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Article

Information Geometry of Complex Hamiltonians and Exceptional Points

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Abstract: Information geometry provides a tool to systematically investigate the parameter sensitivity of the state of a system. If a physical system is described by a linear combination of eigenstates of a complex (that is, non-Hermitian) Hamiltonian, then there can be phase transitions where dynamical properties of the system change abruptly. In the vicinities of the transition points, the state of the system becomes highly sensitive to the changes of the parameters in the Hamiltonian. The parameter sensitivity can then be measured in terms of the Fisher-Rao metric and the associated curvature of the parameter-space manifold. A general scheme for the geometric study of parameter-space manifolds of eigenstates of complex Hamiltonians is outlined here, leading to generic expressions for the metric.

Keywords: information geometry; non-Hermitian Hamiltonian; perturbation theory; Fisher-Rao metric; phase transition; exceptional point; PT symmetry

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1. Introduction

In statistical physics, if a system is in equilibrium with a heat bath at inverse temperature β, then the state of the system is characterised by the canonical phase-space density function:

$$\rho(x|\beta) = \frac{\mathrm{e}^{-\beta H(x)}}{Z(\beta)} \tag{1}$$

where $H(x)$ is the Hamiltonian function on phase space Ω and the partition function $Z(\beta)$ is given by the integral of the Boltzmann weight $\exp(-\beta H)$ over Ω. Systems having sufficiently rich inter-particle interactions can exhibit phase transitions. Typically, a phase transition is associated with the breakdown of the analyticity of one or more thermodynamic quantities, such as specific heat or magnetic susceptibility. The density function in Equation (1), on the other hand, is analytic, and one can legitimately ask in which way a breakdown of analyticity can be extracted from an analytic quantity. Indeed, for a real analytic function, it is not possible to find a breakdown of analyticity in a system having finitely many degrees of freedom, and it is mandatory to consider the operation of a thermodynamic limit.

If the state of a system is described by a density function (or a discrete set of probabilities) that lacks analyticity in the first place, however, then a phase transition can be seen without involving the mathematically cumbersome operation of the thermodynamic limit. Such situations arise in many physical contexts. For example, if an isolated quantum system is in a microcanonical state having support on the level surface of the expectation of the Hamiltonian, then the density of states is not analytic, and one can find thermal phase transitions in small quantum systems [1].

Another important example arises when considering eigenstates, or linear combinations of them, of complex Hamiltonian operators in quantum mechanics. While quantum mechanics traditionally focusses on closed systems described by Hermitian Hamiltonians, recently there has been considerable interest in relaxing the Hermiticity condition to consider more general complex Hamiltonians. For a Hermitian Hamiltonian in finite dimensions, the associated eigenfunctions are analytic in the parameters of the Hamiltonian, and a breakdown of analyticity may be obtained only in infinite dimensions. In the case of a complex Hamiltonian, however, the associated eigenfunctions need not be analytic in the parameters of the Hamiltonian, and phase transitions can be seen in finite matrix Hamiltonians (see, e.g., [2]). This situation is reminiscent of the analysis proposed by Lee and Yang [3,4], where the breakdown of analyticity associated with the canonical density function in Equation (1) can be explained by extending the parameters into a complex domain (see, e.g., [5] for a heuristic but informative exposition of the Lee-Yang theory). In this case, the canonical density function can exhibit lack of analyticity even in a system with finitely many degrees of freedom, in a way that resembles the eigenstates of finite complex Hamiltonians (see also [6] for a related point of view on these issues).

The transition points, or critical points, associated with eigenstates of a complex Hamiltonian are points at which degeneracies occur, that is, points at which not only eigenvalues but also eigenstates coalesce. In the literature, these critical points are often referred to as "exceptional points" (see [7] for a concise and informative overview of the physics of exceptional points). The purpose of the present paper is to investigate properties of eigenstates of complex Hamiltonians around exceptional points, from the viewpoint of inference theory. If a system, say, is in an eigenstate of a complex Hamiltonian, but an experimentalist does not know the exact values of the parameters in the Hamiltonian, then these parameter values can be estimated from observational data. Inference theory concerns the analysis of this data and, in particular, error bounds associated with such estimates. Evidently, if the eigenstate is sensitive to the changes of the parameter values, that is, if the state of the system changes significantly when the Hamiltonian is modified only slightly, then in this regime it is easy to estimate the parameter values. Conversely, if the state of the system is almost unaltered under the changes of the parameters, then in this regime estimation errors will be large. Hence, from the viewpoint of inference theory, we are interested in identifying the parameter sensitivity of the eigenfunctions of complex Hamiltonians. The method of information geometry then allows us to proceed with such an analysis, since it assigns distance measures between eigenstates of the Hamiltonian associated with different parameter values.

The paper is organised as follows. In Section 2, we give a brief overview of the method of information geometry applied to statistical physics for the benefit of readers less acquainted with the material. For a recent review of the use of information geometry in statistical mechanics, and a comprehensive list of references, see [8]. In Section 3, we explain in which way the standard method of information geometry, based on structures of *real* Hilbert space, extends into the case of *complex* Hilbert space. As an example, we consider in Section 4 the Hilbertian manifold generated by an eigenstate of a Hermitian Hamiltonian. In this context, we make use of the idea proposed in [9] of applying first-order perturbation theory to deduce a generic and intuitive form of the Riemannian metric on the manifold. Furthermore, we derive a new type of quantum uncertainty relation that arises naturally from the estimation of parameters in the Hamiltonian. In Section 5, we turn to the analysis of the geometry of the manifold associated with eigenstates of a complex Hamiltonian. Specifically, we derive an expression for the metric using the Rayleigh-Schrödinger perturbation theory on complex Hamiltonians, away from exceptional points. This perturbation expansion, however, breaks down in the vicinity of exceptional points. Thus, in Section 6, we apply generalised perturbation theory, so as to identify the generic structure of the metric close to an exceptional point where two of the eigenstates coalesce. In Section 7, we work out nonperturbatively the metric geometry of the parametric eigenstates in a simple example system, showing the existence of a geometric singularity at the exceptional point. The result is also compared to the perturbative analysis of Section 6.

