Quantum critical surface of the zigzag spin chain under magnetic field: Application to superconducting quantum dots

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We analyze the exact ground state of XXZ zigzag spin chain with applied magnetic field and find the quantum critical surface. Using the theorem of positive semi-definite matrix, we can prove that the ground states for a specific region, are fully polarized state and one magnon states. With Bethe ansatz, we argue that this is the quantum critical state in all cases. A first in the literature, we derive the analytical expression of quantum critical surface for superconducting quantum dots array in the presence of gate voltage.

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Low dimensional spin systems has been an active field of research \cite{1} for many year. Bethe ansatz has been used widely to solve many new families of integrable Hamiltonians of one dimensional systems \cite{2,3,4,5}. A quantum inverse scattering method based on Bethe ansatz has also been developed for dealing with the two-dimensional models \cite{5}. Another method which also enables one to find the exact solutions of various models is the matrix product method $\cite{7,8,9,10}$. For example, it is related to the Affleck-Kennedy-Lieb-Tasaki(AKLT) state $\cite{9,11}$. In this work we are going to apply these two methods to the zigzag spin chain model.

A zigzag spin chain is an one dimensional system of spins with exchange interactions with their nearest neighbors (NN) and next-nearest neighbors (NNN), denoted by $J_1$ and $J_2$ respectively. It is a frustrated system if $J_1J_2<0$ or both of them are positive. In a zigzag spin chain the situation is not clear. Majumdar and Ghosh $\cite{12}$ found that the degenerate dimer states in which neighboring sites form singlets (MG state) are the exact ground states at $\frac{J_2}{J_1}=2$. At $\frac{J_2}{J_1}=-4$, Hanada et.al. \cite{13} found that the uniformly distributed resonant valence bond (UDRVB) state and the fully polarized (FP) state are degenerate ground states. There are also a few other important theoretical works in zigzag spin chain $\cite{14,15,16}$. The zigzag spin chain can be realized in physical systems, such as the oxides, Li$_2$CuO$_2$ (multiferroic) $\cite{18}$ and SrCuO$_2$ $\cite{19}$. In this letter, we find a quantum critical surface on which the FP state is degenerate with the one-magnon states, along with an application to superconducting quantum dots system. Our calculation is based on the concept that the local ground states in a matrix product form can be extended to global ground states.

Model Hamiltonian: We begin with the Hamiltonian of a zigzag spin chain with applied magnetic field,

$$H = \sum_i J_1 [\Delta_1 s_i^z s_{i+1}^z + \frac{1}{2} (s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+)]$$

$$+ \sum_i J_2 [\Delta_2 s_i^z s_{i+2}^z + \frac{1}{2} (s_i^+ s_{i+2}^- + s_i^- s_{i+2}^+)] + B \sum_i s_i^z$$

where $J_1$ and $J_2$ are the NN and, NNN interaction, $\Delta_1(\Delta_2)$ is the anisotropy in $z$ axes for NN(NNN) interaction and $i$ is the label of the lattice site. Furthermore, we use the periodic boundary condition and hence we have the coupling between $s_{i-1}, s_N$ and $s_1, s_2$. We can dissect the Hamiltonian into many local Hamiltonians. Each local Hamiltonian contains three spins. Thus, the original Hamiltonian can be written as

$$H = \sum_{i} h_{i,i+1,i+2} = \sum_{i} (h^0_{i,i+1,i+2} + h^\text{mag}_{i,i+1,i+2}).$$

where $h^0_{i,i+1,i+2} = \frac{1}{2} [\Delta_1 (s_i^z s_{i+1}^z + s_i^z + s_{i+1}^z) + h.c.] + \frac{1}{2} [\Delta_2 (s_i^z s_{i+2}^z + s_i^z + s_{i+2}^z)]$, and $h^\text{mag}_{i,i+1,i+2} = \frac{b}{2+2s_i^z + s_{i+1}^z + s_{i+2}^z}$. $h^0_{i,i+1,i+2}$ is the local Hamiltonian of exchange interaction, and $h^\text{mag}_{i,i+1,i+2}$ is the that of applied magnetic field. We have set $b = \frac{B}{J_2}, f = \frac{J_2}{J_1}$ and made scaling $J_2 = 1$. In $h^\text{mag}$ we have introduced a free parameter $x$ to facilitate later calculation. Note that the Hamiltonian is independent of the value of $x$ if we apply the periodic boundary condition.

