Hyperbolic Deformation Applied to $S = 1$ Spin Chains
— Scaling Relation in Excitation Energy —

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We investigate excitation energies of hyperbolically deformed $S = 1$ spin chains, which are specified by the local energy scale $f_j = \cosh j\lambda$, where $j$ is the lattice index and $\lambda$ is the deformation parameter. The elementary excitation is well described by a quasiparticle hopping model, which is also expressed in the form of hyperbolic deformation. It is possible to estimate the excitation gap $\Delta$ in the uniform limit $\lambda \to 0$, by means of a finite size scaling with respect to the system size $N$ and the deformation parameter $\lambda$.

KEYWORDS: DMRG, scaling analysis, excitation gap, spin-wave velocity, Heisenberg chain, Haldane gap

1. Introduction

A role of numerical study in condensed matter physics is to analyze ground state properties and also low-energy excitations in the thermodynamic limit. Precise determination of the excitation gap is important, since presence of a finite excitation gap corresponds to the finitely correlated property of the system. In numerical analyses of excitation gap, the finite size scaling$^{1,2}$ has been employed. This is because computational resources are limited, and therefore the direct treatment of infinite system is occasionally difficult.  

Density matrix renormalization group (DMRG) method is widely applied to one-dimensional (1D) quantum systems,$^4-7$ since the method provides precise low-lying eigenvalues of large scale systems, up to hundreds or even thousands of sites. Although it is possible to apply DMRG method to systems with periodic boundary conditions (PBC),$^5,8,9$ a majority of applications are performed under the open boundary conditions (OBC). This is because numerical implementation is much easier with the use of OBC. However, presence of boundary corrections often makes precise scaling analyses difficult. To suppress such a corrections, so called the smooth boundary condition has been applied.$^{10-12}$ It is reported that an adiabatic decay of interaction strength toward the system boundary drastically decreases the boundary effect on one-point functions, such as the energy density.

The smooth boundary condition is not applicable when one is interested in elementary excitations. This is because presence of a small energy scale near the boundary induces a fictitious excitation localized around the boundary. We therefore considered to the opposite direction, and proposed the hyperbolic deformation,$^{13,14}$ we introduced position dependence to 1D lattice Hamiltonians, where the energy scale increases toward the both ends of the system. As a consequence of this non-uniform deformation, the excited quasiparticle is weakly bounded around the center of the system. The boundary effect for the excitation energy is reduced, since the quasiparticle does not reach the boundary.

In the previous study, we chiefly applied the hyperbolic deformation to the free Fermionic lattice model, and showed that a two-parameter scaling function exists with respect to the system size $N$ and the deformation parameter $\lambda$.$^{14}$ It is expected that a wide class of 1D systems under the hyperbolic deformation obeys this kind of two-parameter FSS, which could precisely estimate the excitation gap. In this article we investigate the efficiency of this FSS in the context of hyperbolic deformation, when it is applied to correlated systems, such as the $S = 1$ AKLT chain$^{15}$ and the $S = 1$ Heisenberg chain with uniaxial anisotropies (XXZ+D). In the next section we introduce hyperbolically deformed Hamiltonians for these systems. In §3 the form of the two-parameter FSS is shortly reviewed. Numerical results on the spin chains are shown in §4. Conclusions are summarized in the last section.

2. Hyperbolic Deformation

Let us consider a group of 1D quantum spin chains, which are characterized by the non-uniform Hamiltonian

$$
\hat{H}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j\lambda \hat{h}_{j,j+1}, 
$$

(2.1)

where $j$ represents the lattice index, $L$ the system size, and $\lambda$ a nonnegative deformation parameter. The operator $\hat{h}_{j,j+1}$ specifies the interaction between neighboring sites. An example is the bilinear-biquadratic interaction

$$
\hat{h}_{j,j+1} = J \cos \theta \hat{S}_j \cdot \hat{S}_{j+1} + J \sin \theta \left( \hat{S}_j \cdot \hat{S}_{j+1} \right)^2
$$