We remark that while physical effects associated with the existence of exceptional points have been observed in laboratory experiments already as early as 1955 [10], only relatively recently, a controlled experimental investigation is being pursued [11–13]. In particular, investigations into the properties of complex Hamiltonians have increased significantly over the past decade since the observation of Bender and Boettcher that complex Hamiltonians possessing parity-time (PT) reversal symmetry can possess entirely real eigenvalues [14]. Phase transitions associated with the breakdown of PT symmetry of the eigenfunctions at exceptional points have also been predicted or observed in a range of model systems and experiments [15–26], and constitute an interesting and exciting area of application of information geometry. It is our hope that the present paper serves as a concise introduction to the physics of complex Hamiltonians for those who work in the area of information geometry and, at the same time, an introduction to information geometry for those who work in the study of physical systems described by complex Hamiltonians.

2. Information Geometry and Statistical Mechanics

To gain visual insights into the nature of critical points in statistical physics, we follow the mathematical scheme proposed by Rao [27] and consider the square-root map:

$$\rho(x|\beta) \to \xi(x|\beta) = \sqrt{\rho(x|\beta)} \tag{2}$$

It should be evident that the function $\xi(x|\beta)$ belongs to a real Hilbert space $\mathcal{H}$ of square-integrable functions on the phase space Ω of a given system. Thus, with respect to any given choice of coordinates in $\mathcal{H}$, we can think of $\xi(x|\beta)$ for each fixed value of β as a vector $|\xi(\beta)\rangle \in \mathcal{H}$ of unit length satisfying $\langle\xi(\beta)|\xi(\beta)\rangle = 1$. Here, we use the Dirac notation for representing elements of $\mathcal{H}$. If we vary the inverse temperature β, then the vector $|\xi(\beta)\rangle$ representing the thermal equilibrium state at β traverses along a smooth curve on the unit sphere in $\mathcal{H}$. In particular, in the limit $\beta \to \infty$, the equilibrium state $|\xi(\beta)\rangle$ of the system approaches the "ground state" of the Hamiltonian, *i.e.* a state with minimum energy. (Note that unless the parameter is changed adiabatically, the physical state of the system will not traverse the path, $|\xi(\beta)\rangle$ since a rapid change of temperature momentarily brings the state of the system out of equilibrium. Hence, we are not concerned here with the out-of-equilibrium dynamics of the system as such. Rather, we are interested in how an equilibrium configuration at one temperature is related to the equilibrium configuration at another temperature, and this is characterised by the path $|\xi(\beta)\rangle$. Our analysis thus reproduces the dynamical theory only in the adiabatic limit.)

If a system exhibits phase transitions, then the equilibrium curve $|\xi(\beta)\rangle$ can branch out into several curves at the critical points. For example, in the case of the Ising model with vanishing magnetic field, the curve bifurcates at the critical temperature; for the van der Waals model, the curve trifurcates at the critical point. Of course, such a scenario can prevail in the context of the canonical state (1) only if the dimensionality of $\mathcal{H}$ is infinite; nevertheless the concept of a one-dimensional curve residing on an infinite-dimensional unit sphere offers a visual characterisation of the situation.

In the case of a one-parameter family of states $|\xi(\beta)\rangle$, the parametric sensitivity can be measured in terms of the squared "velocity" (metric) and the squared "acceleration" (curvature) of the curve. By squared velocity, which we shall denote by G, we mean the inner product:

$$G = 4\langle\dot{\xi}(\beta)|\dot{\xi}(\beta)\rangle \tag{3}$$

where the dot represents differentiation with respect to β, and the factor of four is purely conventional so that G agrees with the information measure introduced by Fisher [28]. A short calculation shows [29] that in the case of the canonical state (1) we have $G = \Delta H^2$, that is, the variance of the Hamiltonian in the canonical state (1). Hence, in a region where the equilibrium energy uncertainty is small, the state of the system does not change much when the inverse temperature is changed, and this, in turn, means that an accurate estimation of β is difficult. Indeed, from the Cramér-Rao inequality, one finds that the quadratic error $\Delta\beta^2$ of the estimation is bounded below by $(4\Delta H^2)^{-1}$, and one obtains the thermodynamic uncertainty relation [30,31]:

$$\Delta T^{-1}\,\Delta H \geq \frac{k_B}{2} \tag{4}$$

where we have written $\beta = 1/k_B T$, with k_B the Boltzmann constant.

Similarly, the acceleration vector $|\alpha(\beta)\rangle$ of the curve is defined by:

$$|\alpha(\beta)\rangle = |\ddot{\xi}(\beta)\rangle - \frac{\langle\dot{\xi}(\beta)|\ddot{\xi}(\beta)\rangle}{\langle\dot{\xi}(\beta)|\dot{\xi}(\beta)\rangle}\,|\dot{\xi}(\beta)\rangle - \langle\xi(\beta)|\ddot{\xi}(\beta)\rangle\,|\xi(\beta)\rangle \tag{5}$$

where $|\ddot{\xi}(\beta)\rangle = \partial_\beta^2|\xi(\beta)\rangle$. In terms of the acceleration vector, the intrinsic curvature $\mathcal{K}^2$ of the curve $|\xi(\beta)\rangle$ is given by:

$$\mathcal{K}^2 = \frac{16}{G^2}\langle\alpha(\beta)|\alpha(\beta)\rangle \tag{6}$$

In the case of the canonical state (1), a calculation shows [29] that:

$$\mathcal{K}^2 = \frac{\Delta H^4}{(\Delta H^2)^2} - \frac{(\Delta H^3)^2}{(\Delta H^2)^3} - 1 \tag{7}$$

where we have written ΔH^k to mean the k^{th} central moment of the Hamiltonian in the thermal state (1).

