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Random Walk Analysis of the Commensurate-Incommensurate Transition in the Isotropic Spin-1 Chain

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Abstract It has been observed that in the isotropic spin-1 chain a transition in the asymptotic properties of the correlation function (commensurate-incommensurate transition) occurs at the AKLT point. We propose a simple random-walk-type argument, explaining this transition. Also, we consider a modification of the AKLT model, for which this argument can be turned into a rigorous proof.

Keywords Commensurate-incommensurate transition · Isotropic spin-1 chain · AKLT model

1 Introduction

A general isotropic nearest-neighbor spin-1 Hamiltonian on a chain can be written, up to a linear transformation, as

$$H = \sum_k (\cos\theta\, \mathbf{S}_k \cdot \mathbf{S}_{k+1} + \sin\theta (\mathbf{S}_k \cdot \mathbf{S}_{k+1})^2). \tag{1}$$

Here $\mathbf{S} = (S^x, S^y, S^z)$ is the vector of spin components, and $\theta \in [0, 2\pi]$ is a parameter. It is believed that for $-\pi/4 < \theta < \pi/4$ the ground state of this chain is in the Haldane phase [3, 4] characterized by a spectral gap and exponential decay of correlations; the ground state is unique. This is known rigorously to be the case for the special value $\theta_{\mathrm{AKLT}} = \arctan 1/3$ (AKLT model [1]), when, up to a scalar factor, the Hamiltonian has the form

$$H_{\mathrm{AKLT}} = \sum_k P_{k,k+1}, \tag{2}$$

where $P_{k,k+1}$ denotes the projector onto the spin-2 subspace of a pair of neighboring spins. The AKLT Hamiltonian has a unique, finitely correlated VBS-ground state, minimizing the

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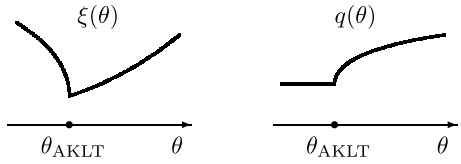

Fig. 1 Correlation length $\xi(\theta)$ and incommensurate wave number $q(\theta)$

energy of each term in (2). Correlations can be found exactly in this state and they are purely exponential; in particular,

$$\langle S_0^\alpha S_n^\beta \rangle = \delta_{\alpha\beta} \frac{4}{3} \left(-\frac{1}{3} \right)^n. \tag{3}$$

For other values of θ the Hamiltonian is frustrated (in the sense that the global ground state does not minimize the energy of single terms in the sum (1)), and one expects the 2-point correlation function to have an approximate form of the Ornstein–Zernike type. In fact, correlation functions of isotropic spin-1 chains were studied numerically by Schollwöck *et al.* [9], and they observed a transition in their qualitative asymptotic properties ("commensurate-incommensurate transition") occurring at the point θ_{AKLT}. Their conclusions can be summarized as follows.

1. Within the Haldane phase, $\theta < \theta_{\mathrm{AKLT}}$ is a "commensurate subphase". The two-point correlation function behaves at large n as

$$\langle S_0^\alpha S_n^\alpha \rangle \sim \mathrm{const} \times (-1)^n \frac{e^{-n/\xi}}{n^{1/2}},$$

where $\xi = \xi(\theta)$ is the correlation length. The correlation length depends continuously on θ, so that $\lim_{\theta \nearrow \theta_{\mathrm{AKLT}}} \xi(\theta) = \xi_{\mathrm{AKLT}} = 1/\ln 3$, and the left-sided derivative

$$\left. \frac{d\xi}{d\theta} \right|_{\theta = \theta_{\mathrm{AKLT}} - 0} = -\infty.$$

2. $\theta > \theta_{\mathrm{AKLT}}$ is an "incommensurate subphase". The correlation function at large n has the form

$$\langle S_0^\alpha S_n^\alpha \rangle \sim \mathrm{const} \times \cos(qn + \phi) \frac{e^{-n/\xi}}{n^{1/2}},$$

with some "incommensurate wave number" $q = q(\theta) \in (\pi, 2\pi/3)$, and a phase shift ϕ. The wave number $q(\theta)$ depends continuously on θ, so that $\lim_{\theta \searrow \theta_{\mathrm{AKLT}}} q(\theta) = q_{\mathrm{AKLT}} = \pi$ and

$$\left. \frac{dq}{d\theta} \right|_{\theta = \theta_{\mathrm{AKLT}} + 0} = +\infty.$$

The correlation length depends continuously on θ, and there is a finite right-sided derivative

$$0 < \left. \frac{d\xi}{d\theta} \right|_{\theta = \theta_{\mathrm{AKLT}} + 0} < +\infty$$

(see Fig. 1).

These features of the spin-1 chain have been studied theoretically in [2, 7–9]: relying on analogies with classical systems [9], on analogies with continuum field theories [2], and on analysis of the static structure factor [7, 8]. It should be mentioned that transitions of the

above sort can be observed in some simple explicitly solvable models, e.g., the free continuum quantum field theory with an appropriate energy-momentum relation, as proposed by Fáth and Sütő in [2]. On the basis of these analogies it was conjectured that the C-IC transition in the spin-1 chain is related to a double degeneracy of roots in some analytic expression, determining the asymptotic of the correlation function; as the perturbation is added to the AKLT Hamiltonian, this degeneracy is lifted either in the real or in the imaginary direction, depending on the sign of the coupling constant. This results in different behavior of the correlation function and suggests that

$$\xi(\theta) - \xi_{\mathrm{AKLT}} \sim \mathrm{const} \times (\theta_{\mathrm{AKLT}} - \theta)^{1/2}, \quad \theta < \theta_{\mathrm{AKLT}}, \tag{4}$$

and

$$q(\theta) - q_{\mathrm{AKLT}} \sim \mathrm{const} \times (\theta - \theta_{\mathrm{AKLT}})^{1/2}, \quad \theta > \theta_{\mathrm{AKLT}}. \tag{5}$$

However, the nature of this degeneracy, and why exactly it is lifted in this way, remained somewhat obscure, as these studies do not derive the asymptotic of the correlation function directly from the initial lattice Hamiltonian. In this paper we propose such a derivation based on random walk considerations.

Namely, using the Kennedy–Tasaki transform, we identify the ground state of the spin-1 chain with a system of interacting random walks on the chain. The resulting $(1 + 1)$-dimensional picture can then be alternatively described by a transfer matrix acting in the spatial direction, which in principle contains all necessary information for computing ground state correlations. After that we consider what appears to be the leading, "one-particle", term in this transfer matrix, ignoring all other terms; this yields a solvable approximation. Its solution exhibits the C-IC transition and has all the expected properties listed above. This argument is presented in Sect. 2. We emphasize, however, that we use here an approximation, which is not exact, and therefore our derivation is only heuristic.

Within our picture, the origin of the C-IC transition at the VBS-point can be explained as follows. The transfer matrix which we derive is not self-adjoint; furthermore, at the wave number $p = 0$, responsible for the asymptotic behavior, the leading eigenvalue of the transfer matrix is degenerate and has a Jordan block: it has geometric multiplicity 1 and algebraic multiplicity 2. When the perturbation is imposed, this degeneracy is lifted, as expected, either in the real or in the imaginary direction, which leads to the conjectured asymptotics.

In Sect. 3 we make an attempt to justify the approximation used in Sect. 2. It has been rigorously proved recently that the massive phase persists for small perturbations of the AKLT model [6, 10]. Namely, near the AKLT point expectations of local observables depend analytically on parameters in the Hamiltonian, and the Hamiltonian has a spectral gap. The proof in [10] is based on a convergent large length scale cluster expansion, and one can expect that by pushing further this expansion one can extract more detailed information about the ground states, in particular proving the C-IC transition. In the present paper, however, we only solve a more modest task. In Sect. 3 we introduce a spin-blocked modification of the AKLT model, which is analytically more tractable, and we rigorously prove the C-IC transition for it. Though this blocked model is rather artificial, it appears to capture the essential features of the C-IC transition in the AKLT chain.

2 Random Walk Representation and the Approximation of Minimal Trajectories

2.1 Kennedy–Tasaki Transformation

We consider the spin-1 chain on a segment $[-L, L]$, with L large. First we consider the non-perturbed AKLT model. It is convenient to perform the non-local unitary Kennedy–Tasaki transformation [6] (KT-transform for short): for any operator A we define the KT-transform $\widetilde{A}$ of A by

$$\widetilde{A} = UAU^{-1},$$

where U is the unitary operator defined by

$$U = \prod_{-L \le j < k \le L} \exp\{i\pi S_j^z S_k^x\}$$

(all factors in this product are commuting reflections).

The KT-transform has the following properties:

$$\begin{aligned}
\widetilde{S}_j^x &= S_j^x \exp\left(i\pi \sum_{k=j+1}^{L} S_k^x\right),\\
\widetilde{S}_j^y &= \exp\left(i\pi \sum_{k=-L}^{j-1} S_k^z\right) S_j^y \exp\left(i\pi \sum_{k=j+1}^{L} S_k^x\right),\\
\widetilde{S}_j^z &= \exp\left(i\pi \sum_{k=-L}^{j-1} S_k^z\right) S_j^z.
\end{aligned} \tag{6}$$

It follows, in particular, that

$$\widetilde{S_j^\alpha S_k^\alpha} = -S_j^\alpha \exp\left(i\pi \sum_{l=j+1}^{k-1} S_l^\alpha\right) S_k^\alpha, \quad \text{if } \alpha = x, z. \tag{7}$$

Furthermore, though the KT-transform is non-local in general, the operator $\widetilde{S_k^\alpha S_{k+1}^\alpha}$ for any α is local, acting only on spins k and $k+1$. Hence for the AKLT model on $[-L, L]$ we have

$$\widetilde{H}_{\mathrm{AKLT},L} = \sum_{k=-L}^{L-1} \widetilde{P}_{k,k+1},$$

where $\widetilde{P}_{k,k+1}$ is a 5-dimensional projector acting on spins k and $k+1$. These projectors can be described as follows. Assume that we work with the standard coordinate representation of the spin-1 variables:

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

and let $|-\rangle, |0\rangle, |+\rangle$ denote the base vectors (eigenvectors of S^z). Consider the four unit vectors

$$\phi^1 = (|0\rangle + \sqrt{2}|+\rangle)/\sqrt{3}, \qquad \phi^2 = (|0\rangle - \sqrt{2}|+\rangle)/\sqrt{3},$$
$$\phi^3 = (-|0\rangle + \sqrt{2}|-\rangle)/\sqrt{3}, \qquad \phi^4 = (-|0\rangle - \sqrt{2}|-\rangle)/\sqrt{3}.$$

