Detection of quantum phase boundary at finite temperatures in two dimensional Kitaev model

Protyush Nandi,1,* Sirshendu Bhattacharyya,2,† and Subinay Dasgupta1,‡

1Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India
2Department of Physics, Raja Ram Mohan Roy Mahavidyalaya, Radhanagar, Hooghly 712406, India

Quantum phase transitions occur when quantum fluctuation destroys order at zero temperature. With an increase in temperature, normally the thermal fluctuation wipes out any signs of this transition. For the two-dimensional Kitaev model, we have identified a physical quantity that shows algebraic divergence at a finite temperature, when an interaction parameter crosses the phase boundary for quantum phase transition. The quantity under consideration is the long time limit of the rate function related to a form of quantum fidelity under the quench of an interaction parameter. The robustness of the divergence makes the phase boundary detectable at any temperature. Our treatment is analytic and restricted to the vortex-free sector.

The dynamics of quantum many-body system at non-zero temperatures has always been an intriguing area of study, primarily because of the interplay between the quantum and the thermal fluctuations [1–3]. The dominance of thermal fluctuation with increasing temperature makes the perception of quantum noise limited to low temperatures only [4–7]. The question is, whether a quantum phase transition (QPT), exclusively driven by quantum fluctuations at zero temperature, has any impact on the behavior of the system at non-zero temperature and whether some physical quantity measured at finite temperature bears the signature of the QPT occurring at zero temperature [8]. Over the past decades, this issue has been addressed through the studies of quantum fidelity. At zero temperature, fidelity generally vanishes in the thermodynamic limit at a quantum critical point as on two sides of this point the ground state wave functions are structurally different (Anderson’s orthogonality catastrophe) [9–14]. At finite temperatures, generalized forms of fidelity have been studied in different systems [15–21], and some of them do detect the QPT through non-analytic signature in their logarithms at small but finite temperatures [15, 16]. However, in all these cases, any non-analytic signature at zero temperature is lost at finite temperature.

The objective of this paper is to look for a quantity that has a robust non-analytic behavior at zero as well as finite temperature while moving across the quantum phase boundary through the quench of a parameter. For this purpose, we consider the Kitaev model on a honeycomb lattice in the vortex-free sector, the ground state of which shows gapless phase and gapped phase separated by a phase transition line. The two phases are also topologically different [22–24]. At a temperature $T$, we perform a sudden quench of the Hamiltonian from $\mathcal{H}$ to $\mathcal{H}'$ at time $t = 0$ and define quantum fidelity as

$$F_t = \frac{\text{Tr} [\rho_t \cdot \rho_0]}{\text{Tr} [\rho_t] \text{Tr} [\rho_0]}$$

where $\rho_0$ is the density matrix at $t = 0$ and $\rho_t$ is the same after the system has evolved for time $t$ under the Hamiltonian $\mathcal{H}$. At zero temperature, this expression reduces to the usual expression for the probability, $|\langle \psi(0)|\psi(t) \rangle|^2$ (where $|\psi(t)\rangle$ is the normalized wave function at time $t$) called the Loschmidt echo and the logarithm of it shows singularities as a function of time, indicating a dynamical quantum phase transition [25]. However, at finite temperatures, there is no such singularity. Since logarithm of $F_t$ is proportional to the system size, we may define a measurable quantity called rate function as,

$$r(t, \beta) = \lim_{N \to \infty} \frac{1}{N} \log F_t$$

We shall prove analytically that the long time limit of this quantity shows a non-analytic behavior at the boundary between gapped and gapless phases at $T > 0$ just as at $T = 0$. The second derivative of the rate function (with respect to the post-quench value of the interaction parameter) diverges algebraically with an exponent of 1/2. According to our knowledge, we identify for the first time a quantity that shows algebraic non-analyticity at the phase boundary at zero and finite temperatures and thus it can serve as an order parameter of this phase transition at any temperature.

