Anomalous behavior of the energy gap in the one-dimensional quantum $XY$ model

Yuuki Yamanaka and Hidetoshi Nishimori

Department of Physics, Tokyo Institute of Technology,
Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan

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Abstract

We show for the one-dimensional quantum $XY$ model with $s = 1/2$ that the energy gap between the ground and first excited states behaves anomalously as a function of the system size at the first-order quantum phase transition. Although it is generally the case that the energy gap closes exponentially at a quantum first-order transition, the gap in the present model behaves non-monotonically as a function of the system size, apparently very irregularly in some cases. This property of the gap is similar to that of the infinite-range quantum $XY$ model, in which the gap closes polynomially, exponentially, or even factorially fast depending on the choice of the series of system sizes toward the thermodynamic limit. This observation is surprising in consideration of the apparent maturity of our understanding of the one-dimensional quantum $XY$ model. Our result is also important from the viewpoint of quantum annealing, where the rate of gap closing determines the efficiency of computation.
I. INTRODUCTION

The ground state of a quantum many-body system changes drastically as a parameter in the Hamiltonian changes across a quantum phase-transition point. This phenomenon is preceded in a finite-size system by the closing of energy gap between the ground and the first excited states as a function of the system size toward the thermodynamic limit. The rate of gap closing is an important measure to characterize a quantum phase transition.

According to the finite-size scaling theory, which applies principally to second-order phase transitions, physical quantities generally behave polynomially as functions of the system size \[1–3\]. In contrast, the gap is expected to close exponentially at a first-order quantum phase transition. The two ground states at both sides of the transition point have significantly different properties in a first-order phase transition, and consequently, their overlap in a finite-size system is very small, typically exponentially small. The overlap of the two states determines the energy gap since the overlap corresponds to the off-diagonal elements of the effective two-level Hamiltonian describing the system around the transition point, and the gap is directly related to the magnitude of the off-diagonal elements. These discussions suggest that the order of quantum phase transition in the thermodynamic limit is generally in one-to-one correspondence with the rate of gap closing toward the thermodynamic limit, polynomially for second order and exponentially for first order \[4, 5\].

Study of the behavior of energy gap is important also from the viewpoint of quantum annealing \[6–12\], in which a system parameter is controlled as a function of time across a quantum transition point. The rate of gap closing directly affects the efficiency of quantum annealing. An exponential closing of the gap implies an exponentially long computation time whereas a polynomial gap leads to a polynomial time \[13, 19\].

Although the above-mentioned correspondence between the order of quantum phase transition and the rate of gap closing generally holds true in most systems, an interesting counterexample has been found by Cabrera and Jullien \[20, 21\] who showed that the first-order quantum phase transition in the one-dimensional transverse-field Ising model with antiperiodic boundary condition accompanies a polynomial closing of the energy gap. See also Ref. \[22\] for essentially the same result. Furthermore, another very anomalous example has been given for the infinite-range quantum \(XY\) model, where the energy gap behaves in many different ways at first-order quantum phase transitions \[23\]. It has been shown there that
many types of energy gap closing, polynomial, exponential, and even factorial closing, co-
exist along an axis in the phase diagram. This example suggests that we should be very
careful to relate the type of quantum phase transition with the rate of gap closing.

In the present paper, we analyze the one-dimensional quantum $XY$ model with $s = 1/2$ and show that this model is another example of anomalous gap behavior. Although it is generally believed that the properties of this one-dimensional model have been well understood [24–31], our detailed analysis leads to the conclusion that the energy gap behaves quite anomalously as the system size change in a very similar way to the case of the infinite-
range quantum $XY$ model.

In the next section, we define the model and analyze the size dependence of the energy gap using both analytical and numerical methods. Our conclusion is given in the final section.

