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ABSTRACT

We investigate the convergence properties of finite-temperature perturbation theory by considering the mathematical structure of thermodynamic potentials using complex analysis. We discover that zeros of the partition function lead to poles in the internal energy and logarithmic singularities in the Helmholtz free energy that create divergent expansions in the canonical ensemble. Analyzing these zeros reveals that the radius of convergence increases at higher temperatures. In contrast, when the reference state is degenerate, these poles in the internal energy create a zero radius of convergence in the zero-temperature limit. Finally, by showing that the poles in the internal energy reduce to exceptional points in the zero-temperature limit, we unify the two main mathematical representations of quantum phase transitions.

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Thermodynamic effects in electronic structure theory become significant when the bandgap is comparable to the temperature. This scenario arises under extreme conditions, such as planetary interiors and laser pulses,¹ or for systems with low-energy excitations, including metals and semiconductors.² Finite-temperature effects also play a role in the emergence of quantum phase transitions, with applications in many-body localization, magnetic phases, and high-temperature superconductivity.^{2,3}

Perturbation theory is the most established *ab initio* approach for finite-temperature systems where electron correlation effects are important.^{4–7} However, for low-order perturbation theory to be reliable and systematically improvable, the corresponding expansion should give a convergent series. Zero-temperature perturbation theory can become divergent when the reference state is a poor approximation to the physical system or when there are near-degeneracies in the reference energies (see Ref. 8 for a review). In contrast, energy degeneracies are less significant at finite temperature than in the zero-temperature expansion,⁹ although the series convergence can often worsen for lower temperatures. Furthermore, finite-temperature perturbation theory can diverge at zero temperature even when the zero-temperature perturbation expansion is convergent.¹⁰ This situation arises for degenerate or incorrect reference states and its manifestation in electronic perturbation theory is known as the Kohn–Luttinger problem.¹¹ However, the general

relationship between the convergence of finite-temperature perturbation theory and its zero-temperature counterpart has not yet been fully established.

The convergence of a perturbation expansion $H = H^{(0)} + \lambda H^{(1)}$ can be mathematically examined by investigating the structure of the energy function $E(\lambda)$ in the complex- λ plane. From complex analysis, the radius of convergence r_c for a perturbation expansion of a function $f(\lambda)$ is determined by the distance of the closest singularity of $f(\lambda)$ to the origin in the complex- λ plane.^{12–15} These singularities represent points where $f(\lambda)$ becomes non-analytic and may correspond to a pole, a branch point, or a more complicated non-analytic feature.^{14,15} The perturbation expansion will converge for the physical system at $\lambda = 1$ when $r_c > 1$ and will diverge for $r_c < 1$. Therefore, understanding the convergence of finite-temperature perturbation theory requires a detailed investigation into the structure of thermodynamic functions in the complex- λ plane.

Complex analysis also plays an important role in the theory of thermodynamic phase transitions. In Lee–Yang theory, zeros of the partition function exist at complex temperatures for finite systems near a phase transition.^{16,17} These zeros converge onto the real axis in the thermodynamic limit and intersect at the critical temperature. The same phenomenon occurs for any complex-valued control parameter,¹⁸ allowing Lee–Yang

theory to be applied to zero-temperature quantum phase transitions.¹⁹ Alternatively, avoided level crossings in finite systems are related to non-Hermitian exceptional points, where two energy levels become identical for a complex control parameter.^{20,21} The distance of an exceptional point to the real-axis controls the “sharpness” of the avoided crossing and, in the thermodynamic limit of a quantum phase transition, the exceptional points converge onto the real axis.²² These exceptional points also play a pivotal role in the convergence of zero-temperature perturbation theory,^{8,21} symmetry breaking in mean-field approximations,^{23,24} and the convergence of quantum criticality in the complete basis set limit.²⁵

In this work, we investigate the convergence of finite-temperature perturbation theory in the canonical ensemble through the lens of complex analysis. We find that the internal energy and Helmholtz free energy are punctuated by poles or logarithmic singularities in the complex- λ plane that determine the radius of convergence of the perturbation series. These singularities are created by Lee–Yang zeros of the partition function and move further from the origin as the temperature increases. Consequently, perturbation expansions converge increasingly rapidly at higher temperatures, even for a divergent zero-temperature expansion. For a degenerate reference, the zeros of the partition function converge onto $\lambda = 0$ for $T \rightarrow 0$, creating a mathematically undefined perturbation expansion that is the origin of the Kohn–Luttinger problem. Finally, we extend these results to directly connect zero-temperature exceptional points and finite-temperature zeros of the partition function in the theory of quantum phase transitions.

We illustrate these ideas using a two-level system representing a spin-1/2 particle in a magnetic field. In the spinor basis of the \hat{S}_z operator, the Hamiltonian is

$$H = \begin{pmatrix} -B_z & -B_x \\ -B_x & B_z \end{pmatrix}, \quad (1)$$

where B_z and B_x are the (real) components of the magnetic field along the z and x directions, respectively. For $B_x = 0$ and $B_z > 0$, the ground state represents an electron aligned in the positive z direction while the excited state represents an electron aligned with the negative z direction. In the $B_z \rightarrow 0$ limit, the electron in its ground state aligns with the positive (negative) x direction for positive (negative) B_x and a quantum phase transition occurs at $B_x = 0$. Any two-state system of this type can be seen as a qubit.