(2.2)

between neighboring $S = 1$ spins, where $J > 0$ is the coupling constant, and where the angle $\theta$ determines the ratio between bilinear and biquadratic interactions. When $\lambda > 0$, the relative bond strength $f_j = \cosh j\lambda$ is position dependent, and the weakest bond is located at the center of the system $j = 0$. The Hamiltonian $\hat{H}(\lambda)$ when $\lambda > 0$ can be regarded as a deformation — the hyperbolic
deformation — from the uniform one $\hat{H}(\lambda = 0)$. The case $\tan \theta = 1/3$ and $J = 1/\cos \theta$ in Eq. (2.2) corresponds to the AKLT interaction.\textsuperscript{15,16} In this case, the deformed Hamiltonian is explicitly written as

$$
\hat{H}^{\text{AKLT}}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j \lambda \left[ \hat{S}_j \cdot \hat{S}_{j+1} + \frac{1}{3} \left( \hat{S}_j \cdot \hat{S}_{j+1} \right)^2 \right],
$$

which can be called as the deformed AKLT chain. Despite of the position dependence in $\hat{H}^{\text{AKLT}}(\lambda)$, the mechanism of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breaking\textsuperscript{17} is preserved, since the Hamiltonian can be written as a linear combination of local projections. The corresponding ground state is the uniform valence-bond-solid state.

A similar uniformity in the ground state is observed for the hyperbolically deformed $S = 1$ antiferromagnetic Heisenberg spin chain, whose Hamiltonian

$$
\hat{H}^{\text{AFH}}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j \lambda \left[ \hat{S}_j \cdot \hat{S}_{j+1} \right],
$$

corresponds to the choice with $J = 1$ and $\theta = 0$ in Eq. (2.2). Even in the case $\lambda > 0$ the expectation value $\langle \hat{S}_j \cdot \hat{S}_{j+1} \rangle$ calculated for the ground state is nearly position independent.\textsuperscript{18} Also the deformed transverse-field Ising model, which is defined by the Hamiltonian

$$
\hat{H}^{\text{TFI}}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j \lambda \left[ \Gamma s_j^z s_{j+1}^z + 4 s_j^x s_{j+1}^x + \Gamma s_j^z s_{j+1}^z \right],
$$

where $s_j=(s_j^x, s_j^y, s_j^z)$ represents the $S = 1/2$ spin at the $j$th site, exhibits a similar uniformity deep inside the system, even at the critical point $\Gamma = 1$.\textsuperscript{19} These uniform property can be qualitatively explained by the path-integral representation of imaginary time evolution $\hat{U} = \exp \left[ -\tau \hat{H}(\lambda) \right]$ under the hyperbolic geometry.\textsuperscript{14}

### 3. Scaling Form for the Excitation Energy

Let us consider the infinitely long and uniform $S = 1$ Heisenberg spin chain, which corresponds to the double limit $\lambda \to 0$ and $L \to \infty$ of $\hat{H}^{\text{AFH}}(\lambda)$ in Eq. (2.4), as a reference system. The model has finite excitation energy $\Delta$ from the singlet ground state, which is known as the Haldane gap.\textsuperscript{20,21} It was reported that the quasiparticle picture well holds for the magnetic excitation.\textsuperscript{22} When only a quasiparticle is present, the energy dispersion of the quasiparticle can be described by the effective Hamiltonian

$$
\hat{H}^{\text{eff}} = -t \sum_j \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + (2t + \Delta) \sum_j \hat{c}_j^\dagger \hat{c}_j
$$

in the vicinity of zero momentum, where $t$ is the hopping parameter, and where $\hat{c}_j^\dagger$ and $\hat{c}_j$ respectively, represent creation and annihilation of the quasiparticle. The eigenvalue of the zero-quasiparticle vacuum is trivially zero, and that of the one-quasiparticle state is larger than zero when $\Delta$ is positive. If more than two quasiparticles are present, interaction terms should be included into the effective Hamiltonian.\textsuperscript{23,24}

We conjecture that such a quasiparticle picture also holds for the hyperbolically deformed Hamiltonian $\hat{H}^{\text{AFH}}(\lambda)$ in Eq. (2.4), and that the effective Hamiltonian can be written as

$$
\hat{H}^{\text{eff}}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j \lambda \left[ -t \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + (2t + \Delta) \left( \hat{c}_j^\dagger \hat{c}_j + \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \right) \right]
$$

in the form of hyperbolic deformation.

