

Yang-Lee Zeros, Semicircle Theorem, and Nonunitary Criticality in Bardeen-Cooper-Schrieffer Superconductivity

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Yang and Lee investigated phase transitions in terms of zeros of partition functions, namely, Yang-Lee zeros [*Phys. Rev.* **87**, 404 (1952); *Phys. Rev.* **87**, 410 (1952)]. We show that the essential singularity in the superconducting gap is directly related to the number of roots of the partition function of a BCS superconductor. Those zeros are found to be distributed on a semicircle in the complex plane of the interaction strength due to the Fermi-surface instability. A renormalization-group analysis shows that the semicircle theorem holds for a generic quantum many-body system with a marginal coupling, in sharp contrast with the Lee-Yang circle theorem for the Ising spin system. This indicates that the geometry of Yang-Lee zeros is directly connected to the Fermi-surface instability. Furthermore, we unveil the nonunitary criticality in BCS superconductivity that emerges at each individual Yang-Lee zero due to exceptional points and presents a universality class distinct from that of the conventional Yang-Lee edge singularity.

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Introduction.—Yang and Lee developed a general approach to understanding phase transitions in terms of zeros, known as Yang-Lee zeros, of the partition function [1,2]. They investigated the distribution of zeros of the partition function of a classical Ising model for an imaginary magnetic field to understand the mathematical origin of nonanalyticity of the ferromagnetic phase transition. The thermal phase transition between the paramagnetic and ferromagnetic phases occurs when the distribution of zeros touches the real axis in the thermodynamic limit. Yang-Lee zeros are also closely related to singularities in thermodynamic quantities accompanied by anomalous scaling [3–8]. This type of singularities in critical phenomena is collectively referred to as the Yang-Lee singularity [9].

The distribution of Yang-Lee zeros governs the critical phenomena in phase transitions [3,10] and is of fundamental importance in statistical physics. The universality of the distribution is encapsulated by the Lee-Yang circle theorem [1,2], which states that the Yang-Lee zeros of the ferromagnetic Ising model are distributed on a unit circle in the complex plane of the fugacity [11–14]. While the Yang-Lee theory has been applied to a wide range of phase transitions in classical [15–18] and quantum [19–28] systems, its application to itinerant electronic systems is limited [20,21]. Itinerant electrons show various types of order arising from Fermi-surface instabilities, including the Bardeen-Cooper-Schrieffer (BCS) superconductivity [29]

as a prime example. Thus, the study of Yang-Lee zeros in the BCS theory is expected to unveil hitherto unnoticed universality in superconductivity.

In this Letter, we develop the Yang-Lee theory of BCS superconductivity to elucidate the nonperturbative nature of the superconducting phase transition in terms of the distribution of zeros of the partition function. We show that the number of roots of the partition function is directly related to the superconducting gap induced by the Fermi-surface instability. In particular, we demonstrate that the Yang-Lee zeros of the partition function are distributed on a semicircle in the complex plane of the interaction strength, where the superconducting phase transition occurs at the edge of the distribution. A previous study [20] on Fisher zeros in pairing fields focuses on a finite-temperature phase transition by making the temperature complex. In contrast, we focus on the zero-temperature quantum phase transition by making the interaction strength complex.

Furthermore, we employ a renormalization group (RG) to investigate the universality of the distribution of Yang-Lee zeros for a generic quantum many-body system with a marginal coupling. In particular, we show the semicircle theorem: Yang-Lee zeros in a quantum many-body system with a marginally relevant coupling are distributed on a semicircle in the complex interaction plane, in contrast to a full circle of the original Lee-Yang circle theorem [1,2]. This general theorem demonstrates that the geometric

shape of the distribution of Yang-Lee zeros is directly connected to the existence of the Fermi-surface instability.

Last, we investigate the nonunitary criticality in BCS superconductivity which originates from the Yang-Lee singularity. By determining the critical exponents, we show that the nonunitary singularity belongs to a universality class distinct from that of the Hermitian superconducting phase transition. The unconventional quantum critical phenomena are caused by exceptional points where a nonanalytic excitation spectrum emerges near the Fermi surface [30].

