Divergent Perturbation Theory and Quantum Phase Transitions at Finite Temperature

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(Dated: March 7, 2022)

We investigate the convergence 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 which create divergent expansions in the canonical ensemble. Analysing these zeros reveals that the radius of convergence increases for higher temperatures. 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.

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

Perturbation theory is the most established ab initio approach for finite-temperature systems where electron correlation effects are important. 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. Furthermore, the series convergence can often worsen for lower temperatures, particularly when the zero-temperature expansions diverge. 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-\( \lambda \) plane. From complex analysis, the radius of convergence \( r_c \) for a perturbation expansion of a function \( f(\lambda) \) is determined by the magnitude of the closest singularity of \( f(\lambda) \) to the origin in the complex-\( \lambda \) plane. 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. 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-\( \lambda \) plane.

Complex analysis already 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. These zeros converge onto the real axis in the thermodynamic limit and intersect at the critical temperature. The same phenomena occurs for any complex-valued control parameter, allowing Lee–Yang theory to be applied to zero-temperature quantum phase transitions. 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. 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. These exceptional points also play a pivotal role in the convergence of zero-temperature perturbation theory.

Here, 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 in the complex-\( \lambda \) plane that determine the radius of convergence of the perturbation series. These poles 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. 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

\[
H = \begin{pmatrix} -B_z & -B_x \\ -B_x & B_z \end{pmatrix},
\]

where \( B_x \) and \( B_z \) are the (real) components of the magnetic field along the \( z \) and \( x \) directions respectively. For \( B_z = 0 \) and \( B_x > 0 \), 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 \( B_x \to 0 \) limit, the electron in its ground state aligns with the positive \( x \) 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.

Zero-Temperature Perturbation Theory. — Within perturbation theory, the Hamiltonian is partitioned into a Hermitian reference Hamiltonian \( H^{(0)} \) and a perturbation \( H^{(1)} \). The time-independent Schrödinger equation is then recast as

\[
H(\lambda)\Psi_\lambda(\lambda) = \left( H^{(0)} + \lambda H^{(1)} \right)\Psi_\lambda(\lambda) = E_\lambda(\lambda)\Psi_\lambda(\lambda),
\]

where \( E_\lambda(\lambda) \) and \( \Psi_\lambda(\lambda) \) are eigenvalues and eigenstates of the Hamiltonian with respect to the control parameter \( \lambda \).
The parameter \( \lambda \) controls the strength of the perturbation. The exact energies and wave functions of the ground and excited states become \( \lambda \)-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

\[
E_k(\lambda) = \sum_{i=0}^{\infty} E_k^{(i)} \lambda^i,
\]

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

When \( H(\lambda) \) is considered in the complex-\( \lambda \) plane, it becomes non-Hermitian and the discrete eigenvalues become unified as a continuous Riemann surface. 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 two energy levels become degenerate and the eigenstates become identical. These non-Hermitian features are related to the onset of dynamic stabilities, avoided level crossings, and quantum phase transitions. Remarkably, following an eigenstate around an exceptional point interconverts the two energy levels in a di-level system.

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

\[
H^{(0)} = \begin{pmatrix} -B_\epsilon & 0 \\ 0 & B_\epsilon \end{pmatrix} \quad \text{and} \quad H^{(1)} = \begin{pmatrix} 0 & -B_\epsilon \\ -B_\epsilon & 0 \end{pmatrix},
\]

with the exact zero-temperature eigenstates

\[
E_{\pm}(\lambda) = \pm \sqrt{B_\epsilon^2 + \lambda^2 B_\epsilon^2}.
\]

These eigenstates form an artificial avoided level crossing along the real-\( \lambda \) axis at \( \lambda = 0 \) that mirrors the true avoided crossing along the real \( B_\epsilon \) axis. The corresponding two-sheeted Riemann surface is shown in Figure 1(a). When the discriminant in Eq. (5) is zero, the eigenstates become degenerate, creating square-root branch points at \( \lambda = \pm B_\epsilon / B_\epsilon \) (black dot). 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.