As a preparation for checking the correspondence between $\hat{H}^{\text{AFH}}(\lambda)$ and $\hat{H}^{\text{eff}}(\lambda)$, the authors investigated one-particle state of $\hat{H}^{\text{eff}}(\lambda)$ in our previous study.\textsuperscript{14} The lowest-energy one-particle state is a shallow bound state, where the quasiparticle does not reaches to the both end of the system when $\lambda$ is sufficiently large. The lowest eigenvalue, which we denote as $\Delta_L(\lambda)$, converges to $\Delta$ in the limit $L \to \infty$ and $\lambda \to 0$. We found that the correction $\Delta_L(\lambda) - \Delta$ satisfies the two-parameter scaling

$$
(L + 1)^2 \frac{\Delta_L(\lambda) - \Delta}{t} = g \left[ \sqrt{\frac{\lambda}{t}} (L + 1)^2 \right]
$$

with respect to the system size $L$ and the deformation parameter $\lambda$. The scaling function $g[y]$ satisfies $g[0] = \pi^2$ and $g[y \gg 1] \sim y/\sqrt{2}$. We conjecture that this scaling form is also applicable for elementary excitation of gapped spin chains in general.

### 4. Two-parameter Scaling Analysis

We perform numerical analysis of the hyperbolically deformed spin chains defined in §2, by means of the DMRG method. In order to avoid the quasi four-fold degeneracy,\textsuperscript{17} we put $S = 1/2$ spins at the both ends of the system;\textsuperscript{22} these boundary spins are not counted when we refer to the system size $L$. For the bond between boundary $S = 1/2$ spin and the neighboring $S = 1$ spin, we set weaker interaction strength $J_{\text{end}} = 0.5088$. Actually the value of $J_{\text{end}}$ is not relevant to the elementary excitation and its energy if $\lambda L$ is sufficiently large. We keep at most $m = 100$ block spin states in the DMRG calculations. Numerical convergence in finite system sweeping is accelerated by use of the wave function prediction method.\textsuperscript{25-28} We explain numerical details in the appendix A.

Concerning to the ground state of the hyperbolically deformed $S = 1$ spin chains that we have introduced, the $z$-component of the total spin is zero. Let us denote the corresponding ground state energy by $E_L^{(0)}(\lambda)$. We also calculate the lowest eigenvalue $E_L^{(1)}(\lambda)$ when the $z$-component of the total spin is one. The magnetic excitation energy is then expressed as their difference

$$
\Delta_L(\lambda) = E_L^{(1)}(\lambda) - E_L^{(0)}(\lambda).
$$

We have used the same notation $\Delta_L(\lambda)$ that appears in Eq. (3.3), since we expect that $\Delta_L(\lambda)$ in Eq. (4.1) also satisfies the scaling relation in Eq. (3.3).
For $H^{HAF}(\lambda)$ in Eqs. (2.4), we confirm the presence of scaling function $g$ under the choice $\Delta = 0.410485$ and $t = 7.381$ after some trials of determining these parameters. Figure 1 shows the scaling result for $\Delta_L(\lambda) - \Delta$ when $L = 100, 200$, and $500$. These data agrees with $\Delta_L(\lambda) - \Delta$ shown by solid curve, which is drawn from the effective one-particle model $H^{eff}(\lambda)$ in Eq. (3.2). We also calculate $\Delta_L(\lambda) - \Delta$ for the deformed AKLT chain defined by $H^{AKLT}(\lambda)$ in Eq. (2.3), and show the result in Fig. 2. For this case the best fit to $H^{eff}(\lambda)$ is realized when $\Delta = 0.7002483$ and $t = 0.51542$. For both Heisenberg and AKLT chains, the quasiparticle picture well holds even under the hyperbolic deformation, and the estimated gaps $\Delta$ by these finite size scalings are consistent with known values.\(^{23, 24, 29, 30}\)