The quantum critical surface from local site Hamiltonian: The local Hamiltonian $h_{123}$, which serves as our starting point, can be diagonalize and the eigenvalues in terms of parameters $x$, $\Delta_{1,2}$ and $f$ are

$$E_0 = \frac{1}{4} (-2b + \Delta_2 + \Delta_1 f),$$

$$E_1 = \frac{1}{4} (2b + \Delta_2 + \Delta_1 f),$$

$$E_2 = \frac{1}{4} (-2 - 2b - \Delta_2) + \frac{b}{2 + x},$$

$$E_3 = \frac{1}{4} (-2 - \Delta_2 + \frac{2bx}{2 + x}),$$

$$E_{4\pm} = \frac{4b - (-2 + \Delta_1 f)(x + 2) \pm \Gamma_+}{8(x + 2)},$$

$$E_{5\pm} = \frac{-4b - (-2 + \Delta_1 f)(x + 2) \pm \Gamma_-}{8(x + 2)},$$

where $\Gamma_+ = \sqrt{\Delta_2^2 + 4b^2}$ and $\Gamma_- = \sqrt{\Delta_2^2 + 4b^2}$. We can express the eigenvalues in terms of $\gamma_0 = \frac{\Delta_1}{\Delta_2}$ and $\gamma_1 = \frac{2b}{\Delta_2}$, as

$$E_0 = \frac{1}{4} (-2b + \Delta_2 + \Delta_1 f),$$

$$E_1 = \frac{1}{4} (2b + \Delta_2 + \Delta_1 f),$$

$$E_2 = \frac{1}{4} (-2 - 2b - \Delta_2) + \frac{b}{2 + x},$$

$$E_3 = \frac{1}{4} (-2 - \Delta_2 + \frac{2bx}{2 + x}),$$

$$E_{4\pm} = \frac{4b - (-2 + \Delta_1 f)(x + 2) \pm \Gamma_+}{8(x + 2)},$$

$$E_{5\pm} = \frac{-4b - (-2 + \Delta_1 f)(x + 2) \pm \Gamma_-}{8(x + 2)},$$

where $\Gamma_+ = \sqrt{\Delta_2^2 + 4b^2}$ and $\Gamma_- = \sqrt{\Delta_2^2 + 4b^2}$. We can express the eigenvalues in terms of $\gamma_0 = \frac{\Delta_1}{\Delta_2}$ and $\gamma_1 = \frac{2b}{\Delta_2}$, as
\[\Gamma_{\pm}^2 = |16b^2(-1 + x)^2 \pm 8b(2 - 2\Delta_2 + \Delta_1 f)(-2 + x + x') + 4(-1 + \Delta_2)^2 - 4\Delta_1(-1 + \Delta_2)f + (8 + \Delta_1^2)f^2|\]

We found that \(E_0(E_1)\) corresponds to the state \(|↓↓↓⟩\) \((|↑↑↑⟩)\), \(E_2\) and \(E_{5\pm}\) correspond to one spin-up states and \(E_3\) and \(E_{3\pm}\) to the one spin-down states. In order to see quantum critical points for entire system, we seek in the spectrum the level crossing between \(FP\) \((\text{whose elements are its eigen states,})\) without affecting \(|↓↓↓⟩\) \((\text{other states because for an infinite spin chain with space inversion symmetry any other states must be two-fold degenerate.})\)

The corresponding eigenvalue of these degenerate states is

\[E_0 = \frac{-2 - \Delta_2 - \Delta_1 f}{4} - \frac{f^2}{16}\]

\textbf{Matrix formulation of the global eigen state:} Here, we generalize the results of local Hamiltonian for arbitrary number of spins. The global Hamiltonian of \(N\) spins can be obtained by the direct sum of local Hamiltonians.

