Hybrid Deformation on Quantum Lattice Hamiltonians

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A group of non-uniform quantum lattice Hamiltonians in one dimension is introduced, which is related to the hyperbolic 1+1-dimensional space. The Hamiltonians contain only nearest neighbor interactions whose strength is proportional to \( \cosh j \lambda \), where \( j \) is the lattice index and where \( \lambda \geq 0 \) is a deformation parameter. In the limit \( \lambda \to 0 \) the Hamiltonians become uniform. Spacial translation of the deformed Hamiltonians is induced by the corner Hamiltonians. As a simple example, we investigate the ground state of the deformed \( S = 1/2 \) Heisenberg spin chain by use of the density matrix renormalization group (DMRG) method. It is shown that the ground state is dimerized when \( \lambda \) is finite. Spin correlation function show exponential decay, and the boundary effect decreases with increasing \( \lambda \).

KEYWORDS: DMRG, Corner Hamiltonian, Regularization, Renormalization Group

1. Introduction

The density matrix renormalization group (DMRG) method has been applied to various problems in low dimensional correlated physics.1–4 The method contains the block spin transformation in its formulation, but the relation with Wilson’s renormalization group (RG) is not clear, since the hierarchy in energy scale is missing in the uniform lattice Hamiltonians. Recently Okunishi considered a group of half-infinite non-uniform systems, whose lattice Hamiltonians

\[
H(\lambda) = \sum_{j=1}^{N} \sum_{j,j+1}^{N} e^{j\lambda} h_{j,j+1} \tag{1.1}
\]

are sum of neighboring interaction terms \( h_{j,j+1} \), where \( j \) is the lattice index and where \( N + 1 \) is the system size.6 He applied numerical RG method to this system, where the application is a one-parameter deformation — the exponential deformation — to the real space RG scheme introduced by Xiang.7,8 It is shown that the energy scale introduced by the deformation parameter \( \Lambda = e^{\lambda} \geq 1 \) regularize the distribution of low energy excitations, even for the models that are gapless when \( \lambda = 0 \) in the large \( N \) limit.

It is possible to introduce Okunishi’s deformation scheme to the DMRG method for the purpose of regularizing low energy excitations. A primitive way is to joint the deformed half-infinite Hamiltonians in Eq. (1.1) at the origin

\[
H^{\text{Joint}}(\lambda) = \sum_{j=-N}^{N} e^{j|\lambda|} h_{j,j+1} \tag{1.2}
\]

to construct the whole system of size \( 2N + 2 \). The interaction strength increases with \( |j| \) toward the boundary of the system, in contrast to the smooth boundary condition proposed by Vekić and White.9 The construction of the above Hamiltonian is, however, rather artificial in the point that one may choose arbitrary increasing function of \( |j| \) instead of \( e^{j|\lambda|} \). In this article we introduce a natural candidate

\[
H^{\cosh}(\lambda) = \frac{1}{2} \sum_{j=-N}^{N} e^{j\lambda} h_{j,j+1} + \frac{1}{2} \sum_{j=-N}^{N} e^{-j\lambda} h_{j,j+1} = \sum_{j=-N}^{N} \cosh(j\lambda) h_{j,j+1}, \tag{1.3}
\]

which keeps some aspects of translational invariance even when \( \lambda > 0 \). It is possible to find a geometric interpretation of \( H^{\cosh}(\lambda) \) as a time boost in the hyperbolic 1+1-dimensional space, as discussed at the end of this article.

In the next section we shortly review the exponential deformation on the lattice Hamiltonian. Eigenvalue distribution is considered in the large system size limit. In §3 we explain the details of the deformed Hamiltonian \( H^{\cosh}(\lambda) \) in Eq. (1.3). It is shown that the lattice translation is related to the deformed corner Hamiltonian. Recursive construction of \( H^{\cosh}(\lambda) \) is also considered. Ground state property of the deformed system is analyzed in §4 in the case of the \( S = 1/2 \) Heisenberg spin chain. It is shown that the spin correlation function of the ground state decays exponentially when \( \lambda \) is finite, and the state is dimerized. The effect of deformation on the quantum entropy is observed. Conclusions are summarized in the last section. Quantum-classical correspondence of the deformed Hamiltonians and several conjectures are discussed.