More generally, consider a generic density function $\rho(x|\theta)$ dependent on one or several parameters, $\{\theta^a\}_{a=1,\ldots,N}$, normalised for all values of $\{\theta^a\}$. Then, for each fixed set of values of $\{\theta^a\}$, the square-root map (2) determines a point $|\xi(\theta)\rangle$ on the unit sphere of Hilbert space. When the values of the parameters are varied, $|\xi(\theta)\rangle$ traverses along an N-dimensional surface $\mathfrak{M}$ on the sphere. A standard result in Riemannian geometry of subspaces then shows that the metric on the subspace $\mathfrak{M}$ is determined by:

$$G_{ab} = 4\langle \partial_a \xi(\theta) | \partial_b \xi(\theta) \rangle \tag{8}$$

where, again, the scale factor of four is purely conventional, and we have written $\partial_a = \partial/\partial\theta^a$. The quadratic form (8) in the statistical context is known as the Fisher-Rao metric. With the expression of the metric tensor (8) at hand, one can proceed to calculate invariant quantities, such as the Ricci curvature, or geodesic curves on $\mathfrak{M}$. For example, given a pair of points θ and θ' on $\mathfrak{M}$, the separation between the two states $|\xi(\theta)\rangle$ and $|\xi(\theta')\rangle$ is given by the distance of the geodesic curve joining these two points on $\mathfrak{M}$. Such a distance then determines the divergence measure between the two states $|\xi(\theta)\rangle$ and $|\xi(\theta')\rangle$, which is more informative than the mere overlap distance $\cos^{-1}(\langle \xi(\theta)|\xi(\theta')\rangle)$.

In the context of statistical mechanics, the curvature of $\mathfrak{M}$ associated with the Fisher-Rao metric is singular along the spinodal curve, which contains the critical point [8]. Typically, on the equilibrium state manifold $\mathfrak{M}$ there is an unphysical region, e.g., a region in which the magnetisation decreases in increasing external field in the Ising model, or a region in which, according to the equation of states, the pressure decreases in increasing volume in the van der Waals model. The spinodal curve gives the boundary of such unphysical regions, and it is along this boundary that the curvature diverges, thus, in some sense, "preventing" a smooth entry into unphysical regions. The method of information geometry, therefore, provides geometric insights into the physics of critical phenomena.

3. Statistical Geometry in Complex Vector Spaces

The geometric analysis of the parametric subspace of the real Hilbert space extends, *mutatis mutandis*, to the complex domain—for example, to the complex Hilbert space of states in quantum mechanics. There are, however, some modifications arising, which we shall discuss now. Consider first the case of a parametric curve $|\xi(\theta)\rangle$ satisfying the normalisation condition $\langle\xi(\theta)|\xi(\theta)\rangle = 1$, where $\langle\xi(\theta)|$ now denotes the Hermitian conjugate of $|\xi(\theta)\rangle$. In the complex case, the condition $\partial_\theta\langle\xi(\theta)|\xi(\theta)\rangle = 0$ does not imply $\langle\dot{\xi}(\theta)|\xi(\theta)\rangle = 0$ owing to the phase factor, so we require a modified expression:

$$|v(\theta)\rangle = |\dot{\xi}(\theta)\rangle - \langle\xi(\theta)|\dot{\xi}(\theta)\rangle\, |\xi(\theta)\rangle \tag{9}$$

for the proper "velocity" vector. The squared velocity (with a factor of four) is then given by:

$$G = 4\left(\langle\dot{\xi}(\theta)|\dot{\xi}(\theta)\rangle - \langle\xi(\theta)|\dot{\xi}(\theta)\rangle\langle\dot{\xi}(\theta)|\xi(\theta)\rangle\right) \tag{10}$$

The simplest situation of a curve $|\xi(\theta)\rangle$ that arises in quantum mechanics is the solution to the Schrödinger equation:

$$\mathrm{i}\hbar|\dot{\xi}\rangle = \hat{H}|\xi\rangle \tag{11}$$

with initial condition $|\xi(0)\rangle$ satisfying $\langle\xi(0)|\xi(0)\rangle = 1$, where the parameter θ represents time. A short calculation then shows that the squared velocity is given by the energy uncertainty:

$$G = \frac{4\Delta H^2}{\hbar^2} \tag{12}$$

which, of course, is merely the statement of the Anandan-Aharanov relation [32]. From the viewpoint of inference theory, we can think of a situation in which a quantum system, prepared in an initial state, is made to evolve under the influence of the Hamiltonian $\hat{H}$. After a passage of time, an experimentalist performs a measurement to estimate how much time has elapsed since its initial preparation. The Cramér-Rao relation then asserts that the quadratic error of time estimation is bounded below by $\hbar^2(4\Delta H^2)^{-1}$, which is just the Heisenberg uncertainty relation (see [29,33] for further details on the problem of time estimation).

More generally, an alternative way of deducing the geometry of a parametric subspace $\mathfrak{M}$ of the quantum state space is to make use of the Fubini-Study geometry of the ambient state space. Here, by a "quantum state space", we mean the space of rays through the origin of the Hilbert space, *i.e.*, the complex projective space. If we write $\mathrm{d}s$ for the line element on the state space of a neighbouring pair of states $|\xi\rangle$ and $|\xi + \mathrm{d}\xi\rangle = |\xi\rangle + |\mathrm{d}\xi\rangle$, then we have the relation:

$$\cos^2 \tfrac{1}{2}\mathrm{d}s = \frac{\langle\xi|\xi + \mathrm{d}\xi\rangle\langle\xi + \mathrm{d}\xi|\xi\rangle}{\langle\xi|\xi\rangle\langle\xi + \mathrm{d}\xi|\xi + \mathrm{d}\xi\rangle} \tag{13}$$

Solving this for $\mathrm{d}s$ and retaining terms of quadratic order, we obtain the Fubini-Study line element:

$$\mathrm{d}s^2 = 4\frac{\langle\xi|\xi\rangle\langle\mathrm{d}\xi|\mathrm{d}\xi\rangle - \langle\xi|\mathrm{d}\xi\rangle\langle\mathrm{d}\xi|\xi\rangle}{\langle\xi|\xi\rangle^2} \tag{14}$$

Now suppose that the state $|\xi\rangle = |\xi(\theta)\rangle$ depends smoothly on a set of parameters $\{\theta^a\}_{a=1,\ldots,N}$, and is normalised to unity for all values of $\{\theta^a\}$. Then, we have $|\mathrm{d}\xi\rangle = |\partial_a\xi\rangle\mathrm{d}\theta^a$, using the summation convention, so that the quantum Fisher-Rao metric on the parameter manifold $\mathfrak{M}$ induced by the ambient Fubini-Study geometry (14) is determined by the line element:

$$\mathrm{d}s^2 = 4\big(\langle\partial_a\xi|\partial_b\xi\rangle - \langle\xi|\partial_a\xi\rangle\langle\partial_b\xi|\xi\rangle\big)\mathrm{d}\theta^a\mathrm{d}\theta^b \tag{15}$$

In other words, the metric tensor is given by:

$$G_{ab} = 4\left(\langle\partial_{(a}\xi|\partial_{b)}\xi\rangle - \langle\xi|\partial_{(a}\xi\rangle\langle\partial_{b)}\xi|\xi\rangle\right) \tag{16}$$

where the brackets in the subscripts denote symmetrisation (which gives the real part of the expression without the symmetrisation). In particular, for $N = 1$ we recover the expression in Equation (10).