To proceed further, we define the Hamiltonian of the Kitaev spin-1/2 model on a honeycomb lattice,

$$\mathcal{H} = \sum_{i,j} J_{\alpha} s^\alpha_i s^\alpha_j$$

where $i, j$ run over all the nearest-neighbouring pairs on the honeycomb lattice, $\alpha$ is 1 or 2 or 3 depending on the location of the sites, as shown in Fig. 1, and $s^\alpha = \sigma^\alpha$, where $\sigma$ are the Pauli spin matrices. This model contains three interaction parameters $J_{\alpha}$. It can be shown that in the vortex-free sector, this Hamiltonian can be written as a sum of commuting Hamiltonians [22–24]

$$\mathcal{H} = \sum_{\vec{q}} \mathcal{H}_{\vec{q}}, \quad \mathcal{H}_{\vec{q}} = a_\vec{q} \sigma_3 + b_\vec{q} \sigma_1$$

where each component of $\vec{q} = (q_x, q_y)$ spans over $(-\pi, \pi)$.
The inverse temperature scaled by Boltzmann constant is \( \beta \) with \( G = \exp(\beta H) \). The decomposition of the Hamiltonian in the Eq (4) enables one to express the density matrix \( \rho = \exp(-\beta H)/\text{Tr}[\exp(-\beta H)] \) in terms of \( \exp(-\beta H_\theta) \) where \( \beta \) is the inverse temperature scaled by Boltzmann constant. To calculate the exponential of \( H_\theta \), we write,

\[
H_\theta = \lambda_\theta G_\theta
\]

with

\[
\lambda_\theta = \sqrt{\lambda_1^2 + \lambda_2^2}, \quad G_\theta = \cos \theta_\theta \sigma_3 + \sin \theta_\theta \sigma_1 \\
\cos \theta_\theta = a_\theta/\lambda_\theta, \quad \sin \theta_\theta = b_\theta/\lambda_\theta
\]

Exploiting the fact \( G_\theta^2 \) is unit matrix, we obtain the quantum fidelity of Eq. (1) and therefrom the rate function, as

\[
r(t, \beta) = -\log 2 + \frac{1}{4\pi^2} \int \! d\vec{q} A_\theta d\vec{q} \]

with

\[
A_\theta = \log \left[ 1 + \tanh^2 \beta \lambda_\theta \left\{ 1 - 2 \sin^2 \lambda_\theta \sin^2 (\theta_\theta - \theta_\theta') \right\} \right]
\]

where \( \lambda_\theta', \theta_\theta' \) refer to the post-quench Hamiltonian. As mentioned earlier, at zero temperature, the tanh term is 1, and \( A_\theta \) shows singularities as a function of time, but at finite temperature no such singularity occurs since the argument of the logarithm never vanishes. The quantity which turns out to be useful is the long-time average of the rate function, defined as

\[
\tilde{r}_a = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau r(t, \beta) \, dt
\]

Using standard results [28] we get

\[
r_a = -3 \log 2 + \frac{1}{4\pi^2} \int \! dq \log(1 + \alpha_\theta q) + \frac{1}{2\pi^2} \int \! dq \log \left[ 1 + \sqrt{1 - \gamma_\theta \sin^2 (\theta_\theta - \theta_\theta')} \right]
\]

where \( \alpha_\theta = \tanh^2 \beta \lambda_\theta, \gamma_\theta = 2 \alpha_\theta/(1 + \alpha_\theta) \).

A few subtle issues need to be discussed. (1) The angle \( \theta (\theta') \) is undefined where \( \lambda (\lambda') \) is zero in the \( \vec{q} \) plane, but this fact will not spoil the integration in Eq. (8) because we may exclude small regions \( R \) and \( R' \) around \( \lambda = 0 \) and \( \lambda' = 0 \) respectively, from the integral and evaluate it in the limit \( R \to 0, R' \to 0 \). (2) In Eq. (10), the quantity \( \lambda \tau' \to \infty \) as \( \tau \to \infty \) since the point \( \lambda' = 0 \) is excluded from the integration. (3) The long time limit of fidelity has also been studied in Ref. [29], but our procedure of calculating the long-time limit is different from theirs. They have first calculated the long-time limit of fidelity and then taken the logarithm to get the rate function while we have taken the long-time limit of the rate function itself, since the experimentally measurable quantity is the rate function [30] and not the fidelity \( F \). (4) When \( \rho_0 \) in Eq. (1) is replaced by the equilibrium density matrix for the post-quench Hamiltonian, namely, \( \rho_0(H') = \exp(-\beta H') \) one gets a measure of fidelity [31, 32] different from ours, since the Hamiltonian being integrable, the \( t \to \infty \) limit of \( \rho_t \) is not the same as \( \rho_0(H') \).

