q-DEFORMATIONS OF QUANTUM SPIN CHAINS WITH
EXACT VALENCE-BOND GROUND STATES

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ABSTRACT
Quantum spin chains with exact valence-bond ground states are of great interest in
condensed-matter physics. A class of such models was proposed by Affleck et al., each
of which is \( su(2) \)-invariant and constructed as a sum of projectors onto definite total spin
states at neighbouring sites. We propose to use the machinery of the \( q \)-deformation of
\( su(2) \) to obtain generalisations of such models, and work out explicitly the two simplest
examples. In one case we recover the known anisotropic spin-1 VBS model while in the
other we obtain a new anisotropic generalisation of the spin-\( \frac{1}{2} \) Majumdar-Ghosh model.

1. Introduction
The study of one-dimensional quantum spin chains continues to flourish, with re-
cent applications to diffusion-limited reactions. In this work the integrability and
quantum group invariance of the spin chain play a crucial role, with the quantum
group deformation parameter \( q \) taking on a simple physical meaning in terms of
the diffusion rates. In this paper we pursue a different application and take up
the \( q \)-deformation of isotropic quantum spin chains with exact valence-bond ground
states.

The interest in valence-bond states originates in proposed mechanisms for high-
\( T_c \) superconductivity. Several one-dimensional chains are known to have ground
states made up of valence-bonds. The primary examples are the spin-\( \frac{1}{2} \) Majumdar-
Ghosh model and the spin-1 valence-bond-solid (VBS) model of Affleck et al. Higher-spin valence-bond models exist on lattices with a higher co-ordination num-
ber, with e.g., a spin-\( \frac{3}{2} \) model on the honeycomb lattice.

A valence-bond between two sites on a lattice is the spin-0 (singlet) combi-
ation of two spin-\( \frac{1}{2} \) states on those sites. For spin-\( \frac{1}{2} \) chains it is a natural concept. In
fact it makes sense for higher spin-\( s \) chains as well, since a spin-\( s \) operator on one
site can be considered as the symmetric combination of \( 2s \) spin-\( \frac{1}{2} \) operators on the
same site. The spin-\( \frac{1}{2} \) Majumdar-Ghosh model involves nearest-neighbour and
next-nearest-neighbour interactions, with Hamiltonian

\[
\mathcal{H}^{M-G} = \sum_{j=1}^{N-2} p_{j,j+1,j+2}^{(3/2)}
\]
where $\mathcal{P}_{j,j+1,j+2}^{(3/2)}$ is the projector onto states with total spin $\frac{3}{2}$ at sites $j$, $j+1$ and $j+2$. The ground states of this model are dimerised, as depicted in Figure 1 for a lattice with $N = 7$ sites, with each dimer representing a valence-bond. That these are indeed ground states, of zero energy, is most evident from the $su(2)$-projector description of the Hamiltonian, since if there is a valence-bond shared between every three neighbouring sites the total spin on those sites can only be $\frac{1}{2}$. For a lattice with even (odd) number of sites, the ground state degeneracy is five (respectively, four) in the case of free boundary conditions, although there are two different ground states in the infinite lattice limit.

On the other hand, the spin-$1$ VBS model involves only nearest-neighbour interactions and has the Hamiltonian

$$
\mathcal{H}_V^{\text{VBS}} = \frac{1}{6} \sum_{j=1}^{N-1} \left[ (S_j \cdot S_{j+1})^2 + 3S_j \cdot S_{j+1} + 2 \right],
$$

where $\mathcal{P}_{j,j+1}^{(2)}$ projects onto states with total spin $2$ at sites $j$ and $j+1$. In this case the groundstates are such that the valence-bonds cover the whole lattice, as depicted in Figure 2. Once again, the nature of the ground states is clear from the projector description of the Hamiltonian, since if there is a valence-bond between any two neighbouring sites, the four spin-$\frac{1}{2}$’s at those sites can only add to spin $0$ or $1$. For this model, the ground state degeneracy is four for finite lattices (with free boundary conditions) with a unique ground state in the infinite lattice limit.