4. Eigengeometry of Hermitian Hamiltonians

Apart from the examples of a one-parameter family of states associated with orbits generated by a Hermitian Hamiltonian $\hat{H}$, there are many other situations of interests in quantum theory where the notion of a statistical manifold $\mathfrak{M}$ plays an important role. For example, the parameters $\{\theta^j\}$ may represent the coordinates for atomic coherent states, in which case Equation (16) determines the metric of the coherent-state manifold (see [34] and references cited therein for a detailed calculation of the geometry of coherent states). Alternatively, and this is the case of interest here, if $|\xi\rangle$ represents an eigenstate of a Hamiltonian $\hat{H}$ such that some of the parameters in $\hat{H}$ can be adjusted, then we obtain another example of a statistical manifold $\mathfrak{M}$. The geometry of $\mathfrak{M}$ can then exhibit nontrivial behaviour for systems describing quantum phase transitions.

In the context of an information-geometric analysis of quantum phase transitions, it has been pointed out in [9] (see also [35,36] for a closely related analysis) that perturbation analysis can be effective in gaining insights into the properties of the metric (16). Traditionally, in the literature on quantum phase transitions, there is a lot of focus on the behaviour of the ground state; however, transitions can occur in a multitude of ways. Here we consider an n^{th} eigenstate of a Hermitian Hamiltonian $\hat{H}(\theta)$:

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle \tag{17}$$

where, for simplicity of notation, we have omitted the θ-dependence of $\hat{H}$, E_n and $|\phi_n\rangle$. Assuming that the eigenvalues of $\hat{H}(\theta)$ are nondegenerate, we can use first-order perturbation theory to deduce that:

$$|\partial_a\phi_n\rangle = \sum_{m\neq n} \frac{\langle\phi_m|\partial_a\hat{H}|\phi_n\rangle}{E_n - E_m}|\phi_m\rangle \tag{18}$$

Substituting this in Equation (16), we find that:

$$G_{ab} = 4\sum_{m\neq n} \frac{\langle\phi_n|\partial_{(a}\hat{H}|\phi_m\rangle\langle\phi_m|\partial_{b)}\hat{H}|\phi_n\rangle}{(E_n - E_m)^2} \tag{19}$$

Observe that the skew-symmetric form obtained from the imaginary part of the expression (19), without the symmetrisation over indices, is just the Berry curvature form appearing in the analysis of geometric phases [37].

To gain intuition about the metric (19), consider the problem of estimating the values of the parameters appearing in the Hamiltonian, when the system is prepared in the n^{th} eigenstate. In a region where the state $|\phi_n\rangle$ is sensitive to the changes of the parameter values, the components of the Fisher-Rao metric (19) are large, and the estimation can be made accurately. If the system exhibits quantum phase transitions, where one or more of the eigenvalues approach the level E_n, then the metric becomes singular. Of course, the perturbation (18) is applicable only away from degeneracies, and hence, in the vicinity of degeneracies, higher-order perturbative analysis is required to identify detailed properties of the metric geometry. In addition, the metric tensor is not invariant under coordinate transformations; hence, for a more comprehensive analysis, one is required to work out an expression for the Ricci scalar. Such an analysis would shed further light on the theoretical study of quantum phase transitions.

An alternative way of interpreting the metric (19) has been suggested in [9], which we shall develop further here, since it is relevant to information-geometric considerations. For $\mathrm{d}\theta \ll 1$, and away from degeneracies, we define the unitary operator according to the prescription:

$$\hat{U} = \sum_n |\phi_n(\theta + \mathrm{d}\theta)\rangle\langle\phi_n(\theta)| \tag{20}$$

Evidently, $\hat{U}$ transports the state $|\phi_n(\theta)\rangle$ into $|\phi_n(\theta + \mathrm{d}\theta)\rangle$. The generators of this evolution are then given by the observables:

$$\hat{X}_a = \mathrm{i}(\partial_a \hat{U})\hat{U}^{-1} \tag{21}$$

It is then a short exercise to show that the Fisher-Rao metric is just the covariance matrix for the observables $\hat{X}_a$ [9].

Suppose that we let $\hat{\Theta}^a$ denote the unbiased estimator for the parameter θ^a. By an unbiased estimator, we mean an operator acting on the states of the Hilbert space with the property that $\langle\phi_n(\theta)|\hat{\Theta}^a|\phi_n(\theta)\rangle = \theta^a$ holds for all values of the parameters. Then, the two operators $\hat{\Theta}^a$ and $\hat{X}_a$ are conjugate to each other. In particular, from the Cramér-Rao inequality we find that the covariance matrix of $\hat{\Theta}^a$ is bounded below by the reciprocal of the Fisher-Rao metric. Hence, the operator pair $(\hat{\Theta}^a, \hat{X}_a)$ for each a satisfies a Heisenberg-like uncertainty relation. As an example, suppose that there is a single control parameter θ in the Hamiltonian and that $\hat{\Theta}$ is the unbiased estimator for θ, satisfying $\langle\phi_n(\theta)|\hat{\Theta}|\phi_n(\theta)\rangle = \theta$. (In general, $\hat{\Theta}$ will not be a self-adjoint operator; see, e.g., [33] for explicit constructions of such examples in a different context.) Suppose, further, that $\lambda^{-1}\hat{X}$ is the self-adjoint operator generating the shift in the parameter θ so that $\mathrm{e}^{-\mathrm{i}\hat{X}\epsilon/\lambda}|\phi(\theta)\rangle = |\phi(\theta+\epsilon)\rangle$ for $\epsilon \ll 1$. Here, λ is a constant such that $\hat{X}\epsilon/\lambda$ is dimensionless. In this situation, since the Fisher information is just the variance of the generator $\hat{X}$, it follows from the Cramér-Rao inequality that the parameter estimate for θ is limited by the variance lower bound of the form:

$$\Delta\Theta^2\,\Delta X^2 \geq \frac{\lambda^2}{4} \tag{22}$$

where by $\Delta\Theta^2$ we mean the variance of $\hat{\Theta}$, and similarly for ΔX^2. It also follows (setting $\lambda = 1$) that:

$$\Delta X^2 = \sum_{m \neq n} \frac{\langle\phi_n|\hat{H}'|\phi_m\rangle\langle\phi_m|\hat{H}'|\phi_n\rangle}{(E_n - E_m)^2} \tag{23}$$

where we have written $\hat{H}' = \partial_\theta \hat{H}$. We remark that Equation (22) represents a new type of uncertainty relation in quantum mechanics that is in principle verifiable in laboratory experiments.

