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

杨-李零点、半圆定理和巴丁-库珀-施里弗超导电性中的非统一临界性

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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.

Yang 和 Lee 根据配分函数的零点，即 Yang-Lee 零点[Phys. Rev. 87, 404 (1952)；Phys. Rev. 87, 410 (1952)]. 我们证明了超导能隙中的本质奇异性与 BCS 超导体配分函数的根的数目直接相关。由于费米表面不稳定性，这些零点分布在相互作用强度的复平面上的一个半圆上。重正化群分析表明，半圆定理适用于一般的具有边缘耦合的量子多体系统，与伊辛自旋系统的李杨圆定理形成鲜明对比。这表明杨-李零点的几何形状与费米表面不稳定性直接相关。此外，我们揭示了 BCS 超导电性中的非统一临界性，这种临界性是由于例外点而出现在每个杨-李零点上的，并给出了一个不同于传统杨-李边缘奇点的普适类。

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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

引言。—杨和李发展了一种用配分函数的零点来理解相变的一般方法，称为杨-李零点[1, 2]. 他们研究了虚磁场的经典伊辛模型配分函数的零点分布，以理解铁磁相变不可解析的数学根源。当零点分布触及热力学极限中的实轴时，在顺磁性和铁磁性相之间发生热相变。杨-李零点也与热力学量中的奇点密切相关
anomalous scaling [3–8]. This type of singularities in critical phenomena is collectively referred to as the
异常标度[3 - 8]。临界现象中这种类型的奇点统称为
Yang-Lee singularity [9].
杨-李奇点[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

杨-李零点的分布决定了相变中的临界现象[3, 10]并且在统计物理学中具有基本的重要性。李-杨圆定理概括了这种分布的普遍性[1, 2]，其中陈述了铁磁伊辛模型的杨-李零点分布在
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
逸度的复平面[11 - 14]。虽然杨-李理论已被广泛应用于经典的相变[15 - 18]和量子[19 - 28]系统，它对巡回电子系统的应用是
limited [20,21]. Itinerant electrons show various types of order arising from Fermi-surface instabilities, including the Bardeen-Cooper-Schrieffer (BCS) superconductivity [29]
有限的[20, 21]。巡回电子显示了费米表面不稳定性产生的各种类型的秩序，包括巴丁-库珀-施里弗(BCS)超导[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.
作为一个主要的例子。因此，对 BCS 理论中杨-李零点的研究有望揭示迄今为止未被注意到的超导普遍性。

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.

在这封信中，我们发展了 BCS 超导的杨-李理论，用配分函数的零点分布来阐明超导相变的非微扰性质。我们证明了配分函数的根的数目与费米表面不稳定性引起的超导能隙直接相关。特别地，我们证明了配分函数的杨-李零点分布在相互作用强度的复平面上的一个半圆上，其中超导相变发生在分布的边缘。先前对配对场中费希尔零点的研究[20]通过使温度变得复杂来关注有限温度相变。相比之下，我们通过使相互作用强度变得复杂来关注零温度量子相变。

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

此外，我们利用重整化群(RG)研究了具有边缘耦合的一般量子多体系统的 Yang- Lee 零点分布的普适性。特别地，我们展示了半圆定理:与原始李-杨圆定理的完整圆相反，具有边缘相关耦合的量子多体系统中的杨-李零点分布在复相互作用平面中的半圆上[1, 2]。这个一般定理证明了几何的

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

杨-李零点分布的形状与费米表面不稳定性的存在直接相关。最后，我们研究了源于杨-李奇异性的BCS超导电性的非统一临界性。通过确定临界指数，我们表明非统一奇点属于一个普适类，不同于厄米超导相变。非常规量子临界现象是由费米子附近出现非解析激发光谱的例外点引起的

surface [30].