Let us check the validity of two-parameter scaling on another model, the $S = 1$ XXZ spin chain with uniaxial anisotropy. Under the hyperbolic deformation, the corresponding Hamiltonian is written as

$$
\hat{H}^{XXZ}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j\lambda \left[ S_j^X S_{j+1}^X + S_j^Y S_{j+1}^Y + \alpha S_j^Z S_{j+1}^Z \right] + D \sum_{j=-L/2+1}^{L/2} \cosh(j - \frac{1}{2})\lambda \left[ S_j^Z \right]^2.
$$

(4.2)

Figure 3 shows the scaling plot when $\alpha = 0.8$ and $D = 0.2$. For this case the scaling parameters are determined as $\Delta = 0.20502$ and $t = 13.01$. Figure 4 is the case when $\alpha = 1$ and $D = 0.2$. For this case we obtain $\Delta = 0.288240$ and $t = 10.77$. Again the two-parameter scaling well holds for $H^{XXZ}(\lambda)$, and the obtained value of $\Delta$ agrees with previous studies.\(^{31-33}\)

A profit of the two-parameter scaling is that the effective hopping parameter $t$ is obtained simultaneously with the gap $\Delta$. It is well known that the spin velocity

$$
v = \sqrt{2t\Delta}
$$

(4.3)

is essential for the thermodynamic property of the spin chains at low temperature.\(^{34}\) (See Appendix B.) From the data in Fig. 1, the velocity at the isotropic Heisenberg point is obtained as $v = 2.462$, which is consistent with $v = 2.4691$ reported by S. Todo.\(^{30}\) At the AKLT
point, the estimated value of the velocity from Fig. 2 is $v = 0.84962$. The value deviates from $v = 0.825$ reported by K. Okunishi et al., and the clarification of this difference is a remaining problem.

5. Conclusion

We have investigated the elementary excitation energy of the hyperbolically deformed $S = 1$ spin chains. Two-parameter scaling for the excitation energy $\Delta_L(\lambda)$ coincides with the effective one-quasiparticle picture in Eq. (3.2), which is also written in the form of hyperbolic deformation. The fact makes it possible to estimate both the bulk gap $\Delta$ and the effective hopping parameter $t$ accurately by introduction of the hyperbolic deformation.

There are some variations of the non-uniform deformation applied to spin chains. A simple example is the exponential deformation introduced by Okunishi. Similar to the hyperbolic deformation, the correlation length becomes finite when the site-dependent energy scale $f_j = e^{\lambda j}$ is introduced. The behavior of the excited quasiparticle from the gapped ground state under this exponential deformation is our interest for future study.

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Appendix A: Numerical Details

We explain several numerical details on the calculation of $E_L^{(0)}(\lambda)$ and $E_L^{(1)}(\lambda)$ in Eq. (4.1) by means of the DMRG method. To simplify the formulation without loosing generality, we consider $\hat{H}(\lambda)$ defined by Eq. (2.1). According to the custom in DMRG, let us split $\hat{H}(\lambda)$ into three parts

$$
\hat{H}(\lambda) = \hat{H}_L(\lambda) + \hat{h}_{0,1} + \hat{H}_R(\lambda),
$$

where $\hat{H}_L(\lambda)$ and $\hat{H}_R(\lambda)$ are, respectively, the left and the right block Hamiltonians, which are defined as

$$
\hat{H}_L(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh j\lambda \, \hat{h}_{j,j+1},
$$

$$
\hat{H}_R(\lambda) = \sum_{j=L/2}^{L-1} \cosh j\lambda \, \hat{h}_{j,j+1}.
$$

These block Hamiltonians satisfy a recursion relation\(^{13}\)

$$
\hat{H}_L(\lambda) = \cosh \lambda \, \hat{h}_{-1,0} - \hat{h}_{-2,-1} + 2 \cosh \lambda \, H_L^*(\lambda)
$$

$$
\hat{H}_R(\lambda) = \cosh \lambda \, \hat{h}_{1,2} - \hat{h}_{2,3} + 2 \cosh \lambda \, H_R^* - H_R^*(\lambda),
$$

where $H_L^*$ and $H_R^*$ represent the block Hamiltonians for the $(L - 2)$-site system

$$
\hat{H}_L^*(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh(j - 1)\lambda \, \hat{h}_{j,j+1},
$$