In this work, we shall study a particular type of quench where the interaction parameters \( J_1 \) and \( J_2 \) of the Kitaev Hamiltonian Eq. (3) is kept fixed at 1, so that the gapless phase exists for \( 0 \leq J_3 \leq 2 \) and the gapped phase, for \( J_3 > 2 \). We quench the parameter \( J_3 \) from \( J_0 \) to \( J \) and study how the rate function \( r_a \) depends on \( J \) when \( J \) approaches 2 from being within the gapless phase.

Thus, the first and second derivatives of the rate function is obtained as (omitting the suffix \( \vec{q} \))

\[
\frac{\partial r_a}{\partial J} = \frac{1}{4\pi^2} \int \! d\vec{q} \frac{\lambda_\theta}{\beta} BC
\]

\[
\frac{\partial^2 r_a}{\partial J^2} = \frac{1}{4\pi^2} \int \! d\vec{q} \frac{\lambda_\theta^2}{\beta^2} \left[ -(1 + \frac{1}{2D}) B^2 C^2 -2\alpha B \sin \theta' \sin(3\theta' - 2\theta) \right]
\]

with \( B = (2 - \gamma)/(D + D'), C = \alpha \sin \theta' \sin(2\theta' - 2\theta) \) and \( D = \sqrt{1 - \gamma \sin^2 (\theta' - \theta)} \).

Numerical integration shows that when \( J \) crosses the phase boundary, there appears a non-analyticity at any finite temperature - the rate function shows a kink, the first derivative remains continuous but undergoes a change of slope, while the second derivative shows power-law divergence with exponent 1/2. The expressions for the first and second derivatives contain \( 1/\lambda \) and \( 1/\lambda^2 \) respectively in the integrand. Indeed, whenever \( J \) lies within the gapless phase, the region of integration includes a point \( \vec{q} = \vec{q}_0 \) where \( \lambda \) vanishes. However, the
presence of this point leads to a non-analyticity only when $J$ is on the phase boundary [33].

We now set out to study analytically the behavior of the rate function as a function of the post-quench parameter $J$. Instead of using Eqs. (12, 13), we shall rather start with the expression of $r_a$ as in Eq. (11). Using the power series expansion of $\log (1 + \sqrt{1 - x})$ for any $x$ in the range $0 < x < 1$, we obtain

$$r_a = -\log 2 + \frac{1}{4\pi^2} \int dq \log (1 + \alpha)$$

$$- \frac{1}{8\pi^2} \sum_{n=1,2,\ldots} c_n \int dq \gamma^n \sin^{2n}(\theta - \theta')$$

with $c_1 = 1$, $c_2 = \frac{3}{8}$, $c_3 = \frac{5}{24}$ etc. We now express the integrand as

$$\gamma^n \sin^{2n}(\theta - \theta') = \left( \frac{\tanh \beta \lambda}{\lambda} \right)^{2n} \left( \frac{2(J-1)^2}{1 + \tanh^2 \beta \lambda} \right)^n \left( \frac{b'}{\lambda'} \right)^{2n}$$

and observe that any non-analytic behavior of this function may arise, if at all, only from a small region around the point where $\lambda' = 0$. The location of this point is given by $\vec{q} = (q_c, q_c)$ with $q_c = \cos^{-1}(J/2)$ for $J \leq 2$. Around this point $\lambda \approx 1$ and in the limit $J \to 2$ we obtain

$$\frac{\partial^2 r_a}{\partial J^2} = - \frac{1}{8\pi^2} \sum_{n=1,2,\ldots} c_n \left( \frac{2 \tanh^2 \beta}{1 + \tanh^2 \beta} \right)^n.$$  

$$\frac{\partial^2}{\partial J^2} \int dq \left( \frac{(J-1)b'}{\lambda'} \right)^{2n}$$