Within perturbation theory, the Hamiltonian is partitioned into a Hermitian reference Hamiltonian $H^{(0)}$ and a perturbation $H^{(1)}$.¹² The time-independent Schrödinger equation is then recast as

$$H(\lambda)\Psi_k(\lambda) = (H^{(0)} + \lambda H^{(1)})\Psi_k(\lambda) = E_k(\lambda)\Psi_k(\lambda), \quad (2)$$

where the parameter λ controls the strength of the perturbation. The exact energies and wave functions of the ground and excited states become λ -dependent functions, with $\lambda = 0$ corresponding to the

reference model and $\lambda = 1$ representing the physical system. Expanding the energy around $\lambda = 0$ gives the power series

$$E_k(\lambda) = \sum_{j=0}^{\infty} E_k^{(j)} \lambda^j, \quad (3)$$

where $E_k^{(j)}$ provides the j th-order perturbation correction. This expansion has a radius of convergence r_c that controls the values of λ where the partial sums of increasing length tend toward the exact value of $E_k(\lambda)$.

When $H(\lambda)$ is considered in the complex- λ plane, it becomes non-Hermitian and the discrete eigenvalues become unified as a continuous Riemann surface.²⁶ This Riemann surface represents a “one-to-many” function, with each sheet representing a different eigenstate. The most common singularities on $E(\lambda)$ are exceptional points (or branch points) where the two energy levels become degenerate and the eigenstates become identical.^{12,13,21,27–29} These non-Hermitian features are related to the onset of dynamic stabilities, avoided level crossings, and quantum phase transitions.²¹ Remarkably, following an eigenstate around an exceptional point interconverts the two energy levels,^{23,26,27,30} a property that has even been realized experimentally.^{31,32}

The reference and perturbation Hamiltonians for the two-level system can be defined as

$$H^{(0)} = \begin{pmatrix} -B_z & 0 \\ 0 & B_z \end{pmatrix} \quad \text{and} \quad H^{(1)} = \begin{pmatrix} 0 & -B_x \\ -B_x & 0 \end{pmatrix}, \quad (4)$$

with the exact zero-temperature eigenstates

$$E_{\pm}(\lambda) = \pm \sqrt{B_z^2 + \lambda^2 B_x^2}. \quad (5)$$

Here, the ground and excited state are defined as $E_1 = E_-$ and $E_2 = E_+$, respectively. These eigenstates form an artificial avoided level crossing along the real- λ axis at $\lambda = 0$ that mirrors the true avoided crossing along the real B_x axis. The corresponding two-sheeted Riemann surface is shown in Fig. 1(a). When the discriminant in Eq. (5) is zero, the eigenstates become degenerate, creating square-root branch points at $\lambda_{\text{bp}} = \pm i B_z / B_x$. Since these exceptional points are the only singularities in $E(\lambda)$, the radius of convergence is $r_c = \left| \frac{B_z}{B_x} \right|$ and the zero-temperature perturbation expansion converges at the physical value $\lambda = 1$ when $|B_x| < |B_z|$.

We now consider a canonical ensemble of non-interacting subsystems, where the partition function of a general N -level system is

$$Z(\lambda) = \sum_{k=1}^N \exp(-\beta E_k(\lambda)). \quad (6)$$

Here, $\beta = (k_B T)^{-1}$ and k_B and T denote the Boltzmann constant and temperature, respectively. The internal energy is

$$U(\lambda) = -\frac{d \ln Z(\lambda)}{d\beta} = \frac{\sum_{k=1}^N E_k(\lambda) \exp(-\beta E_k(\lambda))}{Z(\lambda)}, \quad (7)$$

