = G_{-r}$, the correlation function is given by a determinant

$$\begin{aligned} C^x_{i\,i+r} &= \det\begin{pmatrix} G_{i\,i+1} & G_{i\,i+2} & \cdots & G_{i\,i+r} \\ G_{i+1\,i+1} & G_{i+1\,i+2} & \cdots & G_{i+1\,i+r} \\ \cdots & \cdots & \cdots & \cdots \\ G_{i+r-1\,i+1} & G_{i+r-1\,i+2} & \cdots & G_{i+r-1\,i+r} \end{pmatrix} \\ &= \det\begin{pmatrix} G_{-1} & G_{-2} & \cdots & G_{-r} \\ G_0 & G_{-1} & \cdots & G_{-r+1} \\ \cdots & \cdots & \cdots & \cdots \\ G_{r-2} & G_{r-3} & \cdots & G_{-1} \end{pmatrix} \end{aligned} \tag{2.A.32}$$

which is of size r. Similarly one can evaluate the transverse correlation function defined as

$$\begin{aligned} C^z_{i\,i+r} &= \langle\psi_0|S^z_i S^z_{i+r}|\psi_0\rangle - \left(m^z\right)^2 \\ &= \langle\psi_0|A_i B_i A_{i+r} B_{i+r}|\psi_0\rangle \\ &= (G_{i\,i} G_{i+r\,i+r} - G_{i\,i+r} G_{i+r\,i}) - \left(m^z\right)^2. \end{aligned} \tag{2.A.33}$$

One can now check that,

$$\begin{aligned} m^z &= \langle\psi_0|S^z_i|\psi_0\rangle \\ &= \langle\psi_0|2c^\dagger_i c_i - 1|\psi_0\rangle \\ &= 2\langle\psi_0|c^\dagger_i c_i|\psi_0\rangle - 1 = G_{ii} = G_0 \end{aligned} \tag{2.A.34}$$

so that

$$C^z_{i\,i+r} = -G_{i\,i+r} G_{i+r\,i}. \tag{2.A.35}$$

To evaluate $G_{i\,i+r}$ we consider the inverse Fourier-Bogoliubov transformation (see (2.2.7a), (2.2.7b) and (2.2.13)) given by

$$c^\dagger_i = \sqrt{\frac{1}{N}} \sum_q e^{iqR_i}\left(u_q \eta^\dagger_q + i v_q \eta_{-q}\right) \tag{2.A.36}$$

so that we get

$$c^\dagger_i + c_i = \sqrt{\frac{1}{N}} \sum_q \left(e^{iqR_i} u_q \eta^\dagger_q + e^{-iqR_i} u_q \eta_q - i e^{-iqR_i} v_q \eta^\dagger_{-q} + i e^{iqR_i} v_q \eta_{-q}\right) \tag{2.A.37a}$$

and

$$c_i^\dagger - c_i = \sqrt{\frac{1}{N}} \sum_q \left(e^{iqR_i} u_q \eta_q^\dagger - e^{-iqR_i} u_q \eta_q + i e^{-iqR_i} v_q \eta_{-q}^\dagger + i e^{iqR_i} v_q \eta_{-q} \right). \tag{2.A.37b}$$

Note that u_q and v_q are given by (2.2.17). In the ground state, $G_r = G_{i\,i+r} = \langle \psi_0 | B_i A_{i+r} | \psi_0 \rangle$. At a finite temperature T, $G_r = G_{i\,i+r} = \langle B_i A_{i+r} \rangle_\beta$, where $\langle B_i A_j \rangle_\beta$ denotes an average over the canonical ensemble at temperature $k_B T = 1/\beta$. Thus,

$$\begin{aligned} G_r(\beta) = \frac{1}{N} \sum_q \big[& e^{-iqr} \left\{ \left(u_q^2 + i u_q v_q \right) \langle \eta_q^\dagger \eta_q \rangle + \left(v_q^2 - i u_q v_q \right) \langle \eta_{-q} \eta_{-q}^\dagger \rangle \right\} \\ & - e^{iqr} \left\{ \left(u_q^2 - i u_q v_q \right) \langle \eta_q \eta_q^\dagger \rangle + \left(v_q^2 + i u_q v_q \right) \langle \eta_{-q}^\dagger \eta_{-q} \rangle \right\} \big]. \end{aligned} \tag{2.A.38}$$