Yang-Lee singularity in superconductivity.—We consider a three-dimensional BCS model [30,31]

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \frac{U}{N} \sum_{k,k'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}, \quad (1)$$

where $\xi_k = \epsilon_k - \mu$ is the single-particle energy measured from the chemical potential μ , $\sigma = \uparrow, \downarrow$ is the spin index, and $U = U_R + iU_I$ is the complex-valued interaction strength. The creation and annihilation operators of an electron with momentum k and spin σ are denoted as $c_{k\sigma}^\dagger$ and $c_{k\sigma}$, respectively. The prime in $\sum_{k'}$ indicates that the sum over k' is restricted to $|\xi_{k'}| < \omega_D$, where ω_D is the energy cutoff and N is the number of momenta within this cutoff. Note that the non-Hermitian Hamiltonian (1) is used to investigate Yang-Lee zeros of closed systems as opposed to open systems in Ref. [30].

A non-Hermitian generalization of the BCS theory is made in Ref. [30], where the mean-field BCS Hamiltonian is given by $H_{\text{MF}} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k [\bar{\Delta}_0 c_{-k\downarrow} c_{k\uparrow} + \Delta_0 c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger] + (N/U)\bar{\Delta}_0\Delta_0$, with the superconducting gaps $\Delta_0 = -(U/N)\sum_{kL}\langle c_{-k\downarrow} c_{k\uparrow} \rangle_R$ and $\bar{\Delta}_0 = -(U/N)\sum_{kL}\langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle_R$. Here, ${}_L\langle A \rangle_R := {}_L\langle \text{BCS}|A|\text{BCS} \rangle_R$, where $|\text{BCS} \rangle_R$ and $|\text{BCS} \rangle_L$ are the right and left ground states of the Hamiltonian H_{MF} given by [30]

$$|\text{BCS} \rangle_R = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle, \quad (2)$$

$$|\text{BCS} \rangle_L = \prod_k (u_k^* + \bar{v}_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle, \quad (3)$$

where $|0\rangle$ is the vacuum state for electrons, and u_k, v_k , and \bar{v}_k are complex coefficients subject to the normalization condition $u_k^2 + v_k \bar{v}_k = 1$. These coefficients can be determined in a standard manner and given in Supplemental Material [32]. Since the right and left ground states are not the same, $\Delta_0 \neq \bar{\Delta}_0^*$ and $\bar{v}_k \neq v_k^*$ in general. Here, we take a gauge such that $\bar{\Delta}_0 = \Delta_0$. The Bogoliubov energy spectrum E_k is given by [30] $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$, where $\Delta_k = \Delta_0 \theta(\omega_D - |\xi_k|)$ with $\theta(x)$ being the Heaviside unit-step function. It is worthwhile to note that Δ_0 is

complex in general, so is the energy E_k . In the following, we assume that the density of states ρ_0 in the energy shell is a constant. The gap Δ_0 is then given by

$$\Delta_0 = \frac{\omega_D}{\sinh\left(\frac{1}{\rho_0 U}\right)}, \quad (4)$$

which exhibits an essential singularity at $U = 0$.

The partition function is given by

$$Z = \prod_{k,\sigma} Z_k = \prod_{k,\sigma} (1 + e^{-\beta E_k}), \quad (5)$$

whose absolute value is shown in Fig. 1. Here, β is the inverse temperature. The Yang-Lee zeros of our system are defined by zeros of the partition function in Eq. (5) where $\text{Re}(E_k) = 0$ and $\text{Im}(\beta E_k) = (2n+1)\pi$, $n \in \mathbb{Z}$. This condition is satisfied in the thermodynamic limit if $\text{Re}\Delta_0 = 0$, which agrees with the condition of phase transitions. It follows from this condition that the positions of Yang-Lee zeros satisfy

$$(\rho_0 \pi U_R)^2 + (\rho_0 \pi U_I - 1)^2 = 1, \quad U_R > 0. \quad (6)$$

Note that these points coincide with the exceptional points where H_{MF} is not diagonalizable [30]. The Yang-Lee zeros are distributed on a semicircle in the complex plane of the interaction strength U depicted as the boundary of the gray region in Fig. 1. In the yellow region in Fig. 1, the energy spectrum E_k is gapped and $|Z| \rightarrow 1$ in the zero-temperature limit since $e^{-\beta E_k} \rightarrow 0$ for all momenta k . Note that the distribution of the Yang-Lee zeros touches the real axis at the origin, which is consistent with the fact that the superconducting phase transition occurs at the origin.

