Fluctuations, uncertainty relations, and the geometry of quantum state manifolds

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(Received 4 April 2023; revised 16 July 2023; accepted 6 September 2023; published 27 September 2023)

The complete quantum metric of a parametrized quantum system has a real part (usually known as the Provost-Vallee metric) and a symplectic imaginary part (known as the Berry curvature). In this paper, we first investigate the relation between the Riemann curvature tensor of the space described by the metric, and the Berry curvature, by explicit parallel transport of a vector in Hilbert space. Subsequently, we write a generating function from which the complex metric, as well as higher-order geometric tensors (affine connection, Riemann curvature tensor), can be obtained in terms of gauge-invariant cumulants. The generating function explicitly relates the quantities which characterize the geometry of the parameter space to quantum fluctuations. We also show that for a mixed quantum-classical system both real and imaginary parts of the quantum metric contribute to the dynamics, if the mass tensor is Hermitian. A many-operator generalization of the uncertainty principle results from taking the determinant of the complex quantum metric. We also calculate the quantum metric for a number of Lie group coherent states, including several representations of the SU(1, 1) group. In our examples nontrivial complex geometry results for generalized coherent states. A pair of oscillator states corresponding to the SU(1, 1) group gives a double series for its spectrum. The two minimal uncertainty coherent states show trivial geometry, but, again, for generalized coherent states nontrivial geometry results.

DOI: 10.1103/PhysRevA.108.032218

I. INTRODUCTION

A parametrized quantum system exhibits interesting physics. In such systems a metric structure is induced on the parameter space which is determined by the type of quantum system in question [1]. If the metric is Riemannian, it is then possible to derive an affine connection or a Riemann curvature, quantities which further characterize the geometry of the parameter space. Recently, Smith *et al.* [2] considered the geodesic equation associated with a quantum metric, and arrived at equations of motion similar to those of general relativity. This led to the intriguing suggestion to use parametrized quantum systems in the laboratory to mimic and study space-time physics.

The study of quantum metrics already has a long history. The complex quantum metric of a parametrized quantum system was first derived [1] by Provost and Vallee, and they showed that its real part corresponds to a gauge-invariant Riemannian metric [known as the Provost-Vallee metric (PVM)], while its imaginary part is of symplectic structure. After the discovery [3] of the quantum geometric phase characterizing adiabatic cycles (also known as the Berry phase), it was quickly realized [4] that the imaginary part of the complex quantum metric is the Berry curvature (BC), whose area integral within an adiabatic cycle gives the phase itself. In the study of quantum phase transitions, a useful quantity is the fidelity [5–11], an overlap [Eq. (31)] between quantum states, and the fidelity susceptibility, which is a second derivative of the fidelity. This construction is entirely equivalent to the Provost-Vallee one, which also starts from an overlap of wave functions, and in fact the fidelity susceptibility is the PVM [Eq. (38)]. The quantum metric is also relevant in the modern theory of polarization [12–15], where the metric tensor expresses [16,17] the variance of the polarization in insulators. It can also be connected to linear [18] and nonlinear [19] response functions, and can be used as a gauge to distinguish metals from insulators [20,21]. More recently, the quantum metric has reappeared in the context of topological physics, specifically in the description of the fractional quantum Hall effect [22,23] and of topological insulators [24,25]. Anandan and Aharonov [26] have characterized the geometric phase by the Fubini-Study metric, which was shown [27–29] to be related to the PVM. The PVM is a metric on the parameter space, while the Fubini-Study metric is the metric of the projective Hilbert space of the entire system. It follows that the PVM is the pullback of the Fubini-Study metric with respect to the map defined by the parametrized family of spectral projectors. The Fubini-Study metric was also shown [30] to define a measure of entanglement. Very recently Avdoshkin and Popov [31] derived quantum geometric tensors (including the Christoffel symbol) from a three-point Bargmann invariant [32]. The Bargmann invariant can be interpreted as a cumulant generating function [33], so the formalism of Ref. [31] is related to ours.

In this work we inevstigate the full complex quantum metric. As a start we investigate the relation between the two curvatures which both appear as the characteristic of a parametrized quantum system. The BC appears as the *second derivative* of the scalar product of two quantum states with respect to the parameters, while the four-index Riemann curvature tensor appears as the *fourth derivative*. We clarify the relation between these two quantities by comparing the

parallel transport of a vector in Hilbert space (which is characterized by the BC) against the parallel transport of an ordinary vector (characterized by the Riemann curvature tensor). Subsequently we write down the generating function from which the PVM, as well as higher-order geometric quantities, can be obtained. While it is known that the PVM is related to the second cumulant (variance) of the fluctuations, we point out that higher-order geometric quantities correspond to higher-order cumulants; for example, the affine connection is related to the third cumulant (skew), while the Riemann curvature tensor corresponds to the fourth cumulant (kurtosis). In the fidelity language, this means that higher-order geometric tensors are related to "nonlinear fidelity susceptibilities."

Mixed quantum-classical systems obeying the Born-Oppenheimer approximation were considered [34,35] by Mead and Truhlar. They predicted the "molecular Aharonov-Bohm effect" and introduced the notion of "molecular magnetic field," a gauge field that modifies the force on the nuclei, and whose origin is the BC. In addition, according to the analysis in Ref. [4] the PVM gives rise to a "molecular electric" counterpart of the molecular magnetic field. We revisit this issue, considering the possibility of a complex (Hermitian) mass tensor, and find that the BC also contributes to the molecular electric field (an extra potential term arises, since the antisymmetric part of the complex mass tensor couples to the BC, which is also antisymmetric). Complex mass was first introduced in 1967 by Feinberg [36]. Tachyons are quantum fields with imaginary mass which violate physical principles and such particles are purely hypothetical. However, recently, Hermitian mass matrices have been invoked to explain neutrino oscillations, and generalizations of the Dirac equation in this direction have also been put forth [37]. By diagonalizing the inverse mass tensor, we show that the resulting Born-Oppenheimer-type system is like a "usual" system whose only possible unusual characteristic, in addition to the molecular fields, is that the inverse masses are directionally dependent.