\[H = h \otimes \mathbb{1}_{2N-3} \oplus \hat{h} \otimes \mathbb{1}_{2N-4} \oplus \hat{h} \otimes \mathbb{1}_{2N-5} \oplus \cdots \oplus \mathbb{1}_{2N-2} \otimes h \otimes \mathbb{1}_{2N-3} \otimes h,\]

where each basic element \(h\) is just the local Hamiltonian \(h_{i,i+1,i+2}\) and \(\mathbb{1}_{2N}\) is the identity matrix of rank \(M\). The eigen states of an infinite spin chain can be also found by adding more spins to eigen states of the local Hamiltonian. Consider the matrix

\[m_j = \begin{pmatrix}
|↓⟩_j & |↑⟩_j & 0 \\
0 & 0 & |↓⟩_j \\
0 & f/2 & |↓⟩_j
\end{pmatrix}
\]

representing the spin state at site \(j\). The three degenerate ground states of the local Hamiltonian \(h_{i,j+1,j+2}\) with energies \(E_0\), \(E_2\) and \(E_{5\pm}\) can be expressed as the matrix \(m_j m_{j+1}^\dagger m_{j+2}\). In fact, the matrix elements are the linear combinations of these three eigen states. It is clear that \(M_n = \Pi_{j=1}^N m_j\) gives the states of \(n\) spins. \(h_{i,j+1,j+2}\) operates only on the product \(m_j m_{j+1} m_{j+2}\) (whose elements are its eigen states,) without affecting other matrices. Hence, the operation of Hamiltonian will not alter the form of \(M_n\) and its matrix elements are linear combinations of the eigen states. We can write \(M_n\) in a more compact form

\[M_n = \begin{pmatrix}
|\phi_0^n⟩ & |\phi_1^n⟩ & |\phi_2^n⟩ \\
0 & -f_{n-1} & f_n \|\phi_0^n⟩ \\
0 & -f_n & f_{n+1} \|\phi_0^n⟩
\end{pmatrix}
\]

where \(\|\phi_0^n⟩\) \((|0⟩, |\phi_1^n⟩ = \sum_{j=1}^n f_{n-j+1} |j⟩\) and \(|\phi_2^n⟩ = \sum_{j=1}^n f_{n-j+1} |j⟩\), with \(|0⟩ = |↓↓↓\cdots⟩\) and the coefficients \(f_j\) satisfying the relations \(f_0 \leq 0, f_1 \geq -\frac{f_0}{2}\).

\[k = \cos(\frac{j}{4})\]

satisfies above equations. The first eigen state is the fully polarized (FP) state and the other two can be expressed as the linear combination of two independent one-magnon states: \(|\phi_1^n⟩ = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{ikj} s_j^z |0⟩\) \(|\phi_2^n⟩ = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{-ikj} s_j^z |0⟩\) where \(j\) is the site position. The periodic boundary condition implies that \(Nk = 2\pi n\).

Thus we have constructed the eigen states for a zigzag spin chain of arbitrary length at the surface Eq.23.

\textbf{Proof of the quantum critical surface by positive semi-definite matrix theorem:} We use the theorem of positive semi-definite matrix to show that for spin chain of arbitrary length, the above mentioned three degenerate eigen states are actually the global ground state in certain region. The theorem of positive semi-definite matrix is the following: The necessary and sufficient condition for a real symmetric matrix \(A\) to be positive semi-definite is \(x^T Ax \geq 0\) for all real vectors \(x\). If \(M\) and \(N\) are positive semi-definite, then the sum \(M + N\), and the direct sum \(M \oplus N\), and direct product \(M \otimes N\) are also positive semi-definite.

The FP state and the one-magnon states are the degenerate ground states, if the matrix \((h_{i,j+1,j+2} - E_0)\), with \(E_0\) being their energy, is a positive semi-definite matrix. We begin the proof with a local Hamiltonian with three spins. By setting \(x = \frac{f(1 + \Delta_1)}{2(1 + \Delta_2 + \Delta_1 f)}\), Eq.23 and writing the Hamiltonian \(h_{i,j+1,j+2} - E_0\) in a real and symmetric matrix form, we proceed to prove it is a positive semi-definite matrix. The value \(x^T (h_{i,j+1,j+2} - E_0)x\) where \(x = (x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8)^T\) is any real column matrix, is

\[x^T (h_{i,j+1,j+2} - E_0)x = \frac{1}{4}[f(1 + \Delta_2 + \Delta_1 f + \frac{f^2}{8})x_1^2 + f(\Delta_1 + f)(x_2^2 + x_3^2) + (4 + 4\Delta_2 - \frac{f^2}{2})x_4^2 + 2(x_2 + \frac{f}{2}x_3 + x_5)^2 + 2(x_4 + \frac{f}{2}x_6 + x_7)^2].\]