The essential singularity at the superconducting phase transition is directly linked to the number of roots χ of the

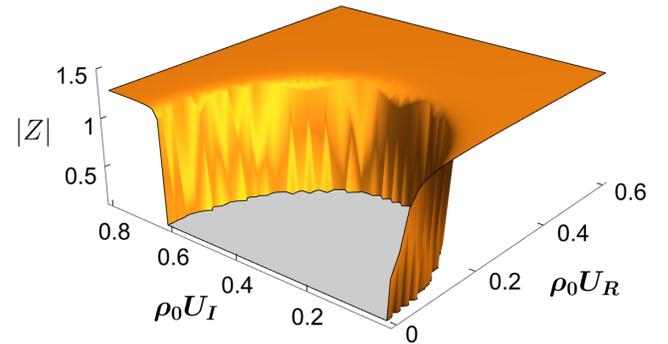


FIG. 1. Absolute value of the partition function Z of the three-dimensional BCS model as a function of the real and imaginary parts of the interaction strength $U = U_R + iU_I$ in the zero-temperature limit. The boundary along which the partition function vanishes is given by Eq. (6). In the gray region inside the phase boundary, the value of the partition function is not shown due to the breakdown of the mean-field approximation [30].

partition function. According to Eq. (5), each factor in the partition function contributes to one root if and only if $\text{Re}(E_k) = 0$ and $\text{Im}(\beta E_k) = (2n + 1)\pi$ for some $n \in \mathbb{Z}$. Therefore, the number of roots of the partition function in the complex energy space is given by the number of integer n satisfying $\text{Im}(\beta E_k) = (2n + 1)\pi$ for $\text{Im}(\beta E_k) \in [0, \beta \text{Im}(\Delta_0)]$ [see Eqs. (12)–(15) in Supplemental Material [32]]. From Eq. (4), we have

$$\chi \simeq \frac{\beta \text{Im}(\Delta_0)}{\pi} = \frac{\beta \omega_D}{\pi \cosh\left(\frac{U_R}{\rho_0 |U|^2}\right)} \quad (7)$$

in the zero-temperature limit, where the spin-degeneracy factor of two is included. Near $U = 0$, the gap takes the form of $\Delta_0 = 2\omega_D \exp[-(1/\rho_0)U]$. Since the phase boundary is tangent to the real axis where $U_I \ll U_R$, we may put $U_I = 0$ in Eq. (7) near the origin, obtaining

$$\chi \simeq \frac{\beta}{\pi} \Delta_0|_{U_I=0}. \quad (8)$$

Equation (8) relates the number of roots χ of the partition function to the superconducting gap Δ_0 on the real axis. The condensation energy $\Delta E = F(\Delta_0) - F(0)$ [33], where F is the free energy, can be obtained from the number of roots χ as [32]

$$\Delta E \simeq -\frac{\pi^2 N \rho_0}{2} \left(\frac{\chi}{\beta}\right)^2 \propto \chi^2. \quad (9)$$

For a general phase transition with spontaneous symmetry breaking and order parameter Δ_0 with the dimension of energy, we have $\Delta E \propto \chi^2$ [34]. The condensation energy is thus directly related to the number of roots χ .

Semicircle theorem.—Here, we show that the semicircular distribution (6) of the Yang-Lee zeros is generic and universal in quantum many-body systems. We consider a general canonical RG equation for a marginal complex interaction:

$$\frac{dV}{dt} = aV^2 + bV^3, \quad (10)$$

where $V = V_R + iV_I \in \mathbb{C}$ is a dimensionless coupling strength which can be taken as $V = \rho_0 U$ in the present case, and $dt = -(d\Xi/\Xi)$ is the relative width of the high-energy shell which is to be integrated out in the Wilsonian RG with Ξ being the energy cutoff. There are two finite fixed points in Eq. (10). One is $V = 0$, which is trivial, and the other is $V = -(a/b)$, which is nontrivial. According to the stability of the nontrivial fixed point, we can classify the RG-flow diagrams into two types depending on the sign of b . The case with $b > 0$ corresponds to an unstable nontrivial fixed point in the Hermitian case and does not exhibit critical phenomena. The other case with $b < 0$ corresponds