These vectors form a regular tetrahedron in $\mathbb{R}^3$, so that the scalar product $\langle \phi^k, \phi^j \rangle = -1/3$ if $k \neq j$. Let ϕ^l_k denote the vector ϕ^l placed at site k. Then the 4-dimensional kernel of the projector $\widetilde{P}_{k,k+1}$ can be described as the subspace spanned by the vectors $\phi^l_k \otimes \phi^l_{k+1}, l = 1, 2, 3, 4$. The four zero-energy ground states of the KT-transformed AKLT model on a finite chain are thus simply the products $\bigotimes_{k=-L}^{L} \phi^l_k, l = 1, 2, 3, 4$. In the pre-transformed AKLT model, the four ground states converge to a single state on local observables in the thermodynamic limit $L \to \infty$. The operators $\exp\{i\pi S^\alpha\}, \alpha = x, y, z$, permute the vectors $\phi^1, \phi^2, \phi^3, \phi^4$ (forming, together with the identity, the group $\mathbb{Z}_2 \times \mathbb{Z}_2$):

$$\begin{aligned} \exp\{i\pi S^x\}: &\quad \phi^1 \leftrightarrow \phi^4, \qquad \phi^2 \leftrightarrow \phi^3, \\ \exp\{i\pi S^y\}: &\quad \phi^1 \leftrightarrow \phi^3, \qquad \phi^2 \leftrightarrow \phi^4, \\ \exp\{i\pi S^z\}: &\quad \phi^1 \leftrightarrow \phi^2, \qquad \phi^3 \leftrightarrow \phi^4. \end{aligned} \tag{8}$$

The formula (3) for correlations in the ground state now easily follows from relations (6); e.g., using (7),

$$\begin{aligned} \langle S^z_0 S^z_n \rangle_L &= -\left\langle \bigotimes_{k=-L}^{L} \phi^1_k,\, S^z_0 \exp\left(i\pi \sum_{k=1}^{n-1} S^z_k \right) S^z_n \bigotimes_{k=-L}^{L} \phi^1_k \right\rangle \\ &= \langle \phi^1, \phi^2 \rangle^{n-1} \langle \phi^1, S^z \phi^1 \rangle^2 = (-1/3)^{n-1} (2/3)^2. \end{aligned}$$

If $\alpha \neq \beta$, then $\widetilde{S^\alpha_0 S^\beta_n}$ transforms the ground state $\bigotimes_{k=-L}^{L} \phi^l_k$ into a vector which has ϕ^m_k's with some $m \neq l$ either for all $k < 0$ or for all $k > n$; it follows that $\langle S^\alpha_0 S^\beta_n \rangle_L \to 0$ as $L \to \infty$.

2.2 Path Space Expansion

Let H be a small perturbation of the AKLT Hamiltonian. Then on a finite chain $[-L, L]$ the expectation in the ground state of H can be found as

$$\langle A \rangle_L = \lim_{t \to +\infty} \frac{\langle \Omega_L, \exp\{-t H_L\} A \exp\{-t H_L\} \Omega_L \rangle}{\langle \Omega_L, \exp\{-2t H_L\} \Omega_L \rangle},$$

where Ω_L is a ground state vector for the unperturbed AKLT Hamiltonian. In terms of the KT-transformed chain,

$$\langle A \rangle_L = \lim_{t \to +\infty} \frac{\langle \bigotimes_{k=-L}^{L} \phi^1_k, \exp\{-t \widetilde{H}_L\} \widetilde{A} \exp\{-t \widetilde{H}_L\} \bigotimes_{k=-L}^{L} \phi^1_k \rangle}{\langle \bigotimes_{k=-L}^{L} \phi^1_k, \exp\{-2t \widetilde{H}_L\} \bigotimes_{k=-L}^{L} \phi^1_k \rangle}. \tag{9}$$

We will derive our random walk representation by expanding the evolution $\exp\{-t \widetilde{H}_L\}$ in this formula in terms of vectors of the form $\bigotimes_{k=-L}^{L} \phi^{l(k)}_k$. (Note that this system of vectors is overcomplete: it contains 4^{2L+1} elements, while the space has dimension 3^{2L+1}; hence there is some arbitrariness in this expansion.)

Though we introduce this expansion with the purpose of analyzing the perturbed AKLT model, before that, in this and the next subsections, we will study it in the case when H is the non-perturbed AKLT Hamiltonian, i.e. $\widetilde{H}_L = \sum_{k=-L}^{L-1} \widetilde{P}_{k,k+1}$. Even in this case, the expansion is rather involved and we will have to restrict our attention to simplest configurations. Then, in Sect. 2.4, we will extend our analysis to the perturbed model.

We start by considering infinitesimal changes of base vectors $\bigotimes_{k=-L}^{L} \phi_k^{l(k)}$ under the evolution $\exp\{-t\widetilde{H}_L\}$, having in mind the formula

$$\exp\{-t\widetilde{H}_L\} = \lim_{t_0 \searrow 0} \left(1 - t_0 \sum_{k=-L}^{L-1} \widetilde{P}_{k,k+1}\right)^{t/t_0}. \tag{10}$$

Let $\widetilde{P}$ be one of the projectors in the above formula; consider its action on vectors of the form $\phi^l \otimes \phi^m$. As mentioned earlier,

$$\widetilde{P}\phi^l \otimes \phi^l = 0. \tag{11}$$

Suppose now that $l \neq m$, e.g., $l = 1, m = 2$. In this case we use the fact that $(1 - \widetilde{P})\phi^1 \otimes \phi^2$ is in the kernel of $\widetilde{P}$ and hence one can write, by symmetry,

$$(1 - \widetilde{P})\phi^1 \otimes \phi^2 = a(\phi^1 \otimes \phi^1 + \phi^2 \otimes \phi^2) + b(\phi^3 \otimes \phi^3 + \phi^4 \otimes \phi^4).$$

A direct calculation shows that $a = -1/3, b = 1/6$. Summarizing, for $l \neq m$ we have

$$\widetilde{P}\phi^l \otimes \phi^m = \phi^l \otimes \phi^m + \frac{1}{3}(\phi^l \otimes \phi^l + \phi^m \otimes \phi^m) - \frac{1}{6} \sum_{p \neq l,m} \phi^p \otimes \phi^p. \tag{12}$$

Formulas (10), (11), (12) completely specify the evolution as acting on configurations $l(k)$, $k = -L, \ldots, L$, associated with vectors $\bigotimes_{k=-L}^{L} \phi_k^{l(k)}$. Infinitesimally, the evolution affects asymmetric bonds, with $l(k) \neq l(k+1)$, and transitions to symmetric states occur independently at these bonds. The constancy of a configuration in time is suppressed by the first term on the r.h.s. of (12). Note the breakdown of the time-reversal symmetry: a non-constant configuration can evolve into a constant one, but not contrariwise.

In order to obtain the random walk picture as an ensemble of trajectories we use a Duhamel-type formula. Let

$$\widetilde{H}_L = \Lambda + J, \tag{13}$$

where Λ is the diagonal part of the operator $\widetilde{H}_L$ w.r.t. the system $\bigotimes_{k=-L}^{L} \phi_k^{l(k)}$, i.e.,

$$\Lambda \bigotimes_{k=-L}^{L} \phi_k^{l(k)} = \left(\sum_{k=-L}^{L-1} (1 - \delta_{l(k),l(k+1)})\right) \bigotimes_{k=-L}^{L} \phi_k^{l(k)}. \tag{14}$$

Then we write

$$e^{-t\widetilde{H}_L} = \sum_{s=0}^{\infty} \int\limits_{0<t_1<\cdots<t_s<t} \cdots \int e^{-t_1\Lambda}(-J)e^{-(t_2-t_1)\Lambda} \cdots (-J)e^{-(t-t_s)\Lambda} dt_1 \cdots dt_s. \tag{15}$$

It is natural to introduce a dual chain, associated with bonds of the initial chain, and specify a configuration by its asymmetric bonds (*defects* for short), separating segments with constant

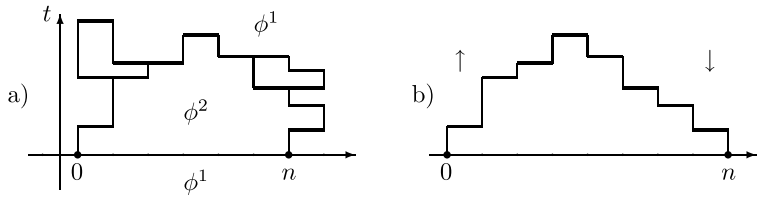

Fig. 2 **a** A typical trajectory. **b** A minimal trajectory

$l(k)$. The evolution is then visualized as that of a (non-constant) number of random walks with a nearest-neighbor interaction, with possible proliferations and pair annihilations, but not creations. The Duhamel formula gives an expansion of the evolution over all possible trajectories. Vertical segments correspond to defects constant in time, resulting from factors $e^{-(t_i-t_{i-1})A}$ in the above formula. Each vertical segment of length t contributes the weight density e^{-t} to the trajectory. Horizontal segments (interactions or jumps of defects) correspond to factors $(-J)$ and contribute the factors $-1/3$ or $1/6$ to the weight. In order to obtain the full expansion one has to sum over all possible configurations and integrate the total product weight density over all positions of horizontal segments.

Now we apply the trajectory expansion to formula (9). Consider the operator $\exp\{-t\widetilde{H}_L\}\widetilde{A}\exp\{-t\widetilde{H}_L\}$, acting on the vector $\bigotimes_{k=-L}^{L}\phi_k^1$ in the numerator. The factor $\exp\{-t\widetilde{H}_L\}$ on the right side preserves the vector $\bigotimes_{k=-L}^{L}\phi_k^1$, so that the evolution becomes non-trivial only after $\widetilde{A}$ is applied. Suppose $A = S_0^z S_n^z$, so that $\widetilde{A} = -S_0^z \exp(i\pi \sum_{l=1}^{n-1} S_n^z) S_n^z$. In this case

$$\widetilde{A}\bigotimes_{k=-L}^{L}\phi_k^1 = -\frac{1}{4}\bigotimes_{k=-L}^{-1}\phi_k^1 \otimes (\phi_0^1 - \phi_0^2)\bigotimes_{k=1}^{n-1}\phi_k^2 \otimes (\phi_n^1 - \phi_n^2)\bigotimes_{k=n+1}^{L}\phi_k^1$$

$$= \frac{1}{4}\sum_{r=0,1}\sum_{s=0,1}(-1)^{s+r}\bigotimes_{k=-L}^{r-1}\phi_k^1\bigotimes_{k=r}^{n+s-1}\phi_k^2\bigotimes_{k=n+s}^{L}\phi_k^1, \tag{16}$$

i.e., $\widetilde{A}$ creates two defects at 0 and n (more precisely, the first one is a linear combination of defects at 0 and 1, and the second one is a linear combination of defects at n and $n+1$). When $\exp\{-t\widetilde{H}_L\}$ is applied again, these two defects give rise to two trajectories, which either extend to the boundary of $[-L, L] \times [-t, t]$ or mutually annihilate; in the latter case they have to be connected to each other. See Fig. 2a. The denominator of (9) in the case of the non-perturbed AKLT model is trivial.