Requiring that the determinant of the complex quantum metric is greater than or equal to zero leads to a many-operator generalization of the Schrödinger uncertainty principle [38], which is a stronger statement than the Heisenberg uncertainty principle (whose many-operator generalization was done by Robertson [39]). We also calculate the metric for three types of Lie group coherent states [40–42]: harmonic oscillator, atomic [SU(2)], and hyperbolic [SU(1, 1)]. Nontrivial complex geometry results from generalized [43,44] coherent states, which are generated from nonextremal starting states, hence they are no longer minimum uncertainty states. This generalization of coherent states was first proposed by Boiteux and Levelut [43], who considered it a purely formal development, but later, Roy and Singh [44] showed that the time-dependent generalization of these generalized coherent states leads to dynamics in which the probability distribution remains undistorted, and the averages perform classical motion. For certain special points in the parameter space even the quantum metric of generalized coherent states can become trivial—points where the complex quantum metric tensor exhibits zero determinant. We analyze the SU(1, 1) case extensively, where different representations of the group correspond [45–50] to different quantum number series. A case of particular interest we treat is a pair of coupled oscillators [47–50], which corresponds to the direct sum of two projective representations of the SU(1, 1) group, corresponding to a spectrum of two series (squeezed vacuum state, squeezed one-photon state). In this case we find that the complex quantum metric is zero for the extremal states of both series; in other words, there are two cases where the geometry is trivial.

Our paper is organized as follows. In Sec. II we give a brief overview of the quantities used to characterize the geometry of curved spaces. In Sec. III we derive the Berry connection and curvature by explicit parallel transport, and compare it to the affine connection and Riemann curvature. In Sec. IV we write down the cumulant generating function which generates gauge-invariant cumulants for a general parametrized quantum system. In Sec. V we investigate a mixed quantum-classical system with a complex mass tensor. Then, in Sec. VI we write the Christoffel symbol in terms of the third gauge-invariant cumulant in our formalism. In Sec. VII we relate geometric tensors and quantum fluctuations to the uncertainty principle. Before concluding in Sec. IX, in Sec. VIII we derive full quantum geometric tensors for coherent states, and identify when the geometries described by the tensors are trivial or not.

II. BACKGROUND: GEOMETRIC TENSORS AND PARALLEL TRANSPORT

In this section we provide some mathematical background [51] used in this work. Given an N-dimensional metric space with coordinates $s_1, \ldots, s_N$, the line element squared can be written as

$$dl^2 = g_{jk} ds^j ds^k, \tag{1}$$

where summation over doubly occurring indices is implied, and g_{ij} denotes the metric tensor. The metric tensor characterizes the geometry of the space and can depend on the coordinates $\{s_i\}$.

The equation for geodesic curves can be obtained by requiring that the integral of the variance of dl along a curve is zero:

$$\delta \int dl = 0. \tag{2}$$

This yields the second-order differential equation

$$g_{ki} \frac{d^2 s^i}{dl^2} = -\frac{ds^i}{dl} \frac{ds^j}{dl} [ij, k], \tag{3}$$

where $[ij, k]$ denotes the Christoffel symbol of the first kind,

$$[ij, k] = \tfrac{1}{2}(\partial_j g_{ik} + \partial_i g_{kj} - \partial_k g_{ij}), \tag{4}$$

where

$$\partial_i g_{kj} = \frac{\partial g_{kj}}{\partial s^i}. \tag{5}$$

The Christoffel symbol of the second kind is defined as

$$\Gamma^l{}_{ij} = \tfrac{1}{2} g^{kl}(\partial_j g_{ik} + \partial_i g_{kj} - \partial_k g_{ij}), \tag{6}$$

where the inverse (or dual) of the metric tensor, g^{ij}, is given by

$$g^{ij} g_{jk} = \delta^i{}_k. \tag{7}$$

The equation for parallel transporting a vector is usually given in terms of the Christoffel symbol of the second kind. If we parallel transport a vector along a curve $s^k(\lambda)$ (parametrized by λ) in a curved space with some metric tensor $g_{ij}(\lambda)$, from which the Christoffel symbol is obtained according to Eq. (6), then the change in the vector in the process is given by

$$\delta V^i(\lambda) = -\Gamma^i{}_{jk}(\lambda) V^j(\lambda) \delta s^k(\lambda). \tag{8}$$

III. BERRY CONNECTION AND BERRY CURVATURE AND THE CHRISTOFFEL SYMBOL AND RIEMANN CURVATURE TENSOR

In the case of parametrized quantum systems there are two "connections" and two "curvatures." The Berry connection has one coordinate index, while the affine connection associated with the parameter space has three. The Berry curvature is a two-index quantity, whereas the Riemann curvature tensor has four indices. The Berry curvature is the imaginary part of the complex quantum metric, which is also a two-index quantity [defined below in Eqs. (40)–(44)].

The Berry connection and curvature correspond [52] to the gauge fields of a fiber bundle. A fiber bundle is constructed by first considering the projected Hilbert space of the parametrized quantum system, where the projection occurs onto the space spanned by a chosen wave function or chosen set of wave functions. The projection removes the phase indeterminacy (for example, if a single state is used, then the projection, $|\Psi(s)\rangle\langle\Psi(s)|$, has no arbitrary phase due to the simultaneous presence of a bra and a ket). A fiber bundle restores the phase by assigning a fiber to each point of the base space (which in this case is the parameter space s). For example, in the case of a single state projection, a typical fiber can be the space on which the phase is easily represented, the S^1 unit circle. In this sense, there is a difference between the Berry connection or curvature (which corresponds to the gauge fields which live on the fibers) and the Christoffel and Riemann curvature tensors (which live on the parameter space s); however, we demonstrate below a useful parallel between these two sets of quantities.

We will argue below that the above discrepancy between the number of indices between the two sets of quantities is due to the projection of the Hilbert space necessary to obtain physically interesting cases (it is conventional to suppress the indices of the projected states). It is in order to cite a few examples. The Berry phase is defined via an integral of one quantum state over an adiabatic cycle, and the state index is usually not explicitly indicated when writing the Berry connection. The state under scrutiny is separated by an energy gap from the other states. A sum over Berry phases over all the states of a complete Hilbert space is zero [53,54]. In the case of the generalization of the Berry phase to a degenerate subset of states by Wilczek and Zee [55], it is the subset of states that is carried around an adiabatic cycle, again, separated from the rest of the states by a gap. In the modern theory of polarization of insulating systems [12–15], a particular kind of Berry phase, a Zak phase [56], is evaluated, which is an integral over the Brillouin zone over an occupied band (or bands) of states. The projection here is justified by the fact that only some bands are occupied; unoccupied bands do not contribute. In the case of time-reversal-invariant topological insulators [57,58], a modified version of the Zak phase is calculated for occupied degenerate Kramers bands. While the gap condition can be relaxed [59], a nontrivial value for a Berry phase or a Wilson loop still requires a projection in Hilbert space.