An anisotropic version of the VBS model was recently proposed in Ref. 6 as a special case of the most general $U_q(su(2))$-invariant spin-$1$ quantum chain. This $q$-deformed version of the VBS model was subsequently investigated by Klümper et al. In this paper we present a natural derivation of this more general model in the framework of $U_q(su(2))$-projectors. We also use this machinery to derive a new generalisation of the spin-$\frac{1}{2}$ Majumdar-Ghosh model. Similar results can be
obtained for the higher spin VBS models of Affleck et al. However, the spin-\(\frac{1}{2}\) and spin-1 cases are special in that the \(U_q(su(2))\) spin matrices are proportional to their \(su(2)\) counterparts and thus the \(q\)-deformed versions of these models can be viewed as anisotropic generalisations.

The paper is arranged as follows. In section 2.1 we rederive the well-known \(U_q(su(2))\)-invariant spin-\(\frac{1}{2}\) XXZ chain. This is the simplest possible \(U_q(su(2))\)-invariant chain, and although not possessing valence-bond ground states, its construction illustrates well the general procedure we follow and serves as a warm up to the derivation of the \(q\)-deformed Majumdar-Ghosh model in section 2.2, which constitutes our main result. Then in section 3 we give the derivation of the \(q\)-deformed spin-1 VBS model.

To first set the notation, we review some relevant facts concerning the quantum algebra \(U_q(su(2))\). This algebra is generated by \(S^z\) and \(S^\pm\), with defining relations \([S^+, S^-] = [2S^z]\) and \([S^z, S^\pm] = \pm S^\pm\), where \([x] \equiv (q^x - q^{-x})/(q - q^{-1})\). The co-product \(\Delta : U_q(su(2)) \rightarrow U_q(su(2)) \otimes U_q(su(2))\) given by

\[
\Delta(S^z) = 1 \otimes S^z + S^z \otimes 1 \\
\Delta(S^\pm) = q^{-S^z} \otimes S^\pm + S^\pm \otimes q^{S^z}
\]

is a homomorphism : \(\Delta(ab) = \Delta(a)\Delta(b)\) and is co-associative : \((1 \otimes \Delta) \circ \Delta = (\Delta \otimes 1) \circ \Delta\). It has a natural extension to \(\Delta^{(n)} : U_q(su(2)) \rightarrow U_q(su(2))^{\otimes (n+1)}\), defined recursively by \(\Delta^{(n)} = ((1^{\otimes (n-1)}) \otimes \Delta) \circ \Delta^{(n-1)}\) and \(\Delta^{(1)} = \Delta\).

The Casimir element, belonging to the centre of \(U_q(su(2))\), is given by \(C = S^- S^+ + [S^z + \frac{1}{2}]^2 - [\frac{1}{2}]^2\), which in the limit \(q \rightarrow 1\) becomes the familiar \(S \cdot S = (S^x)^2 + (S^y)^2 + (S^z)^2\), where \(S^x, S^y\) are such that \(S^\pm = S^x \pm iS^y\). When \(q\) is not a root of unity, the representation theory of \(U_q(su(2))\) is exactly the same as that of \(su(2)\). Namely, the irreducible representations are labelled by the spin \(j\) and are \((2j + 1)\)-dimensional. On the spin-\(j\) representation the Casimir \(C\) takes the value \([j][j+1]\). This equivalence between the representation theory of the \(q\)-deformed and undeformed algebras makes it possible to \(q\)-deform an \(su(2)\) model of Affleck et al. with exact valence-bond ground states by simply replacing \(su(2)\)-projectors with their \(q\)-analogues. These projectors can be obtained from the Casimir \(C\); more specifically, as polynomials in \(\Delta^{(n)}(C)\) where \(n\) is determined by the range of interactions required - \(n = 1\) for nearest-neighbour interactions, \(n = 2\) for nearest- and next-nearest-neighbour interactions, etc.

