# Topological quantum phase transition in the extended Kitaev spin model 

Xiao-Feng Shi, ${ }^{1,2,3}$ Yue Yu, ${ }^{4}$ J. Q. You, ${ }^{1,2,3}$ and Franco Nori ${ }^{2,3,5}$<br>${ }^{1}$ Department of Physics and Surface Physics Laboratory (National Key Laboratory), Fudan University, Shanghai 200433, China<br>${ }^{2}$ Advanced Science Institute, The Institute of Physical and Chemical Research (RIKEN), Wako-shi 351-0198, Japan<br>${ }^{3}$ CREST, Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012, Japan<br>${ }^{4}$ Institute of Theoretical Physics, Chinese Academy of Sciences, P.O. Box 2735, Beijing 100190, China<br>${ }^{5}$ Center for Theoretical Physics, Department of Physics, Center for the Study of Complex Systems, University of Michigan, Ann Arbor, Michigan 48109-1040, USA

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#### Abstract

We study the quantum phase transition between Abelian and non-Abelian phases in an extended Kitaev spin model on the honeycomb lattice, where the periodic boundary condition is applied by placing the lattice on a torus. Our analytical results show that this spin model exhibits a continuous quantum phase transition. Also, we reveal the relationship between bipartite entanglement and the ground-state energy. Our approach directly shows that both the entanglement and the ground-state energy can be used to characterize the topological quantum phase transition in the extended Kitaev spin model.


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## I. INTRODUCTION

Quantum phase transitions, which occur when a driving parameter in the Hamiltonian of the system changes across a critical point, play a central role in the physics of many-body systems. ${ }^{1,2}$ While most quantum phase transitions can be characterized by symmetry breaking, there is also an exception that can only be witnessed by topological order (see, e.g., Refs. 3 and 4). Signatures of topological order in manybody quantum systems can characterize a topological quantum phase transition and include, e.g., the existence of excitations obeying fractional statistics (see, e.g., Ref. 5), ground-state degeneracy related to the topology of the system (instead of the symmetry) (see, e.g., Refs. 3 and 6), and topological entanglement entropy. ${ }^{7,8}$ In particular, the spectral Chern number ${ }^{9}$ serves as a topological number for characterizing a two-dimensional (2D) system of noninteracting (or weakly interacting) fermions with an energy gap. Without closing the gap, energy spectra with different Chern numbers cannot be deformed into each other. ${ }^{10}$ This is because a topological quantum phase transition occurs when changing the Chern number.

Recently, it was shown ${ }^{11,12}$ that the topological quantum phase transition in the Kitaev spin model can be characterized by nonlocal-string order parameters. In an appropriate dual representation, this order parameter can become local and the basic concept of Landau theory of continuous phase transition is also applicable. ${ }^{11}$

In the Kitaev model, a $\frac{1}{2}$ spin is placed at each site of a honeycomb lattice [see Fig. 1(a)] and the interactions between nearest-neighbor spins are highly anisotropic with three types of bonds $J_{x}, J_{y}$, and $J_{z}$. To simplify the site labeling of the honeycomb lattice, one can deform it to a topologically equivalent brick-wall lattice shown in Fig. 1(b). In Refs. 11-13, the topological quantum phase transition of the Kitaev model on a brick-wall lattice was studied for the Hamiltonian:

$$
\begin{align*}
H_{0}= & J_{x} \sum_{n+m=\mathrm{odd}} \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}+J_{y} \sum_{n+m=\mathrm{even}} \sigma_{n, m}^{y} \sigma_{n+1, m}^{y} \\
& +J_{z} \sum_{n+m=\mathrm{even}} \sigma_{n, m}^{z} \sigma_{n, m+1}^{z} \tag{1}
\end{align*}
$$

where $\sigma_{n, m}^{x}, \sigma_{n, m}^{y}$, and $\sigma_{n, m}^{z}$ are the Pauli matrices at the site ( $n, m$ ), with column index $n=0,1,2,3, \ldots, N-1$ and row index $m=0,1,2,3, \ldots, M-1$. A nice Jordan-Wigner transformation was introduced ${ }^{11-13}$ to solve this model and the redundant gauge degrees of freedom were removed. Also, the topological quantum phase transition of the Kitaev model on a decorated honeycomb lattice was studied in Ref. 14 and a chiral spin liquid ground state with spontaneously broken time-reversal symmetry was found.

The phase diagram of the Kitaev model in Eq. (1) consists of two phases: a band insulator phase and a topologically nonuniversal gapless phase. ${ }^{9}$ The insulator phase, as Kitaev has shown by using perturbation theory, ${ }^{9,15}$ is equivalent to a toric code model. ${ }^{16}$ While Abelian anyons can be defined in the insulator phase, the vortices in the gapless phase do not have a well-defined statistics. Applying an external magnetic field as a perturbation, which breaks the time-reversal sym-

b


FIG. 1. (Color online) (a) Honeycomb lattice constructed by two triangular lattices that are connected to each other by three types of bonds $J_{x}, J_{y}$, and $J_{z}$. (b) The brick-wall lattice, which is deformed from the honeycomb lattice in (a). This deformed lattice can be used to label the sites of the honeycomb lattice by column and row indices.
metry in Eq. (1), a gap opens in the gapless phase and the vortices then obey a well-defined non-Abelian anyonic statistics. ${ }^{9}$ The third-order perturbation corresponds to exactly solvable models ${ }^{9,10}$ whose spectrum has recently been extensively studied. ${ }^{17}$

In this paper, we study the following Hamiltonian: ${ }^{10,18,19}$

$$
\begin{align*}
H= & H_{0}+J \sum_{n+m=\text { odd }} \sigma_{n, m}^{x} \sigma_{n+1, m}^{z} \sigma_{n+2, m}^{y} \\
& +J \sum_{n+m=\text { even }} \sigma_{n, m}^{y} \sigma_{n+1, m}^{z} \sigma_{n+2, m}^{x} . \tag{2}
\end{align*}
$$

Hereafter, we call the model in Eq. (2) an extended Kitaev model. We solve this model on a torus, and mainly focus on the quantum phase transition between the phase with Abelian anyons and the phase with non-Abelian anyons. We first apply the Jordan-Wigner transformation to the spin operators and then introduce Majorana fermions to get the ground state of Eq. (2) in the vortex-free sector. We show that the third directional derivative of the ground-state energy is discontinuous at each point on the critical line separating the Abelian and non-Abelian phases, while its first and second directional derivatives are continuous at this point. This implies that the topological quantum phase transition is continuous in this extended Kitaev model. Moreover, at this critical point, we also study the nonanalyticity of the entanglement (i.e., the von Neumann entropy) between two nearestneighbor spins and the rest of the spins in the system. We find that the second directional derivative of the von Neumann entropy is closely related to the third directional derivative of the ground-state energy and it is also discontinuous at the critical point. Our approach directly reveals that both the entanglement measure and the ground-state energy can be used to characterize the topological quantum phase transition in the extended Kitaev model.