2. Exponential Deformation

Consider a group of 1D quantum Hamiltonians

\[
H = \sum_{j=-N}^{N} h_{j,j+1} \tag{2.1}
\]
on the lattice of size \( 2N + 2 \), where \( h_{j,j+1} \) represents the interaction between neighboring sites labeled by \( j \) and \( j + 1 \). A typical example is the antiferromagnetic Heisenberg spin Hamiltonian

\[
H_{H} = J \sum_{j=-N}^{N} s_{j} \cdot s_{j+1}, \tag{2.2}
\]
where \( J \geq 0 \) represents the interaction parameter. Before considering the deformed Hamiltonian \( H^{\text{exp}}(\lambda) \) in Eq. (1.3), let us observe effects of the exponential deformation in Eq. (1.1). For latter convenience we treat the system whose linear size is \( 2N + 2 \). The exponentially deformed Hamiltonian is then written as

\[
H^{\text{exp}}(\lambda) = \sum_{j=-N}^{N} e^{\lambda J} h_{j,j+1},
\]

(2.3)

where the deformation parameter \( \lambda \) is real and positive. \(^{10}\) When \( \lambda = 0 \) the above Hamiltonian \( H^{\text{exp}}(\lambda) \) coincides with the uniform Hamiltonian \( H \) in Eq. (2.1).

It is known that the factor \( \Lambda = e^{\lambda} \) controls the eigenvalue structure. \(^{5,6}\) In order to observe the fact briefly, let us consider the infinite system size limit \( N \rightarrow \infty \). To simplify the discussion we assume that the ground state \( E \) is satisfied. Thus if the eigenvalue \( S \) coincides in Eq. (2.9), and are represented by localized wave functions similar to wavelet basis function. The half-filled state \( |\Phi\rangle \) has finite excitation gap, where \( |\Phi\rangle \) is periodic and satisfies \( S^2|\Phi\rangle = |\Phi\rangle \). When \( \lambda = 0 \) the one-particle eigenfunctions and energy spectrum is explained by the Bloch’s theorem. It is not trivial how such an energy structure is destructed by the introduction of exponential deformation. It is straightforward to generalize the exponential deformation to systems that contain interactions of longer range.

3. Hyperbolic Deformation

The eigenvalue distribution of \( H^{\text{exp}}(\lambda) \) explained in the last section prevents numerical study of the bulk property of the system around the center \( j = 0 \). This is because the energy scale in the left side of the system \( (j < 0) \) is smaller than that at the center, and to apply the DMRG method to such system is difficult. This problem can be avoided if we take an average between \( H^{\text{exp}}(\lambda) \) and \( H^{\text{exp}}(-\lambda) \) as

\[
H^{\text{cosh}}(\lambda) = \frac{1}{2} [H^{\text{exp}}(\lambda) + H^{\text{exp}}(-\lambda)]
\]

(3.1)

It should be noted that presence of periodic eigenstates are not excluded. For example, if there is unique zero-energy eigenstate \( |\Phi\rangle \), it is translationally invariant. This is because Eq. (2.7) shows that \( S|\Phi\rangle \) is also the zero energy state. Thus we can say that if the zero-energy state is unique, it satisfies the translational invariance

\[
S|\Phi\rangle = |\Phi\rangle.
\]

(2.10)

As an extension one can consider degenerated case, where there are two zero-energy eigenstates \( |\Phi_a\rangle \) and \( |\Phi_b\rangle \) that satisfies

\[
|\Phi_a\rangle = S|\Phi_a\rangle,
\]

\[
|\Phi_b\rangle = S|\Phi_b\rangle.
\]

(2.11)

This is the case when there is dimerization in the ground state. This degeneracy would be lifted by the effect of boundary when the system size \( 2N + 2 \) is finite. It is straightforward to extend the argument of degeneracy to trimerized state, etc.

As an example one can consider the deformed tight-binding Hamiltonian

\[
H_{t,b}(\lambda) = \sum_{j=-\infty}^{\infty} e^{\lambda J} [-t (c^\dagger_{j+1} c_j + c^\dagger_j c^\dagger_{j+1}) + (-1)^j \frac{\Delta}{2} (c^\dagger_j c_j - c^\dagger_{j+1} c^\dagger_{j+1})]
\]

(2.12)

for spinless lattice Fermions, where \( t \) represents the hopping parameter and where \( \Delta \) the band gap. Since this Hamiltonian contains oscillating potential, the translation period is 2-site when \( \lambda = 0 \). Thus for this deformed Hamiltonian \( H_{t,b}(\lambda) \) one should modify the relation Eq. (2.4) according to this period. It can be verified that all the one-particle states \( |\Psi\rangle \) satisfy the orthogonality in Eq. (2.9), and are represented by localized wave functions similar to wavelet basis function. The half-filled state \( |\Phi\rangle \) has finite excitation gap, where \( |\Phi\rangle \) is periodic and satisfies \( S^2|\Phi\rangle = |\Phi\rangle \). When \( \lambda = 0 \) the one-particle eigenfunctions and energy spectrum is explained by the Bloch’s theorem. It is not trivial how such an energy structure is destructed by the introduction of exponential deformation. It is straightforward to generalize the exponential deformation to systems that contain interactions of longer range.
We call the deformation from $H$ in Eq. (2.1) to $H^\cosh(\lambda)$ introduced here as the hyperbolic deformation in the following.