2.3 Approximation of Minimal Trajectories

The above two-dimensional picture of weighted random walk trajectories can in principle be alternatively generated by a transfer matrix acting in the "space", rather than "time", direction, which is especially relevant for computing the correlation length. (We can also refer to this alternative description as the "horizontal" evolution, in contrast to the original "vertical" one). However, even for the non-perturbed AKLT model this transfer-matrix is a sufficiently complicated many-body operator, which does not appear to be exactly solvable. This is related to the fact that, while the structure of ground states in the AKLT model is simple, no explicit formulas for excited states are available. Therefore at this point we

introduce our crucial approximation. As shown above, in order to compute $\langle S_0^z S_n^z\rangle_L$ one has to consider trajectories on $[-L, L]\times[0, t]$ originating from $(0, 0)$ and $(n, 0)$. We expect that the entropy of large trajectories is suppressed by their small weight, so that the leading contribution to $\langle S_0^z S_n^z\rangle_L$ comes from shortest finite trajectories connecting the points $(0, 0)$ and $(n, 0)$.

Precisely, we will consider only those trajectories having the smallest possible number of horizontal legs (*minimal* trajectories for short, see Fig. 2b), and neglect all others. In particular, a minimal trajectory can be viewed as a single-valued function on an interval of the lattice $\mathbb{Z}$; it describes jumps and annihilations of defects but not transitions of the kind described by the last term in (12), since they necessarily lead to extra legs. Note that a minimal trajectory always has one maximum and no minima (except for the endpoints), since minima would correspond to creations of pairs of random walks out of vacuum, which do not occur.

The "space-directed" transfer matrix T corresponding to the minimal trajectories is a simple one-particle approximation to the actual total transfer matrix. We can define T as acting on one-defect states characterized by the time coordinate t and the "direction of propagation" $\uparrow$ or $\downarrow$: to the left of the trajectory's maximum the defect moves forward in time, at the maximum it changes direction, and then moves backward. The transition amplitudes for a shift by one lattice spacing can be written as

$$T|\uparrow, t\rangle = -\frac{1}{3}\int_0^{+\infty} e^{-s}\,|\uparrow, t+s\rangle ds - \frac{2}{3}\int_0^{+\infty} e^{-s}\,|\downarrow, t+s\rangle ds,$$
$$T|\downarrow, t\rangle = -\frac{1}{3}\int_0^{+\infty} e^{-s}\,|\downarrow, t-s\rangle ds.$$

As discussion following (15) shows, the contribution to the correlation function from minimal trajectories can be expressed using powers of this operator T. The amplitude $\uparrow\longrightarrow\downarrow$ is twice as large as the others here, because this transition corresponds to the annihilation of two neighboring random walks (in the initial time evolution setup), and this annihilation is caused by a jump of either of them.

As an example, we test now the approximation of minimal trajectories on the correlation function $\langle S_0^z S_n^z\rangle$. By (16),

$$\langle S_0^z S_n^z\rangle = -\frac{1}{4}(c_{n-1} - 2c_n + c_{n+1}), \tag{17}$$

where c_n is the contribution from the term describing two defects separated by exactly n lattice spacings:

$$c_n = \lim_{\substack{L\to\infty\\ t\to+\infty}} \left\langle \bigotimes_{k=-L}^{L} \phi_k^1, \exp\{-t\widetilde{H}_L\} \bigotimes_{k=-L}^{r-1} \phi_k^1 \bigotimes_{k=r}^{n+s-1} \phi_k^2 \bigotimes_{k=n+s}^{L} \phi_k^1 \right\rangle.$$

Now let $c_n^{(\mathrm{mt})}$ be c_n in the approximation of minimal trajectories. It is easy to see that

$$c_n^{(\mathrm{mt})} = \int_0^{+\infty} e^{-t}(T^n)_{|\downarrow,t\rangle,|\uparrow,0\rangle} dt = -3(T^{n+1})_{|\downarrow,0\rangle,|\uparrow,0\rangle}. \tag{18}$$

Since the operator T commutes with translations, it is convenient to apply Fourier transform. When Fourier transformed with respect to t, T becomes a matrix-valued function:

$$\widehat{T}_p\begin{pmatrix}|\uparrow\rangle\\|\downarrow\rangle\end{pmatrix}=-\frac{1}{3}\begin{pmatrix}(1-ip)^{-1} & 0\\ 2(1-ip)^{-1} & (1+ip)^{-1}\end{pmatrix}\begin{pmatrix}|\uparrow\rangle\\|\downarrow\rangle\end{pmatrix},\quad p\in\mathbb{R}. \tag{19}$$

Then

$$\begin{aligned}T^n_{|\downarrow,0\rangle,|\uparrow,0\rangle}&=\frac{1}{2\pi}\int_{-\infty}^{+\infty}(\widehat{T}^n_p)_{\downarrow\uparrow}dp\\&=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{(1+ip)^n-(1-ip)^n}{(-3)^n ip(1+ip)^n(1-ip)^{n-1}}dp\\&=(-3)^{-n},\end{aligned}$$

by a residue computation. Summarizing, in the approximation of minimal trajectories

$$\langle S^z_0 S^z_n\rangle\approx\frac{3}{4}((-3)^{-n}-2(-3)^{-n-1}+(-3)^{-n-2})=\frac{4}{3}(-3)^{-n},$$

which turns out to coincide with the exact value. We emphasize, however, that minimal trajectories constitute only a part of the total expansion and are supposed to yield only approximate values in general (e.g., for the perturbed AKLT model in the next subsection). We are inclined to view the above coincidence as accidental.

2.4 Path Space Expansion and Approximation of Minimal Trajectories for the Perturbed Model

Now consider the perturbed model $H_{\mathrm{AKLT}}+\delta V$, where V is the perturbation and δ a small scalar parameter. The perturbed model is supposed to belong to the family (1). It is convenient to choose

$$V=\sum_k(P^{(0)}_{k,k+1}-1/4), \tag{20}$$

where $P^{(0)}_{k,k+1}$ is the projector to the spin-0 singlet; this is related to the original parametrization (1) by $\tan\theta=1/3+2\delta/3$, so that $\theta-\theta_{\mathrm{AKLT}}=3\delta/5+o(\delta)$. Denote the KT-transform $U(P^{(0)}_{k,k+1}-1/4)U^{-1}$ by $R_{k,k+1}$, so that the KT-transformed Hamiltonian of the perturbed AKLT model can be written as $\sum_k\widetilde{P}_{k,k+1}+\delta\sum_k R_{k,k+1}$.

A direct computation gives

$$R\phi^l\otimes\phi^l=\frac{1}{4}\sum_{n\neq l}\phi^n\otimes\phi^n, \tag{21}$$

and for $l\neq m$

$$R\phi^l\otimes\phi^m=-\frac{1}{4}\phi^l\otimes\phi^m-\frac{1}{12}\sum_n\phi^n\otimes\phi^n. \tag{22}$$

Now we update our trajectory expansion by including the perturbation into the random walk picture. To this end $\delta\sum_k R_{k,k+1}$ should be added to $\sum_k\widetilde{P}_{k,k+1}$ in (10). In order to obtain the modified Duhamel formula we again use the decomposition $\widetilde{H}_{\mathrm{AKLT}}+\delta\widetilde{V}=\Lambda+J$ (similar

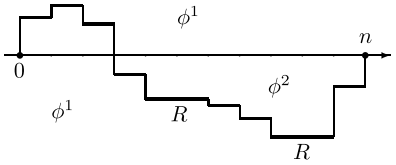

Fig. 3 A minimal trajectory containing R-legs

to (13)), where Λ is the diagonal part of $\widetilde{H}_{\mathrm{AKLT}} + \delta\widetilde{V}$. This new Λ is given by the r.h.s. of (14) multiplied by $1 - \delta/4$. The operator J is modified accordingly, it contains now a contribution from the R terms. The evolution of the perturbed model is then given by the same formula (15).

We discuss now the effect of the changes introduced by the perturbation. The change in the scalar value of Λ is not essential. The change in J is twofold. First, by (22), the amplitude $-1/3$ of a jump is adjusted to $-1/3+\delta/12$, which is not essential either. Second, new transitions arise as a consequence of flipping $\phi^l \otimes \phi^l$ into $\phi^n \otimes \phi^n$ as in (21). In the trajectory expansion, these transitions correspond to new horizontal legs of length 2 (*R-legs* for short) with the amplitude $-\delta/4$. In particular, a pair of random walks separated by two lattice spacings can now be created out of vacuum with a nonzero amplitude. This means that, in the horizontal evolution picture, a trajectory going down can make a "U-turn" and start going up (which was previously impossible). This latter property is crucial for our explanation of the C-IC transition.

We extend our approximation by minimal trajectories to the perturbed model. As before, we define minimal trajectories as those with the total length of horizontal segments having the minimal possible value (see Fig. 3). Minimal trajectories can now also contain R-legs and have several maxima and minima.

The full expansion of the evolution in trajectories is now more complicated; a general (non-minimal) trajectory can have several connected components since creations of pairs are possible. In particular, the denominator in (9) no longer equals 1. It can be argued, however, that the total weight of minimal trajectories connecting $(0,0)$ to $(n,0)$ still provides a reasonable approximation for the correlation function in question. Indeed, viewing the random walk representation as a hard core polymer model, and assuming that weights of trajectories are small so that the low-activity cluster expansion can be performed, one can represent the ratio in (9) via a sum over connected clusters of trajectories. In a cluster there is always one trajectory connecting $(0,0)$ to $(n,0)$, so the weight of minimal trajectories is the leading term in the cluster expansion. In Sect. 3 this argument is made rigorous for a modification of the AKLT model.