We emphasize that the motivation for studying the extended Kitaev model, shown in Eq. (2), is the existence of both gapped Abelian and non-Abelian phases, in sharp contrast to the Kitaev model in Eq. (1), which does not have a gapped non-Abelian phase. In particular, when $\left|J / J_{i}\right| \ll 1$, where $i=x, y$, and $z$, the model in Eq. (2) is equivalent to the Kitaev model in the presence of a weak magnetic field because the third-order perturbation of the magnetic field gives rise to terms in the effective Hamiltonian that have the same form as the $J$ terms in Eq. (2). ${ }^{9,10}$ Furthermore, the extended Kitaev model [Eq. (2)] is exactly solvable, regardless of the strength of the parameter $J$. Thus, it provides a useful exactly solvable model for studying non-Abelian anyons. Moreover, as shown here, this model can analytically reveal the relation between the nonanalyticity of the bipartite entanglement and the nonanalyticity of the ground-state energy at the quantum phase-transition point. Indeed, several numerical calculations for other quantum models (see, e.g., Refs. 20-24) have shown that the measure of quantum entanglement exhibits nonanalyticity at the quantum phase transition, just like the ground-state energy; but no such a relation was analytically derived between the entanglement and the ground-state energy. Here this relation is obtained for the Kitaev-type spin models.

## II. TOPOLOGICAL QUANTUM PHASE TRANSITION

Let us define the Jordan-Wigner transformation ${ }^{25}$

$$
\begin{gather*}
\sigma_{n, m}^{+}=2\left(a_{n, m}^{(s)}\right)^{\dagger} K(n, m) \\
K(n, m)=\prod_{n^{\prime}=0}^{N-1} \prod_{m^{\prime}=0}^{m-1} \sigma_{n^{\prime}, m^{\prime}}^{z} \prod_{n^{\prime}=0}^{n-1} \sigma_{n^{\prime}, m}^{z}, \tag{3}
\end{gather*}
$$

where $s=1$ if the integer $n+m$ is odd and $s=2$ if the integer $n+m$ is even. Also, we introduce the following definitions for Majorana fermions:

$$
\begin{gather*}
i\left[a_{n, m}^{(1) \dagger}-a_{n, m}^{(1)}\right]=c_{n, m}^{(1)}, \\
a_{n, m}^{(1) \dagger}+a_{n, m}^{(1)}=d_{n, m}^{(1)}, \tag{4}
\end{gather*}
$$

for $n+m$ equal to an odd integer, and

$$
\begin{gather*}
i\left[a_{n, m}^{(2) \dagger}-a_{n, m}^{(2)}\right]=d_{n, m}^{(2)}, \\
a_{n, m}^{(2) \dagger}+a_{n, m}^{(2)}=c_{n, m}^{(2)}, \tag{5}
\end{gather*}
$$

for $n+m$ equal to an even integer. When the phase (arising from the Jordan-Wigner transformation) related to each bond between the $(N-1)$ th column and the zeroth column is chosen to be $2 \pi l$ ( $l$ is an integer), the Hamiltonian (2) is reduced to

$$
\begin{align*}
H= & i J_{x} \sum_{n+m=\mathrm{odd}} c_{n, m}^{(1)} c_{n+1, m}^{(2)}-i J_{y} \sum_{n+m=\mathrm{even}} c_{n, m}^{(2)} c_{n+1, m}^{(1)} \\
& +i J_{z} \sum_{n+m=\mathrm{even}} i d_{n, m}^{(2)} d_{n, m+1}^{(1)} c_{n, m}^{(2)} c_{n, m+1}^{(1)}-i J \sum_{n+m=\mathrm{odd}} c_{n, m}^{(1)} c_{n+2, m}^{(1)} \\
& +i J \sum_{n+m=\mathrm{even}} c_{n, m}^{(2)} c_{n+2, m}^{(2)} \tag{6}
\end{align*}
$$

In Eq. (6), the $\frac{1}{2} N M$ operators $i d_{n, m}^{(2)} d_{n, m+1}^{(1)}$, where $n+m$ is an even integer, commute with each other. The ground state is in the vortex-free sector ${ }^{18,26}$ with

$$
\begin{equation*}
d_{n, m+1}^{(1)} d_{n, m}^{(2)} d_{n+2, m+1}^{(1)} d_{n+2, m}^{(2)}=-1 \tag{7}
\end{equation*}
$$

which corresponds to the case with the eigenvalue of each plaquette operator, ${ }^{9}$

$$
\begin{equation*}
W_{(n, m)}=\sigma_{n, m}^{x} \sigma_{n+1, m}^{z} \sigma_{n+2, m}^{y} \sigma_{n, m+1}^{y} \sigma_{n+1, m+1}^{z} \sigma_{n+2, m+1}^{x} \tag{8}
\end{equation*}
$$

equal to one. Thus, we can set the $\frac{1}{2} N M$ operators $i d_{n, m}^{(2)} d_{n, m+1}^{(1)}$ all equal to one in Eq. (6), in order to obtain the ground-state energy. For this quadratic Hamiltonian, the Fourier transformation of $H$ via $c_{n, m}^{(1)}=\frac{2}{\sqrt{N M}} \sum_{\mathbf{k}} e^{i \mathbf{k} \cdot \mathbf{r}_{n m}} c_{\mathbf{k}}^{(1)}$ gives rise to

$$
\begin{gather*}
H=\sum_{\mathbf{k}} \Phi_{\mathbf{k}}^{\dagger} H_{\mathbf{k}} \Phi_{\mathbf{k}} \\
H_{\mathbf{k}}=h_{x}(\mathbf{k}) \sigma^{x}+h_{y}(\mathbf{k}) \sigma^{y}+h_{z}(\mathbf{k}) \sigma^{z} \tag{9}
\end{gather*}
$$

where $\sigma^{x}, \sigma^{y}$, and $\sigma^{z}$ are Pauli matrices, $\Phi_{\mathbf{k}}^{\dagger}=\left(c_{-\mathbf{k}}^{(1)}, c_{-\mathbf{k}}^{(2)}\right)$ with $c_{-\mathbf{k}}^{(j)}=\left(c_{\mathbf{k}}^{(j)}\right)^{\dagger}$, and


FIG. 2. (Color online) Phase diagram of the extended Kitaev spin model, where $J_{x}, J_{y}$, and $J_{z}>0$. The gray region corresponds to the non-Abelian phase and the three triangular (light gray) regions correspond to the Abelian phase. The thick solid, dashed, and dotted lines are $\Lambda_{x}=1+\Lambda_{y}, \Lambda_{y}=1+\Lambda_{x}$, and $\Lambda_{y}=1-\Lambda_{x}$, where $\Lambda_{x} \equiv J_{x} / J_{z}$ and $\Lambda_{y} \equiv J_{y} / J_{z}$. These lines consist of the boundary of the gray region, which are the critical lines separating the Abelian and nonAbelian phases. The thin dotted line intersects the thick solid and dotted lines at the points $\left(\Lambda_{x}, \Lambda_{y}\right)=(1.5,0.5)$ and $(0.5,0.5)$. The direction $l$ has an inclination angle $\varphi$ with respect to the horizontal axis and it indicates the direction along which the driving parameters $\Lambda_{x}$ and $\Lambda_{y}$ vary.

