Phase transitions in the complex plane of physical parameters

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At low temperature, a thermodynamic system undergoes a phase transition when a physical parameter passes through a singularity point of the free energy. This corresponds to the formation of a new order. At high temperature, thermal fluctuations destroy the order. Correspondingly, the free energy is a smooth function of the physical parameter and singularities only occur at complex values of the parameter. Since a complex valued parameter is unphysical, no phase transitions are expected when the physical parameter is varied. Here we show that the quantum evolution of a system, initially in thermal equilibrium and driven by a designed interaction, is equivalent to the partition function of a complex parameter. Therefore, we can access the complex singularity points of thermodynamic functions and observe phase transitions even at high temperature. We further show that such phase transitions in the complex plane are related to topological properties of the renormalization group flows of the complex parameters. This result makes it possible to study thermodynamics in the complex plane of physical parameters.
High-temperature magnetic phase transitions. Spin systems can have ferromagnetic (FM) or antiferromagnetic (AFM) orders at low temperatures, corresponding to positive or negative coupling \( J \) between the spins, respectively. Thus an FM-AFM transition would occur if the coupling \( J \) varies from positive to negative. At high temperatures, thermal fluctuations destroy the magnetic order and hence no phase transition is expected with changing \( J \). Here we study the Ising spin model to demonstrate the FM-AFM transition in the complex plane of the parameter \( J \). The Hamiltonian for the general Ising model is

\[
H = - \sum_{ij} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i, \tag{2}
\]

where \( J_{ij} \) is the coupling between spins \( \sigma_i \) and \( \sigma_j \), \( h \) is the magnetic field, and the signs \( \sigma_i \) take values \( \pm 1 \). At low temperatures, when the coupling changes from positive to negative, the Ising model presents a phase transition from the FM order to the AFM order at zero field. Correspondingly, the Lee-Yang zeros in the complex plane of scaled magnetic field \( z = \exp(2 \pi i \beta J/|J|) \) exhibit different distributions. Note that the distinct features of Lee-Yang zeros distribution in the complex plane persist even at high temperatures \( (T > |J|) \).

To be specific, we study the one-dimensional (1D) Ising model with nearest-neighbor coupling \( J \), which can be exactly solved through the transfer matrix method\(^{10-12} \) (see Supplementary Information). There is no finite temperature phase transition in the 1D Ising model. The Lee-Yang zeros of the 1D Ising model of \( N \) spins have been exactly calculated\(^5 \). We plot the distribution of Lee-Yang zeros in Fig. 2a. For AFM coupling \((J > 0)\), all the zeros lie on the negative real axis (indicated by the red surface) (Fig. 2a). While for the FM coupling \((J < 0)\), the zeros are distributed on an arc of the unit circle (indicated by the blue surface) (Fig. 2a). At the transition point \((J = 0)\), all the Lee-Yang zeros are degenerate at \( z_n = -1 \) (indicated by the green solid ball).

To observe the Lee-Yang zeros and the critical behaviors in the complex plane\(^6 \), we study the time-domain measurement in equation (1) by choosing \( H_t = \sum_i \sigma_i \) and analytically continuing the magnetic field to the complex plane \( h \to h + it/\beta \). In this case, the time-domain measurement corresponds to decoherence of a quantum probe spin coupled to the Ising model\(^7 \) (see physical realizations). Figs. 2b–e plot the time-domain measurement calculated for different coupling parameters \( J \) at fixed inverse temperature \( \beta = 1 \) (which is a high temperature case for the 1D Ising model, since the critical temperature of this model is zero). For AFM coupling \( J = -1 \), the time-domain measurement has no zeros (Fig. 2b) and it is a smooth function of time. On the contrary, for the FM coupling \( J = 1 \), the time-domain measurement shows a number of zeros (Fig. 2c), which have a one-to-one correspondence to the Lee-Yang zeros\(^5 \). Approaching the thermodynamic limit, the Yang-Lee edge singularities (the starting and ending Lee-Yang zeros along the arcs)\(^6 \) lead to critical times in the time-domain observation\(^7 \). To demonstrate this, we perform a finite size scaling analysis on the time-domain measurement and show the scaled results \( \langle L(t) \rangle \) in Figs. 2d & 2e. The profiles of the time-domain measurement in the FM and AFM regions are qualitatively different. For AFM coupling, the scaled measurement is a smooth function of time (Fig. 2d). While for FM coupling, the scaled measurement presents sudden changes at critical times corresponding to the Yang-Lee edge singularities (Fig. 2e). The profiles of the time-domain measurement in the FM and AFM regions cannot be smoothly transformed into each other, which is the signature of the onset of a high-temperature phase transition.