Let us extend the shift operation $S$ and its conjugate $S^\dagger$ to Hamiltonians of finite size systems. A natural way is to consider that the operation modifies the coefficients of the neighboring interactions as follows

$$\cosh j\lambda \to \cosh(j - 1)\lambda.$$  

(3.2)

Then the shift operation on $H^\cosh(\lambda)$ is defined as

$$SH^\cosh(\lambda)S^\dagger = \sum_{j=-N}^{N} \cosh(j - 1)\lambda h_{j,j+1}.$$  

(3.3)

Taking the weighted difference between $H^\cosh(\lambda)$ and $SH^\cosh(\lambda)S^\dagger$ we obtain the relation

$$H^\cosh(\lambda) - \frac{1}{\cosh \lambda} SH^\cosh(\lambda)S^\dagger = \tanh \lambda \sum_{j=-N}^{N} \sinh j\lambda h_{j,j+1} = \tanh \lambda H^\sinh(\lambda),$$  

(3.4)

where $H^\sinh(\lambda)$ introduced here represents deformed Hamiltonian of another type

$$H^\sinh(\lambda) = \sum_{j=-N}^{N} \sinh j\lambda h_{j,j+1},$$  

(3.5)

which is decoupled at the origin $j = 0$. Similar to Eq. (3.4), the deformed Hamiltonian $H^\cosh(\lambda)$ can be obtained from $H^\sinh(\lambda)$ by the following weighted difference

$$H^\sinh(\lambda) - \frac{1}{\cosh \lambda} SH^\sinh(\lambda)S^\dagger = \tanh \lambda H^\cosh(\lambda).$$  

(3.6)

The relations Eqs. (3.4) and (3.6) can be regarded as one parameter deformation to the translational invariance $SHS^\dagger = H$, which is satisfied by the uniform Hamiltonian in Eq. (2.1).

Following the convention in the infinite system DMRG method, let us divide $H^\cosh(\lambda)$ into three parts

$$H^\cosh(\lambda) = H_L(\lambda) + h_{0,1} + H_R(\lambda),$$  

(3.7)

where $H_L(\lambda)$ and $H_R(\lambda)$ are defined as follows

$$H_L(\lambda) = \sum_{j=-N}^{1} \cosh j\lambda h_{j,j+1},$$

$$H_R(\lambda) = \sum_{j=1}^{N} \cosh j\lambda h_{j,j+1}. $$  

(3.8)

We also divide $H^\sinh(\lambda)$ in the same manner

$$H^\sinh(\lambda) = C_L(\lambda) + C_R(\lambda),$$  

(3.9)

where $C_L(\lambda)$ and $C_R(\lambda)$ are defined as follows

$$C_L(\lambda) = \sum_{j=-N}^{1} \sinh j\lambda h_{j,j+1}$$

$$C_R(\lambda) = \sum_{j=1}^{N} \sinh j\lambda h_{j,j+1}. $$  

(3.10)

These are deformations to the corner Hamiltonian, \cite{12, 13} since in the limit $\lambda \to 0$ we obtain the relation

$$\lim_{\lambda \to 0} \frac{C_R(\lambda)}{\sinh \lambda} = \sum_{j=1}^{N} j h_{j,j+1}. $$

(3.11)

We have shown the relation between $H^\cosh(\lambda)$ and $H^\sinh(\lambda)$ for the same system size $2N + 2$. We then focus on recursion relations, which connects systems of different sizes. Let us introduce Baxter’s star notation \cite{12, 13}

$$H^*_R(\lambda) = \sum_{j=2}^{N} \cosh(j - 1)\lambda h_{j,j+1}$$

$$C^*_R(\lambda) = \sum_{j=2}^{N} \sinh(j - 1)\lambda h_{j,j+1}. $$

(3.12)

We then obtain recursion relation

$$C_R(\lambda) = \sum_{j=1}^{N} \sinh[(j - 1)\lambda + \lambda] h_{j,j+1}$$  

(3.13)

$$= \cosh \lambda C^*_R(\lambda) + \sinh \lambda [h_{1,2} + H^*_R(\lambda)],$$

and similarly we obtain

$$H^*_R(\lambda) = \sum_{j=3}^{N} \cosh[(j - 1)\lambda + \lambda] h_{j,j+1}$$  

(3.14)

$$= \cosh [h_{1,2} + H^*_R(\lambda)] + \sinh \lambda C^*_R(\lambda).$$

If we introduce the double star notations

$$H^*_R^{**}(\lambda) = \sum_{j=3}^{N} \cosh(j - 2)\lambda h_{j,j+1}$$

$$C^*_R^{**}(\lambda) = \sum_{j=3}^{N} \sinh(j - 2)\lambda h_{j,j+1}, $$

(3.15)

we can decouple the recursion relations as follows

$$H^*_R(\lambda) = \cosh \lambda h_{1,2} - h_{2,3} + 2 \cosh \lambda H^*_R(\lambda) - H^*_R^{**}(\lambda)$$

$$C_R(\lambda) = \sinh \lambda h_{1,2} + 2 \cosh \lambda C^*_R(\lambda) - C^*_R^{**}(\lambda). $$