$$
\begin{gather*}
h_{x}(\mathbf{k})=-J_{x} \sin \left(\frac{k_{x}}{2}+\frac{k_{y}}{2 \sqrt{3}}\right)+J_{y} \sin \left(\frac{k_{x}}{2}-\frac{k_{y}}{2 \sqrt{3}}\right)-J_{z} \sin \frac{k_{y}}{\sqrt{3}} \\
h_{y}(\mathbf{k})=-J_{x} \cos \left(\frac{k_{x}}{2}+\frac{k_{y}}{2 \sqrt{3}}\right)-J_{y} \cos \left(\frac{k_{x}}{2}-\frac{k_{y}}{2 \sqrt{3}}\right)+J_{z} \cos \frac{k_{y}}{\sqrt{3}} \\
h_{z}(\mathbf{k})=2 J \sin k_{x} \tag{10}
\end{gather*}
$$

Let us define

$$
\begin{equation*}
B_{\mathbf{k}}=\frac{\alpha^{*}(\mathbf{k}) c_{\mathbf{k}}^{(1)}-\left[\varepsilon(\mathbf{k})+2 J \sin k_{x}\right] c_{\mathbf{k}}^{(2)}}{\sqrt{|\alpha(\mathbf{k})|^{2}+\left[\varepsilon(\mathbf{k})+2 J \sin k_{x}\right]^{2}}} \tag{11}
\end{equation*}
$$

where

$$
\begin{equation*}
\alpha(\mathbf{k})=i J_{x} e^{i\left[\left(k_{x} / 2\right)+\left(k_{y} / 2 \sqrt{3}\right)\right]}+i J_{y} e^{-i\left[\left(k_{x} / 2\right)-\left(k_{y} / 2 \sqrt{3}\right)\right]}-i J_{z} e^{-i\left(k_{y} / \sqrt{3}\right)} \tag{12}
\end{equation*}
$$

and

$$
\begin{equation*}
\varepsilon(\mathbf{k})=|\mathbf{h}(\mathbf{k})|=\sqrt{|\alpha(\mathbf{k})|^{2}+4 J^{2} \sin ^{2} k_{x}} . \tag{13}
\end{equation*}
$$

It is straightforward to verify that

$$
\begin{equation*}
\left\{B_{\mathbf{k}}^{\dagger}, B_{\mathbf{k}^{\prime}}\right\}=\delta_{\mathbf{k}, \mathbf{k}^{\prime}} \tag{14}
\end{equation*}
$$

i.e., $B_{\mathbf{k}}^{\dagger}$ and $B_{\mathbf{k}}$ are fermionic operators, and the Hamiltonian (9) can be written as

$$
\begin{equation*}
H=\sum_{\mathbf{k}}\left[\varepsilon(\mathbf{k})-2 \varepsilon(\mathbf{k}) B_{\mathbf{k}}^{\dagger} B_{\mathbf{k}}\right] \tag{15}
\end{equation*}
$$

For Hamiltonian (15), the ground-state energy is $-\sum_{\mathbf{k}} \varepsilon(\mathbf{k})$ and the ground-state $|g\rangle$ obeys $B_{\mathbf{k}}^{\dagger} B_{\mathbf{k}}|g\rangle=|g\rangle$. The energy spectrum $\varepsilon(\mathbf{k})$ is gapless ${ }^{10}$ only when $J_{x}=J_{y}+J_{z}, J_{y}=J_{z}+J_{x}$, or $J_{z}=J_{x}+J_{y}$, which corresponds to the thick solid, dashed,
and dotted lines in Fig. 2, respectively. It should be clarified that for a system with periodic boundary conditions, the Jordan-Wigner transformation has some boundary terms. This means that the physical ground-state wave function for the Kitaev model should be a "gauge" average over all these possible boundary terms. ${ }^{14}$

When $J>0$, the spectral Chern number is one if $J_{x}<J_{y}$ $+J_{z}, J_{y}<J_{z}+J_{x}$, and $J_{z}<J_{x}+J_{y}$, and zero if $J_{x}>J_{y}+J_{z}, J_{y}$ $>J_{z}+J_{x}$, or $J_{z}>J_{x}+J_{y}$ (see Refs. 9 and 10). These two cases correspond to the non-Abelian and Abelian phases in the Kitaev model, and both of them are gapped topological phases. The phase diagram is shown in Fig. 2, where the gray area corresponds to the non-Abelian phase, and the critical lines (denoted as thick solid, dashed, and dotted lines) separate the Abelian and non-Abelian phases. This indicates that the system can experience quantum phase transitions across these three thick lines. Here we rescale the interspin coupling strengths by introducing $\Lambda_{x} \equiv J_{x} / J_{z}, \Lambda_{y} \equiv J_{y} / J_{z}$, and $\Lambda$ $\equiv J / J_{z}$, so as to conveniently characterize the quantum phase transition.

To demonstrate the quantum phase transition, one may reveal the nonanalyticity of the ground-state energy. The ground-state energy per site is

$$
\begin{equation*}
E=-\frac{1}{N M} \sum_{\mathbf{k}} \varepsilon(\mathbf{k})=-\frac{\sqrt{3}}{16 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \varepsilon(\mathbf{k}) \tag{16}
\end{equation*}
$$

where BZ denotes the first Brillouin zone. Its directional derivatives with respect to the driving parameter along any given direction $l$ (see Fig. 2) are

$$
\begin{gather*}
\frac{\partial E}{\partial l}=\cos \varphi \frac{\partial E}{\partial \Lambda_{x}}+\sin \varphi \frac{\partial E}{\partial \Lambda_{y}}, \\
\frac{\partial^{2} E}{\partial l^{2}}=\cos ^{2} \varphi \frac{\partial^{2} E}{\partial \Lambda_{x}^{2}}+\sin 2 \varphi \frac{\partial^{2} E}{\partial \Lambda_{x} \partial \Lambda_{y}}+\sin ^{2} \varphi \frac{\partial^{2} E}{\partial \Lambda_{y}^{2}} \\
\frac{\partial^{3} E}{\partial l^{3}}= \\
\cos ^{3} \varphi \frac{\partial^{3} E}{\partial \Lambda_{x}^{3}}+3 \sin \varphi \cos ^{2} \varphi \frac{\partial^{3} E}{\partial \Lambda_{y} \partial \Lambda_{x}^{2}}  \tag{17}\\
+3 \sin ^{2} \varphi \cos \varphi \frac{\partial^{3} E}{\partial \Lambda_{x} \partial \Lambda_{y}^{2}}+\sin ^{3} \varphi \frac{\partial^{3} E}{\partial \Lambda_{y}^{3}}
\end{gather*}
$$

If the $n$th directional derivative $\partial^{n} E / \partial l^{n} \quad(n=1,2, \ldots)$ is nonanalytical at the critical point $\left(\Lambda_{x}^{c}, \Lambda_{y}^{c}\right)$, and the directional derivatives $\partial^{m} E / \partial l^{m}$ with $0 \leq m<n$ are analytical there, a topological quantum phase transition occurs at this critical point.