We now turn to the main purpose of this section, which is to derive the Berry connection and curvature by explicit parallel transport of a vector in Hilbert space. Our aim is to place emphasis on the connections (no pun intended) and the differences between the Berry connection and curvature on the one hand and the Christoffel symbol and the Riemann curvature tensor on the other.

One way [51] to arrive at the Christoffel symbol and the Riemann tensor is to consider the change in a general vector $\mathbf{V}(s)$ defined on a curved parameter space. $\mathbf{V}(s)$ is a mapping from each point of the parameter space $s_1, \ldots, s_N$ to $V_1, \ldots, V_M$. One can expand the vector in a local basis,

$$\mathbf{V}(s) = V^j(s)\mathbf{e}_j(s), \tag{9}$$

where $V^j(s)$ denotes the components of the vector $\mathbf{V}(s)$ in the local basis and $\mathbf{e}_j(s)$ denotes the members of the basis themselves. In general, a change in $\mathbf{V}(s)$ results from a change in the coefficients themselves as well as a possible change in the basis,

$$\frac{\partial \mathbf{V}(s)}{\partial s^k} = \frac{\partial V^j(s)}{\partial s^k}\mathbf{e}_j(s) + V^j(s)\frac{\partial \mathbf{e}_j(s)}{\partial s^k}. \tag{10}$$

We can expand the derivative in the second term as

$$\frac{\partial \mathbf{e}_j(s)}{\partial s^k} = \Gamma^l{}_{jk}(s)\mathbf{e}_l(s), \tag{11}$$

where the Christoffel symbol, $\Gamma^l{}_{jk}(s)$, is the expansion coefficient. Let us resolve the change in $\mathbf{V}(s)$ into components as

$$\mathbf{e}^l(s) \cdot \frac{\partial \mathbf{V}(s)}{\partial s^k} = \frac{\partial V^l(s)}{\partial s^k} + V^j(s)\Gamma^l{}_{jk}(s). \tag{12}$$

We define the covariant derivative in the k direction as

$$D_k V^l(s) = \frac{\partial V^l(s)}{\partial s^k} + \Gamma^l{}_{jk}(s) V^j(s). \tag{13}$$

From the covariant derivative, it is possible to define the four-index Riemann curvature tensor as

$$(D_j D_k - D_k D_j)V^l(s) = R^l{}_{mkj}(s)V^m(s), \tag{14}$$

where

$$R^l{}_{mkj}(s) = \partial_j \Gamma^l{}_{km}(s) - \partial_k \Gamma^l{}_{jm}(s) + \Gamma^l{}_{jn}(s)\Gamma^n{}_{km}(s) - \Gamma^l{}_{kn}(s)\Gamma^n{}_{jm}(s). \tag{15}$$

Note, the first pair of indices in $R^l{}_{mkj}$ (l and m) rotate the vector components, while the second pair (k and j) are sensitive to the curvature of the surface on which the transport occurs.

In an exactly analogous manner, we can consider a quantum system which is parametrized by a set of variables $s = s_1, \ldots, s_N$, and we can write a general vector in the Hilbert space in some basis,

$$|\Psi(s)\rangle = \sum_\iota |\iota(s)\rangle\langle\iota(s)|\Psi(s)\rangle = \sum_\iota |\iota(s)\rangle \Psi^\iota(s). \tag{16}$$

We use greek indices to label basis states. We can consider a change in this state in the k direction,

$$\partial_k|\Psi(s)\rangle = \sum_\iota [|\iota(s)\rangle\partial_k\Psi^\iota(s) + \partial_k|\iota(s)\rangle\Psi^\iota(s)]. \tag{17}$$

For the directions in the parameter space we use latin indices. Multiplying from the left by another state $\langle\lambda(s)|$ we obtain the change of $\Psi(s)$ in the basis,

$$\begin{aligned}\tilde{D}_k\Psi^\lambda &= \langle\lambda(s)|\partial_k|\Psi(s)\rangle \\ &= \partial_k\Psi^\lambda(s) + \sum_\iota \langle\lambda(s)|\partial_k|\iota(s)\rangle\Psi^\iota(s).\end{aligned} \tag{18}$$

Comparing Eqs. (12) and (18), we see that the two terms on the right-hand side of the equations correspond. The analog of the Christoffel symbol in Eq. (18) is the expression

$$\tilde{\Gamma}^\lambda{}_{\iota k} = \langle\lambda(s)|\partial_k|\iota(s)\rangle. \tag{19}$$

The Berry connection is a special case of $\tilde{\Gamma}^\lambda{}_{\iota k}$. The Berry phase arises from transporting a *single* energy eigenstate around an adiabatic cycle. In other words, the state $|\Psi(s)\rangle$ is itself some energy eigenstate, and the basis used is also the energy eigenbasis, resulting in

$$i\tilde{\Gamma}^0{}_{0k} = i\langle\Psi_0(s)|\partial_k|\Psi_0(s)\rangle. \tag{20}$$

The general connection, $\tilde{\Gamma}^\lambda{}_{\iota k}$, is a three-index quantity because it connects the states indexed by λ and ι by a change in the coordinate s_k. $\tilde{\Gamma}^\lambda{}_{\iota k}$ represents the probability amplitude to go between quantum state λ and ι when a change in the coordinate k is occurring. The Berry connection connects the same states, and this state remains fixed during the entire adiabatic cycle, and the only remaining index is the coordinate one, k. When $\lambda \neq \iota$, and the system is nondegenerate, the quantity $\tilde{\Gamma}^\lambda{}_{\iota k}$ represents nonadiabatic transitions between different quantum states under a change of the coordinate s_k. As such, this quantity plays a central role in the field of nonadiabatic molecular dynamics [60–62]: the nonadiabatic coupling vector is closely related [63] to the Pechukas [64,65] force, the force which acts on the nuclei of a molecular system whose electrons undergo a transition between electronic quantum states, in other words, when the Born-Oppenheimer approximation does not hold.