to a stable nontrivial fixed point in the Hermitian case and is the only one that includes the critical line. The BCS model belongs to this case. The RG-flow diagrams for these cases are shown in Supplemental Material [32]. By applying the Wilsonian RG analysis of the fermionic field theory [35], the RG equation of the BCS model up to the two-loop order including the self-energy correction is written as [32]

$$\frac{dV}{dt} = V^2 - \frac{1}{2}V^3. \quad (11)$$

From Eq. (11), we find $a = 1$ and $b = -1/2$ in the canonical RG equation (10). A similar RG equation has been obtained for the non-Hermitian Kondo model [36]. Note that the sign of the parameter a does not influence the physics of RG flows since we can reverse its sign by the replacement $V \rightarrow -V$. For a system with $b < 0$, there exists a critical line which separates the trivial and nontrivial fixed points. Every point on the critical line flows toward an infinite fixed point $(V_R, V_I) = (-a/(3b), \infty)$. After integrating Eq. (10) and taking the imaginary part, we obtain the critical line as

$$\frac{b\pi}{|a|} + \frac{V_I}{V_R^2 + V_I^2} = \frac{b}{a} \arctan \frac{V_I}{V_R} + \frac{b}{a} \arctan \left(-\frac{bV_I}{a + bV_R} \right). \quad (12)$$

Near the origin, Eq. (12) can be expanded as

$$\frac{V_I}{V_R^2 + V_I^2} + \frac{b\pi}{|a|} = 0. \quad (13)$$

The critical line specified by Eqs. (12) and (13) is located in the right-half complex plane $V_R > 0$ for $a > 0$ and in the left-half complex plane $V_R < 0$ for $a < 0$. Note that the critical line (13) forms a semicircle for all $a \neq 0$ and $b < 0$. For the BCS model, Eq. (13) reduces to $-U_I/[\rho_0(U_R^2 + U_I^2)] + (\pi/2) = 0$, which agrees with the mean-field phase boundary in Eq. (6) along which the Yang-Lee zeros are distributed. This RG result confirms the validity of the mean-field results.

The above analysis of general marginally interacting systems with $a \neq 0$ and $b < 0$ implies that the criticality associated with the Yang-Lee zeros, if exists, can only take place on the semicircle (13) within the perturbative RG framework. This semicircle distribution of Yang-Lee zeros is to be compared with the Lee-Yang circle theorem [2] where the zeros are distributed on a unit circle. The semicircle structure arises from the marginal nature of the coupling strength that induces different RG-flow behaviors between the left-half plane $V_R < 0$ and the right-half plane $V_R > 0$. In fact, such a feature lies at the heart of the Fermi-surface instability in superconductivity.

This semicircle theorem indicates that the nonperturbative properties in the Fermi-surface instability is generally

linked to the geometric shape of the distribution of Yang-Lee zeros. This semicircular distribution of Yang-Lee zeros should appear in diverse systems subject to Fermi-surface instabilities, such as the charge-density wave (CDW) and anisotropic Cooper pairing, since they are described by similar RG equations with marginal couplings [35]. In fact, systems with the CDW instability can be described by a mean-field analysis similar to the BCS theory [37–39].

Nonunitary critical phenomena in superconductivity.—The Yang-Lee zeros in the complex plane are accompanied by nonunitary critical phenomena in BCS superconductivity with a complex-valued interaction. Remarkably, the criticality in the BCS model arises at every point on the phase boundary rather than at the edges alone as in the Ising model.