It can be proved that (see Appendix A)

$$
\begin{gather*}
\left.\frac{\partial E}{\partial l}\right|_{1^{+}}=\left.\frac{\partial E}{\partial l}\right|_{1^{-}} \\
\left.\frac{\partial^{2} E}{\partial l^{2}}\right|_{1^{+}}=\left.\frac{\partial^{2} E}{\partial l^{2}}\right|_{1^{-}}, \tag{18}
\end{gather*}
$$

and

$$
\begin{equation*}
\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{+}}-\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{-}} \simeq \frac{\sqrt{6} \mathcal{D}^{3}}{2 \pi^{2}} \Gamma \tag{19}
\end{equation*}
$$

where

$$
\begin{gather*}
\mathcal{D}=\cos \left(\varphi+\frac{\pi}{4}\right) \\
\Gamma=\int_{0}^{2 \pi} d \theta \frac{1}{Q_{1}+Q_{2} \sin \left(2 \theta+\phi_{1}\right)} \tag{20}
\end{gather*}
$$

$1^{+}$denotes $\left(\Lambda_{x}-\Lambda_{y}\right) \rightarrow 1$ with $\left(\Lambda_{x}-\Lambda_{y}\right)>1$, and $1^{-}$denotes $\left(\Lambda_{x}-\Lambda_{y}\right) \rightarrow 1$ with $\left(\Lambda_{x}-\Lambda_{y}\right)<1$. In Eq. (20),

$$
\begin{gather*}
Q_{1}=\frac{1}{2}\left(4 \Lambda^{2}+\Lambda_{y}^{2}+\Lambda_{y}+1\right) \\
Q_{2}=\frac{1}{4} \sqrt{\left(8 \Lambda^{2}+2 \Lambda_{y}^{2}+2 \Lambda_{y}-1\right)^{2}+3\left(1+2 \Lambda_{y}\right)^{2}}, \\
\phi_{1}=\arctan \left(\frac{8 \Lambda^{2}+2 \Lambda_{y}^{2}+2 \Lambda_{y}-1}{\sqrt{3}\left(1+2 \Lambda_{y}\right)}\right) . \tag{21}
\end{gather*}
$$

Equations (18) and (19) reveal that a continuous topological quantum phase transition occurs across the critical line $\Lambda_{x}$ $=1+\Lambda_{y}$ (denoted by the thick solid line in Fig. 2). Similarly, it can be shown that such a continuous topological quantum phase transition also occurs across the critical lines $\Lambda_{y}=1$ $+\Lambda_{x}$ and $\Lambda_{x}=1-\Lambda_{y}$ (denoted, respectively, by the thick dashed and dotted lines in Fig. 2). As a numerical test, we choose $\Lambda=0.1, \varphi=0$, and $\Lambda_{y}=0.5$ to show this quantum phase transition in Fig. 3, where the range of $\Lambda_{x}$ is chosen by the thin dotted line in Fig. 2. It can be seen in Fig. 3 that the ground-state energy and its first and second directional derivatives are continuous for each $\Lambda_{x}$, while its third directional derivative is nonanalytic at the points $\Lambda_{x}=0.5$ and $\Lambda_{x}=1.5$. These two points satisfy the condition $J_{z}=J_{x}+J_{y}$ and $J_{x}=J_{y}+J_{z}$, respectively. It is obvious that these two points are on the critical lines denoted by the thick dotted and solid lines in Fig. 2.

## III. ENTANGLEMENT

It has been shown that the entanglement also exhibits critical behavior at the quantum phase-transition point for both spin (see, e.g., Refs. 20-22) and fermionic systems (see, e.g., Refs. 23 and 24). Also, it has been shown ${ }^{27,28}$ that there is a general relation between the bipartite entanglement and the quantum phase transition. In this section, we show that the nonanalyticity of the ground-state energy in the extended Kitaev model results from the correlation functions [see Eqs. (25), (29), and (30) for their definitions]. Furthermore, we show that the bipartite entanglement also exhibits nonanalyticity at the quantum phase-transition point and its nonanalyticity is also due to the nonanalyticity of the same correlation functions. This implies that both the ground-state energy and the bipartite entanglement can characterize the quantum phase transition in the Kitaev model.


FIG. 3. (Color online) The ground-state energy per site $E$ (in units of $J_{z}$ ), and its first, second, and third derivatives with respect to $\Lambda_{x}$, where $\Lambda_{y}=0.5, \Lambda=0.1$, and $\varphi=0$ (which corresponds to the horizontal thin dotted line in Fig. 2). It is clear that $E$ and $\partial E / \partial \Lambda_{x}$ are continuous functions but $\partial^{3} E / \partial \Lambda_{x}^{3}$ is discontinuous at the transition points $\Lambda_{x}=0.5$ and 1.5, both shown by the vertical (red) dashed lines.

## A. Correlation functions and nonanalyticity of ground-state energy

From the Hellmann-Feynman theorem, ${ }^{29}$ we have

$$
\begin{align*}
\frac{\partial E}{\partial l}= & \frac{1}{N M} \operatorname{Tr}\left(\rho \frac{\partial H}{\partial l}\right) \\
= & \frac{1}{N M} \cos \varphi \sum_{n+m=\text { odd }} \operatorname{Tr}\left(\rho \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}\right) \\
& +\frac{1}{N M} \sin \varphi \sum_{n+m=\text { even }} \operatorname{Tr}\left(\rho \sigma_{n, m}^{y} \sigma_{n+1, m}^{y}\right), \tag{22}
\end{align*}
$$

where $E$ is the ground-state energy per site given in Eq. (16), $H$ is the Hamiltonian (2) (rescaled by $J_{z}$ ), Tr denotes the trace over the ground-state subspace, and $\rho=|g\rangle\langle g|$ is the density matrix of the system. When $|g\rangle\langle g|$ is traced over all spins except the two spins at $\mathbf{r}_{n, m}$ and $\mathbf{r}_{n^{\prime}, m^{\prime}}$, the reduced density matrix is

$$
\begin{align*}
\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n^{\prime}, m^{\prime}}\right) & =\operatorname{Tr}^{\prime}(|g\rangle\langle g|) \\
& =\frac{1}{4} \sum_{\alpha, \alpha^{\prime}=0}^{3}\langle g| \sigma_{n, m}^{\alpha} \sigma_{n^{\prime}, m^{\prime}}^{\alpha^{\prime}}|g\rangle \sigma_{n, m}^{\alpha} \sigma_{n^{\prime}, m^{\prime}}^{\alpha^{\prime}} \tag{23}
\end{align*}
$$