We can also derive the analog of the Riemann curvature tensor in this case, via

$$(\tilde{D}_k\tilde{D}_l - \tilde{D}_l\tilde{D}_k)\Psi^\lambda = \tilde{R}^\lambda{}_{\mu lk}\Psi^\mu, \tag{21}$$

resulting in

$$\tilde{R}^\lambda{}_{\mu lk} = \partial_k\tilde{\Gamma}^\lambda{}_{\mu l} - \partial_l\tilde{\Gamma}^\lambda{}_{\mu k} + \tilde{\Gamma}^\lambda{}_{\nu k}\tilde{\Gamma}^\nu{}_{\mu l} - \tilde{\Gamma}^\lambda{}_{\nu l}\tilde{\Gamma}^\nu{}_{\mu k}. \tag{22}$$

Equation (22) is identically zero if the indices run over the entire Hilbert space. To show this, we write the s-dependent state $|\iota(s)\rangle$ using a fixed basis, as

$$|\iota(s) = U(s)|\iota_0\rangle, \tag{23}$$

where $|\iota_0\rangle$ denotes a member of the fixed basis, and $U(s)$ is a unitary matrix spanning the entire Hilbert space. The quantum Christoffel symbol becomes

$$\tilde{\Gamma}^\lambda{}_{\iota k} = \langle\lambda_0|U(s)^\dagger\partial_k U(s)|\iota_0\rangle. \tag{24}$$

Using this definition of $\tilde{\Gamma}^\lambda{}_{\iota k}$ it is a relatively simple exercise that $\tilde{R}^\lambda{}_{\mu lk}$, as defined in Eq. (22), is zero. But this only holds if the entire Hilbert space is considered; in other words, a nontrivial quantum Riemann curvature results if the Hilbert space is truncated, meaning that all the indices in Eq. (22) (including the internal ones which are summed) are truncated [53]. Projections of the types discussed above are examples of such truncations. Comparing the sets of Eqs. (14) and (15) and Eqs. (21) and (22), we see that there is a correspondence between the curvature tensor of the parametrized quantum system and the Riemann curvature tensor known from differential geometry.

The four-index tensor $\tilde{R}^\lambda{}_{\mu lk}$ is not a curvature in the sense of the Riemann curvature tensor. To lower the index λ in $\tilde{R}^\lambda{}_{\mu lk}$ one uses not the metric tensor of the parameter space, but that of the Hilbert space of states ($\delta_{\mu\nu}$ for complete orthonormal states). As for contraction the Riemann curvature tensor can be contracted in three ways, because the indices are equivalent, whereas $\tilde{R}^\lambda{}_{\mu lk}$ can only be contracted as

$$\tilde{R}_{lk} = \tilde{R}^\lambda{}_{\lambda lk}. \tag{25}$$

The contraction over the entire Hilbert space leads to zero (for a proof of this statement, see, for example, the introduction of Ref. [54]); however, it is possible to sum over a part of the Hilbert space. The Berry curvature involves only one state, its generalization [55]; the Wilson loop involves a subset of the complete Hilbert space (usually a degenerate subspace). In these cases $\tilde{R}_l k$ is not trivial.

If the metric tensor of the parameter space is invertible, one can raise one of the indices of $\tilde{R}_l k$ as

$$\tilde{R}^j{}_k = g^{jl}\tilde{R}_{lk}, \tag{26}$$

and contract it to get the scalar curvature,

$$\tilde{R} = \tilde{R}^j{}_j. \tag{27}$$

The scalar curvature obtained from the Berry curvature is zero on account of the antisymmetry in the two coordinate indices.

IV. CUMULANT GENERATING FUNCTION FOR QUANTUM STATES

Before stating the cumulant generating function relevant to quantum state manifolds, let us give the definitions of moments and cumulants from the theory of probability. In this section, we use a notation that is closest to the original derivation of Provost and Vallee [1]. In the Appendix we develop a notation in which the relation between moments and cumulants in the case of quantum state manifolds can be made manifest.

Moments and cumulants are quantities which characterize probability distributions. Given a multivariate normalized probability distribution

$$\begin{aligned}&P(x_1,\ldots,x_N) \geqslant 0, \forall x_i, \\ &\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx_1\cdots dx_N P(x_1,\ldots,x_N) = 1,\end{aligned} \tag{28}$$

the Mth moment and the Mth cumulant are obtained from the generating (or characteristic) function, defined as

$$f(k_1,\ldots,k_N)=\int dx_1\cdots dx_N e^{i\sum_{j=1}^{N}k_j x_j}P(x_1,\ldots,x_N), \tag{29}$$

via the derivatives and logarithmic derivatives, respectively, as

$$\mathcal{M}_M=\prod_{j=1}^{N}\frac{1}{i^{m_j}}\frac{\partial^{m_j}}{\partial k_j^{m_j}}f(k_1,\ldots,k_N)\Big|_{k_1=\cdots=k_N=0},$$
$$\mathcal{C}_M=\prod_{j=1}^{N}\frac{1}{i^{m_j}}\frac{\partial^{m_j}}{\partial k_j^{m_j}}\ln f(k_1,\ldots,k_N)\Big|_{k_1=\cdots=k_N=0}, \tag{30}$$

where $\sum_{j=1}^{N}m_j=M$. Cumulants can be written in terms of moments (and vice versa).

We now turn to quantum state manifolds. Consider a family $\{\Psi(s)\}$ of quantum state vectors parametrized smoothly by the n-dimensional variable $s=s_1,\ldots,s_n$. We write the overlap between two wave functions with different s as

$$S(s',s)=\langle\Psi(s')|\Psi(s)\rangle. \tag{31}$$

We define the generating function for gauge-invariant cumulants as

$$\mathcal{C}_{m'_1,\ldots,m'_N;m_1,\ldots,m_N}=(-i)^{M'}(i)^{M}(\partial'_1)^{m'_1}\cdots(\partial'_N)^{m'_N}\partial_1^{m_1}\ldots\partial_N^{m_N}\ln S(s',s)\big|_{s'=s}. \tag{32}$$

In Eq. (32) $M'=m'_1+\ldots+m'_N$ and $M=m_1+\ldots+m_N$, and $\partial_j(\partial'_j)$ denotes a partial derivative with respect to $s_j(s'_j)$. Since this cumulant depends on the parameters of the vector in Hilbert space $|\Psi(s)\rangle$ and its dual $\langle\Psi(s')|$, there are two numbers specifying the order of the cumulant, M', referring to the dual vector $\langle\Psi(s')|$ and M referring to the vector $|\Psi(s)\rangle$. In Sec. VII we show that in the case where the state $|\Psi(s)\rangle$ is generated by simple translation operators, $\mathcal{C}_{m'_1,\ldots,m'_N;m_1,\ldots,m_N}$ correspond exactly to the statistical cumulants given in Eq. (30).