2. Spin-half chains

2.1. The XXZ model

Let \(V = \mathbb{C}^2\) be a spin-\(\frac{1}{2}\) module for \(U_q(su(2))\). The generators \(S^z\) and \(S^\pm\) in this representation take the same form as their (undeformed) \(su(2)\) counterparts, namely

\[
S^z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \quad S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.
\]
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From the definition of the co-product $\Delta$ and the Casimir $C$ we can calculate the element $C^{(2)} = \Delta(C) \in U_q(su(2))^\otimes2$. On the tensor product of two spin-$\frac{1}{2}$ representations, it takes the form

$$C^{(2)} = \begin{pmatrix} q + q^{-1} & 0 & 0 & 0 \\ 0 & q^{-1} & 1 & 0 \\ 0 & 1 & q & 0 \\ 0 & 0 & 0 & q + q^{-1} \end{pmatrix}. $$

This can be expressed alternatively as

$$C^{(2)} = 2(S^x \otimes S^x + S^y \otimes S^y) + (q + q^{-1}) S^z \otimes S^z + \frac{1}{4} (q^{-1} - q) (S^z \otimes 1 - 1 \otimes S^z) + \frac{1}{4} (q + q^{-1}) (1 \otimes 1) \tag{5}$$

in terms of the spin matrices. Let $h_{XXZ}^{(2)} = C^{(2)} - \frac{1}{4} (q + q^{-1}) 1 \otimes 1$ and consider the object

$$\mathcal{H}_{XXZ} = \sum_{j=1}^{N-1} 1 \otimes \cdots \otimes 1 \otimes h_{XXZ}^{(j,j+1)} \otimes 1 \otimes \cdots \otimes 1, \tag{6}$$

where $h_{XXZ}^{(j,j+1)}$ is a copy of $h_{XXZ}$ acting in the $(j, j + 1)$ slot of $V^\otimes N$. It turns out that $\mathcal{H}_{XXZ}$ is a special case of a more general (integrable) Hamiltonian for the XXZ quantum chain with open boundaries and surface fields, and can be written in more usual notation as

$$\mathcal{H}_{XXZ} = \sum_{j=1}^{N-1} 2(S^x_j S^x_{j+1} + S^y_j S^y_{j+1}) + (q + q^{-1}) S^z_j S^z_{j+1} + \frac{1}{4} (q^{-1} - q) (S^z_1 - S^z_N), \tag{7}$$

where $S^x_j$, $S^z_j$ and $S^y_j$ are copies of $S^x$, $S^z$ and $S^y$ acting in the $j$-th slot of $V^\otimes N$.

By construction, it is $U_q(su(2))$-invariant, i.e.

$$[\mathcal{H}_{XXZ}, S^z] = [\mathcal{H}_{XXZ}, S^\pm] = 0,$$

where

$$S^z = \Delta^{(N-1)}(S^z) = \sum_{j=1}^{N} 1 \otimes \cdots \otimes 1 \otimes S^z_j \otimes 1 \otimes \cdots \otimes 1,$$

$$S^\pm = \Delta^{(N-1)}(S^\pm) = \sum_{j=1}^{N} q^{S^z_j} \otimes \cdots \otimes q^{S^z_j} \otimes S^\pm_j \otimes q^{-S^z_j} \otimes \cdots \otimes q^{-S^z_j}, \tag{8}$$

generate $U_q(su(2))$ on $V^\otimes N$. Since on $V \otimes V$ the centre of $U_q(su(2))$ is spanned by $C^{(2)}$ and $1 \otimes 1$, if we replace $h_{XXZ}$ by either of the projectors $P^{(0)}$ or $P^{(1)}$ (in line with the other constructions of spin chains in this paper) we would end up with an equivalent (up to trivial additive and multiplicative constants) quantum chain. It is a happy accident that this most general nearest-neighbour spin-$\frac{1}{2}$ quantum chain with $U_q(su(2))$ symmetry is integrable.
2.2. The q-deformed Majumdar-Ghosh model

As described in the Introduction, the Majumdar-Ghosh model (1) can be constructed as a sum of \( su(2) \)-projectors \( P_{j,j+1,j+2}^{(3/2)} \). Its q-deformation is evidently given by

\[
H^{q\text{-MG}} = \sum_{j=1}^{N-2} P_{j,j+1,j+2}^{(3/2)},
\]

where now \( P_{j}^{(3/2)} \) is a projector onto the spin-\( \frac{3}{2} \) subspace in the decomposition of the \( U_q(su(2)) \)-module \( V \otimes V \otimes V \). As noted also in the Introduction, the equivalence of the representation theory for \( U_q(su(2)) \) and \( su(2) \) (when \( q \) is not a root of unity) implies that all the arguments for the fact that the Majumdar-Ghosh model has exact valence-bond ground states remain valid for the q-deformation.