where $\sigma^{\alpha}\left(\sigma^{\alpha^{\prime}}\right)$ are Pauli matrices $\sigma^{x}, \sigma^{y}$, and $\sigma^{z}$ for $\alpha\left(\alpha^{\prime}\right)$ $=1-3$, and the unit matrix for $\alpha\left(\alpha^{\prime}\right)=0$. When the two spins at $\mathbf{r}_{n, m}$ and $\mathbf{r}_{n+1, m}$ are linked by an $x$-type bond, the reduced density matrix becomes

$$
\begin{equation*}
\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right)=\frac{1}{4}\langle g| \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}|g\rangle \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}+\frac{1}{4} I_{n, m} I_{n+1, m}, \tag{24}
\end{equation*}
$$

where $n+m$ is an odd integer, and $I$ is the unit operator.
Because of translational invariance, the correlation function

$$
\begin{equation*}
\mathcal{G}_{x} \equiv\langle g| \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}|g\rangle \tag{25}
\end{equation*}
$$

is spatially invariant. Thus, Eq. (24) can be written as

$$
\begin{equation*}
\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right)=\frac{I_{n, m} I_{n+1, m}+\mathcal{G}_{x} \sigma_{n, m}^{x} \sigma_{n+1, m}^{x}}{4} \tag{26}
\end{equation*}
$$

where $n+m$ is an odd integer. Similarly, one has

$$
\begin{align*}
& \rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right)=\frac{I_{n, m} I_{n+1, m}+\mathcal{G}_{y} \sigma_{n, m}^{y} \sigma_{n+1, m}^{y}}{4},  \tag{27}\\
& \rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n, m+1}\right)=\frac{I_{n, m} I_{n, m+1}+\mathcal{G}_{z} \sigma_{n, m}^{z} \sigma_{n, m+1}^{z}}{4}, \tag{28}
\end{align*}
$$

with

$$
\begin{align*}
\mathcal{G}_{y} & \equiv\langle g| \sigma_{n, m}^{y} \sigma_{n+1, m}^{y}|g\rangle  \tag{29}\\
\mathcal{G}_{z} & \equiv\langle g| \sigma_{n, m}^{z} \sigma_{n, m+1}^{z}|g\rangle \tag{30}
\end{align*}
$$

where $n+m$ is an even integer for both $\mathcal{G}_{y}$ and $\mathcal{G}_{z}$. Here Eqs. (26)-(28) are the results obtained for the reduced density matrix when the two spins at $\mathbf{r}_{n, m}$ and $\mathbf{r}_{n^{\prime}, m^{\prime}}$ are nearest neighbors. When the two spins at $\mathbf{r}_{n, m}$ and $\mathbf{r}_{n^{\prime}, m^{\prime}}$ are not nearest neighbors, the density matrix is

$$
\begin{equation*}
\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n^{\prime}, m^{\prime}}\right)=\frac{I_{n, m} I_{n^{\prime}, m^{\prime}}}{4} \tag{31}
\end{equation*}
$$

Using the Jordan-Wigner transformation (3), and the definitions (4) and (5) for the Majorana fermions, we can derive that

$$
\begin{equation*}
\mathcal{G}_{x}=\langle g| \sigma_{0,1}^{x} \sigma_{1,1}^{x}|g\rangle=i\langle g| c_{0,1}^{(1)} c_{1,1}^{(2)}|g\rangle \tag{32}
\end{equation*}
$$

From Eqs. (11), (13), and (32) we have

$$
\begin{align*}
\mathcal{G}_{x}= & \frac{\sqrt{3} i}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{\alpha(\mathbf{k})}{\varepsilon(\mathbf{k})} \exp \left(-i \frac{k_{x}}{2}-i \frac{\sqrt{3} k_{y}}{6}\right) \\
= & \frac{-\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{1}{\sqrt{|\alpha(\mathbf{k})|^{2}+4 \Lambda^{2} \sin ^{2} k_{x}}} \\
& \times\left[\Lambda_{x}+\Lambda_{y} \cos k_{x}-\cos \frac{k_{x}+\sqrt{3} k_{y}}{2}\right] \tag{33}
\end{align*}
$$

and

$$
\begin{equation*}
\left|\mathcal{G}_{x}\right| \leq \frac{\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{|\alpha(\mathbf{k})|}{\varepsilon(\mathbf{k})}<\frac{\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{\varepsilon(\mathbf{k})}{\varepsilon(\mathbf{k})}=1 \tag{34}
\end{equation*}
$$

which gives rise to $-1<\mathcal{G}_{x}<1$. Similarly, we have

$$
\begin{align*}
\mathcal{G}_{y}= & \frac{-\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{1}{\sqrt{|\alpha(\mathbf{k})|^{2}+4 \Lambda^{2} \sin ^{2} k_{x}}} \\
& \times\left[\Lambda_{x} \cos k_{x}+\Lambda_{y}-\cos \frac{k_{x}-\sqrt{3} k_{y}}{2}\right] \tag{35}
\end{align*}
$$

with $-1<\mathcal{G}_{y}<1$.
From Eqs. (22), (25), and (29), it follows that

$$
\frac{\partial E}{\partial l}=\frac{1}{2} \cos \varphi \mathcal{G}_{x}+\frac{1}{2} \sin \varphi \mathcal{G}_{y}
$$

$$
\begin{aligned}
\frac{\partial^{2} E}{\partial l^{2}}= & \frac{1}{2} \cos ^{2} \varphi \frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{x}}+\frac{1}{2} \sin ^{2} \varphi \frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{y}} \\
& +\frac{1}{2} \sin \varphi \cos \varphi\left[\frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{y}}+\frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{x}}\right]
\end{aligned}
$$

$$
\frac{\partial^{3} E}{\partial l^{3}}=\frac{1}{2} \cos ^{3} \varphi \frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x}^{2}}+\frac{1}{2} \sin ^{3} \varphi \frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{y}^{2}}
$$

$$
+\frac{1}{2} \cos ^{2} \varphi \sin \varphi\left[2 \frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x} \partial \Lambda_{y}}+\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x}^{2}}\right]
$$

$$
\begin{equation*}
+\frac{1}{2} \cos \varphi \sin ^{2} \varphi\left[2 \frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x} \partial \Lambda_{y}}+\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{y}^{2}}\right] \tag{36}
\end{equation*}
$$