\((h_{i,j+1,j+2} - E_0)\) is a positive semi-definite matrix provided two inequalities below are satisfied simultaneously

\[f(\Delta_1 + f) \geq 0, \quad 4 + 4\Delta_2 - \frac{f^2}{2} \geq 0.\]
Since all the local Hamiltonian \( h_{ij,j'+j'' - E_0} \hat{1} \) are positive semi-definite matrices, so is \( h_{123} \otimes I_2 + I_2 \otimes h_{234} \) and \( H - E_0 \). Thus we conclude that in the region given by inequalities (7), the degenerate ground state is the FP state and one magnon state with \( k \) in Eq. (9). The degenerate ground states are \( |\phi^+_N \rangle = |0 \rangle \), \( |\phi^-_N \rangle = \sum_{m=1}^N e^{ikm}s^+_m |0 \rangle \), \( |\phi^0_N \rangle = \sum_{m=1}^N e^{-ikm}s^-_m |0 \rangle \). We will give argument below that even if outside of the region given by inequalities (7), they are still the degenerate ground states. In the mean time we show the quantum critical surfaces given by Eq. (2) for the case \( \Delta_1 = \Delta_2 = d \) in Fig. (a) and the case \( \Delta_1 = d \) and \( \Delta_2 = 0 \) in Fig. (b). In the region above the surfaces only the FP state is the ground state. There are several interesting features. Firstly, larger \( \Delta_1 \) and \( \Delta_2 \), requires larger magnetic field \( b \). This means that the system is made difficult to be polarized by anisotropy. On the other hand, negative \( f \), ferromagnetic coupling, reduces the value of \( b \) as expected. Eq. (2) is valid for \( f \geq -4 \). Beyond which only the FP state is the ground state. Quantitatively, we see a linear dependence of the energy would have been obtained by varying them independently. This result is

\[
2(E - E_0) a_{x_1,x_2,...,x_n} = 2n(b - \Delta_2 - \Delta_1 f) a_{x_1,x_2,...,x_n} + f \sum_{i=1}^n (a_{x_{i-1},x_{i-1}+1} + a_{x_{i-1},x_{i+1}+1} + a_{x_{i-1},x_{i-1}+1} + a_{x_{i-1},x_{i+1}+1}) + \sum_{i=1}^n (a_{x_{i-1},x_{i-1}+2} + a_{x_{i-1},x_{i+2}}).
\]

With the same method for two-magnon states, we let \( a_{x_1,x_2,...,x_n} = \sum_P P \exp[i \sum_{j=1}^n k_P x_j] \), where \( P \) means permutation of spin sites \( j \). The equation becomes

\[
2(E - E_0) = 2n(b - \Delta_2 - \Delta_1 f) + 2f \sum_{i=1}^n \cos k_i + 2 \sum_{i=1}^n \cos 2k_i.
\]

(9)

If \( k_i \)'s were independent variables, then the lowest energy would have been obtained by varying them independently. The result is

\[
k_i = k = \pm \cos^{-1}(-\frac{f}{4}).
\]

(10)

For \( E = E_0 \) and Eq. (10), we again reach the relation in Eq. (2). Since \( k_i \)'s have other constraints, the energy we thus get is the lower bound. Hence, we conclude that for \( 1 \leq n \leq N \), the FP state and one-magnon states have the lowest energy with the magnetic field given by Eq. (2). It is plausible to assume that this is true for arbitrary
value of $n$. The ansatz gives the excitation energy of magnons as $\Delta E = E - E_0 = 1 + \frac{h}{2} + f \cos k + \cos 2k$. Interestingly, it does not depend on the anisotropy $\Delta_1$ and $\Delta_2$. It vanishes when Eq. (3) is satisfied. Physically, this means that the magnons soften at certain wave vectors, depending on the value of $f$. This phenomena can be detected by neutron scattering or susceptibility measurement.