In order to write the perturbed horizontal transfer matrix, it is convenient to supplement the states $|\uparrow,t\rangle, |\downarrow,t\rangle$ with new states $|R,t\rangle$ describing the walker in the middle of an R-leg. Then R-legs and their amplitudes can be described in the horizontal evolution setup by new transitions

$$|\uparrow,t\rangle \mapsto -\int_0^{+\infty} e^{-(1-\delta/4)s}|R,t+s\rangle ds,$$

$$|\downarrow,t\rangle \mapsto -\int_0^{+\infty} e^{-(1-\delta/4)s}|R,t-s\rangle ds,$$

$$|R,t\rangle \mapsto \frac{\delta}{4}|\uparrow,t\rangle + \frac{\delta}{4}|\downarrow,t\rangle.$$

Also, we update the rates of transitions among states $|\uparrow,t\rangle$ and $|\downarrow,t\rangle$, taking into account (22) (though this adjustment is not essential for the final qualitative picture). The total

transfer matrix (in the approximation of minimal trajectories) thus becomes

$$
\begin{aligned}
T|\uparrow,t\rangle &= -\frac{1-\delta/4}{3}\int_0^{+\infty} e^{-(1-\delta/4)s}\,|\uparrow,t+s\rangle ds \\
&\quad -\frac{2-\delta/2}{3}\int_0^{+\infty} e^{-(1-\delta/4)s}|\downarrow,t+s\rangle ds - \int_0^{+\infty} e^{-(1-\delta/4)s}|R,t+s\rangle ds, \\
T|\downarrow,t\rangle &= -\frac{1-\delta/4}{3}\int_0^{+\infty} e^{-(1-\delta/4)s}|\downarrow,t-s\rangle ds - \int_0^{+\infty} e^{-(1-\delta/4)s}|R,t-s\rangle ds, \\
T|R,t\rangle &= \frac{\delta}{4}|\uparrow,t\rangle + \frac{\delta}{4}|\downarrow,t\rangle,
\end{aligned}
$$

so that in the Fourier-transformed representation it is given by the matrix-valued function

$$
\widehat{T}_p \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \\ |R\rangle \end{pmatrix} = \begin{pmatrix} -\frac{1-\delta/4}{3(1-\delta/4-ip)} & 0 & \delta/4 \\ -\frac{2(1-\delta/4)}{3(1-\delta/4-ip)} & -\frac{1-\delta/4}{3(1-\delta/4+ip)} & \delta/4 \\ -\frac{1}{1-\delta/4-ip} & -\frac{1}{1-\delta/4+ip} & 0 \end{pmatrix} \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \\ |R\rangle \end{pmatrix}.
$$

One eigenvalue of $\widehat{T}_p$ is 0, the other two equal $\lambda_\pm(v(p))$, where

$$
\lambda_\pm(v) = -\frac{1 \pm i\sqrt{v^2 + 18\delta(1+v^2)/(4-\delta)}}{3(1+v^2)}, \tag{23}
$$

and $v(p) = p/(1-\delta/4)$.

2.5 Asymptotic of the Correlation Function for the Perturbed Model

Recall that, as discussed in Sect. 2.3, the correlation function can be represented as a linear combination of contributions from defects separated by exactly n lattice spacings (see (17)). In order to find the asymptotic of $\langle S_0^z S_n^z\rangle$ in the approximation of minimal trajectories, we update our expression for $c_n^{(\mathrm{mt})}$. It is easy to check that an analog of (18) for the perturbed model can be written, e.g., as

$$
c_n^{(\mathrm{mt})} = -T^{n+1}_{|R,0\rangle,|\uparrow,0\rangle} - T^{n+1}_{|R,0\rangle,|\downarrow,0\rangle}.
$$

A direct calculation shows that the r.h.s. equals

$$
\frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\lambda_+^{n+1}(v) - \lambda_-^{n+1}(v)}{\lambda_+(v) - \lambda_-(v)} \frac{dv}{1+v^2}. \tag{24}
$$

The asymptotic of this expression can be found by standard methods. Let

$$
f_\pm(v) = \frac{\lambda_\pm^{n+1}(v)}{(\lambda_+(v) - \lambda_-(v))(1+v^2)}.
$$

The functions $f_\pm$ have branching points at $v = \pm v_0 := \pm\sqrt{-18\delta/(4+17\delta)}$. We make a cut along the segment $[-v_0, v_0]$ and adopt the convention that $f_\pm$ is the branch which corresponds to the $\pm$ sign of the square root in (23) for large real v. We consider now the cases $\delta < 0$ and $\delta > 0$ separately.

1. Commensurate case $\delta < 0$. In this case the segment $[-v_0, v_0] \subset \mathbb{R}$. The integrand in (24) is a single-valued analytic function with poles at $v = \pm i$, therefore using the fast fall-off of $f_\pm$ we can replace the integration along $\mathbb{R}$ by the integration along $i/2 + \mathbb{R}$. Above this line f_+ has no singularities, so $\int_{i/2+\mathbb{R}} f_+(v)dv = 0$. Similarly, $\int_{-i/2+\mathbb{R}} f_-(v)dv = 0$. This shows that (24) is equal to $\pi^{-1}\int_\gamma f_-(v)dv$, where γ is a contour going around the cut $[-v_0, v_0]$, which in turn equals

$$\frac{1}{\pi}\int_{-v_0}^{v_0}(f_-(v-i0) - f_-(v+i0))dv.$$

The two functions in the integrand are real-valued, and the leading contribution to the asymptotic results from the neighborhood of $v = 0$, where $|\lambda_-(v \pm i0)|$ attains the maximum. This maximum is equal to $\frac{1}{3} + \sqrt{\frac{-2\delta}{4-\delta}}$. Using the Laplace method one can show that

$$c_n^{(\mathrm{mt})} = \frac{\mathrm{const}(1 + O(n^{-1}))}{\sqrt{n}}\left(-\frac{1}{3} - \sqrt{\frac{-2\delta}{4-\delta}}\right)^n.$$

The same asymptotic then holds for the approximate value of $\langle S_0^z S_n^z\rangle$, in general agreement with the numerical results and the conjecture (4). For the correlation length we thus get

$$\xi \approx \left(-\ln\left(\frac{1}{3} + \sqrt{\frac{-2\delta}{4-\delta}}\right)\right)^{-1} = \frac{1}{\ln 3} + \frac{\sqrt{30(\theta_{\mathrm{AKLT}} - \theta)}}{2\ln^2 3}(1 + o(\theta_{\mathrm{AKLT}} - \theta)).$$

2. Incommensurate case $\delta > 0$. In this case the segment $[-v_0, v_0] \subset i\mathbb{R}$. Like in the previous case, we have $c_n^{(\mathrm{mt})} = \pi^{-1}\int_\gamma f_-(v)dv$, where γ is a contour going around the cut $[-v_0, v_0]$. It is convenient to make a change of variables: $w = w(v) = \lambda_-(v)$. The inverse relation is

$$v(w) = \frac{i}{3w}\sqrt{(3w+1)^2 + \frac{18\delta}{4-\delta}}.$$

This function has branching points at

$$w = w_{\pm,0} = -\frac{1}{3} \pm i\sqrt{\frac{2\delta}{4-\delta}},$$

corresponding to $v = 0$. The function $\lambda_-(v)$ maps the v-plane cut along $[-v_0, v_0]$ onto the w-plane with a cut connecting $w_{-,0}$ with $w_{+,0}$. A direct computation yields

$$\frac{dv}{(\lambda_+(v) - \lambda_-(v))(1+v^2)} = \frac{3i\,dw}{2w\sqrt{(3w+1)^2 + 18\delta/(4-\delta)}},$$

so

$$\begin{aligned} c_n^{(\mathrm{mt})} &= \frac{3i}{2\pi}\int_{\lambda_-(\gamma)} \frac{w^n dw}{\sqrt{(3w+1)^2 + 18\delta/(4-\delta)}} \\ &= \frac{3i}{\pi}\int_{w_{-,0}}^{w_{+,0}} \frac{w^n dw}{\sqrt{(3w+1)^2 + 18\delta/(4-\delta)}}, \end{aligned}$$

where the latter integration is along any line connecting $w_{-,0}$ to $w_{+,0}$. Deforming appropriately the integration path, we see that the leading contribution to the integral comes from the

endpoints $w_{-,0}, w_{+,0}$, and for large n the asymptotic for the integral (and hence for $\langle S_0^z S_n^z \rangle$) is

$$\mathrm{Re}\,\mathrm{const}\,\frac{w_{+,0}^n}{\sqrt{n}}(1+O(n^{-1})),$$

again in agreement with the numerics and the conjecture (5). The incommensurate wave number is thus found to be

$$q \approx \pi + \arctan(\sqrt{18\delta/(4-\delta)}) = \pi + \frac{\sqrt{30(\theta-\theta_{\mathrm{AKLT}})}}{2}(1+o(\theta-\theta_{\mathrm{AKLT}})),$$

and the correlation length

$$\xi \approx \left(\ln\left(3\sqrt{\frac{4-\delta}{4+17\delta}}\right)\right)^{-1} = \frac{1}{\ln 3} + \frac{15(\theta-\theta_{\mathrm{AKLT}})}{4\ln^2 3}(1+o(\theta-\theta_{\mathrm{AKLT}})).$$

3 Rigorous Proof for a Modification of the AKLT Model

3.1 Modified AKLT Model and the Result

It appears to be rather difficult to rigorously prove the C-IC transition for the AKLT model. In this section we will consider a closely related family of frustration-free isotropic spin-1 chains, where this can be done. These are spin-blocked modifications of the AKLT model, where the size of a block is a parameter which we tune to derive a convergent cluster expansion.

Precisely, fix some integer L. Consider a spin-1 chain $[n+1, n+2L]$ of length $2L$ with free boundary conditions. The AKLT model has a 4-dimensional space of ground states on this chain; let us denote by $P_{n+1,n+2L}$ the projector onto the complementary subspace. Consider the Hamiltonian

$$H^{(L)} = \sum_{k\in\mathbb{Z}} P_{kL+1,(k+2)L}. \tag{25}$$

This can be viewed as a direct analog of the AKLT model, where a single spin is replaced by a block of L spins. For $L=1$ the Hamiltonian $H^{(L)}$ is just the AKLT model. $H^{(L)}$ has the same unique infinite-volume zero energy ground state as the AKLT model; the proof that $H^{(L)}$ has a spectral gap is analogous to the proof for the AKLT model.

We will rigorously prove in this section the C-IC transition for $H^{(L)}$ for L sufficiently large. In this case one can confirm the approximation of minimal trajectories, in the sense that it can be used as a basis for a controllable polymer expansion. We will partly follow the work of Kennedy [5], where he establishes the asymptotic of the correlation functions for the Ising model in a strong magnetic field. We consider the perturbed model $H^{(L)} + \delta V$, where, as before, V is given by (20). It is not difficult to prove that for δ small enough $H^{(L)} + \delta V$ has an exponentially clustering ground state $\langle\cdot\rangle$, which analytically depends on δ (see [10] for the case $L=1$; for other L the proof is identical). We will consider the correlation function $\langle S_0^\alpha S_{Ln}^\alpha \rangle$ and establish its expected properties. We will typically denote by ϵ, c, etc. various auxiliary constants, which can be different in different formulas.

Theorem 1 *Let L be sufficiently large.*

1. (*Commensurate case*) *Let $\delta < 0$ and $|\delta|$ be small enough. Then, as $n \to \infty$,*

$$\langle S_0^\alpha S_{Ln}^\alpha \rangle = c((-1)^{Ln} + O(n^{-1/2}))\frac{e^{-n/\xi}}{n^{1/2}},$$

where, as $\delta \to 0$,

$$\xi(\delta) = (L \ln 3)^{-1} + c_1\sqrt{\delta} + O(\delta) \tag{26}$$

with $c_1 > 0$.