Equation (36) shows that the directional derivatives of the ground-state energy per site are determined by the correlation functions $\mathcal{G}_{\alpha}(\alpha=x, y)$ and their derivatives. Section II shows that $\partial E / \partial l$ and $\partial^{2} E / \partial l^{2}$ are continuous while $\partial^{3} E / \partial l^{3}$ is discontinuous on the critical line, e.g., $\Lambda_{x}=1+\Lambda_{y}$ (i.e., the thick solid line in Fig. 2). Equation (36) reveals that the nonanalyticity of $E$ on the critical line is due to the nonanalyticity of $\mathcal{G}_{\alpha}$. As shown in Appendix B,

$$
\begin{align*}
\left.\mathcal{G}_{\alpha}\right|_{1^{+}} & =\left.\mathcal{G}_{\beta}\right|_{1^{-}}, \\
\left.\frac{\partial \mathcal{G}_{\alpha}}{\partial \Lambda_{\beta}}\right|_{1^{+}} & =\left.\frac{\partial \mathcal{G}_{\alpha}}{\partial \Lambda_{\beta}}\right|_{1^{-}}, \tag{37}
\end{align*}
$$

where $\alpha, \beta=x, y$, and

$$
\begin{gather*}
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x}^{2}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{y}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{y}^{2}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x}^{2}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma \\
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{y}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{y}^{2}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \tag{38}
\end{gather*}
$$

where $\Gamma$ is given in Eq. (20). Equation (38) shows that the spin-spin correlation function $\mathcal{G}_{\alpha}$ can signal the quantum phase transition, similar to the bond-bond correlation function in the original Kitaev model. ${ }^{30}$ From Eqs. (36) and (38), we have

$$
\begin{equation*}
\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{+}}-\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{-}} \simeq \frac{\sqrt{3}(\cos \varphi-\sin \varphi)^{3}}{4 \pi^{2}} \Gamma=\frac{\sqrt{6} \mathcal{D}^{3}}{2 \pi^{2}} \Gamma \tag{39}
\end{equation*}
$$

which is the same as in Eq. (19). This further reveals that the nonanalyticity of the ground-state energy results from the nonanalyticity of the correlation functions $\mathcal{G}_{\alpha}$.

## B. Nonanalyticity of entanglement

We now focus on the bipartite entanglement of the ground state $|g\rangle$ between two spins (at $\mathbf{r}_{n, m}$ and $\mathbf{r}_{n^{\prime}, m^{\prime}}$ ) and the rest of the spins in the system. We use the von Neumann entropy to measure the entanglement between these two spins and the rest of the spins in the system. The von Neumann entropy can be defined by ${ }^{31}$

$$
\begin{equation*}
S_{\alpha}=-\operatorname{Tr}\left[\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right) \log _{2} \rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right)\right] \tag{40}
\end{equation*}
$$

where Tr denotes the trace over the two-spin Hilbert space, and $\alpha=x$ if $n+m$ is an odd integer, and $\alpha=y$ if $n+m$ is an even integer. Also, this entropy can be written as

$$
\begin{equation*}
S_{\alpha}=-\sum \lambda_{i} \log _{2} \lambda_{i} \tag{41}
\end{equation*}
$$

where the sum runs over the four eigenvalues $\lambda_{i}$ of the matrix $\rho\left(\mathbf{r}_{n, m}, \mathbf{r}_{n+1, m}\right)$. From Eqs. (25) and (29), it follows that

$$
\lambda_{1}=\lambda_{2}=\frac{1}{4}\left(1+\mathcal{G}_{\alpha}\right)
$$

$$
\begin{equation*}
\lambda_{3}=\lambda_{4}=\frac{1}{4}\left(1-\mathcal{G}_{\alpha}\right) \tag{42}
\end{equation*}
$$

Thus, we have the entanglement measure

$$
\begin{equation*}
S_{\alpha}=2-\frac{1}{2} \log _{2}\left[\left(1-\mathcal{G}_{\alpha}\right)^{1-\mathcal{G}_{\alpha}}\left(1+\mathcal{G}_{\alpha}\right)^{1+\mathcal{G}_{\alpha}}\right] \tag{43}
\end{equation*}
$$

which is determined by the correlation function $\mathcal{G}_{\alpha}$, similar to the thermal entanglement. ${ }^{32}$

To see the relationship between the entanglement and the quantum phase transition, we analyze the directional derivatives of the von Neumann entropy with respect to the driving parameters along any direction $l$. The first and second directional derivatives of the bipartite entanglement are

$$
\begin{gather*}
\frac{\partial S_{\alpha}}{\partial l}=\frac{\partial \mathcal{G}_{\alpha}}{\partial l} \log _{2} \sqrt{\frac{1-\mathcal{G}_{\alpha}}{1+\mathcal{G}_{\alpha}}} \\
\frac{\partial^{2} S_{\alpha}}{\partial l^{2}}=\frac{\partial^{2} \mathcal{G}_{\alpha}}{\partial l^{2}} \log _{2} \sqrt{\frac{1-\mathcal{G}_{\alpha}}{1+\mathcal{G}_{\alpha}}}-\frac{1}{\ln 2} \frac{\partial \mathcal{G}_{\alpha}}{\partial l} \frac{1}{1-\mathcal{G}_{\alpha}^{2}}, \tag{44}
\end{gather*}
$$

where

$$
\begin{gather*}
\frac{\partial \mathcal{G}_{\alpha}}{\partial l}=\cos \varphi \frac{\partial \mathcal{G}_{\alpha}}{\partial \Lambda_{x}}+\sin \varphi \frac{\partial \mathcal{G}_{\alpha}}{\partial \Lambda_{y}} \\
\frac{\partial^{2} \mathcal{G}_{\alpha}}{\partial l^{2}}=\cos ^{2} \varphi \frac{\partial^{2} \mathcal{G}_{\alpha}}{\partial \Lambda_{x}^{2}}+\sin 2 \varphi \frac{\partial^{2} \mathcal{G}_{\alpha}}{\partial \Lambda_{x} \partial \Lambda_{y}}+\sin ^{2} \varphi \frac{\partial^{2} \mathcal{G}_{\alpha}}{\partial \Lambda_{y}^{2}} \tag{45}
\end{gather*}
$$

From Eqs. (37), (38), (43), and (44), we have

$$
\begin{gather*}
\left.S_{\alpha}\right|_{1^{+}}=S_{\alpha 1^{-}}, \\
\left.\frac{\partial S_{\alpha}}{\partial l}\right|_{1^{+}}=\left.\frac{\partial S_{\alpha}}{\partial l}\right|_{1^{-}}, \tag{46}
\end{gather*}
$$

and

$$
\begin{gather*}
\left.\frac{\partial^{2} S_{x}}{\partial l^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} S_{x}}{\partial l^{2}}\right|_{1^{-}} \simeq \frac{\sqrt{3} \Gamma \mathcal{D}^{2}}{\pi^{2}} \log _{2} \sqrt{\frac{1-\mathcal{G}_{x}^{c}}{1+\mathcal{G}_{x}^{c}}} \\
\left.\frac{\partial^{2} S_{y}}{\partial l^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} S_{y}}{\partial l^{2}}\right|_{1^{-}} \simeq-\frac{\sqrt{3} \Gamma \mathcal{D}^{2}}{\pi^{2}} \log _{2} \sqrt{\frac{1-\mathcal{G}_{y}^{c}}{1+\mathcal{G}_{y}^{c}}} \tag{47}
\end{gather*}
$$

where

$$
\begin{equation*}
\mathcal{G}_{\alpha}^{c}=\mathcal{G}_{\alpha \mid 1^{+}}=\left.\mathcal{G}_{\alpha}\right|_{1^{-}} . \tag{48}
\end{equation*}
$$