and the Helmholtz free energy is

$$F(\lambda) = -\frac{1}{\beta} \ln Z(\lambda). \quad (8)$$

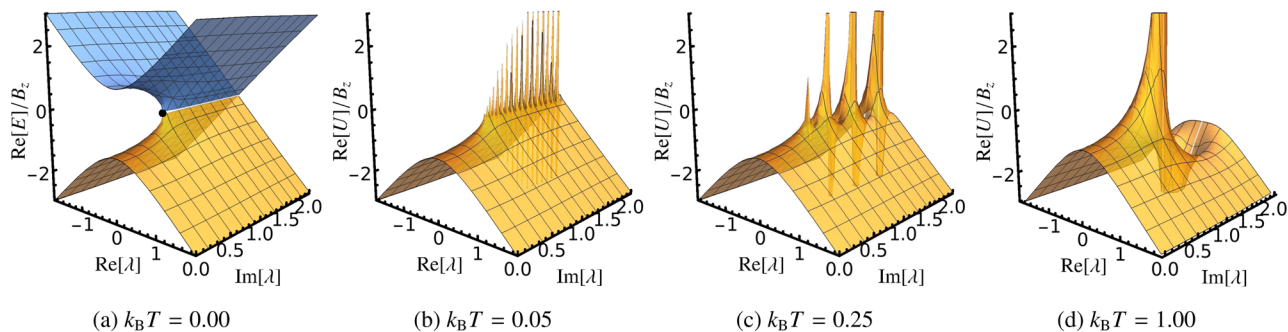


FIG. 1. Internal energy for the two-level Hamiltonian [Eq. (4)] in the canonical ensemble as a function of the perturbation strength λ for $B_x = \frac{3}{2}B_z$. (a) The zero-temperature ground and excited state energies form a two-sheeted Riemann surface with square-root branch points at $\lambda = \pm i B_z/B_x$ (black dot). (b)–(d) At finite temperature, the internal energy features a sequence of poles corresponding to zeros of the partition function $Z(\lambda)$, with the spacing increasing at higher temperature. The distance of the closest pole to the origin determines the radius of convergence for a perturbation expansion of the internal energy.

The perturbation series for these thermodynamic potentials are given by Taylor expansions around $\lambda = 0$,⁶ i.e.,

$$U(\lambda) = \sum_{j=0}^{\infty} U^{(j)} \lambda^j \quad \text{and} \quad F(\lambda) = \sum_{j=0}^{\infty} F^{(j)} \lambda^j, \quad (9)$$

where the individual corrections are, e.g.,

$$U^{(j)} = \frac{1}{j!} \left. \frac{\partial^j U(\lambda)}{\partial \lambda^j} \right|_{\lambda=0}. \quad (10)$$

The radius of convergence is then controlled by the distance of the closest singularity to the origin in the complex- λ plane.

Singularities in $U(\lambda)$ at non-zero temperature can be identified by inspecting the general form of Eq. (7). One possibility is that $U(\lambda)$ has a singularity at values of λ corresponding to exceptional points in the zero-temperature energy. We find that this is not the case because a thermodynamic summation, including every discrete eigenstate, removes singularities caused by exceptional points. This property is shown for the partition function in the Appendix and can be extended to the numerator of the internal energy.

On the other hand, $Z(\lambda)$ can become zero in the complex- λ plane, creating poles in the internal energy that dictate the radius of convergence for the perturbation expansion. At large temperatures, we find $Z(\lambda) \rightarrow 1$ for all λ . However, if we consider low temperatures near a degeneracy between $E_1(\lambda)$ and $E_2(\lambda)$, the partition function approximates to

$$Z(\lambda) \approx e^{-\beta E_1(\lambda)} [1 + e^{-\beta(E_2(\lambda) - E_1(\lambda))}]. \quad (11)$$

Zeros of $Z(\lambda)$ then occur when $e^{-\beta(E_2(\lambda) - E_1(\lambda))} = -1$, giving an infinite set of possible solutions that satisfy

$$E_2(\lambda) - E_1(\lambda) = \underbrace{k_B T(2n+1)\pi i}_{\omega_n} \quad \forall \quad n \in \mathbb{Z}. \quad (12)$$

In other words, zeros of the partition function for low- T occur when the real components of $E_1(\lambda)$ and $E_2(\lambda)$ are degenerate and the difference in the imaginary components is equal to the

Matsubara frequencies ω_n .³³ For $T \rightarrow 0$, the Matsubara frequencies form a continuum along the imaginary axis and zeros of the partition function occur whenever the real components are degenerate, regardless of the imaginary components. In this limit, the zeros of the partition function form a continuum along the locus of points where the real component of the lowest excitation energy is zero. These points include non-Hermitian branch cuts on the ground-state energy surface as well as Hermitian conical intersection seams. The same zeros of $Z(\lambda)$ create logarithmic singularities in the Helmholtz free energy, meaning that $F(\lambda)$ and $U(\lambda)$ have an identical radius of convergence.

In the two-level system, the internal energy is given in terms of the perturbation strength λ as

$$U(\lambda) = - \frac{\sqrt{B_z^2 + \lambda^2 B_x^2} \sinh(\beta \sqrt{B_z^2 + \lambda^2 B_x^2})}{\cosh(\beta \sqrt{B_z^2 + \lambda^2 B_x^2})}, \quad (13)$$

where the denominator represents the partition function $Z(\lambda) = \cosh(\beta \sqrt{B_z^2 + \lambda^2 B_x^2})$. Plotting the internal energy at various temperatures in Figs. 1(b)–1(d), we find that the square-root branch cut in the zero-temperature energy is lost for $T \neq 0$. Instead, there are a sequence of poles with a separation that increases for higher temperatures. Solving $Z(\lambda) = 0$, the positions of these poles is

$$\lambda_{\text{pole}} = \pm i \frac{B_z}{B_x} \sqrt{1 + \frac{\pi^2 k_B^2 T^2}{4B_z^2} (4n+1)^2} \quad \forall \quad n \in \mathbb{Z}. \quad (14)$$

Therefore, the poles extend along the imaginary axis and their spacing decreases with temperature. When $T \rightarrow 0$, the poles tend toward a continuum extending outward from the zero-temperature exceptional points, corresponding to the line where the real components of the ground- and excited-state energies are degenerate. Ultimately, this continuum of poles recovers the branch cut on the lowest-energy sheet of the zero-temperature Riemann surface [Fig. 1(a)].