Gauge invariance can be shown via substituting a wave function

$$|\tilde{\Psi}(s)\rangle=\exp(-i\alpha(s))|\Psi(s)\rangle, \tag{33}$$

a state with a modified phase, $\alpha(s)$, which depends on the parameter set s. The overlap becomes

$$\tilde{S}(s',s)=\ln\langle\tilde{\Psi}(s')|\tilde{\Psi}(s)\rangle=\ln\langle\Psi(s')|\Psi(s)\rangle+i(\alpha(s')-\alpha(s)). \tag{34}$$

While cumulants with either M or M' zero are not gauge invariant, all other cases (including cumulants which correspond to the geometric tensors of interest) are independent of $\alpha(s)$.

The gauge-invariant quantum metric tensor of Provost and Vallee [1] is easily generated. We first relabel the cumulants of order $M=1$ and $M'=1$ as

$$C_2(j;k)=C_{0,\ldots,0,m'_j=1,0,\ldots,0;0,\ldots,0,m_k=1,0,\ldots,0}. \tag{35}$$

Evaluating $C_2(j;k)$ using Eq. (32), we obtain

$$C_2(j;k)=\gamma_{jk}-\beta_j\beta_k, \tag{36}$$

where

$$\gamma_{jk}=\langle\partial_j\Psi(s)|\partial_k\Psi(s)\rangle,\quad \beta_j=-i\langle\Psi(s)|\partial_j\Psi(s)\rangle. \tag{37}$$

β_j is the Berry connection in the state $\Psi(s)$. The metric tensor g_{jk} and the Berry curvature σ_{jk} are given by

$$g_{jk}(s)=\mathrm{Re}C_2(j;k),\ \ \sigma_{jk}(s)=\mathrm{Im}C_2(j;k). \tag{38}$$

g_{jk} (σ_{jk}) is symmetric (antisymmetric) in its indices. The second cumulant in ordinary statistics gives only a real correlation matrix. In the quantum case the particular structure of the scalar product of the probability amplitudes of quantum states ($S(s',s)$) is what gives rise to the additional imaginary antisymmetric component.

V. A BORN-OPPENHEIMER SYSTEM WITH HERMITIAN INVERSE MASS TENSOR

One area in which the study of the PVM and the BC proved crucially important was for mixed quantum-classical systems, in which the quantum subsystem remains in one quantum state throughout the dynamics (Born-Oppenheimer approximation). Mead and Truhlar showed that the BC gives rise to the "molecular magnetic field," which is measurable in several types of experiments, for example, pseudorotation of triatomic molecules [66,67].

In this section we show, on the one hand, that the metric tensor as well as its derivative (a three-index quantity related to the Christoffel symbol) appears in mixed quantum-classical systems. In addition, we also show that a complex inverse mass tensor leads to a "molecular electric field" which depends not only on the PVM, but also the BC.

We consider a molecular system consisting of electrons and nuclei. Since nuclei are at least three orders of magnitude heavier than electrons, the dynamics of molecules are often studied by invoking the Born-Oppenheimer approximation, which assumes that electrons remain in one electronic state (the ground state). We first write the Hamiltonian (fully quantum) as

$$\hat{H}_{\mathrm{tot}}=\frac{1}{2}\sum_{jk}Q^*_{jk}\hat{P}_j\hat{P}_k+\hat{h}(\hat{\xi};\hat{s}), \tag{39}$$

where $\hat{s}_j$ and $\hat{P}_j=i\partial_{s_j}$ represent the positions and momenta of the nuclei, $\hat{\xi}$ denote the electronic coordinates collectively (s denotes the nuclear coordinates collectively), and $h(\hat{\xi};\hat{s})$ is the Hamiltonian of the electrons. Q^*_{ij} denotes the complex conjugate of the inverse mass tensor. We assume that the inverse mass tensor has real and imaginary parts,

$$Q_{jk}=Q'_{jk}+iQ''_{jk}. \tag{40}$$

From the Hermiticity of the kinetic energy, it follows that $Q'_{jk}=Q'_{kj}$, and $Q''_{jk}=-Q''_{kj}$.

In the Born-Oppenheimer approximation one writes the total wave function as

$$\Psi_{\mathrm{tot}}(\xi;s)=\psi_{\mathrm{nuc}}(s)\phi_0(\xi;s), \tag{41}$$

where $\psi_{\mathrm{nuc}}(\hat{X})$ denotes the nuclear wave function, and $\phi_0(\hat{\xi};\hat{X})$ denotes the ground-state electronic wave function,

satisfying

$$\hat{h}(\xi;s)\phi_0(\xi;s) = E_0(s)\phi_0(\xi;s). \tag{42}$$

The effective Hamiltonian acting on the nuclei that results is

$$\hat{H}_{\text{eff}} = \int d\xi \phi_0^*(\xi;s)\hat{H}_{\text{tot}}\phi_0(\xi;s). \tag{43}$$

The effective Hamiltonian can be shown to be

$$\hat{H}_{\text{eff}} = \sum_{jk} \frac{Q_{jk}^*}{2}(\hat{P}_j - A_j(s))(\hat{P}_k - A_k(s)) + \Phi(s) + E_0(s), \tag{44}$$

where $A_j(s)$ and $\Phi(s)$ denote a vector potential and a scalar potential, respectively, defined as

$$\begin{aligned} A_j(s) &= -i\int d\xi \phi_0^*(\xi;s)\partial_j\phi_0(\xi;s), \\ \Phi(s) &= \frac{1}{2}\sum_{jk} Q_{jk}^* C_2(j;k) \\ &= \frac{1}{2}\sum_{jk}(Q'_{jk}g_{jk}(s) + Q''_{jk}\sigma_{jk}(s)). \end{aligned} \tag{45}$$

$g_{jk}(s)$ denotes the quantum metric tensor, derived in the previous section. In Eq. (45) the real part of the mass tensor couples to the PVM, and the imaginary part couples to the BC. Even though the mass tensor has an imaginary component, the terms in the effective Hamiltonian obtained above are all real, so the above potential corresponds to a classical system with a modified potential (modified "molecular electric field").