Equation (47) shows that the bipartite entanglement is nonanalytic with its second directional derivative $\partial^{2} S_{\alpha} / \partial l^{2}$ discontinuous at the critical line $\Lambda_{x}=1+\Lambda_{y}$ (denoted by the thick solid line in Fig. 2). Because $-1<\mathcal{G}_{\alpha}<1$, it follows from Eq. (44) that the discontinuity of $\partial^{2} S_{\alpha} / \partial l^{2}$ is due to the discontinuity of $\partial^{2} \mathcal{G}_{\alpha} / \partial l^{2}$. Similarly, it can be shown that $\partial^{2} S_{\alpha} / \partial l^{2}$ also exhibits a discontinuity on the critical lines $\Lambda_{y}=1+\Lambda_{x}$ and $\Lambda_{x}=1-\Lambda_{y}$ (denoted by the thick dashed and dotted lines in Fig. 2) which is due to the discontinuity of


FIG. 4. (Color online) The bipartite entanglement (i.e., the von Neumann entropy) $S_{x}$, and its first and second derivatives with respect to $\Lambda_{x}$, where $\Lambda_{y}=0.5, \Lambda=0.1$, and $\varphi=0$ (which corresponds to the horizontal thin dotted line in Fig. 2). Obviously, $S_{x}$ and $\partial S_{x} / \partial \Lambda_{x}$ are continuous functions but $\partial^{2} S_{x} / \partial \Lambda_{x}^{2}$ is discontinuous at the transition points $\Lambda_{x}=0.5$ and 1.5 , both shown by the vertical (red) dashed lines.
$\partial^{2} \mathcal{G}_{\alpha} / \partial l^{2}$ on these lines. As in Fig. 3, we choose $\Lambda=0.1, \varphi$ $=0$, and $\Lambda_{y}=0.5$ as a typical example to show $S_{x}$, and its first and second derivatives with respect to $\Lambda_{x}$ (see Fig. 4). It is clear that $S_{x}$ and its first derivative $\partial S_{x} / \partial \Lambda_{x}$ are continuous as a function of $\Lambda_{x}$ but its second derivative $\partial^{2} S_{x} / \partial \Lambda_{x}^{2}$ is discontinuous at the quantum phase-transition points $\Lambda_{x}=0.5$ and $\Lambda_{x}=1.5$.

As shown above, both the nonanalyticity of the groundstate energy and that of the bipartite entanglement are due to the nonanalyticity of the spin-spin correlation functions. This reveals that the ground-state energy and the bipartite entanglement are closely related with each other, and both of them can be used to characterize the topological quantum phase transition in the extended Kitaev spin model.

## IV. CONCLUSION

In conclusion, we have studied the topological quantum phase transition between Abelian and non-Abelian phases in the extended Kitaev spin model on a honeycomb lattice. From the ground-state energy, we show that this model displays a continuous quantum phase transition on the critical lines separating the Abelian and non-Abelian phases, where the third derivative of the ground-state energy is discontinu-
ous. Also, we use the von Neumann entropy as a measure of bipartite entanglement to study this topological quantum phase transition. Our results show that the bipartite entanglement is also nonanalytic on the same critical lines as the ground-state energy. Moreover, we show that the discontinuity of the second derivative of the bipartite entanglement is related to the discontinuity of the third derivative of the ground-state energy. Our approach directly reveals that both the entanglement and the ground-state energy can be used to characterize the topological quantum phase transition in this Kitaev model.

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## APPENDIX A

This appendix focuses on the analyticity of the first, second, and third directional derivatives of the ground-state energy on the critical line denoted by the thick solid line in Fig. 2. From Eq. (16), the derivative of the ground-state energy with respect to $\Lambda_{x}$ is

$$
\begin{align*}
\frac{\partial E}{\partial \Lambda_{x}} & =-\frac{\sqrt{3}}{16 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{\partial}{\partial \Lambda_{x}} \varepsilon(\mathbf{k}) \\
& =-\frac{\sqrt{3}}{16 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} \\
& =-\frac{\sqrt{3}}{16 \pi^{2}} \int_{D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})}-\frac{\sqrt{3}}{16 \pi^{2}} \int_{\mathrm{BZ}-D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} \tag{A1}
\end{align*}
$$

where

$$
\begin{equation*}
A=\Lambda_{x}+\Lambda_{y} \cos k_{x}-\cos \left(\frac{k_{x}+\sqrt{3} k_{y}}{2}\right) \tag{A2}
\end{equation*}
$$

and $D$ denotes two small regions in the first Brillouin zone, i.e., half of the disk with radius $\epsilon$, which is centered at ( $\pi$, $-\pi / \sqrt{3})$, and half of the disk with radius $\epsilon$, which is centered at $(-\pi, \pi / \sqrt{3})$, where $\epsilon \ll 1$. When $\Lambda_{x}-\Lambda_{y}=1, \varepsilon(\mathbf{k})$ becomes zero only at the points $(\mp \pi, \pm \pi / \sqrt{3})$, so $\int_{\mathrm{BZ} \text { - } D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})}$ is analytic because BZ-D is the region excluding $D$ in the first Brillouin zone. For the integral in the region $D$, we can approximate it as

$$
\begin{align*}
\int_{D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} & \int_{0}^{2 \pi} d \theta \int_{0}^{\epsilon} K d K \frac{\Delta+K^{2} S_{1}}{\sqrt{\Delta^{2}+K^{2} S_{2}}} \\
= & \int_{0}^{2 \pi} d \theta\left[\sqrt{\Delta^{2}+\epsilon^{2} S_{2}}-|\Delta|\right] \frac{\Delta}{S_{2}} \\
& +\int_{0}^{2 \pi} d \theta\left[\frac{1}{3}\left(\Delta^{2}+\epsilon^{2} S_{2}\right)^{3 / 2}-|\Delta|^{3}\right] \frac{S_{1}}{S_{2}^{2}} \\
& -\int_{0}^{2 \pi} d \theta \frac{S_{1} \Delta^{2} \sqrt{\Delta^{2}+\epsilon^{2} S_{2}}}{S_{2}^{2}}+\int_{0}^{2 \pi} d \theta|\Delta|^{3} \frac{S_{1}}{S_{2}^{2}} \tag{A3}
\end{align*}
$$