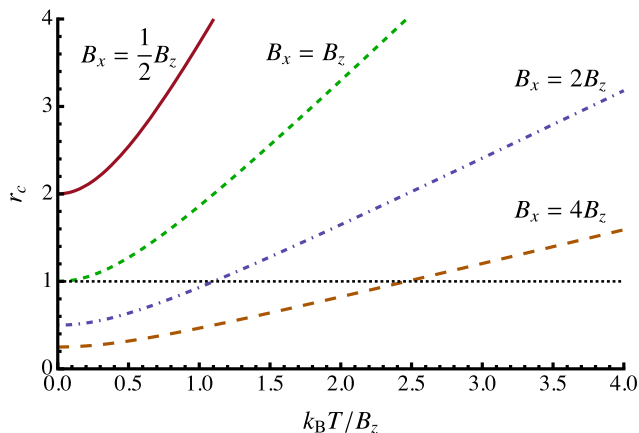


FIG. 2. Radius of convergence r_c for U and F in the two-level system. Different B_x values show that divergent systems at $T = 0$ will converge at $\lambda = 1$ for a sufficiently high T .

The closest pole to the origin corresponds to $n = 0$, giving the radius of convergence

$$r_c = \left| \frac{B_z}{B_x} \sqrt{1 + \frac{\pi^2 k_B^2 T^2}{4B_z^2}} \right|. \quad (15)$$

In the $T \rightarrow 0$ limit, this radius of convergence tends toward the expected value for the ground-state energy perturbation series and scales quadratically with respect to T (see Fig. 2). On the other hand, for $T \rightarrow \infty$, we recover the asymptotic behavior $r_c \sim \frac{\pi k_B T}{2B_x}$. Therefore, the perturbation series will always converge at a sufficiently large T as long as B_x is finite.

Remarkably, we find that the finite-temperature perturbation series in the two-level system can converge at non-zero temperatures even when the zero-temperature expansion diverges. This scenario is illustrated in Fig. 3 for the internal energy and Helmholtz free energy with $B_x = \frac{3}{2}B_z$. The temperature at which the thermodynamic perturbation expansion becomes convergent at $\lambda = 1$ can

TABLE I. Perturbation expansions of U and F for the two-level system with $B_x = \frac{3}{2}B_z$, evaluated at $\lambda = 1$. Only terms with even order have a non-zero contribution. These series diverge at $k_B T = 0.5B_z$ and converge at $k_B T = 1.5B_z$.

Order	$U(\lambda = 1)/B_z$		$F(\lambda = 1)/B_z$	
	$k_B T = 0.5$	$k_B T = 1.5$	$k_B T = 0.5$	$k_B T = 1.5$
0	-0.964 03	-0.582 78	-1.009 07	-1.350 94
2	-2.207 52	-1.733 69	-2.093 61	-2.006 57
4	-1.342 09	-1.427 01	-1.572 97	-1.916 37
6	-2.407 45	-1.530 24	-2.029 38	-1.936 67
8	-0.964 56	-1.494 87	-1.558 83	-1.931 45
10	-2.959 66	-1.507 01	-2.081 18	-1.932 89
12	-0.187 59	-1.502 84	-1.475 85	-1.932 48
Exact	-1.800 12	-1.503 89	-1.803 14	-1.932 57

be identified by solving $r_c > 1$, giving $k_B T > \frac{2}{\pi} \sqrt{B_x^2 - B_z^2}$ in the two-level system. For $B_x = \frac{3}{2}B_z$, the perturbation expansion becomes convergent at $k_B T = 0.711763B_z$, as indicated by the vertical gray lines in Fig. 3. Numerical results indicating the accuracy of the low-order corrections either side of this temperature are given in Table I. (Note that only terms of even order contribute to the expansion.) The numerical data in Fig. 3 and Table I demonstrate that the Helmholtz free energy and internal energy start to diverge at the same temperature, confirming that the zeros of the partition function (common to both thermodynamic potentials) are the origin of these divergences.