2. (*Incommensurate case*) *Let $\delta > 0$ and δ be small enough. Then, as $n \to \infty$,*

$$\langle S_0^\alpha S_{Ln}^\alpha \rangle = c(\cos(qn + \phi) + O(n^{-1/2}))\frac{e^{-n/\xi}}{n^{1/2}},$$

where, as $\delta \to 0$,

$$\xi(\delta) = (L \ln 3)^{-1} + O(\delta)$$

and

$$q(\delta) = L\pi + (L \ln 3)^2 c_1\sqrt{\delta} + O(\delta). \tag{27}$$

The constant c_1 in (27) is the same as in (26).

We remark that in the incommensurate case we only claim a linear bound for $\xi(\delta)$, because a more precise asymptotic requires a higher order perturbation theory.

The remainder of Sect. 3 is the proof of this theorem. In Sect. 3.2 we consider the path–space expansion for our model. In Sect. 3.3 we reduce the asymptotic of the correlation function to a "one-particle" expression, which is essentially a perturbation of the expression obtained by considering only minimal trajectories. In Sect. 3.4 we study this one-particle expression and finish the proof.

3.2 Beginning of the Proof: Path Space Expansion

We use again the Kennedy–Tasaki transform (as defined on the initial non-rescaled chain). Consider first the non-perturbed Hamiltonian (25). Let $Q_{k,k+1}$ denote the KT-transform of the projector $P_{kL+1,(k+2)L}$. The operator $Q_{k,k+1}$ acts on spins $kL+1, \dots, (k+2)L$ and projects onto the orthogonal complement to the four-dimensional subspace spanned by $\bigotimes_{s=kL+1}^{(k+2)L} \phi^l$, $l = 1, 2, 3, 4$. It is convenient to introduce blocked spins Φ_k, describing the state of the original spins $\phi_{kL+1}, \dots, \phi_{(k+1)L}$. Denote $\Phi_k^l = \bigotimes_{s=kL+1}^{(k+1)L} \phi^l$, $l = 1, 2, 3, 4$. If L is large then the system of four vectors Φ^l, $l = 1, 2, 3, 4$, is close to an orthogonal system, with the scalar product between two vectors

$$\lambda = \langle \Phi^l, \Phi^m \rangle = (-3)^{-L} \tag{28}$$

for $l \neq m$. Our goal will be to make an expansion w.r.t. the products $\bigotimes_k \Phi_k^{l(k)}$, similarly to the expansion w.r.t. $\bigotimes_k \phi_k^{l(k)}$ in the previous section. The Hamiltonian $H^{(L)}$ has been chosen so that for $Q_{k,k+1}$ we have relations similar to (11), (12) for $\widetilde{P}_{k,k+1}$:

$$\begin{aligned} &Q\Phi^l \otimes \Phi^l = 0, \\ &Q\Phi^l \otimes \Phi^m = \Phi^l \otimes \Phi^m - a(\Phi^l \otimes \Phi^l + \Phi^m \otimes \Phi^m) - b\sum_{r \neq l,m} \Phi^r \otimes \Phi^r, \end{aligned} \tag{29}$$

where the coefficients a, b depend on L through λ,

$$a = \frac{\lambda(1+\lambda+2\lambda^2)}{(1+\lambda)(1+3\lambda^2)}, \qquad b = \frac{\lambda^2(1-\lambda)}{(1+\lambda)(1+3\lambda^2)}. \tag{30}$$

Note that the coefficients a, b are small if L is large, in particular

$$a(L) = (-3)^{-L}(1 + O((-3)^{-L})). \tag{31}$$

We thus get the same random walk picture as in the previous section, but on a larger scale and with different coefficients.

Now we make an expansion about minimal trajectories, following Kennedy. As shown in the previous section, the value of the correlation function is given by the sum of all trajectories connecting the point $(0, 0)$ with $(n, 0)$. For each trajectory, consider its projection to the space lattice. For each k between 0 and n, the segment $[k, k+1]$ is either the projection of a unique leg of the trajectory, or the projection of more than one legs. We group the latter segments $[k, k+1]$ into connected families, and call them (one-dimensional) polymers. Between polymers the trajectory is a minimal trajectory, and in the Fourier modes representation the transfer operator is, like in (19), a 2×2-matrix-valued function

$$\widehat{T}_p \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} = a \begin{pmatrix} (1-ip)^{-1} & 0 \\ 2(1-ip)^{-1} & (1+ip)^{-1} \end{pmatrix} \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix}, \quad p \in \mathbb{R}, \tag{32}$$

where a is given by (30). We take into account the contribution from polymers by introducing transfer matrices $W^{(s)}$, acting on the same states $|\uparrow, t\rangle, |\downarrow, t\rangle$ as T and describing the total contribution of polymers of length s with the given incoming and outgoing states. We therefore write, using again Fourier transform,

$$\langle S_0^\alpha S_{Ln}^\alpha \rangle = \int_{\mathbb{R}} f_n(p) dp, \tag{33}$$

where

$$f_n(p) = \sum_{\substack{n_k=1,2,\dots,\\ s_k=1,2,\dots \\ \sum n_k + \sum s_k = n}} \widehat{W}_{\text{in},p}^{(s_0)} \widehat{T}_p^{n_1} \widehat{W}_p^{(s_1)} \widehat{T}_p^{n_2} \widehat{W}_p^{(s_2)} \cdots \widehat{T}_p^{n_{\max}} \widehat{W}_{\text{fin},p}^{(s_{\max})} + \widehat{W}_{\text{in+fin},p}^{(n)}. \tag{34}$$

Here we single out the 1×2-matrix $\widehat{W}_{\text{in},p}^{(s_0)}$ and 2×1-matrix $\widehat{W}_{\text{fin},p}^{(s_{\max})}$, corresponding to polymers at the boundaries of the trajectory; the values $s_0, s_{\max}$ are the lengths of their projections to the segment $[0, n]$. The last term $\widehat{W}_{\text{in+fin},p}^{(n)}$ is the contribution from polymers extending all the way from 0 to n.

Our assumption that L is large implies that a, b in (30) can be made arbitrarily small; from this one can derive exponential estimates for the weights of polymers (see [5]):

$$\| W_{t_2,t_1}^{(s)} \| \le \epsilon^s a^s e^{-c|t_1-t_2|}, \tag{35}$$

$$\| W_{\#,t_2,t_1}^{(s)} \| \le \epsilon^s a^s e^{-c|t_1-t_2|}, \tag{36}$$

where $\# = \text{in}, \text{fin}$ or $\text{in} + \text{fin}$. Here c is a positive constant which can be chosen independent of L, while ϵ can be chosen arbitrarily small for large enough L. The crucial point in deriving

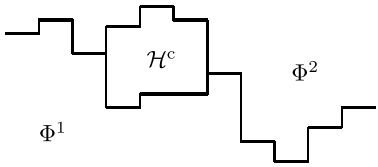

Fig. 4 A piece of a trajectory corresponding to $\widetilde{H}^{(L)} + \delta\widetilde{V}$

these estimates is that polymers have, by definition, extra horizontal legs, each of which has a small factor a or b.

Using Fourier transform, we see that the operators $\widehat{W}^{(s)}_p$, $\widehat{W}^{(s)}_{\#,p}$ depend analytically on p in a vicinity of the real axis, and we have there estimates

$$\|\widehat{W}^{(s)}_p\| \le \epsilon^s a^s, \qquad \|\widehat{W}^{(s)}_{\#,p}\| \le \epsilon^s a^s. \tag{37}$$

It is essential that for p close to 0, $\widehat{W}^{(s)}_p$ is small compared to $\widehat{T}^s_p$.

Here and below we shall assume that the thermodynamic limit has been performed both in time and space; this can be done by standard cluster expansion since we have good cluster estimates.

For the perturbed Hamiltonian $\widetilde{H}^{(L)} + \delta\widetilde{V}$ the expansion is more complicated. In the general case $\delta \neq 0$, in each single site Hilbert space of the spin blocked lattice we have to consider also the fifth, complementary subspace, $\mathcal{H}^c = (\mathbb{C}^3)^L \ominus (\bigoplus_{l=1}^4 \{\Phi^l\})$. Whereas in the non-perturbed case the evolution preserves the set of vectors of the form $\bigotimes_k \Phi^{l(k)}_k$, the perturbation $\delta\widetilde{V}$ creates transitions to and from states containing excitations from $\mathcal{H}^c$.

We use an analog of the Duhamel formula (15). Like in Sect. 2, we define Λ as the diagonal part of the non-perturbed Hamiltonian $\widetilde{H}^{(L)}$ with respect to product basis vectors. The difference is that now we also have to take into account the complementary subspaces $\mathcal{H}^c$, so that the decomposition is rather into subspaces of the form $(\bigotimes_{k\in X}\{\Phi^{l(k)}_k\}) \otimes (\bigotimes_{k\notin X}\mathcal{H}^c_k)$, where $X \subset \mathbb{Z}$. Note that $\mathcal{H}^c \otimes \{\Phi^l\}$ and $\mathcal{H}^c \otimes \mathcal{H}^c$ are eigenspaces of Q with the eigenvalue 1, hence, similarly to (14), $(\bigotimes_{k\in X}\{\Phi^{l(k)}_k\}) \otimes (\bigotimes_{k\notin X}\mathcal{H}^c_k)$ is an eigenspace of Λ with the eigenvalue $\sum_{k,k+1\in X}(1-\delta_{l(k),l(k+1)})$.

Now let $J = \widetilde{H}^{(L)} - \Lambda$, then we have

$$e^{-t(\widetilde{H}^{(L)}+\delta\widetilde{V})} = \sum_{s=0}^{\infty} \int\limits_{0<t_1<\cdots<t_s<t} \cdots \int e^{-t_1\Lambda}(-J-\delta\widetilde{V})e^{-(t_2-t_1)\Lambda}\cdots$$
$$\times\cdots(-J-\delta\widetilde{V})e^{-(t-t_s)\Lambda}dt_1\cdots dt_s. \tag{38}$$

We keep Λ and J independent of δ.

We can introduce trajectories as boundaries separating space–time regions with different Φ^l and $\mathcal{H}^c$ (see Fig. 4). As pointed out above, transitions to and from regions with $\mathcal{H}^c$ are caused by the perturbation $\delta\widetilde{V}$. In fact, every horizontal leg bordering an $\mathcal{H}^c$-region carries δ associated with corresponding terms $\delta R_{k,k+1}$ in $\delta\widetilde{V}$. Some horizontal legs can have length 2, as a result of terms $\delta R_{k,k+1}$ coupling neighboring blocks of the rescaled lattice. Anyway, the number of δ's associated with an $\mathcal{H}^c$-region is at least of the order of its horizontal length, so that typical $\mathcal{H}^c$-regions tend to be short provided δ is small enough. A large vertical length is also unfavorable for an $\mathcal{H}^c$-region, since sites with states from $\mathcal{H}^c$ are excited for Λ and hence decrease exponential factors $e^{-(t_{l+1}-t_l)\Lambda}$ in the Duhamel expansion.