**Application to superconducting quantum dot system:** Here we derive the analytical expression of the quantum critical surface of a superconducting quantum dots (SQD) array with NN and NNN tunneling and Coulomb interaction in the presence of gate voltage in every superconducting dot. The quantum critical surface separate the charge density wave phase of lower commensurability ($n = 1/2$), which corresponds to a anti-ferromagnetic phase of a spin chain; from a higher commensurability state ($n = 1$, or integer numbers of Cooper pair in every dot,) which corresponding to the FF phase. Therefore, we use the relation between $b$ and $f$ evaluated in the previous section to study the quantum critical surface between these two phases. The quantum fluctuations are controlled by the system parameters like charging energy of SQD and the Josephson coupling ($E_J$). In the SQD model [21], we consider the finite range $E_J$ and Coulomb interaction which have experimental support [22–25]. The model Hamiltonian of our study consists of different interactions, $H = H_{J1} + H_{J2} + H_{EC0} + H_{EC1} + H_{EC2}$. We recast our basic Hamiltonians in the spin language around the charge degeneracy point. $H_{J1} = 2E_{J1}\sum_i(S_i^+S_{i+1}^- + h.c.)$, $H_{J2} = 2E_{J2}\sum_i(S_i^+S_{i+2}^- + h.c.)$, $H_{EC0} = E_{EC0}\sum_i(2S_i^Z + E_c)^2 \approx 2hE_{EC0}\sum_i2S_i^Z$, $H_{EC1} = 4E_{Z1}\sum_iS_{i+1}^Z$, $H_{EC2} = 4E_{Z2}\sum_iS_i^Z S_{i+2}^Z$, where $H_{J1}$ and $H_{J2}$ are Josephson energy Hamiltonians respectively for NN and NNN Josephson tunneling between the SQD and $H_{EC0}, H_{EC1}, H_{EC2}$ are the Hamiltonians for on-site, NN and NNN charging energies of the SQD. $h = \frac{2\pi}{E_{EC0}}$ is a parameter which allows tuning the system to a degeneracy point by means of gate voltage. When $E_{EC0} \gg E_J$, sequential tunnelling of Cooper pair across the SQD is not a energetically favorable process. One must consider the cotunneling effect, i.e., the higher order expansion in $\frac{E_{EC0}}{E_J}$, which reduce the intersite Coulomb charging energy and also increase the NNN $E_J$ [21, 26, 27]. This results in new tunneling energies: $E_{J2} \rightarrow E_{J2} + E_{J2}^2/2E_{EC0}$, and $E_{Z1} \rightarrow E_{Z1} - 3E_{J1}^{1/2}/16E_{EC0}$.

Now we present the analytical expression of quantum critical surface for the presence and absence of cotunneling effect, following the relation $b$ and $f$ in Eq.(2). The analytical expression of quantum critical surface in the absence of cotunneling effect are the following

\[2hE_{C0} = 2E_{J2} + 4(E_{Z1} + E_{Z2}) + \frac{E_{J2}^2}{4E_{EC0}}\]

while that in the presence of cotunneling effect is

\[2hE_{C0} = 2E_{J2} + 4(E_{Z1} + E_{Z2}) + \frac{E_{J2}^2}{4E_{EC0}} + \frac{E_{J2}^4}{16E_{EC0}^2} + \frac{E_{J2}^4}{8E_{EC0}^3} \].

We have already calculated the quantum critical surface on which FP state and one magnon state are degenerate. Here the one vacant site of Cooper pair in the SQD lattice array corresponds to one magnon state and Mott insulating state with integer numbers of Cooper pairs in each lattice site corresponds to the FP state. The applied gate voltage on each SQD of the array corresponds to the applied magnetic field. The charging energy corresponds to the anisotropy of the exchange interaction of the spin system. For large gate voltage, the SQD is in the insulating state. Interestingly, the charging energy tends to reverse this trend by destabilizing the state of integer numbers of Cooper pairs in each lattice site and makes the system conducting. The analytical expression for the quantum critical surface for the SQD array is the first in the literature.

**Conclusions:** We have found the quantum critical surface of a zigzag spin chain under magnetic field by using the theorem of positive semi-definite matrix and Bethe-ansatz methods. We have also find the quantum critical surface of superconducting quantum dots system by using our analytical methods.

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