To obtain the projector \( P_{j}^{(3/2)} \) we first construct the matrix representative of \( C^{(3)} \equiv \Delta^{(2)}(C) \), which has eigenvalues \( \{ \frac{3}{2}, \frac{7}{2} \} \) and \( \{ \frac{1}{2}, \frac{5}{2} \} \), each with multiplicity four, being eigenvalues on irreducible spin-\( \frac{3}{2} \) (two copies) and spin-\( \frac{5}{2} \) modules respectively.

It is then clear that the projector is

\[
P_{j}^{(3/2)} = \frac{C^{(3)} - \{ \frac{3}{2}, \frac{7}{2} \}(1 \otimes 1 \otimes 1)}{\{ \frac{1}{2}, \frac{5}{2} \} - \{ \frac{3}{2}, \frac{7}{2} \}}.
\]

The element \( C^{(3)} \) in \( U_q(su(2))^{\otimes 3} \) can be constructed in an analogous way to \( C^{(2)} \), using the definitions of \( C \) and \( \Delta \). In the spin-\( \frac{1}{2} \) representation the result can be written in the form

\[
C^{(3)} = (q + q^{-1}) (1 \otimes S^x \otimes S^x + 1 \otimes S^y \otimes S^y + S^x \otimes S^x \otimes S^x 1 + S^y \otimes S^y \otimes 1) \\
+ 2(q - q^{-1})(S^x \otimes S^x \otimes S^z + S^x \otimes S^y \otimes S^z - S^z \otimes S^x \otimes S^x - S^z \otimes S^y \otimes S^y) \\
+ 2(S^x \otimes 1 \otimes S^x + S^y \otimes 1 \otimes S^y + S^z \otimes 1 \otimes S^z) \\
+ (q^2 + q^{-2})(1 \otimes S^z \otimes S^z + S^z \otimes S^z \otimes 1) \\
+ \frac{1}{2} (q^2 - q^{-2}) (1 \otimes 1 \otimes S^z - S^z \otimes 1 \otimes 1) \\
+ \frac{(1 + q^2)(1 + q + q^2)^2}{2q^2(1 + q)^2} (1 \otimes 1 \otimes 1).
\]

It then follows that the Hamiltonian for the q-deformed Majumdar-Ghosh model is

\[
H^{q\text{-MG}} = \frac{1}{1 + q^2 + q^{-2}} \sum_{j=1}^{N-2} \left\{ (q + q^{-1}) (S_j \cdot S_{j+1} + S_{j+1} \cdot S_j + 2S_j \cdot S_{j+2}) \\
+ 2(q - q^{-1}) (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) S_{j+2}^z - S_j^z (S_{j+1}^x S_{j+2}^x + S_{j+1}^y S_{j+2}^y)) \\
+ (q^2 + q^{-2} - q - q^{-1}) (S_{j+1}^x S_{j+2}^x + S_{j+1}^y S_{j+2}^y) \\
+ \frac{1}{2} (q^2 - q^{-2}) (S_N^x + S_{N-1}^x - S_1^x - S_2^x) \right) + \frac{1}{2} (N - 2).
\]

Note the presence of boundary terms, as in the XXZ chain, and also of three-spin interactions. The constant term can of course be dropped, but is naturally present.
to make the ground state energy zero for chains of all length $N$. This generalisation of the Majumdar-Ghosh model differs from that given by Shastry and Sutherland which includes only two-spin interactions\cite{2}, and which is presumably not $U_q(su(2))$-invariant.

The $q$-deformed Majumdar-Ghosh Hamiltonian is $U_q(su(2))$-invariant by construction. We note that the most general spin-$\frac{1}{2}$ $U_q(su(2))$-invariant Hamiltonian with next-nearest neighbour interactions can be constructed by starting from a linear combination of $C^{(3)}$ and $(C^{(3)})^2$ (which together with the identity generate the centre of $U_q(su(2))$ on $V^{\otimes 3}$). Amongst all such chains one can expect to find one which is integrable, whose periodic version is the next highest conserved quantity of the XXZ Hamiltonian.