The perturbation analysis indicated above can also be applied to obtain an expression for the curvature of a curve associated with a one-parameter family of eigenstates $|\phi_n(\theta)\rangle$ of a parametric Hamiltonian $\hat{H}(\theta)$. In the one-parameter case, Equation (18) reduces to:

$$|\dot{\phi}_n\rangle = \sum_{m \neq n} \frac{\langle\phi_m|\hat{H}'|\phi_n\rangle}{E_n - E_m}|\phi_m\rangle \tag{24}$$

Assuming that $\hat{H}(\theta)$ is nondegenerate, the second-order term in perturbation series gives:

$$|\ddot{\phi}_n\rangle = 2\sum_{m\neq n}\left[\sum_{l\neq n}\frac{\langle\phi_m|\hat{H}'|\phi_l\rangle\langle\phi_l|\hat{H}'|\phi_n\rangle}{(E_n-E_m)(E_n-E_l)} - \frac{\langle\phi_n|\hat{H}'|\phi_n\rangle\langle\phi_m|\hat{H}'|\phi_n\rangle}{(E_n-E_m)^2}\right]|\phi_m\rangle \tag{25}$$

which shows that $\langle\phi_n|\ddot{\phi}_n\rangle = 0$. In this case, the expression for the intrinsic curvature becomes:

$$\mathcal{K}_n^2 = \frac{\langle\ddot{\phi}_n|\ddot{\phi}_n\rangle}{\langle\dot{\phi}_n|\dot{\phi}_n\rangle^2} - \frac{\langle\ddot{\phi}_n|\dot{\phi}_n\rangle\langle\dot{\phi}_n|\ddot{\phi}_n\rangle}{\langle\dot{\phi}_n|\dot{\phi}_n\rangle^3} \tag{26}$$

Substitution of Equations (24) and (25) in Equation (26) then gives the expression for the curvature, which, in turn, can be used (*cf.* [38]) to derive a higher-order correction to the uncertainty lower bound in Equation (22).

5. Information Geometry for Complex Hamiltonians

We now wish to examine the statistical manifold $\mathfrak{M}$ associated with eigenstates of a complex Hamiltonian $\hat{K}$ for which $\hat{K}^\dagger \neq \hat{K}$. Complex Hamiltonians are traditionally used to describe decay and scattering phenomena [39–43]. They are also used in the context of open systems as effective Hamiltonians. More recently, complex Hamiltonians that fulfil certain antilinear symmetries have attracted a lot of attention, owing to the facts that such Hamiltonians may possess entirely real eigenvalues and that depending on the parameter values in the Hamiltonian there can be a phase transition where a pair of real eigenvalues degenerates and turns into a complex conjugate pair [15–26]. As indicated above, such a critical point is where the associated eigenstates also coalesce, thus constituting an example of an exceptional point. Here we are interested in the geometry of the statistical manifold $\mathfrak{M}$ associated with such a Hamiltonian exhibiting one or more phase transitions.

To proceed, let $\hat{K} = \hat{H} - \mathrm{i}\hat{\Gamma}$, where $\hat{H}^\dagger = \hat{H}$ and $\hat{\Gamma}^\dagger = \hat{\Gamma}$, be a complex Hamiltonian with eigenstates $\{|\phi_n\rangle\}$ and nondegenerate eigenvalues $\{\kappa_n\}$:

$$\hat{K}|\phi_n\rangle = \kappa_n|\phi_n\rangle \quad \text{and} \quad \langle\phi_n|\hat{K}^\dagger = \bar{\kappa}_n\langle\phi_n| \tag{27}$$

Additionally, it will be convenient to introduce eigenstates of the adjoint matrix $\hat{K}^\dagger$:

$$\hat{K}^\dagger|\chi_n\rangle = \bar{\kappa}_n|\chi_n\rangle \quad \text{and} \quad \langle\chi_n|\hat{K} = \kappa_n\langle\chi_n| \tag{28}$$

The reason for introducing the additional states $\{|\chi_n\rangle\}$ is because the eigenstates $\{|\phi_n\rangle\}$ of $\hat{K}$ are in general not orthogonal, and hence conventional projection techniques so commonly used in many calculations of quantum mechanics, in particular, in perturbation theory, are not effective when dealing with the eigenstates of a complex Hamiltonian [43–48]. With the introduction of the states $\{|\chi_n\rangle\}$, however, we have the relations:

$$\langle\chi_n|\phi_m\rangle = \delta_{nm}\langle\chi_n|\phi_n\rangle \quad \text{and} \quad \sum_n \frac{|\phi_n\rangle\langle\chi_n|}{\langle\chi_n|\phi_n\rangle} = \mathbb{1} \tag{29}$$

which hold in finite dimensions away from degeneracies.