(16)

Indeed, this equality will not work for $r_a$, for $\partial r_a / \partial J$ and even for $\partial^2 r_a / \partial J^2$ away from the singular point. Numerical results also support this equality (Fig. 2). Hence, we only need to calculate the integral

$$I_n \equiv (J - 1)^{2n} \int_{q_x, q_y = -\pi}^{\pi} dq_x dq_y \left( \frac{b'}{\lambda'} \right)^{2n}, \ n = 1, 2, \ldots$$

(17)

Let us transform to the variables $u = (q_x + q_y)/2$, $v = (q_x - q_y)/2$ and get

$$I_n = 4(J - 1)^{2n} \int_{u=0}^{\pi/2} du \int_{v=-\pi}^{\pi} dv \left( \frac{b'}{\lambda'} \right)^{2n}$$

(18)

by using the invariance of the integral under $u \to \pi \pm u$, $v \to \pi \pm v$. Recall that $\theta$ and $\theta'$ are defined by Eq. (7), and the expressions for $a$ and $b$ are now $a = 1 - 2 \cos u \cos v$, $b = 2 \cos u \sin v = b'$, $a' = J - 2 \cos u \cos v$. The crucial step is to express the integrand as

$$\left( \frac{b'}{\lambda'} \right)^{2n} = \left( \frac{\mu}{4J} \right)^n, \frac{(z^2 - 1)^{2n}}{z^n (z - \frac{\mu}{J})^n (z - \frac{\mu}{J})^n}$$

with $z = \exp(iv)$ and $\mu = 2 \cos u$. This gives

$$I_n = -4i(J - 1)^{2n} \int_{u=0}^{\pi/2} du \oint F^{(n)}dz$$

(20)

where $\oint$ stands for integral over unit circle, and

$$F^{(n)}(z) = \frac{\mu^n}{z^{n+1}} \left( \frac{z^2 - 1}{z - \frac{\mu}{J}} \right)^n$$

For $u < q_c$, the poles inside the unit circle are $z_1 = 0$ and $z_2 = J/\mu$, while for $u > q_c$, the poles inside are $z_1 = 0$ and $z_3 = \mu/J$. Denoting the residue of $F^{(n)}$ at $z_i$ as $R_i^{(n)}$ for $i = 1, 2, 3$,

$$I_n = \frac{8\pi(J - 1)^{2n}}{(4J)^n} \sum_{i=1}^{3} \int_{0}^{\pi/2} R_i^{(n)} du$$

(21)

As we are interested only in the behavior of rate function when the post-quench parameter $J$ approaches the value 2 within the gapless phase, we introduce a parameter $\epsilon$ by

$$J = 2 - \epsilon^2, \ \epsilon = \sqrt{2 - J}$$
so that \( q_c = \cos^{-1}(1 - \epsilon^2/2) = \epsilon + \frac{1}{12}\epsilon^3 + \cdots \).

At high temperatures, only the first term in the summation in Eq. (14) is dominant and the residues can be easily calculated as

\[
R_1^{(1)} = \frac{J^2 + \mu^2}{J}, \quad R_2^{(1)} = \frac{J^2 - \mu^2}{J}, \quad R_3^{(1)} = \frac{\mu^2 - J^2}{J}
\]

(22)

This gives, up to leading order in \( \epsilon \),

\[
I_1 = \pi^2 - \pi^2 \epsilon^2 - \frac{8\pi^3}{3} \epsilon^3
\]

(23)

implying that \( \partial^2 I_1 / \partial J^2 = -2\pi / \sqrt{2-J} \). Let us express \( I_n \) also as a power series:

\[
I_n = a_0 + a_1 \epsilon + a_2 \epsilon^2 + a_3 \epsilon^3 + \cdots
\]