We further study the high-temperature AFM-FM phase transition in the time-domain measurement for a two-dimensional (2D) Ising model. Specifically, we consider a 2D Ising model in a square lattice with nearest neighbor coupling \( J \). This model under zero field is exactly solvable\(^13-15 \) and has a finite-temperature phase transition at \( \beta_c = 0.44/|J| \). Fig. 3 shows the time-domain measurement in the 2D...
cosh 2

cosh 4

The partition function has no Lee-Yang zeros on the unit circle (|z| = |exp(2βh)| = 1)\(^2\) and therefore the time-domain measurement has no zeros (Fig. 3a). While for the FM coupling, the time-domain measurement presents a number of zeros (equal to the number of spins) corresponding to the Yang-Lee edge singularities for the FM coupling (Fig. 3d). Thus a phase transition with varying the coupling constant \(J\) occurs at a temperature higher than the critical temperature (\(β < 0.44/|J|\)).

Renormalization group theoretic analysis. The renormalization group (RG) method, a powerful tool for studying conventional phase transitions, can be applied to the phase transitions in the complex plane of physical parameters. Since the phase of any complex number is defined modulo \(2\pi\), the RG flows of complex parameters can present novel topological structures.

As an example we first consider the 1D Ising model and define the dimensionless parameters \(K_0 = \beta J\) and \(h_0 = i Jh\). The renormalization of the model can be exactly formulated by blocking two neighboring spins into one (Fig. 4a)\(^1\). By continuation of the dimensionless external field to a purely imaginary value \(h_0 = iτ_0/2\) (the physical external field is zero), the exact RG flow equations become\(^1\)

\[
\begin{align*}
\tau_1(τ_0,K_0) &= τ_0 - iν_0 \ln \left( \frac{\cosh(2K_0 + iτ_0/2)}{\cosh(2K_0 - iτ_0/2)} \right) \\
K_1(τ_0,K_0) &= \frac{1}{4} \ln \left( \frac{\cosh(4K_0) + \cos τ_0}{1 + \cos τ_0} \right)
\end{align*}
\]

where the coupling \(K_1\) remains real after renormalization. Since \(τ\) is defined modulo \(2\pi\), the parameter space can be identified with the surface of an infinitely long cylinder with unit radius. The original system corresponds to the parameter curve \(K = K_0\) and \(-π < τ_0 < π\), and therefore the winding number \(W_1\) defined to be the number of times the parameter curve wraps around the cylinder, is 1 (Fig. 4b).

The parameter curve is renormalized according to the RG flow equations. Since \(K_1(τ_0,K_0) = K_1(τ_0,K_0,−K_0)\) in Eq. (3), the distinct behaviors of the FM and AFM Ising chains are encoded entirely in different RG flows of \(τ\). This is illustrated in Figs. 4c–h. Figs. 4c, 4e & 4g show that after successive renormalization, the winding number in the FM case \((K_0 = 1/8)\) becomes 2, 4, 8, ... On the contrary, the winding number in the AFM case \((K_0 = −1/8)\) is zero after renormalization (Figs. 4d, 4f & 4h). The RG flow becomes trivial at the phase transition point \(K_0 = 0\), which corresponds to the infinite temperature limit, and the winding number remains unchanged \((W_1 = 1)\) after the renormalization. In summary, the winding numbers for different couplings after \(k\) steps of renormalization are

\[
W_{\#} → W_{\#}^{(k)} = \begin{cases} 
0 & \text{for} \ K_0 < 0 \\
1 & \text{for} \ K_0 = 0 \\
2^k & \text{for} \ K_0 > 0
\end{cases}
\]

The different topologies of the RG flows demonstrate unambiguously the high-temperature phase transition with varying the coupling parameter.