With the use of the biorthogonal states, the notion of an associated state can be introduced: For an arbitrary state $|\psi\rangle$, we define the associated state $|\tilde{\psi}\rangle$ according to the following relations:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \quad \Leftrightarrow \quad \langle\tilde{\psi}| = \sum_n \bar{c}_n\langle\chi_n| \tag{30}$$

We shall let Equation (30) determine the duality relation on the state space. Additionally, for convenience we assume that $\langle\chi_n|\phi_n\rangle = 1$ holds for all n. Under this convention, the states are no longer normalised, *i.e.*, $\langle\psi|\psi\rangle > 1$, but we can assume that:

$$\langle\tilde{\psi}|\psi\rangle = \sum_n \bar{c}_n c_n = 1 \tag{31}$$

At an exceptional point, however, the convention $\langle\chi_{EP}|\phi_{EP}\rangle = 1$ breaks down for the following reason. Suppose that the two eigenstates $|\phi_k\rangle$ and $|\phi_l\rangle$ "meet" at $|\phi_{EP}\rangle$. Evidently, the biorthogonality condition implies that $\langle\chi_l|\phi_k\rangle = 0$ and $\langle\chi_k|\phi_k\rangle \neq 0$, but $\langle\chi_l|$ and $\langle\chi_k|$ will both approach $\langle\chi_{EP}|$ so that we have $\langle\chi_{EP}|\phi_{EP}\rangle = 0$. This feature is often referred to as "self-orthogonality" in the literature. To complete the basis for the eigenspace belonging to the degenerate eigenstate, one needs to introduce associated eigenvectors, or so-called *Jordan vectors*. We will return to this issue in the discussion of exceptional points in the section to follow, but for now, we assume that the states are away from degeneracies.

Away from exceptional points, and based on the convention that $\langle\chi_n|\phi_n\rangle = 1$, the overlap distance s between the two states $|\xi\rangle$ and $|\eta\rangle$ is now given by the expression:

$$\cos^2 \tfrac{1}{2}s = \frac{\langle\tilde{\xi}|\eta\rangle\langle\tilde{\eta}|\xi\rangle}{\langle\tilde{\xi}|\xi\rangle\langle\tilde{\eta}|\eta\rangle} \tag{32}$$

In particular, if $|\eta\rangle = |\xi\rangle + |\mathrm{d}\xi\rangle$ is a neighbouring state to $|\xi\rangle$, then expanding Equation (32) and retaining the terms of quadratic order, we obtain the following form of the Fubini-Study line element:

$$\mathrm{d}s^2 = 4\frac{\langle\tilde{\xi}|\xi\rangle\langle\widetilde{\mathrm{d}\xi}|\mathrm{d}\xi\rangle - \langle\tilde{\xi}|\mathrm{d}\xi\rangle\langle\widetilde{\mathrm{d}\xi}|\xi\rangle}{\langle\tilde{\xi}|\xi\rangle^2} \tag{33}$$

We remark that an analogous expression for the metric appears in [49]; however, Equation (33) is different from the metric obtained in [49], since we have chosen a different definition for an associated state $\langle\tilde{\xi}|$.

With the alternative expression in Equation (33) for the Fubini-Study metric at hand, we are in a position to investigate the metric geometry of the eigenstates of complex Hamiltonians. To begin, recall that for the identification of the local metric geometry of the statistical manifold $\mathfrak{M}$ associated with an eigenstate $|\phi_n\rangle$ of a Hamiltonian $\hat{K}$ we need to determine the perturbation $|\partial_a\phi_n\rangle\mathrm{d}\theta^a$ of the state associated with a small change in the parameter values. For this purpose, we shall follow closely the approach of [40]. Specifically, with the convention $\langle\chi_n|\phi_n\rangle = 1$ and the help of the biorthogonal states $(\{|\phi_n\rangle\}, \{|\chi_n\rangle\})$, we consider the perturbation of an eigenstate away from degeneracies. Then the eigenvalues and eigenvectors can be expanded in a Taylor series in the perturbation parameter, much as in the Hermitian case. Taylor expanding the Hamiltonian $\hat{K}(\theta)$, the eigenstate $|\phi_n(\theta)\rangle$, and the eigenvalue $\kappa_n(\theta)$ at θ in the eigenvalue equation, we obtain:

$$(\hat{K} + \partial_a\hat{K}\mathrm{d}\theta^a + \cdots)(|\phi_n\rangle + |\partial_a\phi_n\rangle\mathrm{d}\theta^a + \cdots) = (\kappa_n + \partial_a\kappa_n\mathrm{d}\theta^a + \cdots)(|\phi_n\rangle + |\partial_a\phi_n\rangle\mathrm{d}\theta^a \cdots) \tag{34}$$

where we have omitted explicit θ dependencies. Equating the terms linear in $\mathrm{d}\theta$, we find:

$$(\hat{K} - \kappa_n)|\partial_a \phi_n\rangle = \partial_a \kappa_n |\phi_n\rangle - \partial_a \hat{K}|\phi_n\rangle \tag{35}$$

So far, the result is identical to that for a Hermitian Hamiltonian. However, the lack of orthogonality of the eigenstates prevents us from using the projector $\hat{\Phi}_m = |\phi_m\rangle\langle\phi_m|$ to further simplify the expression. Nevertheless, if we multiply $\hat{\Pi}_m = |\phi_m\rangle\langle\chi_m|$ from the left and rearrange terms, we find:

$$(\kappa_m - \kappa_n)\hat{\Pi}_m|\partial_a \phi_n\rangle = (\partial_a \kappa_n)\delta_{mn}|\phi_m\rangle - \langle\chi_m|\partial_a \hat{K}|\phi_n\rangle|\phi_m\rangle \tag{36}$$

For $n = m$, we are led to the expression (*cf.* [46]):

$$\partial_a \kappa_n = \langle\chi_n|\partial_a \hat{K}|\phi_n\rangle \tag{37}$$

To obtain an expression for $|\partial_k \phi_n\rangle$, in [40] the operator $(\hat{K} - \kappa_n \mathbb{1})^{-1}$ is applied from the left in Equation (35). This approach, however, is problematic on account of the fact that $(\hat{K} - \kappa_n \mathbb{1})$ is degenerate and thus not invertible. The result of [40] can nevertheless be justified if we make the assumption that the perturbation vector $|\partial_a \phi_n\rangle \mathrm{d}\theta^a$ is orthogonal to the dual vector $|\chi_n\rangle$. With this assumption, which turns out to be the correct one, for $n \neq m$ we divide both sides of Equation (36) by $\kappa_m - \kappa_n$ and sum over $m \neq n$ to obtain:

$$|\partial_a \phi_n\rangle = \sum_{m \neq n} \frac{\langle\chi_m|\partial_a \hat{K}|\phi_n\rangle}{\kappa_n - \kappa_m}|\phi_m\rangle \tag{38}$$

where we have made use of the condition, $\langle\chi_m|\mathrm{d}\phi_m\rangle = 0$.