**FIG. 1:** Internal energy for the two-level Hamiltonian [Eq. (4)] in the canonical ensemble as a function of the perturbation strength \( \lambda \) for \( B_\epsilon = \frac{1}{2} B_\epsilon \). (a) The zero-temperature ground and excited state energies form a two-sheeted Riemann surface with square-root branch points at \( \lambda = \pm B_\epsilon / B_\epsilon \) (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 internal energy for the two-level Hamiltonian [Eq. (4)] in the canonical ensemble as a function of the perturbation strength \( \lambda \) for \( B_\epsilon = \frac{1}{2} B_\epsilon \). (a) The zero-temperature ground and excited state energies form a two-sheeted Riemann surface with square-root branch points at \( \lambda = \pm B_\epsilon / B_\epsilon \) (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.
of a zero-temperature branch point. This property is shown for the partition function in the Supplemental Material and can be extended to the numerator of the internal energy. On the other hand, $Z(\lambda)$ can become zero in the complex-$\lambda$ plane, creating poles in the internal energy that dictate the radius of convergence for the perturbation expansion. At large temperatures, we find $Z(\lambda) \to 1$ for all $\lambda$. However, if we consider low temperatures near a degeneracy between $E_1(\lambda)$ and $E_2(\lambda)$, the partition function approximates to

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

(10)

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

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

(11)

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 $\omega_n$. For $T \to 0$, 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. 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 analytically in terms of the perturbation strength $\lambda$ as

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

(12)

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

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

(13)

Therefore, we see that the poles extend along the imaginary axis and their spacing decreases with temperature. When $T \to 0$, the poles tend towards a continuum extending outwards from the zero-temperature exceptional points, ultimately recovering the branch cut on the zero-temperature Riemann surface [Figure 1(a)].

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

$$r_c = \frac{B_z}{B_x} \sqrt{1 + \frac{\pi^2 k_B^2 T^2}{4 B_x^2}}.$$  

(14)

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

Remarkably, these results suggest that finite-temperature perturbation expansions are more likely to converge than their zero-temperature counterpart. In fact, at a sufficiently high temperature, a perturbation expansion of $U(\lambda)$ or $F(\lambda)$ will converge even if the zero-temperature perturbation expansion diverges. This scenario is illustrated in Figure 3 for the internal energy and Helmholtz free energy of the two-level system with $B_z = \frac{1}{2} B_x$. For these parameters, the ground-state perturbation corrections tend towards the divergent zero-temperature energy expansion in the $T \to 0$ limit. In contrast, the low-order perturbation corrections in the large-$T$ limit provide an excellent agreement with the exact results.

The temperature at which the thermodynamic perturbation expansion becomes convergent at $\lambda = 1$ can be identified by solving $r_c > 1$, giving $k_B T > \frac{7}{2} \sqrt{B_x^2 - B_z^2}$. For $B_z = \frac{1}{2} B_x$, this means that the perturbation expansion becomes convergent for $k_B T = 0.711763 B_z$, as indicated by the vertical gray lines in Figure 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). Significantly, the numerical data in Figure 3 and Table I demonstrate that the Helmholtz free energy and internal energy start to diverge at the same temperature, as expected. This result confirms that the poles of the partition function, which are common to both energy formulae, are the origin of these divergences.

**Relationship to Quantum Phase Transitions.**— Having identified the branch cut as the zero-temperature limit of zeros of the partition function in the two-level system, 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. 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 $B_z \to 0$. For a fixed value of $B_z > 0$, 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 $(S_z)$ at $\lambda = 0$, as shown in Figure 4 (left and middle panels respectively). For $B_z \neq 0$, a complex-conjugate pair of exceptional points exist in the complex-$\lambda$ plane, creating an avoided level crossing on the real axis (Figure 4; right panel). As expected, these zero-temperature exceptional points converge onto the real axis in the $B_z \to 0$ 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-$\lambda$ 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 partition function to converge onto the real axis in the $T \to 0$ and $B_z \to 0$ 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 $T \to 0$, these zeros form a continuum along the branch cut that terminates at the exceptional point. Therefore, in the $B_z \to 0$ limit, we find that 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 $T \to 0$, they must also converge onto the real axis as $B_z \to 0$, creating the expected behaviour 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.

Discussion. — We have shown that divergent finite-temperature perturbation theory is driven by poles 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 temper-
FIG. 4: 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 $B_x = 1$.

...through the lens of complex analysis. Recently, Lee–Yang zeros and exceptional points have been independently realised in experiments.\textsuperscript{28,29,35,36} 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 new aspects of non-Hermitian physics.

H.G.A.B. acknowledges Pierre-François Loos for enlightening discussions in the early stages of this work and David Tew for supporting this research. H.G.A.B. was supported by New College, Oxford through the Astor Junior Research Fellowship. Y.S. was supported by a Summer Research Studentship from Hertford College, Oxford.

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