We now examine the critical exponents and the universality class of the Yang-Lee singularity. The correlation function

$$\begin{aligned} C(\mathbf{x}) &= {}_L \langle c_{\sigma}^{\dagger}(\mathbf{x}) c_{\sigma}(0) \rangle_R \\ &:= {}_L \langle \text{BCS} | c_{\sigma}^{\dagger}(\mathbf{x}) c_{\sigma}(0) | \text{BCS} \rangle_R \end{aligned} \quad (14)$$

can be calculated from the Fourier transformation

$$C(\mathbf{x}) \simeq -\frac{1}{N} \sum_{\mathbf{k}}' \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}} e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (15)$$

Here, we restrict the sum over \mathbf{k} to the energy shell since we are concerned with the long-range behavior of the correlation function. We expand $\xi_{\mathbf{k}}$ near the Fermi surface as $\xi_{\mathbf{k}} = v_F(k - k_F)$, where v_F is the Fermi velocity, k_F is the Fermi momentum, and $k = |\mathbf{k}|$. On the phase boundary (6), the correlation function (15) shows a power-law decay as

$$\lim_{x \rightarrow \infty} C(\mathbf{x}) \simeq \frac{A(l)}{l^{3/2}} + i \frac{B(l)}{l^{3/2}} \propto x^{-3/2}, \quad (16)$$

where $x = |\mathbf{x}|$, $l := (\text{Im}\Delta_0/v_F)x$ is a dimensionless length scale, and $A(l)$ and $B(l)$ are real functions that oscillate with l without decay (see Supplemental Material [32] for details). The anomalous power of $\frac{3}{2}$ arises from the exceptional points of the system, and should be compared with the power of 2 for the normal-metal phase [40]. When the gap closes at the exceptional points, the dispersion relation near the Fermi surface is given by

$$E_{\mathbf{k}} \simeq \sqrt{v_F^2 k^2 - (\text{Im}\Delta_0)^2}. \quad (17)$$

Near the exceptional points $k_E := (\text{Im}\Delta_0/v_F)$, the dispersion relation reduces to $E_{\mathbf{k}} \sim \sqrt{k - k_E}$, in sharp contrast with the Hermitian counterpart which exhibits a linear dispersion relation near a gapless point. It is this square-root excitation spectrum that induces the anomalous decay of the correlation function near the phase boundary.

From the correlation function (16), we find the anomalous dimension $\eta = 1/2$ from $C(\mathbf{x}) \propto x^{-D+2-\eta}$ on the phase boundary, where D is the dimension of the system [40].

The correlation function decays exponentially near the phase boundary. If we shift U by an infinitesimal amount δU along the real axis from the phase boundary, the correlation function can also be calculated from Eq. (15), giving

$$\lim_{x \rightarrow \infty} C(\mathbf{x}) \propto [A(l) + iB(l)] \frac{\exp\left(-\frac{l}{\xi}\right)}{l^{3/2}}, \quad (18)$$

where the correlation length $\xi \propto (\rho_0 \delta U)^{-1}$ diverges on the phase boundary, and hence we obtain the critical exponent $\nu = 1$ from $\xi \propto (\delta U)^{-\nu}$ [40] (see Supplemental Material [32] for the derivation). Near the phase boundary, the dynamical critical exponent z is defined as

$$\text{Re}\Delta_0 \propto \xi^{-z}. \quad (19)$$

From the expression of Δ_0 in Eq. (4), we find that $\text{Re}\Delta_0 \propto \xi^{-1} \propto \delta U$. Hence, we have $z = 1$.

The correlation length in the Hermitian case takes the form of

$$\xi \propto \exp\left(\frac{1}{\rho_0 \delta U}\right). \quad (20)$$

This behavior is distinct from that of the quantum phase transition in the non-Hermitian case since ξ^{-1} in Eq. (20) cannot be expanded as a power series of $\rho_0 \delta U$, indicating that the exceptional points lead to a distinct universality class in the non-Hermitian system.