II. ENERGY GAP AS A FUNCTION OF THE SYSTEM SIZE

A. Model system and its ground state

We study the one-dimensional quantum $XY$ model with $s = 1/2$ in transverse and longitudinal fields, $\Gamma$ and $h$, respectively, with a periodic boundary,

$$\hat{H} = -\frac{1}{2} \sum_{j=1}^{N-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) - \frac{1}{2} (\sigma_1^x + \sigma_N^x) - \Gamma \sum_{j=1}^{N} \sigma_j^z - h \sum_{j=1}^{N} \sigma_j^x. \quad (1)$$

We will have quantum annealing in mind in which the longitudinal filed $h$ is controlled as a function of time for a given fixed value of the transverse field $\Gamma$. It does not lose generality to assume $\Gamma \geq 0$. A first-order quantum transition takes place at $h = 0$ between the phases with positive expectation value of $\sigma_j^x$ (for $h > 0$) and negative expectation value (for $h < 0$) as long as $0 \leq \Gamma < 1$, as shown in Fig. 1 [24–31]. This expectation value jumps at $h = 0$, which is the reason that we call this a first-order phase transition. We aim to clarify the system-size dependence of the energy gap at this first-order phase transition at $h = 0$. Notice that the term of longitudinal field in Eq. (1), $-h \sum_j \sigma_j^x$, induces transitions between states with even and odd values of the $z$-component of total spin $S_{tot}^z = \frac{1}{2} \sum_j \sigma_j^z$, although the other terms in the Hamiltonian conserve the even-odd parity of the eigenvalue of $S_{tot}^z$. It is therefore legitimate to study the energy gap between the ground state and the first excited state, one of which has an odd value of $S_{tot}^z$ and the other has even $S_{tot}^z$, if we consider
FIG. 1. Phase diagram of the model system Eq. (1), which undergoes a first-order phase transition across the bold line between the phases with positive and negative expectation values of $\sigma_j^z$.

quantum annealing in which we drive the system by changing the longitudinal field from $h > 0$ to $h < 0$ across $h = 0$. We therefore study the properties of the system Eq. (1) exactly at the transition point $h = 0$.

Equation (1) with $h = 0$ can be diagonalized by the standard procedure [24–31]. After the Jordan-Wigner transformation, the Hamiltonian is expressed in the term of spinless Fermions as

$$\hat{H} = \sum_{j=1}^{N} \left( c_{j+1}^\dagger c_j - c_j^\dagger c_{j+1} \right) - 2\Gamma \sum_{j=1}^{N} \left( c_j^\dagger c_j - \frac{1}{2} \right),$$

(2)

where the Fermion operators satisfy a periodic boundary condition, $c_{N+j} = c_j$, if the total number of Fermions $N_c = \sum_j c_j^\dagger c_j$ is odd, and an antiperiodic condition applies, $c_{N+j} = -c_j$, when $N_c$ is even. After the Fourier transformation, Eq. (2) is diagonalized as

$$\hat{H} = \sum_k \left[ -2(\cos k + \Gamma)c_k^\dagger c_k + \Gamma \right],$$

(3)

where the values of $k$ depend on the boundary condition; $k = k_1$, for periodic boundary $c_{N+j} = c_j \ (N_c \text{ odd})$ and $k = k_2$ for antiperiodic boundary $c_{N+j} = -c_j \ (N_c \text{ even})$ with

$$k_1 = 0, \pm \frac{2}{N}\pi, \pm \frac{4}{N}\pi, \cdots, \pm \frac{N-2}{N}\pi, \pi$$

(4)

$$k_2 = \pm \frac{1}{N}\pi, \pm \frac{3}{N}\pi, \cdots, \pm \frac{N-1}{N}\pi.$$  

(5)

We have assumed that $N$ is even.

We now carefully analyze the ground state in preparation to evaluate the energy gap. An apparent candidate of the ground state is the state where all states with wave numbers
satisfying

\[ \cos k > -\Gamma \]  

are occupied. We show that this presumed ground state indeed satisfies the relation between the total number of Fermions \( N_c \) and the boundary condition for the Fermion operators, \( c_{N+j} = c_j \) for odd \( N_c \) and \( c_{N+j} = -c_j \) for even \( N_c \) for each series of wave numbers Eqs. (4)-(5). As should be clear from Fig. 2, the series of wave numbers \( k_1 \) of Eq. (4) is consistent with odd \( N_c \). Similarly, \( k_2 \) is consistent with even \( N_c \) as indicated in Fig. 3. Thus, those two states in Figs. 2 and 3 are the candidates of the ground state. Whichever having a lower energy is the true ground state. Notice that the parity of \( N_c \) coincides with the parity of \( S_{\text{tot}}^z \) up to a constant \( N/2 \),

\[ S_{\text{tot}}^z = \frac{1}{2} \sum_{j=1}^{N} \sigma_j^z = \sum_{j=1}^{N} \left( c_j^\dagger c_j - \frac{1}{2} \right) = N_c - \frac{N}{2}. \]  

(7)

This fact is closely related with the aforementioned statement that we consider the gap between states with even and odd values of \( S_{\text{tot}}^z \), which amounts to the gap between the states with even and odd values of \( N_c \).