3. The $q$-deformed spin-1 VBS model

Now let $V = \mathfrak{su}^1$, a spin-1 module for $U_q(su(2))$. In this representation, $S^z$ and $S^\pm$ take the form

$$S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad S^+ = \sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad S^- = \sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

As described in the Introduction, the spin-1 VBS model\cite{3} of Affleck et al.\cite{2} can be constructed as a sum of $su(2)$ projectors $P^{(2)}$. Once again, its $q$-deformation is clear; being

$$\mathcal{H}^{q\text{VBS}} = \sum_{j=1}^{N-1} P^{(2)}_{j,j+1},$$

where $P^{(2)}$ is now a projector onto the spin-2 subspace in the decomposition of $V \otimes V$ as a $U_q(su(2))$-module.

As before, $P^{(2)}$ can be obtained from the Casimir $C$, this time as

$$P^{(2)} = \frac{C^{(2)}}{[2][3]} \left( \frac{C^{(2)} - [2][3] \otimes 1}{[2][3] - [2]} \right),$$

since 0, [2] and [2][3] are the eigenvalues of $C^{(2)} = \Delta(C)$ on irreducible modules of spin 0, 1 and 2, respectively. The construction of $C^{(2)}$ goes as before, via the definitions of $\Delta$ and $C$. Its matrix representative in the present case is a lot more laborious to work out than in the spin-$\frac{1}{2}$ case, with the result expressible as

$$C^{(2)} = (q + q^{-1})(S^z \otimes S^z + S^y \otimes S^y) - \frac{1}{4}(q + q^{-1})^2(q - q^{-1})(S^z \otimes 1 - 1 \otimes S^z) + \frac{1}{4}(q + q^{-1})^2(S^z \otimes S^z + \frac{1}{2}(q + q^{-1})(q - q^{-1})^2((S^z)^2 \otimes 1 + 1 \otimes (S^z)^2)) + (2 - q - q^{-1}) \{(1 \otimes S^z)(S^x \otimes S^x + S^y \otimes S^y)(S^z \otimes 1) - (S^z \otimes 1)(S^x \otimes S^x + S^y \otimes S^y)(1 \otimes S^z)\} - \frac{1}{2}(q - q^{-1}) \{(S^z \otimes S^z + S^y \otimes S^y)(S^z \otimes 1 - 1 \otimes S^z) - (S^z \otimes 1 - 1 \otimes S^z)(S^x \otimes S^x + S^y \otimes S^y)\} - \frac{1}{2}(q + q^{-1})^2(q - q^{-1})((S^z)^2 \otimes S^z - S^z \otimes (S^z)^2) + 2(q + q^{-1})(1 \otimes 1)(15)$$
in terms of the spin matrices. If we let \( C^{(2)}_{j,j+1} = (q + q^{-1})(S^x_j S^x_{j+1} + S^y_j S^y_{j+1}) + \cdots \) be a copy of \( C^{(2)} \) acting on the \((j, j + 1)\) slot of \( V^\otimes N \) then the Hamiltonian for the \( q \)-deformed VBS model is given by

\[
H^{q\text{VBS}} = \left( [2][3][3] - 1 \right)^{-1} \sum_{j=1}^{N-1} C^{(2)}_{j,j+1} \left( C^{(2)}_{j,j+1} - [2] \right). \tag{16}
\]

Since the matrix representatives of \( S^z, S^x \) and \( S^y \) in the spin-1 representation are proportional to their (undeformed) \( su(2) \) counterparts, the Hamiltonian \( H^{q\text{VBS}} \) can be written wholly in terms of the latter after appropriate rescalings.