On the other hand, it is also possible for a finite-temperature expansion to become divergent in the $T \rightarrow 0$ limit while the corresponding zero-temperature expansion is convergent. In this scenario, there is a mismatch between the $T \rightarrow 0$ limit of $U^{(n)}$ and the corresponding zero-temperature ground-state correction $E_1^{(n)}$, known as the Kohn and Luttinger problem.¹¹ This issue originally

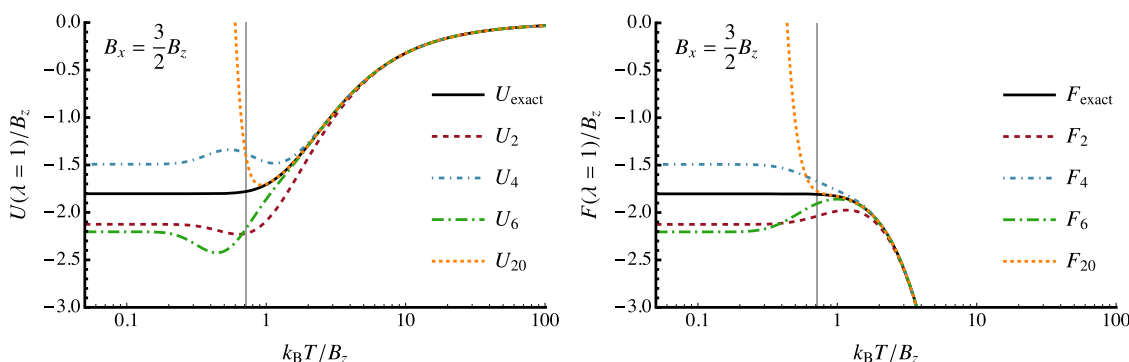


FIG. 3. Low-order perturbation expansions of the internal energy (left) and the Helmholtz free energy (right) for the two-level system with $B_x = \frac{3}{2}B_z$, evaluated at $\lambda = 1$. Here, U_k or F_k denotes a partial sum of the perturbation expansion up to the k th-order. The vertical gray line at $k_B T = 0.711763B_z$ indicates the lowest temperature where the perturbation expansions become convergent.

suggested that the formulation of finite-temperature electronic perturbation theory may be incorrect, inspiring a comprehensive reformulation that expands all thermodynamic potentials on an equal footing.^{7,34–36} However, Hirata subsequently demonstrated that the Kohn–Luttinger problem still persists by showing that $U^{(1)}$ and $U^{(2)}$ tend toward the wrong limit when the degeneracy is lifted at first order,¹⁰

$$\lim_{T \rightarrow 0} U^{(1)} = \mathbb{E}[E_k^{(1)}] \neq E_1^{(1)}, \quad (16a)$$

$$\lim_{T \rightarrow 0} U^{(2)} = -\infty \neq E_1^{(2)}, \quad (16b)$$

where $\mathbb{E}[E_k^{(1)}]$ is the average of the first-order corrections for the degenerate reference states k . These limits give a zero radius of convergence at zero temperature and Hirata concluded that the Kohn–Luttinger problem “originates from the non-analyticity of the Boltzmann factor at $T = 0$.”¹⁰

Applying our analysis in the case of a degenerate reference state, we find that the zeros of the partition function must converge onto $\lambda = 0$ for $T \rightarrow 0$. Therefore, the zero-temperature continuum of poles in $U(\lambda)$ intersects $\lambda = 0$ and the radius of convergence becomes zero, in agreement with Ref. 10. In contrast to zero-temperature perturbation theory, this feature arises from the properties of the partition function and only requires a degeneracy in the zeroth-order ground state; it does not assume anything about the convergence properties of the zero-temperature eigenstates. The presence of a non-analytic pole in $U(\lambda)$ at $\lambda = 0$ then leads to an inherently divergent perturbation expansion. Consequently, we can refine Hirata’s concluding statement to say that the Kohn–Luttinger problem *originates from a singularity in a thermodynamic potential at $\lambda = 0$ created by a zero of the partition function for $T \rightarrow 0$.*

However, this analysis does little to explain the origin of differences between the results of zero-temperature and finite-temperature perturbation theory in the Kohn–Luttinger problem. To elucidate this further, we fix $B_z = 0$ in the two-level system to give degenerate reference states where the zero-temperature energies converge exactly at first-order,

$$E_{\pm}(\lambda) = \pm B_x \lambda. \quad (17)$$

The corresponding internal energy is

$$U(\lambda) = -B_x \lambda \tanh\left(\frac{B_x \lambda}{k_B T}\right) \quad (18)$$

with poles at

$$\lambda_{\text{pole}} = \pm i \frac{\pi k_B T}{2 B_x} (4n + 1) \quad \forall n \in \mathbb{Z}. \quad (19)$$

The radius of convergence is then directly proportional to T and finite-temperature perturbation theory will diverge for $T \rightarrow 0$, even though the zero-temperature energies are convergent.