![sink](sink)

FIG. 2. Wave numbers for the presumed ground state in the case of \( k_1 \) on the complex-\( k \) plane. The black points express occupied wave numbers, and the white ones are for unoccupied states.

The ground-state energy is given by the value of Eq. (3), where \( c_k^\dagger c_k = 1 \) for \( k \) satisfying Eq. (6) and \( c_k^\dagger c_k = 0 \) otherwise. If \( N_c \) is even, \( k \) takes the values \( k_1 \) of Eq. (4), and \( k = k_2 \) of Eq. (5) if \( N_c \) is odd. The true ground-state energy is given by one of these possibilities,
FIG. 3. Occupied wave numbers are shown in black for the presumed ground state and unoccupied ones are in white for the wave-number series \( k_2 \).

\( k = k_1 \) or \( k = k_2 \). The first excited state is the other one. We can therefore calculate the energy gap as follows,

\[
\Delta = \left| \sum_{k_1} ' [-2(\cos k + \Gamma)] - \sum_{k_2} ' [-2(\cos k + \Gamma)] \right|,
\]

where \( \sum ' \) stands for the summation over the wave number satisfying Eq. (6).

Let us rewrite Eq. (8). The wave number series \( k_1 \) is represented as

\[
k_1 = 0, \pm \frac{2j}{N} \pi, \pi \quad (j = 1, 2, \cdots \frac{N-2}{2}).
\]

We denote by \( n \) the upper bound of \( k_1 \) appearing in the summation specified by Eq. (6). Then,

\[
\sum_{k_1} ' \cos k = 1 + 2 \sum_{j=1}^{n} \cos \frac{2j}{N} \pi = \frac{\sin (2n+1)\pi}{\sin \frac{\pi}{N}}.
\]

Similarly,

\[
k_2 = \pm \frac{2j-1}{N} \pi \quad (j = 1, 2, \cdots \frac{N}{2})
\]

and

\[
\sum_{k_2} ' \cos k = \frac{\sin 2m\pi}{\sin \frac{\pi}{N}},
\]
where \( m \) refers to the upper limit of \( k_2 \).

Next, we calculate \( n \) and \( m \). From Eq. (6),

\[
\begin{align*}
    n &= \left\lfloor \frac{Nx}{2\pi} \right\rfloor, \\
    m &= \left\lfloor \frac{Nx}{2\pi} + \frac{1}{2} \right\rfloor,
\end{align*}
\]  

where

\[
x = \cos(-\Gamma).
\]  

We divide the quantities inside the integer-part symbol of Eq. (13) into integer and decimal parts,

\[
    \frac{Nx}{2\pi} = \left\lfloor \frac{Nx}{2\pi} \right\rfloor + \delta_1 = n + \delta_1 \quad (0 \leq \delta_1 < 1) \\
    \frac{Nx}{2\pi} + \frac{1}{2} = \left\lfloor \frac{Nx}{2\pi} + \frac{1}{2} \right\rfloor + \delta_2 = m + \delta_2 \quad (0 \leq \delta_2 < 1).
\]  

Then, when \( 0 \leq \delta_1 < \frac{1}{2}, \delta_2 = \delta_1 + \frac{1}{2} \) and the energy gap becomes, using Eqs. (10) and (12),

\[
\Delta = 2 \left| \Gamma \cos \frac{\pi}{2N} (1 - 4\delta_1) + \sqrt{1 - \Gamma^2} \sin \frac{\pi}{2N} (1 - 4\delta_1) \cos \frac{\pi}{2N} - \Gamma \right|.
\]  

When \( \frac{1}{2} \leq \delta_1 < 1, \delta_2 = \delta_1 - \frac{1}{2} \) and the gap is

\[
\Delta = 2 \left| \Gamma \cos \frac{\pi}{2N} (3 - 4\delta_1) + \sqrt{1 - \Gamma^2} \sin \frac{\pi}{2N} (3 - 4\delta_1) \cos \frac{\pi}{2N} - \Gamma \right|.
\]  

**B. Evaluation of the energy gap**

Typical examples of the energy gap as a function of the system size are shown in Figs. 4 to 8, which have been drawn by direct numerical evaluations of Eqs. (17) and (18). These figures look very similar to those for the infinite-range quantum XY model [23], some of which are plotted in Figs. 9 to 11. It is worth remembering that, in the infinite-range model, the gap can be tuned to close polynomially, exponentially, or factorially by an appropriate choice of the series of system sizes for a given fixed value of \( \Gamma \) [23].
FIG. 4. System-size dependence of the energy gap for $\Gamma = 0.1$.