The average fermion occupation at temperature T

$$\langle \eta_q^\dagger \eta_q \rangle_\beta = \langle \eta_{-q}^\dagger \eta_{-q} \rangle_\beta = \left(\exp(\beta \cdot 2\omega_q) + 1 \right)^{-1}$$

so that,

$$\begin{aligned} G_r(\beta) &= \frac{1}{N} \sum_q e^{iqr} \left(1 - 2u_q^2 + 2 i u_q v_q \right) \tanh(\beta \omega_q) \\ &\overset{N \to \infty}{\to} \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iqr} \left(\frac{1 + \overline{\lambda} e^{iq}}{1 + \overline{\lambda} e^{-iq}} \right)^{1/2} \tanh(\beta \omega_q). \end{aligned} \tag{2.A.39}$$

For ground state $\tanh(\beta \omega_q / 2) = 1$, we have

$$G_r = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iqr} \left(\frac{1 + \overline{\lambda} e^{iq}}{1 + \overline{\lambda} e^{-iq}} \right)^{1/2}. \tag{2.A.40}$$

One can now evaluate the following values G_r for some special values of $\overline{\lambda}$, e.g.,

$$G_r = \begin{cases} \frac{2}{\pi} \frac{(-1)^r}{2r+1} & \text{for } \overline{\lambda} = 1 \\ \delta_{r,-1} & \text{for } \overline{\lambda} = \infty \\ \delta_{r,0} & \text{for } \overline{\lambda} = 0 \end{cases}$$

etc.

In order to evaluate the determinant (2.A.32), let us define

$$\begin{aligned} D_p &= G_{i\,i-1+p} = G_{p-1} \\ &= \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iq(p-1)} \left(\frac{1 + \overline{\lambda} e^{iq}}{1 + \overline{\lambda} e^{-iq}} \right)^{1/2} \tanh(\beta \omega_q) \\ &= \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iqp} \left(\frac{1 + \overline{\lambda}^{-1} e^{-iq}}{1 + \overline{\lambda}^{-1} e^{iq}} \right)^{1/2} \tanh(\beta \omega_q). \end{aligned} \tag{2.A.41}$$

In terms of this, (2.A.32) is rewritten as

$$C^x_{i\,i+r} = \det \begin{pmatrix} D_0 & D_{-1} & \cdots & D_{-r+1} \\ D_1 & D_0 & \cdots & D_{-r+2} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{pmatrix}. \tag{2.A.42}$$

This Toeplitz determinant can be evaluated by using the Szegö's theorem [393] (see also Ref. [144]), which stated as follows. We refer to Ref. [268] for the proof.

Szegö's Theorem *Assume that* $\hat{D}(e^{iq})$ *and* $\ln \hat{D}(e^{iq})$ *are continuous cyclic functions of* q *for* $q \in [-\pi, \pi]$. *Let*

$$D_p = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \hat{D}\big(e^{iq}\big) e^{-iqp}, \qquad d_p = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln \hat{D}\big(e^{iq}\big) e^{-iqp}.$$

The Toeplitz determinant

$$\Delta_r = \det \begin{pmatrix} D_0 & D_{-1} & \cdots & D_{-r+1} \\ D_1 & D_0 & \cdots & D_{-r+2} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{pmatrix}$$

is given by

$$\lim_{r\to\infty} \frac{\Delta_r}{e^{rd_0}} = \exp\left[\sum_{p=1}^{\infty} p d_{-p} d_p\right], \tag{2.A.43}$$

whenever the sum in (2.A.43) *converges*.