表面[30]。

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

总的来说很复杂，能量 Ek 也是如此。在下面，我们假设能量壳层中的态密度 ρ0 是一个常数。间隙 δ0 由下式给出

$$\Delta = \frac{\omega_D}{\rho_0 U}; \tag{4}$$

δ ωD；(4)

ρ 0U

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

超导中的杨-李奇异性。—我们考虑一个三维 BCS 模型[30, 31]

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

它在 U 0 处表现出一个本质奇点。

The partition function is given by

配分函数由下式给出

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

z = YZk = Y(1+e β Ek)； = (5)

k； σ

$k;\sigma$

σ

$k;$

$\sum \dagger \quad \underline{U} \sum , \dagger \dagger$

X U X ,

whose absolute value is shown in Fig. 1. Here, β is the inverse temperature. The Yang-Lee zeros of our system are

其绝对值如图 2 所示。1。这里，β 是温度的倒数。我们系统的杨–李零点是

$$H \quad \xi_k c_{k\sigma} c_{k\sigma} - \quad c_{k\uparrow} c_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}; \quad (1)$$

$k\sigma \qquad k;k'$

$c_{k\uparrow} c_{k\downarrow} c_{k'\downarrow} c_{k'\uparrow}$; (1)

where ξ_k $\epsilon_k - \mu$ is the single-particle energy measured from the chemical potential μ, σ $\uparrow$; $\downarrow$ is the spin index,

其中，ξ_k ϵ_k μ 是从化学势 μ 测量的单粒子能量，σ $\uparrow$；$\downarrow$ 是旋转指数，

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 $c^\dagger$

而 U U_R iU_I 是复值相互作用强度。动量为 k 且自旋为 σ 的电子的产生和湮灭算符记为 c

and $c_{k\sigma}$, respectively. The prime in $\sum'_k$ indicates that the

和 $c_{k\sigma}$。k 中的撇表示

define d by zeros of the partition function in Eq. (5) where $\mathrm{Re}(E_k) = 0$ and $\mathrm{Im}(\beta E_k) = (2n + 1)\pi, n \in \mathbb{Z}$. This con-

由方程中配分函数的零点定义。(5) 其中 $\mathrm{Re}(E_k) = 0$，$\mathrm{Im}(\beta E_k) = (2n + 1)\pi$，$n \in \mathbb{Z}$。这个 con-

dition is satisfied in the thermodynamic limit if $\mathrm{Re}\Delta_0$ 0,

如果re δ 0 0，热力学极限满足条件，

which agrees with the condition of phase transitions. It follows from this condition that the positions of Yang-Lee zeros satisify

这符合相变的条件。从这个条件可以得出，杨-李零

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].

k 上的 sum 限于 ξk < ωD，其中 ωD 为能量截止值，N 为该截止值内的动量数。注意，非厄米哈密顿量(1) 是用来研究杨李零点的封闭系统，而不是开放系统在参考。[30]。

A non-Hermitian generalization of the BCS theory is made in Ref. [30], where the mean-field BCS Hamiltonian

参考文献[1]对 BCS 理论作了非埃尔米特推广。[30]，其中平均场 BCS 哈密顿量

is given by $H = \xi c^\dagger c + [\Delta c c +$ P P P P

由 H = ξ c c+ [δ c c+给出 M F MF

点的位置满足

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

(ρ 0 π UR)2+(ρ 0 π UI 1)2 = 1; UR > 0。(6)

Note that these points coincide with the exceptional points where $H_{\rm MF}$ 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 $Z \to 1$ in the zero-temperature

注意，这些点与 HMF 不可对角化的例外点重合[30]。杨-李零点分布在相互作用强度 U 的复平面上的一个半圆上。1。在图中的黄色区域。1 在零温下，能谱 Ek 是有隙的，Z → 1

$\Delta_0 c_{k\uparrow} c_{-k\downarrow}] + (N/U)\Delta_0\Delta_0$, with the superconducting gaps $\Delta_0 = -(U/N)\sum_k {}_L\langle c_{-k\downarrow} c_{k\uparrow}\rangle_R$ and $\bar{\Delta}_0 = -(U/N)\sum_k {}_L\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle_R$. Here, ${}_L\langle A\rangle_R \coloneqq {}_L\langle \mathrm{BCS}|A|\mathrm{BCS}\rangle_R$, where