The perturbation term of Equation (38) formally resembles the expression in Equation (18) of its Hermitian counterpart. However, there are important differences, including the fact that the perturbation is not orthogonal to the state $|\phi_n\rangle$, *i.e.*, $\langle\phi_n|\partial_a \phi_n\rangle \neq 0$, but rather $\langle\chi_n|\partial_a \phi_n\rangle = 0$. It follows that under this assumption the perturbation will necessarily change the overall complex phase of the eigenstate. This is nevertheless natural under the geometry of the state space formulated from Equation (33).

The metric geometry of the parameter space can now be determined if we substitute Equation (38) in Equation (33):

$$G_{ab} = 4 \sum_{m \neq n} \frac{\langle\chi_m|\partial_{(a} \hat{K}|\phi_n\rangle\langle\phi_n|\partial_{b)} \hat{K}|\chi_m\rangle}{(\bar{\kappa}_n - \bar{\kappa}_m)(\kappa_n - \kappa_m)} \tag{39}$$

With the expression in Equation (39) at hand, we are able to investigate the geometry of the statistical manifold associated with eigenstates of complex Hamiltonians, away from degeneracies. Incidentally, this expression for the metric is in line with the analysis of geometric phases associated with the eigenstates of complex Hamiltonians [50–53]. Since the perturbative result of Equation (39) is only valid away from degeneracies, in the next section we shall investigate the generic behaviour close to the exceptional point by employing a more refined perturbative technique.

6. Geometry Close to Exceptional Points

In the case of a Hermitian Hamiltonian, the first-order perturbation used to derive expression (19) for the metric breaks down near degeneracies, and one has to consider higher-order perturbations. In the case of a complex Hamiltonian, the situation is more severe on account of the fact that the Rayleigh-Schrödinger perturbation theory breaks down altogether in the vicinities of exceptional points. Nevertheless, for a given Hamiltonian, one can expand the eigenstates and eigenvalues in the form of a Newton-Puiseux series in order to identify the metric geometry close to exceptional points (see, for example, [54,55] for effective use of the Newton-Puiseux expansion for the investigation of properties of the eigenstates of complex Hamiltonians in the vicinities of exceptional points; see, also, [56,57] for a more general discussion on related mathematical ideas). This line of investigation, therefore, leads to a new application of information geometry in the sensitivity analysis of physical systems characterised by Hermitian or more generally complex Hamiltonians (we remark that properties of exceptional points of higher order, where more than two eigenstates coalesce, can be quite intricate; see, e.g., [58,59]).

Let us illustrate how such an analysis can be applied to deduce the nature of geometric singularities close to exceptional points. For more details on perturbation theory around exceptional points, see, e.g., [57] and the references cited therein. As indicated above, at an exceptional point, two or more eigenvalues and the corresponding eigenstates coalesce, that is, the Hamiltonian is not diagonalisable. Here, we consider the most common case, where two eigenvalues and the corresponding eigenstates coalesce. At such an exceptional point, there is a two-fold degenerate eigenvalue κ_{EP} and a single eigenvector $|\phi_{EP}\rangle$, which is orthogonal to the corresponding left eigenvector: $\langle\chi_{EP}|\phi_{EP}\rangle = 0$. However, one can define an associated vector, the so-called Jordan vector, denoted $|\phi^J_{EP}\rangle$, fulfilling the relation:

$$\hat{K}|\phi^J_{EP}\rangle = \kappa_{EP}|\phi^J_{EP}\rangle + |\phi_{EP}\rangle \tag{40}$$

Similarly, the left Jordan vector can be defined according to the relation:

$$\hat{K}^\dagger|\chi^J_{EP}\rangle = \bar{\kappa}_{EP}|\chi^J_{EP}\rangle + |\chi_{EP}\rangle \tag{41}$$

The Jordan vector $|\phi^J_{EP}\rangle$ and the eigenvector $|\phi_{EP}\rangle$ span the two-dimensional eigenspace corresponding to the degenerate eigenvalue κ_{EP}. Note that the Jordan vector is not uniquely defined by Equation (40). However, the ambiguity can be removed by choosing appropriate normalisation conditions [57]. In fact, it will be convenient to normalise the states such that:

$$\langle\chi_{EP}|\phi^J_{EP}\rangle = \langle\chi^J_{EP}|\phi_{EP}\rangle = 1 \tag{42}$$

and that:

$$\langle\chi^J_{EP}|\phi^J_{EP}\rangle = 0 \tag{43}$$

As already indicated, conventional Rayleigh-Schrödinger perturbation theory breaks down around an exceptional point, and in general, the eigenvalues and eigenvectors are not analytic functions of the perturbation parameter. That is, they cannot be expanded in a Taylor series. In the general case, they can nevertheless be expanded into a power series with fractional exponents, which is known as a Puiseux series. While in general one has to distinguish different cases of perturbation behaviours [60], the most common, generic behaviour around an exceptional point at which two eigenvectors coalesce is that the eigenvalues and eigenvectors can be expanded in a power series with half-integer exponents.

Let $\epsilon \ll 1$ denote a small perturbation parameter that measures the deviation away from the exceptional point. Expanding the Hamiltonian, the eigenvalues, and eigenvectors to lowest order in ϵ in the eigenvalue equation yields:

$$(\hat{K}_{EP} + \epsilon\hat{K}' + \cdots)(|\phi_{EP}\rangle + |\phi'\rangle\epsilon^{\frac{1}{2}} + \cdots) = (\kappa_{EP} + \kappa'\epsilon^{\frac{1}{2}} + \cdots)(|\phi_{EP}\rangle + |\phi'\rangle\epsilon^{\frac{1}{2}} + \cdots) \tag{44}$$