For this example, the derivatives required for the first- and second-order corrections to the internal energy are

$$\frac{\partial U}{\partial \lambda} = -\frac{B_x^2 \lambda}{k_B T} \operatorname{sech}^2\left(\frac{B_x \lambda}{k_B T}\right) - B_x \tanh\left(\frac{B_x \lambda}{k_B T}\right), \quad (20a)$$

$$\frac{1}{2} \frac{\partial^2 U}{\partial \lambda^2} = -\frac{B_x^2}{k_B T} \operatorname{sech}^2\left(\frac{B_x \lambda}{k_B T}\right) \left[1 - \frac{B_x \lambda}{k_B T} \tanh\left(\frac{B_x \lambda}{k_B T}\right)\right]. \quad (20b)$$

Both functions are mathematically undefined at $\lambda = T = 0$, and the value obtained by perturbation theory will depend on the order in which this limit is approached. For the first-order correction, two possible limits are

$$\lim_{T \rightarrow 0^+} \left(\lim_{\lambda \rightarrow 0^+} \frac{\partial U}{\partial \lambda} \right) = 0 \quad \text{and} \quad \lim_{\lambda \rightarrow 0^+} \left(\lim_{T \rightarrow 0^+} \frac{\partial U}{\partial \lambda} \right) = -B_x, \quad (21)$$

as illustrated in Fig. 4(a). The first case corresponds to the zero-temperature limit of finite-temperature perturbation theory (red curve), recovering the average of the zero-temperature first-order corrections as described in Ref. 10. In contrast, the second case represents a perturbation expansion of the zero-temperature internal energy (blue curve) and recovers the expected behavior $\lim_{T \rightarrow 0} U^{(1)} = E_1^{(1)}$. Similarly, the two limits for the second-order correction yield

$$\lim_{T \rightarrow 0^+} \left(\lim_{\lambda \rightarrow 0^+} \frac{1}{2} \frac{\partial^2 U}{\partial \lambda^2} \right) = -\infty \quad \text{and} \quad \lim_{\lambda \rightarrow 0^+} \left(\lim_{T \rightarrow 0^+} \frac{1}{2} \frac{\partial^2 U}{\partial \lambda^2} \right) = 0, \quad (22)$$

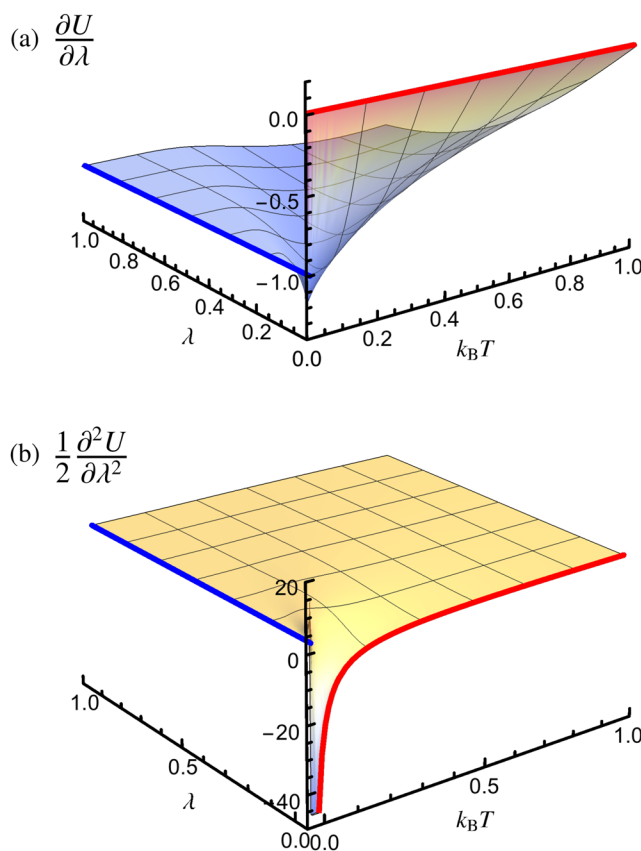


FIG. 4. (a) First-order and (b) second-order contributions to the internal energy in the degenerate two-level system [Eq. (17)] with $B_z = 0$ and $B_x = 1$. Different values at $(\lambda, T) = (0, 0)$ result from taking the $T \rightarrow 0$ and $\lambda \rightarrow 0$ limits in different orders, as illustrated by the red ($\lambda \rightarrow 0$) and blue ($T \rightarrow 0$) curves.

as illustrated in Fig. 4(b). Again, the first case recovers the divergent finite-temperature behavior described in Ref. 10, while the second case tends to the second-order correction of the exact ground state.

These results suggest that the Kohn–Luttinger problem is fundamentally an order-of-limits issue that arises because the internal energy with degenerate reference states is non-analytic for $\lambda = 0$ and $T = 0$ and the derivatives required for perturbation theory are mathematically undefined. Because this situation arises from zeros of the partition function, the divergence depends on the degeneracy of the reference states regardless of their coupling through the perturbation. Therefore, this problem cannot be removed by simply using degenerate perturbation theory.³⁷ Instead, it appears that the only resolution is to remove the degeneracy using an alternative reference or partitioning, as recently proposed in Ref. 38.

Finally, having identified a relationship between branch cuts of the zero-temperature eigenstates and zeros of the partition function in the $T \rightarrow 0$ limit, a natural question is whether this concept can be extended to unify Lee–Yang theory with the convergence of exceptional points onto the real axis at quantum phase transitions. Previous work by Cejnar and co-workers has investigated this connection by associating non-Hermitian degeneracies with point charges and connecting the position of these degeneracies in the complex plane with zeros of a Coulombic partition function.^{39,40} However, we are not aware of any direct connection between Lee–Yang zeros and zero-temperature exceptional points at quantum phase transitions.