$$
\hat{H}_R^*(\lambda) = \sum_{j=L/2}^{L-1} \cosh(j - 1)\lambda \, \hat{h}_{j,j+1},
$$

and where $H_L^{**}$ and $H_R^{**}$ represent those for $(L - 4)$-site systems

$$
\hat{H}_L^{**}(\lambda) = \sum_{j=-L/2+1}^{L/2-1} \cosh(j - 2)\lambda \, \hat{h}_{j,j+1},
$$

$$
\hat{H}_R^{**}(\lambda) = \sum_{j=L/2}^{L-1} \cosh(j - 2)\lambda \, \hat{h}_{j,j+1}.
$$

The recursion relation Eq. (A.3) is useful when one performs the infinite system DMRG iteration for the preparation of the block Hamiltonians to start the following finite system DMRG sweeps. It is also possible to perform the infinite system DMRG method for a uniform spin chain $\lambda = 1$, and increase $\lambda$ afterword adiabatically during the following finite system DMRG sweeps.

A special care, which should be taken for the hyperbolically deformed system, is the subtraction of the energy expectation value from the Hamiltonian. Since the factor $\cosh j\lambda$ increases rapidly with respect to $|j|$, the value of $E_L^{(0)}(\lambda)$ becomes huge when $\frac{L}{2}\lambda$ is large. This is a cause of numerical error. Thus we shift the origin of the energy so that the ground-state energy becomes almost zero. This energy shift can be performed during the finite size sweeping. First we obtain the ground state $|\Psi_0\rangle$ diagonalizing the Hamiltonian $\hat{H}(\lambda)$, which is represented as the super-block Hamiltonian in DMRG formulation. We calculate the expectation value $\langle \hat{h}_{j,j+1} \rangle$ for each bond between the active two sites between the left and the right blocks. Every time we calculate $\langle \hat{h}_{j,j+1} \rangle$, we subtract $\cosh \lambda j \langle \hat{h}_{j,j+1} \rangle$ from the bond Hamiltonian, and create the renormalized block Hamiltonians after this subtraction. Within several sweeps the numerical error in $\langle \hat{h}_{j,j+1} \rangle$ almost vanishes, and the ground state energy calculated for the Hamiltonian under the energy shift

$$
\hat{H}(\lambda) - \langle \hat{H}(\lambda) \rangle = \sum_{j=-L/2+1}^{L/2-1} \cosh j\lambda \left( \hat{h}_{j,j+1} - \langle \hat{h}_{j,j+1} \rangle \right)
$$

becomes zero within the tiny numerical error. When we put $S = \frac{L}{2}$ boundary spins, we also perform this energy shift for the additional boundary interactions.

Appendix B: Spin Velocity

We shortly review a physical interpretation of the spin velocity $v = \sqrt{2t\Delta}$ in Eq. (4.3). In special relativity the energy $E$ of a particle that has momentum $p$ and mass $m$ is given by $E = \sqrt{p^2c^2 + m^2c^4}$, where $c$ is the velocity of light. Expanding by $p$ one obtains the non relativistic...
approximation

\[ E \sim mc^2 + \frac{p^2}{2m} = mc^2 + \frac{p^2c^2}{2mc^2}. \quad \text{(B-1)} \]

On the other hand, the dispersion of \( H_{\text{eff}} \) in Eq. (3.1) is given by

\[ E_{\text{eff}} = \Delta + 2t(1 - \cos k), \]

where \( k \) is the wave number of the quasiparticle. Expanding by \( k \) one obtains

\[ E_{\text{eff}} \sim \Delta + \frac{tk^2}{2} = \Delta + \frac{k^2}{2} \frac{\Delta}{2\Delta}. \quad \text{(B-2)} \]

It should be noted that both the lattice constant and \( k \) are dimensionless. Thus \( mc^2 \) corresponds to \( \Delta \), and \( p \) corresponds to \( k \). Comparing Eq. (B-1) and Eq. (B-2), one finds that the light velocity \( c \) corresponds to a dimensionless velocity \( v = \sqrt{2t\Delta} \), which is nothing but the velocity of the spin wave when the system is gapless.

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