FIG. 5. System-size dependence of the energy gap for $\Gamma = 0.3$.

FIG. 6. System-size dependence of the energy gap for $\Gamma = 1/\sqrt{5}$.
FIG. 7. System-size dependence of the energy gap for $\Gamma = 0.9999$.

FIG. 8. System-size dependence of the energy gap for $\Gamma = 1/2$.

FIG. 9. System-size dependence of the energy gap for the infinite-range model with $\Gamma = \pi/10$ and $\hbar = 0$. 
of Figs. 4 to 8 with Figs. 9 to 11 strongly suggests that the same may be true for the one-dimensional model. We will discuss it in more detail below.

There are several important points to notice in these results. First, a slight change in $\Gamma$ leads to drastically different behavior. In order to understand it, it is useful to reduce the formulas for the gap, Eqs. (17) and (18), to simpler forms for some values of $\Gamma$. For example, when $\Gamma = \frac{1}{2}$, $x = \cos^{-1}(-\Gamma) = 2\pi/3$, and hence $Nx/2\pi = N/3$. Then, for $N = 3l$ ($l \in \mathbb{N}$), $\delta_1 = 0$ according to Eq. (15), and the gap of Eq. (17) has a simple expression

$$\Delta = \sqrt{3} \tan \frac{\pi}{2N}. \quad (20)$$

When $N = 3l + 1$ and $3l + 2$, $\delta_1 = 1/3$ and $2/3$, respectively, and Eq. (17) for $\delta_1 = 1/3$
becomes

\[
\Delta = 2 \left| \frac{1}{2} \cos \frac{\pi}{6N} - \frac{\sqrt{3}}{2} \sin \frac{\pi}{6N} \cos \frac{\pi}{2N} - \frac{1}{2} \right|
\]  \hspace{1cm} \text{(21)}

and Eq. (18) for \( \delta_1 = 2/3 \) is

\[
\Delta = 2 \left| \frac{1}{2} \cos \frac{\pi}{6N} + \frac{\sqrt{3}}{2} \sin \frac{\pi}{6N} \cos \frac{\pi}{2N} - \frac{1}{2} \right|
\]  \hspace{1cm} \text{(22)}

Equations (21) and Eq. (22) show the same system-size dependence for large \( N \) because \( \cos \frac{\pi}{6N} \gg \sin \frac{\pi}{6N} \). Thus, the gap as a function of the system size follows essentially two separate curves as seen in Fig. 8. A similar argument applies to \( x = \cos^{-1}(\Gamma) = \frac{l\pi}{j} \) with \( l, j \in \mathbb{N} \) satisfying \( \frac{1}{2} \leq l/j < 1 \), the latter condition coming from \( 0 \leq \Gamma < 1 \). In such a case

\[
Nx = \frac{lN}{2j},
\]  \hspace{1cm} \text{(23)}

and \( \delta_1 \) assumes a fixed value for selected series of system sizes. For instance, for the series \( N = ji \) \( (i \in \mathbb{N}) \), \( \delta_1 = 0 \) or \( \frac{1}{2} \), and for \( N = ji + 1 \), \( \frac{2Nl}{2j} = li/2 + l/2j \) and hence \( \delta_1 = \frac{l}{2j} \) or \( \frac{1}{2} + \frac{l}{2j} \), where \( \frac{1}{4} < \frac{1}{2j} < \frac{1}{2} \). Each of the series \( N = ji \) and \( N = ji + 1 \) gives a simple curve of \( \Delta \). Similar discussions apply to other series of the form \( N = ji + \text{const} \). Therefore, for some rational values of \( \cos^{-1}(\Gamma)/\pi \), the gap as a function of the system size follows a finite number of different curves. For irrational \( \cos^{-1}(\Gamma)/\pi \), this argument does not apply, and the behavior of the gap looks irregular. This difference between rational and irrational values of \( \cos^{-1}(\Gamma)/\pi \) may be one of the reasons why the behavior of the gap changes drastically as \( \Gamma \) changes.