We further consider the RG flows of the 2D Ising model in a square lattice. By continuation of the external field to a purely imaginary value of \(h = it/2\), the approximate RG flow equations read\(^1\) (See Supplementary Information for derivation)
Figure 4 | Renormalized parameters of the 1D Ising model with a purely imaginary field. (a), Real-space renormalization scheme. In each renormalization step the spins on every other site are traced out, which effectively combines pairs of neighboring spins into block spins with renormalized coupling and external field. (b), The un-renormalized parameters. The spin coupling \( K \) and evolution time \( \tau \) (i.e., imaginary part of the external field) form a space identical to the surface of an infinitely long cylinder. When the imaginary field \( \tau \) is varied at a fixed value of \( K = K_0 \), the curve winds about the cylinder once and so the winding number \( W_\theta = 1 \). (c–h), Under RG flow, the original curve depicted in (a) would transform differently in the different parameter regimes of \( K_0 \). Figs. 5a, c & e present the renormalized parameters under one, two and three applications of the renormalization transformation for the FM case \((K_0 = 1/8)\). Figs. 5b, d & f present the results for the AFM case \((K_0 = -1/8)\). The vertical dashed lines indicate \( \tau = 0 \mod (2\pi) \), which are identified as the same line when represented on an infinitely long cylinder. The winding numbers can be directly inferred from the number of times the renormalized curve crosses this line.

\[
\begin{align*}
\tau_1(t_0, K_0) &\approx t_0 - \frac{i}{2} \ln \left( \frac{\cosh (4K_0 + i t_0 / 2) \cosh^2(2K_0 + i t_0 / 2)}{\cosh (4K_0 - i t_0 / 2) \cosh^2(2K_0 - i t_0 / 2)} \right), \\
K_1(t_0, K_0) &\approx \frac{3}{16} \ln \left( \frac{\cosh (8K_0) + \cos (t_0)}{1 + \cos (t_0)} \right).
\end{align*}
\]

Fig. 5 presents the RG flows of the parameters in the FM and AFM cases. Figs. 5a, c & e present the renormalized parameters under one, two and three applications of the renormalization transformation for the FM case \((K_0 = 1/8)\). Figs. 5b, d & f present the results for the AFM case \((K_0 = -1/8)\). The winding numbers of the different cases after \( k \) steps of renormalization are

\[
W_\theta = \begin{cases} 
(5/2)^k & \text{for } K_0 > 0, \\
1 & \text{for } K_0 = 0, \\
(5/2)^{k-1}/2 & \text{for } K_0 < 0
\end{cases}
\]

where \([x]\) is the integer part of \( x \). The winding number of the parameters under RG reflects the different topologies intrinsic to the RG flow equations in the different parameter regimes.

Transverse-field Ising model. The models considered above are all classical models in which different components of the Hamiltonian commute. A natural question arises about whether the high-temperature phase transitions with complex parameters would exist also for quantum models. To address this question, we study the 1D transverse-field Ising model. The model contains \( N \) spin-1/2 with nearest neighbor interaction \((\lambda_j)\) along the \( x \)-axis and under a transverse field \((\lambda_2)\) along the \( z \)-axis, described by the Hamiltonian

\[
H = \lambda_1 H_1 + \lambda_2 H_2 = \lambda_1 \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x + \lambda_2 \sum_{j=1}^{N} \sigma_j^z,
\]