We next consider the pair correlation function

$$\begin{aligned} &\rho_2(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2; \mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2) \\ &= {}_L \langle c_{\sigma_1}^{\dagger}(\mathbf{r}_1) c_{\sigma_2}^{\dagger}(\mathbf{r}_2) c_{\sigma'_2}(\mathbf{r}'_2) c_{\sigma'_1}(\mathbf{r}'_1) \rangle_R, \end{aligned} \quad (21)$$

where $(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2)$ and $(\mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2)$ are the positions and spins of electrons that form Cooper pairs. Setting $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{R}$ and $\mathbf{r}'_1 = \mathbf{r}'_2 = 0$ and taking the limit $|\mathbf{R}| \rightarrow \infty$, we find that ρ_2 converges to a nonzero value on the phase boundary as

$$\lim_{R \rightarrow \infty} \rho_2(\mathbf{R}\uparrow, \mathbf{R}\downarrow; 0\downarrow, 0\uparrow) = -\frac{(\text{Im}\Delta_0)^2}{U^2} \neq 0. \quad (22)$$

This nonvanishing pair correlation function is characteristic of nonunitary critical phenomena, where the correlation function of the order parameter may diverge at long distance [3]. We can also use Eq. (22) to define the critical exponent δ as

$$\lim_{R \rightarrow \infty} \rho_2(\mathbf{R}\uparrow, \mathbf{R}\downarrow; 0\downarrow, 0\uparrow) \propto |\mathbf{R}|^{-\delta}. \quad (23)$$

We have $\delta = 0$ here, which is also unique to the nonunitary critical phenomena.

The compressibility also shows critical behavior associated with the Yang-Lee singularity. By analyzing the compressibility $\kappa = (\partial^2 F / \partial \mu^2)$ near the phase boundary where $F = -(1/\beta) \log Z$ is the free energy of Bogoliubov quasiparticles, we have

$$\kappa = -N \int_{-\omega_D}^{\omega_D} \rho_0 d\xi_k \frac{\Delta_0^2}{(\xi_k^2 + \Delta_0^2)^{3/2}}. \quad (24)$$

On the phase boundary (6), the compressibility κ diverges. Therefore, we define another critical exponent ζ near the phase boundary as

$$\kappa \propto (\delta U)^{-\zeta}, \quad (25)$$

with $\zeta = 1/2$ in this system. This critical behavior also arises from the nonanalytic square-root dispersion relation near the exceptional points. In fact, the critical exponents η and ζ are equal to each other for a general fractional-power dispersion relation $(k - k_E)^{1/n}$, which includes the case of higher-order exceptional points [32].

These power-law behaviors in the nonunitary critical phenomena constitute a new Yang-Lee universality class distinct from that of the Yang-Lee edge singularity [3]. From the RG analysis, each point on the phase boundary (12) except for the origin flows to $(\rho_0 U_R, \rho_0 U_I) = (\frac{2}{3}, \infty)$, while the origin remains invariant in the RG flow. Hence, the points on the phase boundary except for the origin represent a universality class different from that at the origin.

Conclusion.—We have investigated the Yang-Lee zeros in BCS superconductivity and found that the Yang-Lee zeros are distributed on the semicircular phase boundary in the complex plane of the interaction strength. We find that the nonperturbative nature of the order parameter and thermodynamic quantities are directly connected to the number of roots of the partition function, which allows us to understand superconducting quantum phase transitions from the analytic property of the partition function. We have performed the RG analysis of generic many-body fermionic systems with marginal interactions and shown that the semicircle distribution of Yang-Lee zeros is a universal phenomenon in Fermi systems. We have also explored the Yang-Lee critical behavior and obtained critical exponents of the nonunitary criticality.

The Yang-Lee zeros and the corresponding singularity studied in this Letter are not only an interesting mathematical property but can also be tested experimentally. In fact, the non-Hermitian BCS model can be realized in open quantum systems [30,41]. The complex-valued interaction strength describes the effect of two-body loss in ultracold

atoms. For example, inelastic two-body losses can be induced by utilizing Feshbach resonances [42–44] or photoassociation [45,46]. Since the dissipation in these cases only involves atomic loss, the eigenvalue spectrum and the exceptional points of the Lindblad equation including the jump terms are the same as those of the corresponding non-Hermitian Hamiltonian without the jump terms [47]. Hence, we believe the nonunitary critical phenomena introduced in this Letter should also be observed in open quantum systems.

While we have focused on the quantum phase transition, it is worthwhile to investigate how the Yang-Lee singularity is connected to a superconducting phase transition at finite temperature. We also expect that Yang-Lee zeros can emerge in other non-Hermitian many-body systems such as a non-Hermitian Bose-Hubbard model [48].

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