The next point is that the envelope of the curve of the gap is proportional to the inverse of the system size as suggested in Fig. 12, where \( N\Delta \) is drawn as a function of \( N \) for \( \Gamma = 0.1 \). This fact can be verified analytically as follows. If we differentiate the quantities inside the symbol of absolute value in Eqs. (17) and (18) with respect to \( \delta_1 \) assuming that \( \delta_1 \) takes continuous values, we find that this derivative does not vanish if \( \Gamma < \cos(\pi/N) \). This means that the gap does not reach its extremum at an intermediate value in the range \( 0 \leq \delta_1 < 1 \). For example, if \( 0 \leq \delta_1 < \frac{1}{2} \), we find by setting the above-mentioned derivative to 0,

\[
\sin \left[ \alpha - \frac{\pi}{2N}(1 - 4\delta_1) \right] = 0,
\]  \hspace{1cm} \text{(24)}

11
where $\alpha$ is defined by $\cos \alpha = \Gamma$. The argument of the above sinusoidal function never vanishes if $0 \leq \delta_1 < \frac{1}{2}$ and $\Gamma < \cos(\pi/N)$. The gap therefore assumes its local maximum or minimum at the end points of the range, $\delta_1 = 0, \frac{1}{2},$ or $1$. By comparing the values of the gap at these end points, we find that the peak value of the gap is $2\sqrt{1-\Gamma^2} \tan(\pi/2N)$. This result suggests that, by choosing an appropriate series of system sizes corresponding to the peaks, we can find power-law dependence of the energy gap on the system size, $2\sqrt{1-\Gamma^2} \tan(\pi/2N) \approx \sqrt{1-\Gamma^2} / N$, for sufficiently large $N$. Therefore, the gap can be chosen to decrease in a power law at a first-order quantum phase transition, contrary to the usual case with an exponential law.

The third observation is that we may be able to choose a series of system sizes such that the gap closes very rapidly. The reason is that the expressions inside the absolute value symbol of Eqs. (17) and (18) oscillate between positive and negative values as suggested in Figs. (4) to (7) except for the special case of rational $\cos^{-1}(-\Gamma)/\pi$ mentioned above. This implies that the gap, obtained after taking the absolute value, reaches 0 if $N$ is allowed to take continuous values. Then, it may be possible to choose appropriate values of $N$ close to such zeros of the gap that give very small, possibly exponentially small, values of the gap. If this is indeed correct, which we failed to prove rigorously unlike the case of the infinite-range quantum $XY$ model [23], the rate of gap closing can be tuned to behave exponentially by an appropriate choice of the series of system sizes.

Last, Eq. (8) simplifies considerably when $\cos(\pi/N) < \Gamma$ because, in such a case, the summations over $k_1$ and $k_2$ in Eq. (8) run over all allowed values of these wave numbers.
except for $k_1 = \pi$. Then, the gap reduces to a simple form,

$$\Delta(\Gamma, N) = \left| \sum_{k_1} [-2(\cos k + \Gamma)] - 2(1 - \Gamma) - \sum_{k_2} [-2(\cos k + \Gamma)] \right| = 2(1 - \Gamma). \quad (25)$$

This last expression is independent of $N$ as is observed in Fig. 7 in the range $\cos(\pi/N) < \Gamma$ or $N < 222$.

III. CONCLUSION

We have studied the energy gap of the one-dimensional quantum XY model with $s = 1/2$ to show that the energy gap at the first-order transition point behaves quite anomalously as a function of the system size toward the thermodynamic limit. This resembles the property of the energy gap of the infinite-range quantum XY model, where the gap decreases in many different ways, polynomially, exponentially, or factorially, depending on the choice of the series of system sizes [23]. It is surprising that such an anomaly has been found in the well-studied one-dimensional model. It is an interesting problem to investigate what aspects of these one-dimensional and infinite-range models are the key to the anomalous behavior. The continuous symmetry is one of the common features of these models, but we should carefully investigate if this is the most essential property. From the viewpoint of implementation of quantum annealing, it is reassuring that the energy gap can be tuned to decrease polynomially as a function of system size even when the lower bound closes very quickly because the right choice of the series of system sizes allows us to avoid the problematic rapid closing of the gap. This also means that that one should be careful to interpret the results obtained from numerical simulations or other methods for a limited series of system sizes for systems that cannot be solved exactly.

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