where

$$
\begin{gather*}
\Delta=\Lambda_{x}-\Lambda_{y}-1, \\
S_{1}=P_{1}+P_{2} \sin \left(2 \theta+\phi_{2}\right), \\
S_{2}=Q_{1}+Q_{2} \sin \left(2 \theta+\phi_{1}\right), \tag{A4}
\end{gather*}
$$

and

$$
\begin{gather*}
Q_{1}=\frac{\Lambda_{x} \Lambda_{y}+4 \Lambda^{2}+\Lambda_{x}-\Lambda_{y}}{2}, \\
Q_{2}=\frac{1}{4} \sqrt{\left(2 \Lambda_{x} \Lambda_{y}+8 \Lambda^{2}-\Lambda_{x}+\Lambda_{y}\right)^{2}+3\left(\Lambda_{x}+\Lambda_{y}\right)^{2}}, \\
P_{1}=\frac{\Lambda_{y}+1}{4} \\
P_{2}=\frac{1}{4} \sqrt{\Lambda_{y}^{2}-\Lambda_{y}+1} \\
\phi_{1}=\arctan \left(\frac{2 \Lambda_{x} \Lambda_{y}+8 \Lambda^{2}-\Lambda_{x}+\Lambda_{y}}{\sqrt{3}\left(\Lambda_{x}+\Lambda_{y}\right)}\right) \\
\phi_{2}=\arctan \left(\frac{2 \Lambda_{y}-1}{\sqrt{3}}\right) \tag{A5}
\end{gather*}
$$

From Eq. (A3), we have

$$
\begin{align*}
& \left.\int_{D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})}\right|_{1^{+}} \simeq \frac{\epsilon^{3}}{3} \int_{0}^{2 \pi} d \theta \frac{S_{1}}{S_{2}^{2}} \\
& \left.\int_{D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})}\right|_{1^{-}} \simeq \frac{\epsilon^{3}}{3} \int_{0}^{2 \pi} d \theta \frac{S_{1}}{S_{2}^{2}} \tag{A6}
\end{align*}
$$

where $1^{+}$denotes $\Lambda_{x}-\Lambda_{y} \rightarrow 1$ with $\Lambda_{x}-\Lambda_{y}>1$, and $1^{-}$denotes $\Lambda_{x}-\Lambda_{y} \rightarrow 1$ with $\Lambda_{x}-\Lambda_{y}<1$. When $\epsilon \rightarrow 0$, it follows from Eq. (A6) that $\int_{\mathrm{BZ}-D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} \rightarrow 0$ on the critical line $\Lambda_{x}$ $=1+\Lambda_{y}$ (i.e., the thick solid line in Fig. 2). Thus, from Eq. (A1), we have

$$
\begin{equation*}
\left.\frac{\partial E}{\partial \Lambda_{x}}\right|_{1^{+}}=\left.\frac{\partial E}{\partial \Lambda_{x}}\right|_{1^{-}} . \tag{A7}
\end{equation*}
$$

Similarly,

$$
\begin{equation*}
\left.\frac{\partial E}{\partial \Lambda_{y}}\right|_{1^{+}}=\left.\frac{\partial E}{\partial \Lambda_{y}}\right|_{1^{-}} . \tag{A8}
\end{equation*}
$$

From Eqs. (17), (A7), and (A8), it follows that

$$
\begin{equation*}
\left.\frac{\partial E}{\partial l}\right|_{1^{+}}=\left.\frac{\partial E}{\partial l}\right|_{1^{-}} . \tag{A9}
\end{equation*}
$$

Using the same procedure as above, we can obtain

$$
\begin{gather*}
\left.\frac{\partial^{2} E}{\partial l^{2}}\right|_{1^{+}}=\left.\frac{\partial^{2} E}{\partial l^{2}}\right|_{1^{-}}, \\
\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{+}}-\left.\frac{\partial^{3} E}{\partial l^{3}}\right|_{1^{-}} \simeq \frac{\sqrt{3} \Gamma}{4 \pi^{2}}(\cos \varphi-\sin \varphi)^{3}, \tag{A10}
\end{gather*}
$$

where

$$
\begin{equation*}
\Gamma \equiv \int_{0}^{2 \pi} d \theta \frac{1}{Q_{1}+Q_{2} \sin \left(2 \theta+\phi_{1}\right)} \tag{A11}
\end{equation*}
$$

## APPENDIX B

This appendix gives results regarding the analyticity of the correlation function $\mathcal{G}_{\alpha}(\alpha=x, y)$, and its first and second directional derivatives on the critical line denoted by the thick solid line in Fig. 2. Similar to Eq. (A1), one can divide the integral in Eq. (33) into two parts:

$$
\begin{align*}
\mathcal{G}_{x}= & -\frac{\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}} d^{2} k \frac{A}{\varepsilon(\mathbf{k})}=-\frac{\sqrt{3}}{8 \pi^{2}} \int_{D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} \\
& -\frac{\sqrt{3}}{8 \pi^{2}} \int_{\mathrm{BZ}-D} d^{2} k \frac{A}{\varepsilon(\mathbf{k})} \tag{B1}
\end{align*}
$$

where $A$ is given in Eq. (A2). Using the same procedure for Eqs. (A9) and (A10), we can derive from Eq. (B1) that

$$
\begin{equation*}
\left.\mathcal{G}_{x}\right|_{1^{+}}=\left.\mathcal{G}_{x}\right|_{1^{-}}, \tag{B2}
\end{equation*}
$$

and

$$
\begin{gather*}
\left.\frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{x}}\right|_{1^{+}}=\left.\frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{x}}\right|_{1^{-}}, \\
\left.\frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{y}}\right|_{1^{+}}=\left.\frac{\partial \mathcal{G}_{x}}{\partial \Lambda_{y}}\right|_{1^{-}}, \\
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x}^{2}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{y}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{x}}{\partial \Lambda_{y}^{2}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \tag{B3}
\end{gather*}
$$

where $\Gamma$ is given in Eq. (A11).

From Eq. (35), we can obtain

$$
\begin{gathered}
\left.\mathcal{G}_{y}\right|_{1^{+}}=\left.\mathcal{G}_{y}\right|_{1^{-}}, \\
\left.\frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{x}}\right|_{1^{+}}=\left.\frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{x}}\right|_{1^{-}}, \\
\left.\frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{y}}\right|_{1^{+}}=\left.\frac{\partial \mathcal{G}_{y}}{\partial \Lambda_{y}}\right|_{1^{-}}
\end{gathered}
$$

$$
\begin{gather*}
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x}^{2}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{x} \partial \Lambda_{y}}\right|_{1^{-}} \simeq \frac{\sqrt{3}}{2 \pi^{2}} \Gamma, \\
\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{y}^{2}}\right|_{1^{+}}-\left.\frac{\partial^{2} \mathcal{G}_{y}}{\partial \Lambda_{y}^{2}}\right|_{1^{-}} \simeq-\frac{\sqrt{3}}{2 \pi^{2}} \Gamma . \tag{B4}
\end{gather*}
$$

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