It is also possible to diagonalize the Hermitian mass tensor, and end up with a more straightforward expression:

$$\hat{H}_{\text{eff}} = \sum_r \frac{\hat{\Pi}_r^2}{2M_r} + \Phi(s) + E_0(s), \tag{46}$$

where

$$\hat{\Pi}_r = \sum_j U_{jr}(\hat{P}_j - A_j(s)), \tag{47}$$

where U diagonalizes Q, and M_r are the inverse eigenvalues. The potential adopts the form

$$\Phi(s) = \sum_r \frac{\tilde{g}_r(s) + \tilde{\sigma}_r(s)}{M_r}, \tag{48}$$

where

$$\begin{aligned} \tilde{g}_r(s) &= \sum_{jk}(U_{jr}U_{kr}^*)'g_{jk}(s), \\ \tilde{\sigma}_r(s) &= \sum_{jk}(U_{jr}U_{kr}^*)''\sigma_{jk}(s). \end{aligned} \tag{49}$$

In the form of Eq. (46) the effective Hamiltonian is not very different from systems with an "effective mass," since the kinetic energy has the usual from, apart from exhibiting directionally dependent masses, and the BC term only affects the potential in which the particle is moving. It is interesting that in the original Hamiltonian [Eq. (39)], the imaginary part of the complex Hermitian mass tensor appears in the kinetic energy; however, after invoking the Born-Oppenheimer approximation, it only affects the potential energy.

VI. THREE-INDEX QUANTITIES: THE QUANTUM CHRISTOFFEL SYMBOL

We now consider the three-index quantity of the form

$$C_3(j;kl) = (-i\partial_{j'})(i\partial_k)(i\partial_l)\ln S(s',s)|_{s'=s}. \tag{50}$$

$C_3(j;kl)$, like $C_2(j;k)$, is complex and takes the form

$$\begin{aligned} C_3(j;kl) = i\langle\partial_j\Psi|\partial_{kl}^2\Psi\rangle - \langle\Psi|\partial_{kl}^2\Psi\rangle\beta_j \\ +\gamma_{jl}\beta_k + \gamma_{jk}\beta_l - 2\beta_j\beta_k\beta_l. \end{aligned} \tag{51}$$

It is possible to show that

$$\partial_l C_2(j;k) = \frac{1}{2i}(C_3(jl;k) - C_3(j;kl)) \tag{52}$$

by directly taking the derivative of $C_2(j;k)$ [as defined in Eq. (36)] with respect to s_l, and substituting Eq. (51) in the right-hand side of Eq. (52). Using this result, we now define the quantum extension of the Christoffel symbol as

$$\begin{aligned} [jl;k]_q &= \frac{1}{2}(\partial_j C_2(l;k) + \partial_l C_2(k;j) - \partial_k C_2(j;l)) \\ &= \frac{1}{4i}(C_3(jl;k) - C_3(l;kj) + C_3(lk;j) - C_3(k;jl) \\ &\quad - C_3(kj;l) + C_3(j;lk)). \end{aligned} \tag{53}$$

The quantum Christoffel symbol is the analog of the expression in Eq. (4), with the full quantum metric substituted in place of g_{jk}. In addition, the quantum Christoffel symbol evaluates to a sum of various third-order cumulants. Equation (53) establishes a definite relation between quantum fluctuations and the Christoffel symbol.

The usual Christoffel symbol of the first kind, which results from taking the derivative of the PVM, is given by

$$\text{Re}[jl;k]_q = [jl;k], \tag{54}$$

and

$$\text{Im}[jl;k]_q = \tfrac{1}{2}(\partial_j\sigma_{lk} + \partial_l\sigma_{kj} - \partial_k\sigma_{jl}). \tag{55}$$

In the usual Christoffel symbol [Eq. (6)], the first and the last terms change sign upon exchanging indices j and k, and in $\text{Im}[jl;k]_q$ exactly the opposite happens. For this reason, using $[jl;k]_q$, we can write the force associated with the potential $\Phi(\hat{X})$ as

$$\begin{aligned} F_l = -\frac{1}{2}\sum_{jk} Q_{jk}^*[jl;k]_q, \\ -\frac{1}{2}\sum_{jk}(Q'_{jk}\text{Re}[jl;k]_q + Q''_{jk}\text{Im}[jl;k]_q). \end{aligned} \tag{56}$$

The force is thus dependent on the extended quantum Christoffel symbol. The broader conclusion is that in the most general case the parallel transport of a vector in the parameter space s proceeds via not only the derivative of the PVM, but also of the BC. A quantum Christoffel symbol of the second kind can only be defined if the complex quantum metric

$C_2(j;k)$ is invertible. In that case the definition in Eq. (6) can be used.

Since it is always possible to take further derivatives according to Eq. (52), and the resulting higher-order cumulants can then be combined to conform to expressions of higher-order geometric tensors (for example, the Riemann curvature tensor), geometric tensors of any order can be expressed as quantum fluctuations of the same order.

VII. GEOMETRIC TENSORS, QUANTUM FLUCTUATIONS, AND THE UNCERTAINTY PRINCIPLE

In this section we investigate how quantum fluctuations are related to geometric tensors. The most straightforward example [1] involves states generated by commuting operators $\{\hat{A}_j\}$, from some quantum state $|\Psi_0\rangle$, as

$$|\Psi\rangle = \exp\left(i\sum_j s_j\hat{A}_j\right)|\Psi_0\rangle. \tag{57}$$

Apart from the fluctuations in $|\Psi_0\rangle$, this example can be considered classical. Substituting Eq. (57) into Eq. (32), we obtain ordinary statistical cumulants [Eq. (30)]. The metric tensor g_{jk} is simply the second statistical cumulant; σ_{jk} is zero in this case. $C_3(jk;l)$ only has a real part and corresponds to the third-order statistical cumulant (the skew).