δ0ck↑CK,↓]+(n/u)δ0δ0，超导间隙 δu/n' c 和 δu/np' kl⟨c†c 在 L⟨A⟩R ≔ L⟨BCS|A|BCS⟩R 这里，其中

limit since $e^{-\beta E_k} \to 0$ for all momenta k. Note that the

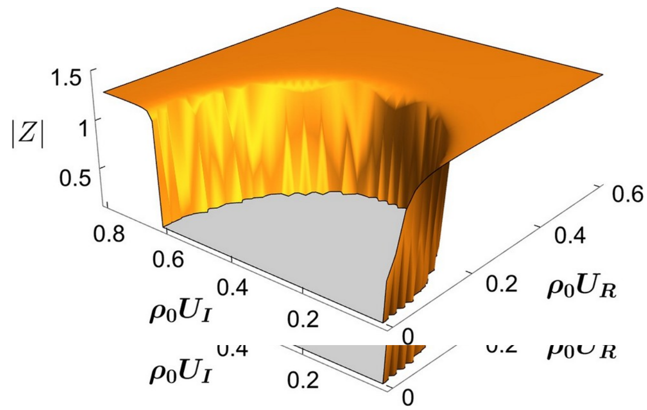
从 eβEk→0 开始对所有动量 k 进行限制，注意

the origin, which is consistent with the fact that the superconducting phase transition occurs at the origin.

原点，这与超导相变发生在原点的事实是一致的。

The essential singularity at the superconducting phase

超导相的本质奇点



|BCS⟩$_R$ and |BCS⟩$_L$ are the right and left ground states of the Hamiltonian H_{MF} given by [30]

BCS R 和 BCS L 是哈密顿 HMF 的右和左基态，由下式给出[30]

$$|\mathrm{BCS}\rangle_R = \prod (u_k + v_k c^\dagger \; c^\dagger \;)|0\rangle; \tag{2}$$

|BCS⟩R = Y(英国+vkc c+)|0⟩; (2)

$$|\mathrm{BCS}\rangle_L = \prod (u^*_k + \bar{v}^*_k c^\dagger \; c^\dagger_{k\downarrow})|0\rangle; \tag{3}$$

|bcs⟩l = y(u ∗ k+v ∗ KC ck↓)|0⟩; (3)

where 0 is the vacuum state for electrons, and u_k; v_k, and $\bar{v}_k$ are complex coefficients subject to the normalization condition u^2 $v_k\bar{v}_k$ 1. These coefficients can be deter- mined 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 $\bar{v}_k \neq v$ in general. Here, we

其中 0 是电子的真空状态，uk；vk 和 k 是复系数，服从归一化条件 u2 vkv k 1。这些系数可以用标准方式确定，并在补充材料中给出[32]。由于左右基态不一样，δ0≠δ∗ 0 和 v k≠ v 一般情况下。在这里，我们

take a gauge such that $\bar{\Delta}$ Δ . The Bogoliubov energy

取一个量规，使 δ δ。博戈柳波夫能源公司

spectrum E_k is given by [30] $E_k \equiv_0 \; \xi^2 + \Delta^2$, where

频 谱 Ek 由 下 式 给 出 [30]ek

=qﬃ ξ ﬃﬃ2ﬃﬃﬃ+ﬃﬃﬃﬃﬃ δ ﬃﬃﬃﬃﬃ2ﬃﬃ，哪里

Δ_k $\Delta_0\theta$ $\omega_D - \xi_k$ with θ x being the Heaviside unit-step function. It is worthwhile to note that Δ_0 is

δk δ0 θ ωD ξk θ x 是亥维赛单位阶跃函数。值得注意的是，δ0为

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

图一。三维 BCS 模型的配分函数 Z 的绝对值，作为零温度极限下相互作用强度 U UR iUI 的实部和虚部的函数。分区所沿的边界

phase boundary, the value of the partition function is not shown due to the breakdown of the mean-field approximation [30].

相界，由于平均场近似的分解，配分函数值没有显示出来
[30]。

partition function. According to Eq. (5), each factor in the partition function contributes to one root if and only if Re E_k 0 and Im βE_k $2n$ 1 π for some

配分函数。根据等式。(5)，配分函数中的每个因子贡献一个根当且仅当 Re Ek 0 和 Im βEk 2n 1 π 对某些

( ) = ( ) = (+

$n \in Z$. Therefore, the number of roots of the partition

( ) = ( ) = (+

n ∈ Z。因此，划分的根的数目

function in the complex energy space is given by the

复能量空间中的函数由

number of integer n satisfying Im βE_k $2n$ 1 π for Im $\beta E_k \in 0$; βIm Δ_0 [see Eqs. (12)–(15) in Supplemental Material [32]]. From Eq. (4), we have