(24)

so that

\[
\frac{\partial^2 I_n}{\partial J^2} = -\frac{a_1}{4} \cdot \frac{1}{(2-J)^{3/2}} + \frac{3a_3}{4} \cdot \frac{1}{\sqrt{2-J}} + \cdots
\]

It is important to note that the divergence behavior is controlled by the coefficients \( a_1 \) and \( a_3 \) only. It can be shown that for any value of \( n \), \( a_1 = 0 \) and \( a_3 \neq 0 \), so that \( \partial^2 I_n / \partial J^2 \sim 1 / \sqrt{2-J} \) [33]. In view of Eq. (16), this completes the proof that at any temperature

\[
\frac{\partial^2 r_n}{\partial J^2} \sim \frac{1}{\sqrt{2-J}}
\]

(25)

To conclude, we explore the finite temperature behavior of the two-dimensional Kitaev model and observe power-law divergence of the second derivative of a form of mixed state fidelity across the gapped to gapless transition. A similar quantity has been previously observed to show logarithmic divergence in zero temperature [34]. In our case, the power-law divergence originates only from the second derivative of the integral in Eq. (17) which is independent of temperature. That is why thermal fluctuation can never suppress this divergence. Some related results may also be mentioned here without details. (i) If the pre-quench value of \( J_0 \) is chosen to be in the gapped phase, the divergence with respect to variation of \( J \) remains unchanged. (ii) No singularity in rate function is observed when it is studied as a function of \( J_0 \) (which is not surprising, since the right-hand side of Eq. (15) does not show any non-analytic behavior at \( \lambda = 0 \)). (iii) If we choose \( J_1 \neq J_2 \), then the divergence appears when \( J \) crosses the two phase boundaries located at \( |J_1 - J_2| \) and \( J_1 + J_2 \).

The fact that the quantity is insensitive to thermal fluctuations makes it a potential candidate to be studied experimentally. Moreover, such quantities having divergence at the quantum phase boundary at any temperature is very likely to be found in other models as well. Therefore, at any temperature, it can be treated as an order parameter of the quantum phase transition. However, as we have remained within the vortex-free sector of the Kitaev model, a question arises as to whether excitation of vortices at finite temperatures destroys the singularity in the rate function \( r_n \). This opens up a future direction of study especially when analytic treatment at finite temperatures is being performed recently [35]. It would also be interesting to explore how this rate function behaves for other integrable Hamiltonians in one- and two-dimensions. Work in this line is under progress. For now, we report that in the case of one-dimensional Ising model under the quench of the transverse field the singularity in fidelity (as defined by Eq. (1)) appears when the post-quench value of the field crosses the critical point. This indicates that the robustness of the singularity may persist in all dimensions. However the generic nature of the divergence is yet to be uncovered.

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* protyush18@gmail.com
† sirs.bh@gmail.com
‡ subinay.dasgupta@gmail.com

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Supplemental Material: Detection of quantum phase boundary at finite temperatures in two dimensional Kitaev model

WHY THE QUANTITY $r'' \equiv \partial^2 r/\partial J^2$ DIVERGES ONLY AT THE PHASE BOUNDARY?

The quench under consideration is from $(J_1, J_2, J_3) = (1, 1, J_0)$ to $(1, 1, J)$ and we have from Eq. (13)

$$r'' = \partial^2 r_a/\partial J^2 = \int_{q_x,q_y=-\pi}^{\pi} \mathcal{F} dq_x dq_y$$

with

$$\mathcal{F} = \frac{1}{4\pi^2 \lambda^2} \left[ -\left( 1 + \frac{1}{2D} \right) B^2 C^2 - 2\alpha B \sin \theta' \sin (3\theta' - 2\theta) \right]$$

(S1)

According to Eq. (7)

$$\lambda \cos \theta = 1 - \cos q_x - \cos q_y$$

$$\lambda \sin \theta = -\sin q_x + \sin q_y$$

$$\lambda' \cos \theta' = J - \cos q_x - \cos q_y$$

$$\lambda' \sin \theta' = -\sin q_x + \sin q_y$$

(S2)