Further insight can be gained via considering a state generated by assuming that the set of operators $\{\hat{A}_j\}$ are noncommuting (generators of a Lie group). To start, we study the fluctuations near the origin of the parameter space, by taking s to zero in Eq. (32). In this case, the cumulants will have imaginary parts. The second-order cumulant looks like

$$\begin{aligned} g_{jk} &= \tfrac{1}{2}\langle[\hat{A}_j,\hat{A}_k]_+\rangle_0 - \langle\hat{A}_j\rangle_0\langle\hat{A}_k\rangle_0, \\ \sigma_{jk} &= \tfrac{1}{2}\langle[\hat{A}_j,\hat{A}_k]_-\rangle_0, \end{aligned} \tag{58}$$

where $[,]_+$ ($[,]_-$) indicates an anticommutator (commutator), and $\langle\rangle_0$ indicates average over the state $|\Psi_0\rangle$. A nontrivial Berry phase is a result of noncommuting generators.

It is instructive to consider the matrix $C_2(j;k)$ for a system with a two-dimensional parameter space, where there are only two generators, $\hat{A}_1$ and $\hat{A}_2$. In this case, the quantities $C_2(1;1)$ and $C_2(2;2)$ are simply the variances of operators $\hat{A}_1$ and $\hat{A}_2$. Since the quantity $C_2(j;k)$ is itself a variance, and therefore has a determinant greater than or equal to zero, we obtain

$$\sigma_j^2\sigma_k^2 \geqslant \left|\tfrac{1}{2}\langle[\hat{A}_j,\hat{A}_k]_+\rangle_0 - \langle\hat{A}_j\rangle_0\langle\hat{A}_k\rangle_0\right|^2 - \left|\tfrac{1}{2}\langle[\hat{A}_j,\hat{A}_k]_-\rangle_0\right|^2. \tag{59}$$

This equation is a form of the uncertainty relation, known as the Schrödinger uncertainty relation [38], which is a stronger form of this principle than the well-known one due to Heisenberg. Considering now the general case of an arbitrary number of dimensions, a multidimensional generalization of the uncertainty principle can be obtained via

$$\det[C_2(j;k)] \geqslant 0. \tag{60}$$

This form of the uncertainty principle places a constraint on the variances $\sigma_1,\ldots,\sigma_N$ if the parameter space is N dimensional. The many-operator version of the Heisenberg uncertainty relation was first derived by Robertson [39].

If the determinant of $C_2(j;k)$ is zero, it means that the complex metric $C_2(j;k)$ cannot be inverted. This also means that a Christoffel symbol of the second kind cannot be constructed, and that the parameter space, when considered together with the quantum fluctuations, has a trivial geometry; the entire parameter space represents the same point (all distances are zero). In the next section we give examples of both cases.

VIII. COHERENT-STATE EXAMPLES

In this section we will analyze the geometry of quantum systems using coherent states. Reviews of this subject are found in Refs. [41,42,68]. After deriving the uncertainty relation in a coherent-state context, we will consider three well-known examples of coherent states associated with Lie groups. They are known as Glauber, SU(2), and SU(1, 1) coherent states. Glauber coherent states are associated with the Weyl-Heisenberg group [69]. Glauber coherent states are minimum uncertainty states of a quantum harmonic oscillator. SU(2) coherent states are constructed using angular momentum operators. The generators of the SU(1, 1) group can be obtained by modifications of the SU(2) algebra. An interesting connection [45,46] exists between the SU(2) and SU(1, 1) groups. The SU(2) space corresponds to a sphere, which is a compact space. The basis states of the SU(2) correspond to the bound states of the Pöschl-Teller potential. The modifications leading to the SU(1, 1) algebra lead to a noncompact group space (a hyperboloid) and the modified basis states correspond to the scattering states of the same potential. The SU(1, 1) group space has several projections, which correspond to different series of quantum numbers. In the case of SU(1, 1) we will consider several representations of the group space below, including the case when the group space is the universal covering space of the hyperboloid, as well as projections thereof.

Before turning to our concrete examples, we give a brief overview of coherent states. Our purpose here is to calculate and analyze the quantum geometric tensor associated with coherent states, but we believe it is in order to give the general steps of their construction in a Lie group context.

Given is a Lie group G with a Lie algebra consisting of the identity $\hat{I}$ and two sets of generators, $\{\hat{A}_i\}$ and $\{\hat{B}_i\}$. The original coherent states [42] are minimum uncertainty states whose starting point is an *extremal* state. The set $\{\hat{A}_i\}$ together with the identity forms the stability subgroup of G, which we call H, consisting of operators which leave the extremal state invariant. The set $\{\hat{B}_i\}$, the complement of H in G, consists of operators which do not leave the extremal state invariant, and include at least one operator, which eliminates the extremal state. In practice, this means that the extremal state is an eigenstate of the operators included in H, with definite quantum numbers, and the operators of the complement of H in G are ladder (raising and lowering, or creation and annihilation) operators. Coherent states are then constructed by applying

the shift operator, $\hat{D}(s)$,

$$|s\rangle = \hat{D}(s)|0\rangle, \hat{D}(s) = \exp\left(\sum_j s_j \hat{B}_j\right), \tag{61}$$

to the extremal state. The argument of the exponential operator $D(s)$ consists of a sum over operators of the complement of H in G, and the parameters s_j are coordinates designating points on the geometrical space of the quotient group G/H. The complex metric can be written [70] as

$$C_2(j;k) = \sum_{m\neq 0} \langle 0|[\hat{D}^\dagger(s)\partial_j \hat{D}(s)]^\dagger|m\rangle\langle m|\hat{D}^\dagger(s)\partial_k \hat{D}(s)|0\rangle. \tag{62}$$

It is also possible to construct *generalized* [43,44] coherent states via acting with the displacement operator on a state which is not extremal, but still an eigenstate of the stability group. Such states are no longer minimum uncertainty states, but they are interesting, because their time-dependent generalization corresponds [44] to the averages moving according to classical dynamics, while the full quantum distribution remains rigid. Other generalizations of the original coherent-state formalism include a variety of squeezed states [42,47–49].