The Hamiltonian \( \text{[16]} \) (or rather, one equivalent to it up to an additive and a multiplicative constant) was first proposed in Ref. 6 as potentially having exact valence-bond ground states. In that paper, the most general \( U_q(su(2)) \)-invariant spin-1 Hamiltonian was written down as

\[
H^{\text{spin}} = \sum_{j=1}^{N-1} O_{j,j+1}(a, b),
\]

with the Hamiltonian on two sites \( O(a, b) \) being the most general linear combination of \( C^{(2)} \) and \( (C^{(2)})^2 \) (which together with the identity generate the centre of \( U_q(su(2)) \) in \( V \otimes V \)). The operator \( O(a, b) \) has three eigenvalues \( E_k(a, b) \) corresponding to the three spin-\( k \) representations \( (k = 0, 1, 2) \) in the decomposition of \( V \otimes V \). The Hamiltonian proposed corresponds to a choice of parameters \( a = \tilde{a} \) and \( b = \tilde{b} \) such that \( E_0(\tilde{a}, \tilde{b}) = E_1(\tilde{a}, \tilde{b}) \). Since one can always shift \( O(\tilde{a}, \tilde{b}) \) by a constant to make \( E_0(\tilde{a}, \tilde{b}) = E_1(\tilde{a}, \tilde{b}) = 0 \), it is essentially the projector \( P^{(2)} \). The projector nature of this special choice of \( O(a, b) \) was first discussed in Ref. 7 where the ground state properties of \( H^{q\text{VBS}} \) were calculated. In particular, the ground state is unique, there is a finite gap to excitations, and correlations decay exponentially. We turn now to the properties of the \( q \)-deformed Majumdar-Ghosh model.

### 4. Properties of the \( q \)-deformed Majumdar-Ghosh model

The ground state correlation functions of the Majumdar-Ghosh model are particularly simple due to the exact dimerised ground states.\[4\] For ease of comparison with the earlier results, we consider the generalised Hamiltonian \( \text{[12]} \) for even \( N \) with periodic boundary conditions, so that the surface terms ensuring the \( U_q(su(2)) \) invariance vanish. In this case the ground state is two-fold degenerate with eigenvectors

\[
\phi_1 = [1, 2] [3, 4] \cdots [N - 1, N], \tag{17}
\]

\[
\phi_2 = [2, 3] [4, 5] \cdots [N, 1], \tag{18}
\]

where

\[
[l, m] = \frac{1}{\sqrt{1 + q^2}} (|l \downarrow m - q^{-1} l \uparrow m). \tag{19}
\]
For each state the ground state energy is zero. The ground state wave function is given by either of the functions \( \Psi^\pm = \phi_1 \pm \phi_2 \), which ensure translational symmetry. The matrix element \( \langle \phi_1 | \phi_2 \rangle \) vanishes as

\[
\langle \phi_1 | \phi_2 \rangle = (-1)^{N/2} 2 (q + q^{-1})^{-N/2},
\]

so the states \( \phi_1, \phi_2 \) become orthogonal in the thermodynamic limit for \( q \) real. On the other hand, \( \langle \phi_1 | \phi_1 \rangle = \langle \phi_2 | \phi_2 \rangle = 1 \).

Various spin-spin correlations can be considered. In particular, the correlation associated with Néel order is defined by

\[
C_n^\pm = \langle \Psi^\pm | S_1^z S_{1+n}^z | \Psi^\pm \rangle.
\]

In the \( N \to \infty \) limit with \( q = 1 \), \( C_1^\pm = -\frac{1}{2} \) with \( C_n^\pm = 0 \) for \( n > 1 \), indicating the absence of Néel long-range order. However, in the same limit away from \( q = 1 \), \( C_n^\pm = (-1)^n \frac{1}{2} \), independent of \( q \). Thus the anisotropy induces a form of long-range Néel order.

As a final remark, we note that the model remains massive as a function of \( q \). In general there is a symmetry in the eigenspectrum about the value \( q = 1 \) with the eigenvalues satisfying \( E(q) = E(1/q) \). Thus confining our attention to the region \( 0 \leq q \leq 1 \), we see that the gap \( \Lambda \) opens up from the value \( \Lambda \approx \frac{1}{4}(0.236) \) at \( q = 1 \) to the exact value \( \Lambda = 2 \) (even \( N \)) or \( \Lambda = 1 \) (odd \( N \)) at \( q = 0 \) where the Hamiltonian is trivial.

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