In general, a single trajectory as defined above can be described by different terms in the Duhamel expansion (38). Inside an $\mathcal{H}^c$-region there may be additional transitions between

different $\mathcal{H}^c$ states; they are caused by the perturbation $\delta\widetilde{V}$. However, each instance of such a transition brings in an extra factor δ, so it is unfavorable to have many transitions.

The above considerations show that for δ small enough, $\mathcal{H}^c$-regions tend to be small. One can show that they can be controlled with exponential estimates.

Apart from introducing $\mathcal{H}^c$-regions, the perturbation $\delta\widetilde{V}$ changes transition amplitudes between Φ^l-regions. Like in Sect. 2, the significant change is the appearance of "U-turns" (the piece of the trajectory including the lowest horizontal leg in Fig. 4). We expect these U-turns to make the leading contribution to the asymptotic of the correlation function to first order in δ. Note that the order of $\mathcal{H}^c$-regions is at least δ^2, so they will not contribute to the first-order asymptotic.

Since $\delta\widetilde{V}$ creates excitations of the vacuum, a general trajectory (boundary between regions) will consist of many connected components. If δ is small, then these connected components form a dilute gas. A typical configuration consists of one "big" component remaining from the non-perturbed case and connecting points $(0, 0)$ and $(n, 0)$, and many "small" components forming "islands" in the sea of Φ^1 states.

The cluster expansion represents the correlation function as an expansion over connected clusters of connected trajectories (see Kennedy [5]). A cluster consists of the "big" trajectory (connecting $(0, 0)$ and $(n, 0)$) and a number of small "islands" which overlap in such a way that the whole set is connected. We can therefore view a cluster as a perturbed minimal trajectory.

Now we can extend to the perturbed Hamiltonian the representation of the correlation function by transfer matrices T and $W^{(s)}$. We divide again the segment $[0, n]$ into minimal trajectories alternating with intervals having more complex structure (polymers). In general, a polymer includes now a piece of the "big" trajectory and a number of "small" trajectories. It is not difficult to check that the weight clusters into the product over minimal trajectories and polymers, so that we can define T and $W^{(s)}$. The exponential estimates (37) then still hold as long as $|\delta|$ is small enough.

It is convenient to have T independent of δ, so we slightly modify the above definition by putting all the contribution of the perturbation into polymers $W^{(s)}$. More precisely, a trajectory can be a minimal one but contain some legs whose weight involves $\delta\widetilde{V}$. In this case we consider these legs as belonging to polymers and modify $W^{(s)}$ accordingly. In particular, the lowest horizontal leg in Fig. 4 has to belong to a polymer, since the corresponding transition can only occur as a result of $\delta\widetilde{V}$.

The full expansion for $W^{(s)}$ is rather complicated, but for our qualitative first order perturbation theory we will need to consider essentially only the leading term in $W^{(1)}_{\uparrow\downarrow}$ given by the simplest U-turn, as represented by the lowest leg in Fig. 4.

3.3 Asymptotic of the Correlation Function: Reduction to a "One-Particle" Leading Term

In order to find the asymptotic of the correlation function we divide the total set of momenta into two subsets, a bounded neighborhood Ω of the origin, and the remainder $\mathbb{R} \setminus \Omega$, whose contribution will be negligible. For momenta in Ω the perturbation is small. If operators in the expansion (34) were scalars rather than 2×2 matrices, then $f_n(p)$ could be represented using the partition function of the dilute gas of polymers $\widehat{W}^{(s)}$ in the segment $[0, n]$, which would imply $f_n(p) = c_{1,p}c^n_{2,p}(1 + O(\epsilon^n))$ with some $\epsilon < 1$ (see [5]). We now give an analog of this asymptotic in our 2×2-matrix setting.

Lemma 1 *Let $\Omega \subset \mathbb{R}$ be a fixed bounded open set containing the origin. For any $\epsilon_1 > 0$, one can chose L sufficiently large so that for δ sufficiently small the following holds*:

(a) *For $p \in \Omega$, uniformly in p*

$$f_n(p) = \eta^{\mathrm{t}}_{\mathrm{in},p} G_p^n \eta_{\mathrm{fin},p} + O((a\epsilon_1)^n); \tag{39}$$

here $\eta_{\mathrm{in},p}$, $\eta_{\mathrm{fin},p}$ are 2-dimensional vectors, G_p is a 2×2-matrix, and

$$\|(G_p - \widehat{T}_p)\widehat{T}_p^{-1}\| \le \epsilon_1. \tag{40}$$

Furthermore, $\eta_{\mathrm{in},p}$, $\eta_{\mathrm{fin},p}$ and G_p depend analytically on p and δ in some complex neighborhoods of Ω and 0, respectively; these neighborhoods don't depend on L, and the bound (40) extends to these neighborhoods.

(b) *For $p \in \mathbb{R}\setminus\Omega$, uniformly in p*

$$|f_n(p)| = O((a(1+p^2)^{-1/2} + a\epsilon_1)^n).$$

Remark 1 Part (a) says that for $p \in \Omega$ the leading term in the asymptotic is the first term on the r.h.s. of (39), since it is essentially of order $(a(1+p^2)^{-1/2})^n$ by (40) and (32). On the other hand, part (b) ensures that the contribution of momenta $p \notin \Omega$ is small compared to p near 0, since for $p \notin \Omega$ we have $(1+p^2)^{-1/2} < c_\Omega$ for some $c_\Omega < 1$.

Proof (a) We start by writing

$$f_n(p) = \sum_{\substack{s_0, s_{\max}, r=1,2,\dots \\ s_0+s_{\max}+r=n}} \widehat{W}^{(s_0)}_{\mathrm{in},p} A_{r,p} \widehat{W}^{(s_{\max})}_{\mathrm{fin},p} + \widehat{W}^{(n)}_{\mathrm{in+fin},p},$$

where

$$A_{r,p} = \sum_{\substack{n_k=1,2,\dots \\ s_k=1,2,\dots \\ \sum n_k+\sum s_k=r}} \widehat{T}_p^{n_1} \widehat{W}_p^{(s_1)} \widehat{T}_p^{n_2} \widehat{W}_p^{(s_2)} \cdots \widehat{T}_p^{n_{\max}}. \tag{41}$$

It has already been stated in (37) that $\widehat{W}^{(n)}_{\mathrm{in+fin},p} = O((a\epsilon_1)^n)$, if L is large enough and δ small enough.

Fix $p \in \Omega$; in what follows we mostly omit p from the notation. It is convenient to introduce operators B_r by

$$A_r = B_r B_{r-1} \cdots B_1.$$

We will show that B_r converge to a limit G so that $\|B_r - G\| = O(\epsilon^r)$. We can rewrite (41) as

$$A_r = \widehat{T} A_{r-1} + \widehat{T} \sum_{s=1}^{r-2} \widehat{W}^{(s)} A_{r-s-1}.$$

Multiplying by A_{r-1}^{-1} on the right (we will see shortly that A_r are invertible), we get

$$B_r = \widehat{T} + \widehat{T} \sum_{s=1}^{r-2} \widehat{W}^{(s)} B_{r-s}^{-1} B_{r-s+1}^{-1} \cdots B_{r-1}^{-1}. \tag{42}$$

This is an equation that can be solved by iterations. Precisely, consider the map

$$\mathcal{F}(B) = \widehat{T} + \widehat{T} \sum_{s=1}^{\infty} \widehat{W}^{(s)} B^{-s}.$$

Using the inevitability of $\widehat{T}$ (which is uniform for momenta $p \in \Omega$) and the exponential smallness of $\widehat{W}^{(s)}$, one easily proves that $\mathcal{F}$ is a contraction in a small neighborhood of the operator $\widehat{T}$. Hence, iterations of $\mathcal{F}$ yield a sequence converging exponentially fast to the fixed point G of $\mathcal{F}$. The difference between $\mathcal{F}$ and the transformation defined by the r.h.s. of (42) is of order $O(\epsilon^r)$, so one can easily see that B_r converge to G exponentially fast.

Now let us write A_r in the form

$$A_r = G^r C_r.$$

We have

$$C_r = G^{-r} B_r G^{r-1} C_{r-1} = C_{r-1} + G^{-r}(B_r - G)G^{r-1} C_{r-1}.$$

Since B_r converge to G exponentially fast, we conclude that C_r also converge to some limit C_∞ exponentially fast.

Now write f_n in the form

$$f_n = \sum_{\substack{s_0, s_{\max}=1,2,\dots \\ s_0+s_{\max}\le n}} (\widehat{W}_{\text{in}}^{(s_0)} G^{-s_0}) G^n (G^{-s_{\max}} C_\infty \widehat{W}_{\text{fin}}^{(s_{\max})}) + \sum_{\substack{s_0, s_{\max}, r=1,2,\dots \\ s_0+s_{\max}+r=n}} \widehat{W}_{\text{in}}^{(s_0)} G^r (C_r - C_\infty) \widehat{W}_{\text{fin}}^{(s_{\max})} + \widehat{W}_{\text{in+fin}}^{(n)}.$$

Using the exponential convergence of C_r and (37), we see that the last two terms here are $O((a\epsilon_1)^n)$. Consider the sums

$$\eta_{\text{in}}^{\text{t}} := \sum_{s_0=1}^{\infty} \widehat{W}_{\text{in}}^{(s_0)} G^{-s_0}, \qquad \eta_{\text{fin}} := \sum_{s_{\max}=1}^{\infty} G^{-s_{\max}} C_\infty \widehat{W}_{\text{fin}}^{(s_{\max})}.$$

These sums are also exponentially convergent, and the first term in the above expansion of f_n equals $\eta_{\text{in}}^{\text{t}} G^n \eta_{\text{fin}} + O((a\epsilon_1)^n)$.

In order to see that $\eta_{\text{in},p}$, $\eta_{\text{fin},p}$ and G_p extend analytically to neighborhoods of Ω and $\delta = 0$ independent of L, notice that all operation we have performed to find $\eta_{\text{in},p}$, $\eta_{\text{fin},p}$, G_p preserve analyticity, and that the exponential estimates (35), (36) ensure that (37) holds in a complex neighborhood of Ω independent of L. This concludes the proof of part (a).

(b) This estimate follows easily using (37). □

Fix some $p_0 > 0$. Using Lemma 1, if L is sufficiently large and δ sufficiently small, then

$$\langle S_0^\alpha S_{Ln}^\alpha \rangle = \int_{-p_0}^{p_0} \eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} dp + O((ca)^n), \tag{43}$$

where $c = (1 + (1 + p_0^2)^{-1/2})/2 < 1$. If the coupling constant $\delta = 0$, then $\langle S_0^\alpha S_{Ln}^\alpha \rangle = c_1(-3)^{-Ln}$ with $c_1 \neq 0$, and by (31) for large enough L the last term in the above formula is $o((-3)^{-Ln})$. This implies that the leading asymptotic is determined by the first term, and

$$\int_{-p_0}^{p_0} \eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} dp = c_1(1 + o(1))(-3)^{-Ln}. \tag{44}$$

This means in particular that $\eta_{\text{in},p}$, $\eta_{\text{fin},p}$ do not vanish identically, and, since they are analytic in δ, this applies to small nonzero δ as well.