The two-level spin-1/2 model provides a model of a quantum phase transition in the limit $B_z \rightarrow 0$. For a fixed value of $B_x > 0$, this quantum phase transition occurs at $\lambda = 0$, with the spin flipping its alignment from the negative- x direction ($\lambda < 0$) to the positive- x direction ($\lambda > 0$). This transition is demonstrated by a derivative discontinuity in the zero-temperature energy and a discontinuous jump in $\langle S_x \rangle$ at $\lambda = 0$, as shown in Fig. 5 (left and middle panels, respectively). For $B_z \neq 0$, a complex-conjugate pair

of exceptional points exists in the complex- λ plane (Fig. 5: right panel), creating an avoided level crossing on the real axis. As expected, these zero-temperature exceptional points converge onto the real axis in the $B_z \rightarrow 0$ limit corresponding to the quantum phase transition.

This physical phase transition is mathematically equivalent to the analysis of finite-temperature perturbation theory in the complex- λ plane. Therefore, we can use it to directly connect Lee–Yang zeros at quantum phase transitions with zero-temperature exceptional points. Because the quantum phase transition only occurs when $T = 0$ for $B_z = 0$, we expect the zeros of the partition function to converge onto the real axis in the $T \rightarrow 0$ and $B_z \rightarrow 0$ limit. We have already shown that zeros of the partition function for $T \neq 0$ and $B_z \neq 0$ occur along the imaginary axis extending out from the zero-temperature exceptional point. For $T \rightarrow 0$, these zeros form a continuum along the branch cut that terminates at the exceptional point. Therefore, in the $B_z \rightarrow 0$ limit, the convergence of the exceptional points onto the real axis also causes the zeros of the partition function to move closer to the real axis. The position of these zeros still has a complex component for $T \neq 0$ and the internal energy is smooth along the real axis. However, when the zeros of the partition function converge onto the exceptional points for $T \rightarrow 0$, they must also converge onto the real axis as $B_z \rightarrow 0$, creating the expected behavior for a quantum phase transition.

As a result, the convergence of Lee–Yang zeros and exceptional points onto the real axis arises from the same mathematics, providing a unified perspective on quantum phase transitions in the complex plane. The exceptional point in the zero-temperature energy is simply the zero-temperature continuum limit of the poles in the internal energy caused by zeros of the partition function. This result is a formal mathematical connection, in contrast to the previous Coulombic analogy between non-Hermitian degeneracies and zeros of the partition function.^{39,40}

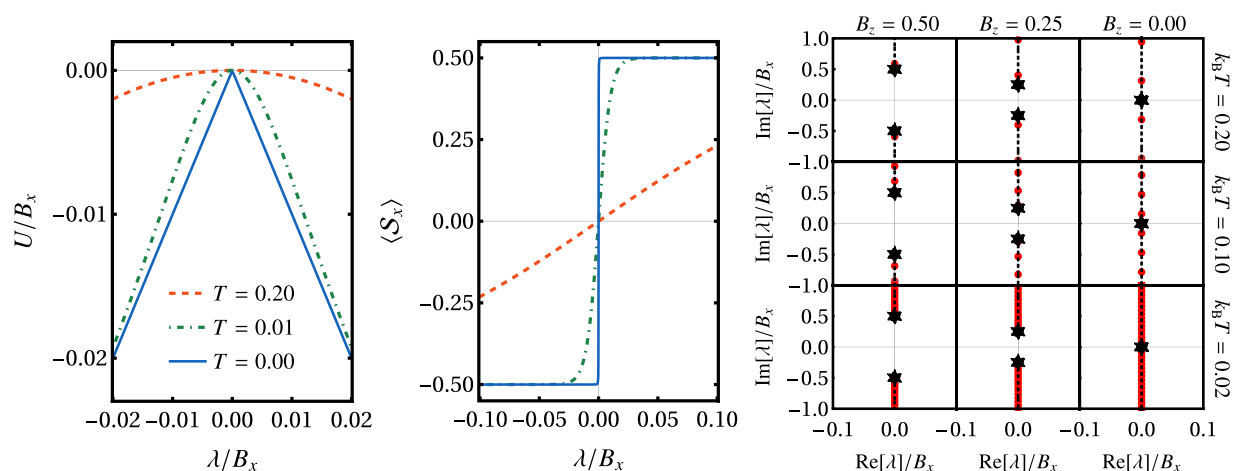


FIG. 5. A quantum phase transition occurs at $\lambda = 0$ in the two-level system with $T = 0$ and $B_z = 0$. Left: Internal energy at different temperatures, showing the quantum phase transition at $T = 0$ as a gradient discontinuity in the energy. Middle: Variation of the spin expectation value at the quantum phase transition. Right: Relationship between the exceptional points of the energy and zeros of the partition function for various values of B_z and $k_B T$ with $B_x = 1$.