where \( \sigma_j^{x/z} \) is the Pauli matrix of the \( j \)-th spin along the \( x/y/z \)-axis. This model is exactly solvable\(^{16}\). It has a quantum phase transition between a magnetic ordered phase for \( |\lambda_1| > |\lambda_2| \) and a disordered phase for \( |\lambda_1| < |\lambda_2| \) at zero temperature, but has no finite-temperature phase transition for any parameters on the real axis. By defining the dimensionless magnetic field \( \tilde{h} = \lambda_2/\lambda_1 \), the Lee-Yang zeros are determined by \( \text{Re}(h)^2 + \text{Im}(h)^2 = 1 + [(n + 1/2)\pi/|\beta|]^2 \), \( \text{Re}(h) \approx 1 \). Therefore, the zeros are located on circles and have cutoff at singularity edges \( \text{Re}(h) = \pm 1, \text{Im}(h) = \pm [(n + 1/2)\pi/|\beta|] \) (see Fig. 6a). When the temperature approaches zero \((|\beta| \to \infty)\), the Lee-Yang zeros are on the unit circle. When the temperature is high \((|\beta| \ll 1)\), the radii of the circles are \( \sqrt{1 + [(n + 1/2)\pi/|\beta|]^2} \gg 1 \). Therefore, the zeros are distributed, approximately, along horizontal lines with interval \( |\pi/|\beta|\). The fact that the Lee-Yang zeros exist only in the parameter range of \( |h| \leq 1 \) indicates that the time-domain measurement of the system would present phase
transitions between the two parameter regions, $|\lambda_2| > |\lambda_1|$ and $|\lambda_2| < |\lambda_1|$. Specifically, the time-dependent measurement can be devised as $L(t) = Z^{-i\beta} \text{Tr} \left( \exp(-\beta H \cos \omega t) \right)$, which is the partition function with a complex external field (AFM case). The contour plot of the time-domain measurement as a function of external field and time are presented in Fig. 6b. To demonstrate the phase transitions more clearly, we plot in Fig. 6c the time-domain measurement as a function of external field for different times. Since the zeros are bounded in the range $|h| \leq 1$ with Yang-Lee edge singularities at $\text{Re}(h) = \pm 1$, $\text{Im}(h) = \pm (n + 1/2)\pi/\beta$, the time-dependent measurement has a sharp change when we tune the parameter from $|h| \leq 1$ to $|h| > 1$ at times $\text{Im}(h) = \pm (n + 1/2)\pi/\beta$ (see Fig. 6c).

**Physical realization.** The time-domain measurement in equation (1) resembles the Loschmidt echo\(^{10,15}\), or equivalently, decoherence of a central spin coupled to the system. Thus we may implement the time-domain measurement by coupling the system to a central spin through the probe-system interaction $\{1\} \langle 1 | \otimes H(t) + |1\} \langle 1 | \otimes H(t)$ ($S_z = |1\} \langle 1 | - |\bar{1}\} \langle \bar{1} |$) and measuring the central spin coherence. Essentially, the coherence of the probe spin is a complex phase factor associated with a real Boltzmann probability for each state of the system. Therefore the probe spin coherence measurement amounts to continuation of a physical parameter to the complex plane. If we initialize the central spin in a superposition state $|1\} + |\bar{1}\}$ and the system in a thermal equilibrium state described by the canonical density matrix, $\rho = Z^{-i\beta} \text{Tr} \left( \exp(-\beta H) \right)$, the probe spin coherence is

$$\langle S_x \rangle = \langle S_y \rangle = \text{Tr} \left[ e^{-\beta H} \epsilon^{\bar{1}} \epsilon^{1} e^{-i[H(t)]} / \text{Tr} \left[ e^{-\beta H} \right] \right].$$ (8)