3.4 Analysis of the "One-Particle" Leading Term

We have thus reduced the analysis of the asymptotic of the correlation function to the analysis of the asymptotic of the integral $\int_{-p_0}^{p_0} \eta^{\mathrm{t}}_{\mathrm{in},p} G_p^n \eta_{\mathrm{fin},p} dp$. We refer to it as a "one-particle expression" since it describes the evolution by just 2×2-matrices G_p.

Let

$$G_p = \begin{pmatrix} g_{\uparrow\uparrow,p} & g_{\uparrow\downarrow,p} \\ g_{\downarrow\uparrow,p} & g_{\downarrow\downarrow,p}. \end{pmatrix}$$

and consider first the case $\delta = 0$. It is easy to see from the construction of G_p that in this case $g_{\uparrow\downarrow,p} = 0$ and hence

$$\begin{aligned} G_p^n &= \begin{pmatrix} g_{\uparrow\uparrow,p}^n & 0 \\ g_{\downarrow\uparrow,p} \sum_{k=1}^n g_{\uparrow\uparrow,p}^{k-1} g_{\downarrow\downarrow,p}^{n-k} & g_{\downarrow\downarrow,p}^n \end{pmatrix} \\ &= \begin{pmatrix} g_{\uparrow\uparrow,p}^n & 0 \\ g_{\downarrow\uparrow,p} \frac{g_{\uparrow\uparrow,p}^n - g_{\downarrow\downarrow,p}^n}{g_{\uparrow\uparrow,p} - g_{\downarrow\downarrow,p}} & g_{\downarrow\downarrow,p}^n \end{pmatrix}. \end{aligned}$$

Using the space-reflection symmetry, one can furthermore conclude that

$$g_{\uparrow\uparrow,p} = g_{\downarrow\downarrow,-p}. \tag{45}$$

In particular, $g_{\uparrow\uparrow,0} = g_{\downarrow\downarrow,0}$.

We can rewrite (44) as

$$\begin{aligned} &\int_{-p_0}^{p_0} \eta_{\mathrm{fin},\uparrow,p} \eta_{\mathrm{in},\uparrow,p} g_{\uparrow\uparrow,p}^n dp + \int_{-p_0}^{p_0} \eta_{\mathrm{fin},\downarrow,p} \eta_{\mathrm{in},\downarrow,p} g_{\downarrow\downarrow,p}^n dp \\ &\quad + \int_{-p_0}^{p_0} \eta_{\mathrm{fin},\uparrow,p} \eta_{\mathrm{in},\downarrow,p} g_{\downarrow\uparrow,p} \frac{g_{\uparrow\uparrow,p}^n - g_{\downarrow\downarrow,p}^n}{g_{\uparrow\uparrow,p} - g_{\downarrow\downarrow,p}} dp = c_1 (1 + o(1)) (-3)^{-Ln}. \end{aligned} \tag{46}$$

Consider the first integral on the l.h.s. Using Lemma 1 we can show that this integral is $O((c/3)^{Ln})$ with some $c < 1$, by deforming the path of integration connecting $-p_0$ and p_0. Indeed, by Lemma 1, $g_{\uparrow\uparrow,p}$ is a small perturbation of $\widehat{T}_{\uparrow\uparrow,p} = a(1-ip)^{-1}$, so we can make $|g_{\uparrow\uparrow,p}|$ smaller than 3^{-L} by slightly bending the path near $p = 0$ into the upper half-plane.

The same applies to the second integral on the l.h.s., only in this case the path should be deformed into the lower half-plane.

Now we consider the last integral. As $g_{\uparrow\uparrow,0} = g_{\downarrow\downarrow,0}$, the integrand has a zero in the denominator at $p = 0$. This zero is of first order, since $g_{\uparrow\uparrow,0}$ and $g_{\downarrow\downarrow,0}$ are perturbations of $\widehat{T}_{\uparrow\uparrow,p} = a(1-ip)^{-1}$ and $\widehat{T}_{\downarrow\downarrow,p} = a(1+ip)^{-1}$, respectively. We can divide the integrand into two parts, corresponding to the two terms in the numerator, and then deform the path of integration in the resulting two integrals in different directions, compensating this by adding the residue in one case:

$$\begin{aligned} &\int_{-p_0}^{p_0} \eta_{\mathrm{fin},\uparrow,p} \eta_{\mathrm{in},\downarrow,p} g_{\downarrow\uparrow,p} \frac{g_{\uparrow\uparrow,p}^n - g_{\downarrow\downarrow,p}^n}{g_{\uparrow\uparrow,p} - g_{\downarrow\downarrow,p}} dp \\ &\quad = 2\pi i \operatorname{res}_{p=0} \frac{\eta_{\mathrm{fin},\uparrow,p} \eta_{\mathrm{in},\downarrow,p} g_{\downarrow\uparrow,p} g_{\uparrow\uparrow,p}^n}{g_{\uparrow\uparrow,p} - g_{\downarrow\downarrow,p}} + o((c/3)^{Ln}) \\ &\quad = \pi i \frac{\eta_{\mathrm{fin},\uparrow,0} \eta_{\mathrm{in},\downarrow,0} g_{\downarrow\uparrow,0} g_{\uparrow\uparrow,0}^n}{g'_{\uparrow\uparrow,0}} + o((c/3)^{Ln}), \end{aligned}$$

where $g'_{\uparrow\uparrow,0}$ is the derivative at $p = 0$. Comparing this with the l.h.s. of (46), we see that

$$g_{\uparrow\uparrow,0} = g_{\downarrow\downarrow,0} = (-3)^{-L}. \tag{47}$$

Now consider the model with a small $\delta \neq 0$.

Lemma 2 *If L is large enough, then*

$$(-3)^{-L} \frac{dg_{\uparrow\downarrow,0}}{d\delta}\bigg|_{\delta=0} < 0. \tag{48}$$

Proof The operator G was found in the previous lemma as the solution of the fixed point equation $B = \mathcal{F}(B, \delta)$. Using the implicit function theorem, we see that

$$\frac{dG}{d\delta} = \left(\mathbf{1} - \frac{\partial \mathcal{F}}{\partial B}\right)^{-1} \frac{\partial \mathcal{F}}{\partial \delta}.$$

Using the expansion for $\partial\mathcal{F}/\partial B$, one easily shows that (48) is equivalent to

$$(-3)^{-L} \frac{\partial \mathcal{F}_{\uparrow\downarrow,0}(G, \delta)}{\partial \delta}\bigg|_{\delta=0} < 0. \tag{49}$$

We have

$$\frac{\partial \mathcal{F}(G, \delta)}{\partial \delta} = \widehat{T} \sum_{s=1}^{\infty} \frac{d\widehat{W}^{(s)}}{d\delta} G^{-s}. \tag{50}$$

Since $g_{\uparrow\downarrow} = 0$ at $\delta = 0$, we have

$$\frac{\partial \mathcal{F}_{\uparrow\downarrow,0}}{\partial \delta}\bigg|_{\delta=0} = \widehat{T}_{\uparrow\uparrow,0} \sum_{s=1}^{\infty} \frac{d\widehat{W}^{(s)}_{\uparrow\downarrow,0}}{d\delta} g^{-s}_{\downarrow\downarrow,0}\bigg|_{\delta=0}. \tag{51}$$

In order to compute the derivative $d\widehat{W}^{(s)}_{\uparrow\downarrow,0}/d\delta$ at $\delta = 0$, we have to consider only those terms in the expansion for $\widehat{W}^{(s)}_{\uparrow\downarrow,0}$, which are first order in δ, i.e. where the transition caused by $\delta\widetilde{V}$ occurs at a single place. For $s = 1$, the simplest such case corresponds to the simple U-turn as represented by the lowest leg in Fig. 4. We compute now the contribution to $d\widehat{W}^{(1)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ from this term.

In the time evolution picture the simple U-turn corresponds to the transition

$$\dots \Phi^1 \otimes \Phi^1 \otimes \Phi^1 \dots \mapsto \dots \Phi^1 \otimes \Phi^2 \otimes \Phi^1 \dots \tag{52}$$

(assuming that the time $t < 0$; if $t > 0$, then Φ^1 and Φ^2 should be exchanged since $\widetilde{S^\alpha_0 S^\alpha_{Ln}}$ flips the spins at $t = 0$). Recall that $\widetilde{V} = \sum_k R_{k,k+1}$, and let A be the part of this sum consisting of the $L - 1$ terms acting on the block Φ^1 flipped into Φ^2. Consider the expansion

$$A\Phi^1 = \sum_{l=1}^{4} \kappa_l \Phi^l + v',$$

where $v' \in \mathcal{H}^c$. Using the asymptotic orthogonality (28), one computes that for $l \neq 1$

$$\begin{aligned}\kappa_l &= \langle A\Phi^1, \Phi^l\rangle - \langle A\Phi^1, \Phi^1\rangle\langle \Phi^1, \Phi^l\rangle + O(\lambda^2 L)\\ &= \frac{8(L-1)}{3}(-3)^{-L} + O((-3)^{2L}L).\end{aligned}$$

The transition (52) can also be caused by the two terms $R_{k,k+1}$ coupling the flipped Φ^1 to its neighbors, but the contribution from these boundary terms is $O(L^{-1})$ compared to that from the bulk terms.

Now taking into account Duhamel formula (38) and evaluating the Fourier transform at $p = 0$, we conclude that the contribution to $d\widehat{W}^{(s)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ from the simple U-turn is $-\kappa_2 \int_0^\infty e^{-t}dt(1 + O(L^{-1}))$, which is $-\frac{8}{3}(-3)^{-L}(L + O(1))$. Recall that G is a perturbation of $\widehat{T}$, so that $g_{\downarrow\downarrow,0}$ has the same sign as $\widehat{T}_{\downarrow\downarrow,0}$ $(= \widehat{T}_{\uparrow\uparrow,0})$. This implies (49), and hence (48), provided the simple U-turn makes the leading contribution to the expansion (51).

We briefly argue now that this is the case.

One can somewhat simplify the combinatorics by noticing that configurations including $\mathcal{H}^c$-excitations don't contribute to $d\widehat{W}^{(s)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$, since one needs to apply $\delta\widetilde{V}$ at least twice, to create as well as annihilate the excitation. Moreover, though the expansion for $\widehat{W}^{(s)}$ in general involves clusters of trajectories (a piece of the "big" trajectory combined with "small" trajectories), each "small" trajectory occurs as a result of the perturbation and hence carries a factor δ. However, for the contribution to $W^{(s)}_{\uparrow\downarrow}$ to be nonzero, the "big" trajectory must also include at least one transition caused by the perturbation. This shows that the clusters contributing to $d\widehat{W}^{(s)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ are trivial in the sense that they contain only a piece of the "big" trajectory and no "small" trajectories. Summarizing, for the analysis of $d\widehat{W}^{(s)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ one has to consider only single connected trajectories (not clusters), which describe transitions only between states Φ^l (not $\mathcal{H}^c$). Moreover, the perturbation $\delta\widetilde{V}$ is always associated with the lowest horizontal leg of the trajectory.