(3.16)

These relations would be of use when one applies numerical renormalization group methods \cite{1, 2, 6, 13} to the deformed Hamiltonian $H^\cosh(\lambda)$ in order to obtain its eigenstates.

4. Numerical Observations

One might conjecture that the hyperbolic deformation violates uniform property of the system, since the bond interaction strength is modified. But for the ground state this intuition is not always true. For example, one can show that the valence bond solid (VBS) state of $S = 1$ spin chains is not violated by the hyperbolic (or even exponential) deformation. We observe another example, the ground state of the deformed $S = 1/2$ Heisenberg spin chain in this section.

Figure 1 shows the nearest neighbor spin correlation function $\langle s_i^z s_{i+1}^z \rangle$ calculated for the ground state of 400-site system when $\lambda = 0, 0.05,$ and $0.1$. We keep $m = 130$ states at most for the block spin variables in the calculation by the finite system DMRG method. When
The correlation function shows even-odd oscillation with respect to \( j \), and the oscillation slowly decays from the boundary to the center of the system. It is known that the decay is in power low, which represents the gapless nature of the undeformed \( S = \frac{1}{2} \) Heisenberg chain. When \( \lambda \) is finite, the oscillation is strongly stabilized, and the boundary effect disappears rapidly.

\[ \lambda = 0 \text{ the correlation function show even-odd oscillation} \]

Figure 2 shows the correlation function \( (-1)^{2j+1} \langle s_{j-1}^z s_{j+1}^z \rangle \) with respect to the distance \( 2j + 1 \).

When \( \lambda = 0.05 \) and \( \lambda = 0.1 \) we observe exponential decay. The correlation length \( \xi \) obtained from the decay rate is almost inverse proportional to \( \lambda \) as shown in Fig. 3, where \( \xi \lambda \sim 0.134 \) is satisfied. These calculated results suggest that the hyperbolic deformation enhances the local property of the system. To confirm this locality, we calculate the entanglement entropy. Figure 4 shows the bipartite entropy \( S \) at the center of 400-site system. The value of \( S \) decrease exponentially with \( \lambda \), where \( S = 1.145 \) at the infinite \( \lambda \) limit.

5. Conclusions and Discussions

We have investigated the effect of hyperbolic deformation on 1D quantum lattice Hamiltonians. Numerical analysis on the deformed \( S = \frac{1}{2} \) Heisenberg model shows that the deformation introduces dimerization in the ground state, and the local property is enhanced. The entanglement entropy becomes finite even in the large system size limit when \( \lambda > 0 \).

Though the calculated system is one-dimensional it can possess a dimerized ground state, because shift of dimerized pattern introduces macroscopic increase of energy expectation value; the dimer order might survive in finite temperature. In this sense the deformed system has property of higher dimensional systems.

It would be interesting to consider whether the ground state is exactly represented by a matrix product state of finite matrix dimension in the infinite \( \lambda \) limit. We conjecture that integer spin Heisenberg spin chains under strong hyperbolic deformation have such finite dimensional matrix product ground states, if appropriate boundary conditions are imposed.

The hyperbolic deformation can be used for scaling analysis of the ground state of undeformed system. The two parameter scaling proposed by Tagliacozzo et al., where the controllable parameters are the system
size $N$ and the kept number of block spin states $m$, can be modified to the scaling analysis with respect to $\lambda$ and $m$. More simply, if one keeps sufficient number of $m$ in numerical calculation, the finite size scaling with respect to $N$ can be replaced by the finite $1/\lambda$ scaling.

Let us cast our eye to the quantum-classical correspondence. If one considers the Trotter decomposition\textsuperscript{24,25} of the deformed Hamiltonian $H^{\cosh}(\lambda)$, one finds that the Hamiltonian describes real or imaginary time boost in the hyperbolic $1 + 1$-dimensional space, which has constant negative curvature. It is known that classical lattice models on the hyperbolic 2D space tend to show gaussian universality in their phase transition.\textsuperscript{16–23} This suggests that if $H^{\cosh}(\lambda)$ describes quantum phase transition of second order, it would subject to Gaussian universality class. Such a geometric interpretation may draw deformation of various type, such as spherical deformation $H^{\sin}(\lambda)$.

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