In this work, we have shown that divergent finite-temperature perturbation theory is driven by singularities created by Lee–Yang zeros of the partition function that move further into the complex plane as the temperature increases. Therefore, perturbation theory is more likely to be convergent at higher temperatures. This result suggests that extrapolating analytic continuations of the perturbation corrections at higher temperatures to $T = 0$, in a similar approach to Refs. 41–43, may provide improved accuracy when the zero-temperature expansion is divergent. Alternatively, because the divergent perturbation expansions at $T \neq 0$ arise from poles, the internal energy will be particularly well-suited to resummation techniques based on Padé approximants.^{12,13,44} For a degenerate reference, we find that the poles in the internal energy converge onto $\lambda = 0$ in the $T \rightarrow 0$ limit, creating a mathematically undefined perturbation expansion that is the origin of the Kohn–Luttinger problem.

Finally, by extending our analysis to quantum phase transitions in the spin-1/2 model, we have demonstrated a direct mathematical connection between finite-temperature Lee–Yang zeros and zero-temperature exceptional points. This unifying connection provides a more complete picture of quantum phase transitions through the lens of complex analysis. Recently, Lee–Yang zeros and exceptional points have been independently realized in experiments.^{31,32,45,46} The possibility of experimentally probing the conversion of Lee–Yang zeros into an exceptional point at low temperatures is an exciting prospect for the discovery and verification of exotic non-Hermitian chemical physics.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are openly available at <https://doi.org/10.5287/bodleian:zr4eaB46w>.

APPENDIX: ANALYTICITY OF $Z(\lambda)$ NEAR ALGEBRAIC BRANCH POINTS

Consider the partition function $Z(\lambda)$ of an N -level system in the vicinity of an k th order algebraic branch point λ_{bp} (where $k > 1$). In this region, the states that are not involved in the branch point provide a smooth, analytic contribution $\mathcal{Z}(\lambda)$ and the partition function to be decomposed as

$$Z(\lambda) = \mathcal{Z}(\lambda) + \sum_{j=1}^k \exp(-\beta E_j(\lambda)), \quad (\text{A1})$$

where the states indexed by j coincide at the branch point. To establish whether $Z(\lambda)$ is analytic at λ_{bp} , we consider the first derivative

$$\frac{dZ(\lambda)}{d\lambda} = \frac{d\mathcal{Z}(\lambda)}{d\lambda} - \beta \sum_{j=1}^k \frac{dE_j(\lambda)}{d\lambda} \exp(-\beta E_j(\lambda)). \quad (\text{A2})$$

Near the k th-order branch point, the corresponding energy levels behave as

$$E_j(\lambda) \approx E_{\text{bp}} + a(\lambda)^{\frac{1}{k}} \exp\left(\frac{2\pi i j}{k}\right) \quad (\text{A3})$$

for some smooth real function $a(\lambda)$ with $a(\lambda_{\text{bp}}) = 0$. For example, in the two-level system considered in this letter, the energy levels near the branch point $E_{\pm}(\lambda) = \pm(B_z^2 + \lambda^2 B_x^2)^{1/2}$ correspond to $a(\lambda) = B_z^2 + \lambda^2 B_x^2$ and $k = 2$. The non-analyticity of the zero-temperature energy levels for $\lambda \rightarrow \lambda_{\text{bp}}$ then arises from the derivatives

$$\frac{dE_j(\lambda)}{d\lambda} = \frac{1}{k} \frac{da(\lambda)}{d\lambda} a(\lambda)^{\left(\frac{1}{k}-1\right)} \exp\left(\frac{2\pi i j}{k}\right), \quad (\text{A4})$$

where clearly the $a(\lambda)^{\left(\frac{1}{k}-1\right)}$ term diverges in the limit $\lim_{\lambda \rightarrow \lambda_{\text{bp}}} a(\lambda) = 0$ for $k > 1$. Inserting Eq. (A3) into Eq. (A2) and considering the $\lambda \rightarrow \lambda_{\text{bp}}$ limit then yields

$$\frac{dZ(\lambda)}{d\lambda} \approx \frac{d\mathcal{Z}(\lambda)}{d\lambda} - \beta \frac{1}{k} \frac{da(\lambda)}{d\lambda} a(\lambda)^{\left(\frac{1}{k}-1\right)} \exp(-\beta E_{\text{bp}}) \underbrace{\sum_{j=1}^k \exp\left(\frac{2\pi i j}{nk}\right)}_0. \quad (\text{A5})$$

Because $\sum_{j=1}^k \exp\left(\frac{2\pi i j}{nk}\right) = 0$, we find that $\frac{dZ(\lambda)}{d\lambda}$ remains finite at the branch point even though the zero-temperature energy levels are non-analytic. This derivation can be trivially extended to show that high-order derivatives of the partition function are also finite at a branch point. Consequently, the partition function is a complex analytic function of λ , even in the presence of non-analytic algebraic branch points in the zero-temperature energy levels. A similar approach can be applied to the numerator of the internal energy.

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