Recall that extra horizontal legs (compared to minimal trajectories) bring additional small factors to the weight of the trajectory. By (29), (30), horizontal legs of length 1 are associated with the coefficient $a = (-3)^{-L}(1 + O(-3)^{-L})$, and horizontal legs of length 2 are associated with the coefficient $b = (-3)^{-2L}(1 + O(-3)^{-L})$, so that each unit of extra horizontal length contributes a factor $O((-3)^{-L})$ to the weight.

Consider polymers of length 1 (i.e., $s = 1$). Trajectories contributing to $d\widehat{W}^{(1)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ and different from the simple U-turn considered above have extra horizontal length, so their total contribution is smaller than that from the simple U-turn, provided L is large enough.

Let $s = 2$. In this case the simplest trajectory contributing to $d\widehat{W}^{(2)}_{\uparrow\downarrow,0}/d\delta|_{\delta=0}$ is a single leg of length 2, corresponding to the transition

$$\cdots \Phi^1 \otimes \Phi^1 \otimes \Phi^1 \otimes \Phi^1 \cdots \mapsto \cdots \Phi^1 \otimes \Phi^2 \otimes \Phi^2 \otimes \Phi^1 \cdots.$$

This transition is produced by the term $R_{k,k+1}$ coupling two neighboring Φ^1's, and the corresponding weight is $O((-3)^{-2L})$. Other trajectories have extra legs and hence smaller weight. By Lemma 1, $g_{\downarrow\downarrow,0} = (-3)^{-L}(1 + O(\epsilon_1))$, so the $s = 2$ term in the expansion (51) is not greater than $O(L^{-1})$ times the $s = 1$ term.

For $s > 2$, polymers have at least $s - 2$ extra horizontal legs so that by choosing L large one can make the s'th term in (51) exponentially small in s. □

We return to the integral $\int_{-p_0}^{p_0} \eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} dp$, which gives by (43) the asymptotic of the correlation function $\langle S_0^\alpha S_{Ln}^\alpha \rangle$. In the remainder we will occasionally use the notation

$$G = \begin{pmatrix} g_{\uparrow\uparrow} & g_{\uparrow\downarrow} \\ g_{\downarrow\uparrow} & g_{\downarrow\downarrow} \end{pmatrix},$$

where dependence on p and δ is suppressed.

We have

$$G^n = \begin{pmatrix} (g_{\uparrow\uparrow} - w_-)w_+^n + (w_+ - g_{\uparrow\uparrow})w_-^n & g_{\uparrow\downarrow}(w_+^n - w_-^n) \\ g_{\downarrow\uparrow}(w_+^n - w_-^n) & (g_{\downarrow\downarrow} - w_-)w_+^n + (w_+ - g_{\downarrow\downarrow})w_-^n \end{pmatrix} \times ((g_{\uparrow\uparrow} - g_{\downarrow\downarrow})^2 + 4g_{\uparrow\downarrow}g_{\downarrow\uparrow})^{-1/2},$$

where

$$w_\pm = \frac{1}{2}(g_{\uparrow\uparrow} + g_{\downarrow\downarrow} \pm \sqrt{(g_{\uparrow\uparrow} - g_{\downarrow\downarrow})^2 + 4g_{\uparrow\downarrow}g_{\downarrow\uparrow}}).$$

As in our case G, η_{in} and η_{fin} are analytic in p in a complex neighborhood of the segment $[-p_0, p_0]$, we see that the integrand in $\int_{-p_0}^{p_0} \eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} dp$ is an analytic expression, which has singularities (branching points) at those values of p, where

$$(g_{\uparrow\uparrow} - g_{\downarrow\downarrow})^2 + 4g_{\uparrow\downarrow}g_{\downarrow\uparrow} = 0. \tag{53}$$

For large L, there will be exactly two such values p, located near 0 at a distance of order $\sqrt{\delta}$. Indeed, if $\delta = 0$, then (53) becomes $g_{\uparrow\uparrow} = g_{\downarrow\downarrow}$, and this holds for $p = 0$ only. By continuity, for small δ the equality (53) can hold only for some p in a small neighborhood of the origin, and we can determine these p using the asymptotic of G at small p and δ. As shown above (see (45), (47)), for $\delta = 0$ we have $g_{\uparrow\uparrow,p} = g_{\downarrow\downarrow,-p} = (-3)^{-L} + c_1 p + O(p^2)$ with some constant c_1. Furthermore, for small δ we have

$$g_{\uparrow\downarrow}g_{\downarrow\uparrow} = c_2\delta(1 + O(\delta) + O(p)),$$

where, by Lemma 2, $c_2 < 0$. Equation (53) thus takes the form

$$(2c_1 p + O(p^2) + O(\delta))^2 + 4c_2\delta(1 + O(\delta) + O(p)) = 0,$$

and has two solutions,

$$p = \pm\frac{\sqrt{-c_2\delta}}{c_1}(1 + O(\sqrt{\delta})). \tag{54}$$

The constant c_1 is nonzero, because by Lemma 1 at large L the operators G_p approach $\widehat{T}_p$ together with their derivatives in p, and $\widehat{T}_{\uparrow\uparrow,p} = (-3)^{-L} + i(-3)^{-L}p + O(p^2)$, so c_1 must be close to $i(-3)^{-L}$.

We write

$$\eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} = f_+(p) + f_-(p),$$

where $f_\pm$ is the part containing $w_\pm^n$. We deform, as before, the segment of integration $[-p_0, p_0]$ in the integral $\int_{-p_0}^{p_0} \eta_{\text{in},p}^{\text{t}} G_p^n \eta_{\text{fin},p} dp$ slightly into the upper half-plane, then

$\int f_+(p)dp = O((c/3)^{Ln})$, with some $c < 1$. The remaining part, $\int f_-(p)dp$, would be as small if we deformed the line of integration in the opposite direction; so we can write

$$\int_{-p_0}^{p_0} \eta^{\mathrm{t}}_{\mathrm{in},p} G^n_p \eta_{\mathrm{fin},p} dp = \int_\gamma f_-(p)dp + O((c/3)^{Ln}),$$

where γ is a contour encircling the singularities (54).

Like in Sect. 2, it is convenient to make the change of variables $w = w_-(p)$. As shown above, in a small neighborhood of the origin the function $w_-(p)$ is two-valued with the two branching points (54), and it maps this neighborhood onto a neighborhood of the point $(-3)^{-L}$. We will show now that, on this latter small neighborhood, the inverse analytic function also has two branching points at

$$w_{\pm,0} = (-3)^{-L} \pm \sqrt{c_2\delta} + O(\delta). \tag{55}$$

These branching points can be found as $w_\pm(p)$, where p are zeros of the derivative: $w'_\pm(p) = 0$, i.e.

$$g'_{\uparrow\uparrow} + g'_{\downarrow\downarrow} \pm \frac{(g_{\uparrow\uparrow} - g_{\downarrow\downarrow})(g'_{\uparrow\uparrow} - g'_{\downarrow\downarrow}) + 2(g_{\uparrow\downarrow}g_{\downarrow\uparrow})'}{\sqrt{(g_{\uparrow\uparrow} - g_{\downarrow\downarrow})^2 + 4g_{\uparrow\downarrow}g_{\downarrow\uparrow}}} = 0.$$

If we look for zeros of the form $p = r\sqrt{\delta}$, with $r = O(1)$ and $\delta \to 0$, we get

$$O(\delta) \pm \frac{(2c_1 r\sqrt{\delta} + O(\delta))(2c_1 + O(\sqrt{\delta})) + O(\delta)}{\sqrt{(2c_1 r\sqrt{\delta} + O(\delta))^2 + 4c_2\delta + O(\delta^{3/2})}} = 0.$$

This has two solutions $r = O(\sqrt{\delta})$, one for each branch of $w_\pm(p)$. The corresponding branching points of the inverse function $p = p(w)$ are therefore

$$w_{\pm,0} = w_\pm(O(\delta)) = (-3)^{-L} \pm \sqrt{c_2\delta} + O(\delta).$$

In a neighborhood of $w = (-3)^{-L}$ the function $p = p(w)$ has two branches which we fix by making a cut connecting the two branching points found above.

Now we make the change of variables in the contour integral:

$$\int_\gamma f_-(p)dp = \int_{\gamma_1} f_-(p(w))p'(w)dw.$$

Here γ_1 is a contour in the w-plane, encircling the cut. Consider possible singularities in the integrand on the r.h.s. The derivative $p'(w)$ has singularities at the branching points $w_{\pm,0}$ so that

$$p'(w) = \mathrm{const}\,(w - w_{\pm,0})^{-1/2}(1 + O((w - w_{\pm,0})^{1/2})).$$

Also, the function $f_-(p)$ has a singularity in the factor $((g_{\uparrow\uparrow} - g_{\downarrow\downarrow})^2 + 4g_{\uparrow\downarrow}g_{\downarrow\uparrow})^{-1/2}$, but it cancels with the zero of $p'(w)$. We conclude that we can deform the contour γ_1 so that it goes along the cut between $w_{-,0}$ and $w_{+,0}$. Since we can arbitrarily choose this cut, the leading contribution to the integral comes from the endpoints $w_{\pm,0}$ and their neighborhoods. Near $w_{\pm,0}$ we have $f_-(p(w))p'(w) = \mathrm{const}\, w^n(w - w_{\pm,0})^{-1/2}(1 + O((w - w_{\pm,0})^{1/2}))$, where the

constant is independent of n. Combining this with the fact that the integral in question is the leading term in the correlation function, we finally get

$$\langle S_0^\alpha S_{Ln}^\alpha \rangle = c_- \frac{1 + O(n^{-1/2})}{n^{1/2}} w_{-,0}^n + c_+ \frac{1 + O(n^{-1/2})}{n^{1/2}} w_{+,0}^n.$$

The asymptotic for $w_{\pm,0}$ is given by (55) and, by Lemma 2, $c_2 < 0$. Now all the claims of the theorem follow from the above formula. If $\delta < 0$, then this is the commensurate case: the term with $w_{+,0}$ prevails, $w_{+,0}$ is real (this follows from the reality of $\langle S_0^\alpha S_{Ln}^\alpha \rangle$). The case $\delta > 0$ is the incommensurate case; the branching points $w_{\pm,0}$ have imaginary components and they are complex conjugate to each other by the reality of $\langle S_0^\alpha S_{Ln}^\alpha \rangle$.

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