( ) = (+

( ) ( )

对于 Im βEk ∈ 0，满足 Im βEk 2n 1 π 的整数 n 的个数；βImδ0[见等式。补充材料中的(12)–(15) [32]].来自 Eq。(4)，我们有

( ) = (+

( ) (

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]

到一个稳定的非平凡不动点，并且是唯一包含临界线的不动点。BCS 模型就属于这种情况。补充材料中显示了这些情况的 RG 流程图[32]。通过应用费米场理论的威

$$\chi \simeq \frac{\beta \mathrm{Im}(\Delta_0)}{\rho U/2} \simeq \frac{\beta\omega_D}{\rho U/2} \tag{7}$$

尔逊 RG 分析[35]，包括自能校正的 BCS 模型的 RG 方程直到两个环路阶被写为[32]

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

$dt = V\ 2V(1\mp)$ (

π $= \pi \cosh \frac{U_R}{\pi \cosh}$

π (你是

0| |

0| |

in the zero-temperature limit, where the spin-degeneracy factor of two is included. Near U 0, the gap takes the

在零温度极限下，自旋简并因子为 2。在 U 0 附近，间隙取

form of Δ_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

δ0 2ωD exp 1/ρ0U 的形式。由于相位边界与 UI ≪ UR 所在的实轴相切，因此我们可以将 UI = 0 放入等式。(7) 在原点附近，获得

$$\chi \simeq \frac{\beta}{-} \Delta_0 | \quad . \tag{8}$$

_ x ≃ β Δ / . (8)

0

From Eq. (11), we find a 1 and b −1/2 in the canonical RG equation (10). A similar RG equation has
来自 Eq。(11)，我们在正则 RG 方程中找到 a 1 和 B1/2(10)。类似的 RG 方程有
been obtained for the non-Hermitian Kondo model [36]. Note that the sign of the parameter a does not influence the
得到了非厄米 Kondo 模型[36]。请注意，参数 a 的符号不影响
physics of RG flows since we can reverse its sign by the

Equation (8) relates the number of roots χ of the partition function to the superconducting gap Δ_0 on the real axis.
等式(8) 将配分函数的根数 x 与实轴上的超导间隙 δ0 联系起来。

replacement $V \to -V$. For a system with $b < 0$, there exists a critical line which separates the trivial and nontrivial fixed
RG 流的物理性质，因为我们可以通过替换 V→v 来反转其符号。对于 b < 0 的系统，存在一条临界线来区分平凡和非平凡的固定值
points. Every point on the critical line flows toward an infinite fixed point $(V_R; V_I) = (-a/(3b); \infty)$. After inte-
分。临界线上的每一点都流向一个无限固定点(VR; VI)=(a/(3b); ∞).在互联网之后

the critical line as

关键一行是

$b\pi$

V_I b

$b\pi$

五 b

$\frac{V_I}{\hbar}$ $\frac{b}{b}$

$\underline{bV_I}$ bVI

The condensation energy $\Delta E = F(\Delta_0) - F(0)$ [33], where

冷凝能 δE = F(δ0)F(0)[33]，在哪里

$|a|$ + V^2 + V^2 = a arctan

+a$\sqrt{2}$+=V2 a

arctan V

+ a arctan

+ a arctan

$a + bV$

a+bV。

F is the free energy, can be obtained from the number of

f 是自由能，可以从数 R 中得到

roots χ as [32]

根 x as[32]

R I R R

我 稀有

稀有

(12)

(12)

ΔE $\pi^2 N\rho_0$ χ ^{2} $\propto$

2

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

δ E π 2n ρ 0 x 2∝2。

原点附近，Eq。(12)
可以扩展为

$$\simeq - \frac{2}{\quad} \beta \bar{\beta} \chi \quad (\ )$$

$$\frac{V_I}{} \quad b\pi$$

$$\frac{五\, b\,\pi}{V^2 + V^2 + |a|} = 0. \qquad (13)$$

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.

对于自发对称性破缺的一般相变，序参量 δ0 以能量为量纲，我们得到 δE∝ x 2[34]。因此，凝聚能与根数 x 直接相关。

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

半圆定理。—在这里，我们展示了半圆形分布(6)、杨-李零点是量子多体系统中普遍存在的。我们认为