Equating terms corresponding to different powers of ϵ and using Equations (40)–(43), we find that the two eigenstates $|\phi_\pm\rangle$ can be expanded in the vicinity of an exceptional point in the form:

$$|\phi_\pm\rangle = n\left(|\phi_{EP}\rangle + \kappa'_\pm\,\epsilon^{\frac{1}{2}}\,|\phi^J_{EP}\rangle + O(\epsilon)\right) \tag{45}$$

where:

$$\kappa'_\pm = \pm\sqrt{\langle\chi_{EP}|\hat{K}'|\phi_{EP}\rangle} \tag{46}$$

A perturbative expression similar to Equation (45) holds for the left eigenvector. The resulting left and right eigenvectors are automatically orthogonal; however, they are only defined up to a normalisation constant n. It is convenient to normalise these vectors according to the usual biorthogonal convention away from the exceptional point: $\langle\chi_\pm|\phi_\pm\rangle = 1$. From this, we find:

$$|\phi_\pm\rangle \approx \frac{1}{\sqrt{2\kappa'}\epsilon^{1/4}}\left(|\phi_{EP}\rangle + \kappa'\,\epsilon^{\frac{1}{2}}\,|\phi^J_{EP}\rangle\right), \quad \langle\chi_\pm| \approx \frac{1}{\sqrt{2\kappa'}\epsilon^{1/4}}\left(\langle\chi_{EP}| + \kappa'\,\epsilon^{\frac{1}{2}}\,\langle\chi^J_{EP}|\right) \tag{47}$$

A calculation then shows that:

$$|\mathrm{d}\phi_+\rangle = \frac{1}{4\sqrt{\kappa'}}\left(-\epsilon^{-\frac{5}{4}}|\phi_{EP}\rangle + \kappa'\,\epsilon^{-\frac{3}{4}}\,|\phi^J_{EP}\rangle\right)\mathrm{d}\epsilon = \frac{1}{4\epsilon}\,|\phi_-\rangle\mathrm{d}\epsilon \tag{48}$$

and hence that:

$$\langle\widetilde{\mathrm{d}\phi_+}| = \frac{1}{4\epsilon}\langle\chi_-|\mathrm{d}\epsilon \tag{49}$$

From Equations (48) and (49), we thus find the expression of the metric close to an exceptional point of the second order where two eigenstates coalesce:

$$G = \frac{1}{4\epsilon^2} \tag{50}$$

on account of Equation (33). It should be remarked that the result of Equation (50) is generic, *i.e.*, it is independent of the model. It can therefore be viewed as providing the scaling property of the metric close to an exceptional point of second order, in a manner analogous to the scaling behaviour of the metric near critical points in statistical mechanics of phase transitions [61].

7. Discussion and Summary

We conclude by remarking that although in the foregoing material, we have placed some emphasis on perturbative analysis for the geometry surrounding exceptional points so as to obtain generic expressions for the metric, if a model is specified, then typically there is no need for evoking the perturbative approach since the metric can be computed exactly. As an example, take the 2×2 Hamiltonian, $\hat{K} = \hat{\sigma}_x - \mathrm{i}\gamma\hat{\sigma}_z$. This Hamiltonian is PT-symmetric and has real eigenvalues in the region $\gamma^2 < 1$ where the eigenstates are also PT-symmetric. Specifically, the eigenstates of $\hat{K}$ and $\hat{K}^\dagger$ are given by:

$$|\phi_\pm\rangle = n_\pm \begin{pmatrix} 1 \\ \mathrm{i}\gamma \pm \sqrt{1-\gamma^2} \end{pmatrix}, \qquad |\chi_\pm\rangle = n_\mp \begin{pmatrix} 1 \\ -\mathrm{i}\gamma \pm \sqrt{1-\gamma^2} \end{pmatrix} \tag{51}$$

where $n_\pm^2 = (1 \mp \mathrm{i}\gamma/\sqrt{1-\gamma^2})/2$. A straightforward calculation then shows that the information metric associated with the curve, say, $|\phi_+(\gamma)\rangle$, is given by:

$$G = \frac{1}{(1-\gamma^2)^2} \tag{52}$$

on account of the relations:

$$|\mathrm{d}\phi_+\rangle = -\frac{\mathrm{i}\,\mathrm{d}\gamma}{2(1-\gamma^2)}|\phi_-\rangle, \qquad \langle\widetilde{\mathrm{d}\phi_+}| = \frac{\mathrm{i}\,\mathrm{d}\gamma}{2(1-\gamma^2)}\langle\chi_-| \tag{53}$$

The nonperturbative expression in Equation (52) shows exactly how the metric diverges as one approaches the critical point $\gamma_c = 1$. It can be easily verified that Equation (52) also holds when the singularity is approached from the region $\gamma^2 > 1$. To compare this exact result with the perturbative analysis presented in the previous section, let us write $\gamma = \gamma_c - \epsilon$. Then we find:

$$G = \frac{1}{4\epsilon^2 + 4\epsilon^3 + \epsilon^4} = \frac{1}{4\epsilon^2}\left(1 - \epsilon + \frac{3}{4}\epsilon^2 - \cdots\right) \tag{54}$$

thus recovering the perturbative result of Equation (50) in leading order of ϵ.

More generally, any curve of the form $|\psi(\gamma)\rangle = c_+|\phi_+(\gamma)\rangle + c_-|\phi_-(\gamma)\rangle$ with fixed coefficients $c_\pm$ in this system possesses the metric (52) and will exhibit a curvature singularity at $\gamma = 1$. In the region $\gamma^2 \gg 1$, on the other hand, we have $G \ll 1$, and thus estimation of the parameter γ becomes unfeasible.

In summary, we began our paper with a brief review of the idea of information geometry applied to classical statistical mechanics formulated on real Hilbert spaces, and showed how the approach extends into complex Hilbert spaces. This paves the way towards the investigation of the geometry of a parametric family of eigenstates of quantum Hamiltonians. We have also reviewed the perturbative approach of [9] and extended the results so as to derive a new class of uncertainty relations of Equation (22) in quantum mechanics arising from the estimation of the parameters appearing in the Hamiltonian. We then applied the perturbation analysis of the eigenstates of non-Hermitian Hamiltonians developed in [40] to derive the expression in Equation (39) for the metric on the parameter space. This metric is induced from the ambient Fubini-Study geometry of the state space; the derivation of the Fubini-Study metric in the Hermitian context is well known, however, for our purposes we were required to derive an alternative representation in Equation (33) for the metric using the biorthogonal framework. We then worked out an example system that admits an exceptional point and showed how a Puiseux series can be applied to deduce, qualitatively, the behaviour of the metric in the vicinity of an exceptional point. The result obtained in Equation (50) shows the existence of a geometric singularity at the exceptional point.

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Conflicts of Interest

The authors declare no conflict of interest.

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