We first observe that if $\vec{q}$ is replaced by $-\vec{q}$, the quantities $\theta, \theta'$ becomes $-\theta, -\theta'$. Also, such reversal of sign of $\theta, \theta'$ keeps $\mathcal{F}$ invariant. Thus, it is sufficient to integrate only over the region $-\pi < q_x \leq \pi, 0 \leq q_y < \pi$ (shaded region in Fig. S1a) and write

$$\partial^2 r/\partial J^2 = 2 \int_{q_x=-\pi}^{\pi} \int_{q_y=0}^{\pi} \mathcal{F} dq_x dq_y$$

(S3)

For any $J$ consider a circle of radius $R$ around the point where $\lambda' = 0$ (We shall call this point as node). The location of this node is given by $q_x = q_y = -1/(J/2)$. The quantity $\mathcal{F}$ diverges at the node and decreases as one moves away from it. When $J$ lies well inside the gapless region, the shaded integration region covers such circles for $R = 0$ to a fairly large value. However, when $J$ is close to the phase boundary, the shaded region cannot cover the whole circle unless the radius $R$ is too small (Fig. S1). It is seen numerically (but is difficult to verify analytically), that the values of $\mathcal{F}$ plotted over a full circle sums up to zero, although being asymmetric about zero. Hence after integration, $r''$ vanishes when $J$ is well-inside the gapless region. However, when $J$ is close to the phase boundary, the integration is over part of a circle and the cancellation of $\mathcal{F}$ values does not occur. Hence, $r''$ does not vanish. This effect is aggravated by the fact that $\mathcal{F}$ attains numerically larger values over a wider region when $J$ is close to the phase boundary, as can be easily seen from Fig. S1.

EVALUATION OF THE INTEGRAL $I_n$

To evaluate the integral $I_n$ as defined in Eq. (17), we look at Eq. (21) and observe that the residue at $z_2$ is

$$R_2^{(n)}(z) = \frac{1}{(n-1)!} \left[ \frac{\partial^{n-1}}{\partial z^{n-1}} \left( (z - z_2)^n F^{(n)} \right) \right]_{z = z_2}$$

(S4)

We define

$$G(z) = \frac{\mu(z^2 - 1)^2}{z(z - \frac{B}{2})}$$

so that

$$(z - z_2)^n F^{(n)} = \frac{G^n}{z}$$

and observe that

$$\frac{\partial^{n-1}(G^n/z)}{\partial z^{n-1}} = \frac{G}{z} \left( n \left( \frac{\partial G}{\partial z} \right)^{n-1} + \mathcal{T} \right)$$

(S5)

where $\mathcal{T}$ contains the other terms that will necessarily involve $G^k/z$ as a factor with $k \geq 1$. 
Obviously, \( (G/z)_{z=z_2} = R_2^{(1)} \). Also,

\[
(G)_{z=z_2} = -\frac{\epsilon^2}{2} + \frac{u^2}{2} + \frac{\epsilon^2 u^2}{4} - \frac{\epsilon^4}{8} - \frac{u^4}{8} + \text{(higher order terms)}
\]

and

\[
\frac{\partial G}{\partial z} \bigg|_{z=z_2} = 2J + \frac{\mu^2}{J}
\]

Hence, up to leading order terms in \( \epsilon \),

\[
R_2^{(n)} \approx \frac{1}{(n-1)!} n4^{n-1} R_2^{(1)}
\]

Using Eqs. (S6) and (S5) in Eq. (S4) and then performing the integration over \( u \) in Eq. (21) we can conclude that the second integral in Eq. (21) contributes an \( \epsilon^3 \) term but no term linear in \( \epsilon \). Similar conclusion will hold for the residue at \( z = z_3 \) too. This implies \( a_1 = 0 \) and \( a_3 \neq 0 \), which in turn shows from Eq.(16) that at any temperature

\[
\frac{\partial^2 r_\lambda(\beta)}{\partial J^2} \sim \frac{1}{\sqrt{2-J}}
\]