If $[H_1 H] = 0$, the time-domain measurement $L(t) = Z^{-i\beta} \text{Tr} \left( \exp(-\beta H) \epsilon^{1} e^{-i[H(t)]} \right)$, which is equal to the probe spin coherence with a probe-bath coupling $H_{gb} = S_z \otimes H_1$, i.e., $H_1 = - H_1 = H/2$. Or if $[H_1 H] \neq 0$ but $[H_1 H, H] = [H_1 H, H_1] = 0$, the time-domain measurement can also be factored as $L(t) = Z^{-i\beta} \text{Tr} \left( \exp(-\beta H) \epsilon^{1} e^{-i[H(t)]} \right)$ (See Supplementary Information for details) and can be implemented by the probe spin coherence with
a modified probe-bath coupling $H_I = H_I/2 - H$ & $H_I = -H/2 - H$. If $[H, H_I] = is H_I$, the time-domain measurement can be written as $L(t) = -Z^{-\frac{1}{2}}[\exp(-it H_I/2)\exp(-\beta H)\exp(-\beta H_I/2)]$ (See Supplementary Information for details), which can be implemented by probe spin decoherence with a probe-bath coupling $H_I = \sin(\theta)H_I/2s - H$ & $H_I = -\sin(\theta)H_I/2s - H$. In the general case, the time-domain measurement in equation (1) can be written as $L(t) = Z^{-\frac{1}{2}}[\exp(-it H_I/2)\exp(-\beta H)\exp(-\beta H_I/2)]$, with $e^{-\beta H} = \exp(-\beta H_I)/\exp(-\beta H-IH_I/2)$ & $T \exp(-\beta H_I/2) = T \exp(-it H_I/2)\exp(-\beta H)\exp(-\beta H_I/2)$, where $T$ & $t$ are the time-ordering and anti-ordering operators. If one initializes the bath in a canonical state $\rho = \exp(-\beta H')\exp(-\beta H-IH_I/2)$, the time-domain measurement can be implemented by probe spin decoherence with probe-bath coupling $H_I = H_I/2 - H$ & $H_I = -H/2 - H$, up to a normalization factor (see Supplementary Information for details). The physical realization of the modified Hamiltonians $H'$ & $H_I'$ is non-trivial.

Note that the time-domain measurement in equation (1) is similar to the measurement of the characteristic function of the work distribution in a quantum quench19-21, which plays a central role in the fluctuation relations in non-equilibrium thermodynamics22-26. The probe spin decoherence realization of the time-domain measurement can also be related to the quench dynamics where the evolution of the system can be controlled under different Hamiltonians for different periods of time27.

Summary. We have shown that the quantum evolution of a system originally in thermodynamic equilibrium is equivalent to the partition function of the system with a complex parameter. By choosing different forms of coupling we have a systematic way to realize the continuation of an arbitrary physical parameter to the complex plane. The time-domain measurement allows us to study a variety of zeros of the partition function. More importantly, we can access the singularity points of thermodynamic functions in the complex plane of physical parameters and therefore observe phase transitions at high temperatures. The physical realization of the time-domain measurement may be nontrivial but in principle it can be implemented by probe spin decoherence or quantum quench experiments. This discovery makes it possible to study thermodynamics in the complex plane of physical parameters.

Methods

The 1D Ising spin model was exactly diagonalized by the transfer matrix method28-31. The evaluation of the partition function after the transformation becomes a trivial problem of diagonalization of a $2 \times 2$ matrix. The probe spin coherence (which has been formulated in terms of partition functions*) was similarly calculated. Similarly, by applying the transfer matrix method, the 2D Ising model with magnetic field was mapped to a 1D Ising model with a transverse field28-31. For a 2D Ising model in a finite magnetic field, it was mapped by the transfer matrix method to a 1D Ising model with both longitudinal field and transverse field28-31, which was then numerically diagonalized. Therefore, the partition function and hence the probe spin coherence for the 2D Ising model in finite magnetic field were obtained. We derived the exact RG equations of the 1D Ising model and approximate RG equations for the 2D Ising model in square lattice for real parameters32-36. By analytic continuation we obtained the RG equations in the complex plane of the physical parameters and analyzed the RG flows of the complex parameters. The 1D Ising model with a transverse magnetic field was exactly solved37 and the partition function and time-domain measurement were then calculated.

Full methods are included in the Supplementary Information.

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Author contributions

R.B.W. conceived the idea, designed project, formulated the theory, and supervised the project. B.B.W. studied magnetic phase transitions in the Ising models and calculated the RG flows of the 2D Ising model. H.C.P. discovered the topological features of the RG flows of the 1D model. S.W. studied the transverse-field Ising model. B.B.W. & R.B.L. wrote the manuscript. All authors discussed the results and the manuscript.

Additional information

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