Applying this theorem to (2.A.41) and (2.A.42), one finds that the longitudinal correlation function behaves as $C^x_{i\,i+r} \approx Ae^{-r/\xi}$ for $r \gg 1$ and the correlation length ξ is given by

$$\begin{aligned} \frac{1}{\xi} &= -d_0 = -\int_{-\pi}^{\pi} \frac{dq}{2\pi} \frac{1}{2} \ln\left(\frac{1+\overline{\lambda}^{-1} e^{-iq}}{1+\overline{\lambda}^{-1} e^{iq}}\right) - \int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln \tanh(\beta\omega_q) \\ &= \begin{cases} \int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln \coth(\beta\omega_q) & \text{for } \overline{\lambda} > 1 \\ \int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln \coth(\beta\omega_q) - \ln \overline{\lambda} & \text{for } \overline{\lambda} < 1 \end{cases}. \end{aligned} \tag{2.A.44}$$

(Note that, when $\overline{\lambda} < 1$, one needs additional algebras because $\ln \hat{D}(e^{iq})$ is not cyclic with respect to q. See Ref. [265].) Substituting (2.2.16) for ω_q and recovering the lattice constant a and scale of energy Γ, one can write (2.A.44) as

$$\frac{1}{\xi} = \begin{cases} \int_0^{\pi/a} \frac{dq}{\pi} \ln \coth \beta\Gamma \sqrt{1 + 2\overline{\lambda}\cos qa + \overline{\lambda}^2} & \text{for } \overline{\lambda} > 1 \\ \int_0^{\pi/a} \frac{dq}{\pi} \ln \coth \beta\Gamma \sqrt{1 + 2\overline{\lambda}\cos qa + \overline{\lambda}^2} - \frac{1}{a} \ln \overline{\lambda} & \text{for } \overline{\lambda} < 1 \end{cases}. \tag{2.A.45}$$

Let us now define $\Delta = |1-\overline{\lambda}|/2\Gamma a^2$ and $c = 2\Gamma a$. By making $a \to 0$ with fixing β, Δ and c, and defining a new variable of integral $y = \beta c q$, we reach an expression for the continuous limit [338]

$$\frac{1}{\xi} = \frac{1}{\beta c} f\left(\beta \Delta c^2\right), \tag{2.A.46}$$

where

$$f(x) = \begin{cases} \int_0^\infty \frac{dy}{\pi} \ln \coth \frac{\sqrt{y^2+x^2}}{2} & \text{for } x > 0 \\ \int_0^\infty \frac{dy}{\pi} \ln \coth \frac{\sqrt{y^2+x^2}}{2} - x & \text{for } x < 0 \end{cases}. \tag{2.A.47}$$

One can easily show that the function $f(x)$ is not only continuous but also smooth at $x = 0$. This fact shows that the transverse Ising chain has no singularity at finite temperatures. In special cases, $f(x)$ takes following forms:

$$f(x) = \begin{cases} \sqrt{\frac{2x}{\pi}} e^{-x} & (x \to \infty) \\ \frac{\pi}{4} & (x = 0) \\ -x + \sqrt{2|x|}\pi e^{-|s|} & (x \to -\infty) \end{cases}. \tag{2.A.48}$$

Substituting this in (2.A.46) and recovering the original parameters, one obtains

$$\frac{1}{\xi} = \begin{cases} \frac{1}{a}\sqrt{\frac{T}{\pi}(\overline{\lambda}-1)} e^{-2(\overline{\lambda}-1)/T} & (\overline{\lambda} > 1,\ T \to 0) \\ \frac{\pi}{4}\frac{T}{2a} & (\overline{\lambda} = 1) \\ \frac{1-\overline{\lambda}}{a} + \frac{1}{a}\sqrt{\frac{T}{\pi}(1-\overline{\lambda})} e^{-2(1-\overline{\lambda})/T} & (\overline{\lambda} < 1,\ T \to 0) \end{cases}. \tag{2.A.49}$$

At the zero temperature, one finds $\xi = a/(1-\overline{\lambda})$ for $\overline{\lambda} < 1$, so that the exponent ν turns out to be 1.

The result (2.A.49) implies that the low temperature phase of the transverse Ising chain is divided into three phases by crossover lines $T \approx |\overline{\lambda} - 1|$. We show a schematic phase diagram in Fig. 2.10.

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2013, XI, 403 p. 117 illus., Softcover
ISBN: 978-3-642-33038-4