To summarize, our construction of coherent states and the calculation of the quantum geometric tensor in Secs. VIII B, VIII C, and VIII D will proceed via the following steps:

(i) Identify the stability group and its complement.

(ii) Identify states which are eigenstates of the operators of the stability group.

(iii) Apply the shift operator to eigenstates of the stability group.

(iv) Calculate the quantum geometric tensor.

For the case of SU(1, 1) we will first analyze (Sec. VIII D) single-valued representations of the group which correspond to the universal covering space of the hyperboloid. It is also possible to construct projective representations in which the groups are multivalued. In Sec. VIII E we give one example of this. The reader should note that the group theoretical approach to potential problems is a very colorful subject, whose mathematical intricacies are beyond the scope of this work, but excellent references exist to quench unsatisfied further curiosity [45,46,71].

A. Uncertainty principle in terms of coherent states

We can derive an uncertainty relation of the Schrödinger type for Lie group coherent states of the form of Eq. (61). These relations will include only the operators of the coset space, and we show that it remains valid at any point on the geometrical space G/H. We can write the operator

$$\hat{D}^\dagger(s)\partial_k \hat{D}(s) = \sum_l A_{kl}(s)\hat{B}_l, \tag{63}$$

where $A_{kl}(s)$ is a matrix which depends on the coordinates s. This linear combination includes only operators of the coset space. Therefore, we can write $C_2(j;k)$ as

$$C_2(j;k) = \langle 0|[\hat{D}^\dagger(s)\partial_j \hat{D}(s)]^\dagger \hat{D}^\dagger(s)\partial_k \hat{D}(s)|0\rangle. \tag{64}$$

Using Eq. (63) we can write $C_2(j;k)$ as

$$C_2(j;k) = \sum_{lm} A^\dagger_{jl}(s)A_{km}(s)\langle 0|\hat{B}^\dagger_l \hat{B}_m|0\rangle. \tag{65}$$

The general complex variance can be written as

$$C_2(j;k) = \sum_{lm} A^\dagger_{jl}(s)A_{km}(s)C_2^{(0)}(l;m). \tag{66}$$

Taking the determinant leads to

$$\mathrm{Det}[C_2] = \mathrm{Det}[A^\dagger(s)A(s)]\mathrm{Det}[C_2^{(0)}]. \tag{67}$$

Since $\mathrm{Det}[A^\dagger A]$ is greater than or equal to zero, and we already know that this is so for $\mathrm{Det}C_2^{(0)}$ from the uncertainty relation, it follows that

$$\mathrm{Det}[C_2] \geqslant 0. \tag{68}$$

Alternatively, it follows that the usual uncertainty relation will hold anywhere in the parameter space.

B. Glauber coherent states

For Glauber coherent states the relevant group is the Weyl-Heisenberg group [69], which consists of elements $\{\hat{I}, \hat{n}, \hat{a}^\dagger, \hat{a}\}$, where $\hat{a}$ ($\hat{a}^\dagger$) denotes the annihilation (creation) operator, and $\hat{n} = \hat{a}^\dagger\hat{a}$. The stability group is $\{\hat{I}, \hat{n}\}$. Minimum uncertainty coherent states are generated using the shift operator, as

$$|\alpha\rangle = \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a})|0\rangle, \tag{69}$$

where $\alpha = \alpha_1 + i\alpha_2$ (the complex plane) is the parameter space. We will also consider generalized Glauber states, constructed from an excited harmonic oscillator state,

$$|\alpha\rangle_m = \exp(\alpha\hat{a}^\dagger - \alpha^*\hat{a})|m\rangle. \tag{70}$$

Using Eq. (62), the result for the quantum geometric tensor is

$$C_2 = \begin{pmatrix} 2m+1 & i \\ -i & 2m+1 \end{pmatrix}. \tag{71}$$

For $m > 0$ the metric is invertible and there exists a nontrivial complex metric; however, for $m = 0$ the metric is not invertible, and the geometry is trivial. Stated differently, coherent states constructed starting from extremal states give rise to a trivial geometry, whereas generalized coherent states are endowed with a nontrivial geometry.

C. SU(2) (atomic) coherent states

The Lie group of angular momentum G is generated by the angular momentum Lie algebra, $\mathfrak{g} = \{\hat{J}_x, \hat{J}_y, \hat{J}_z\}$, which obeys the commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hat{J}_k, \tag{72}$$

where i, j, k denote a cyclic permutation of the coordinates x, y, z. For later use we also define the raising and lowering operators,

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y. \tag{73}$$

A convenient basis is formed by the states $|j, m\rangle$, which satisfy

$$\hat{J}^2|j,m\rangle = j(j+1)|j,m\rangle, \;\; \hat{J}_z|j,m\rangle = m|j,m\rangle, \tag{74}$$

and for which

$$j = \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \ldots,$$
$$m = -j, -j+1, -j+2, \ldots, j-2, j-1, j. \quad (75)$$

The Casimir operator of the group G, $\hat{J}^2$, is defined as

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2. \quad (76)$$

The stability group H of the group G is the subgroup generated by rotations about the z axis (subalgebra $\mathfrak{h} = \{\hat{J}_z\}$). The coset space of G/H corresponds to a sphere (which we can parametrize by angles θ, ϕ).

A generalized coherent state ($|\tau\rangle$) can be generated by the SU(2) shift operator

$$D(\tau) = \exp(\tau \hat{J}_+) \exp(\beta \hat{J}_z) \exp(-\tau^* \hat{J}_-), \quad (77)$$

where

$$\tau = \tan\frac{\theta}{2} e^{i\phi}, \;\; \beta = \ln(1 + |\tau|^2), \quad (78)$$

by acting on a basis state

$$|\tau\rangle = D(\tau)|j, m\rangle. \quad (79)$$

The usual atomic coherent states, which are minimum uncertainty states, are generated by the above procedure from the extremal basis functions of which in this case there are two: the lower and upper bounds of the series of spherical harmonic solutions ($m = -j$ or $m = j$).

After some algebra it is possible to show that

$$D(\tau)^\dagger \partial_\theta D(\tau) = \frac{1}{2}\left[e^{-i\phi}\hat{J}_+ - e^{i\phi}\hat{J}_-\right],$$
$$D(\tau)^\dagger \partial_\phi D(\tau) = \frac{-i\sin\theta}{2}\left[e^{-i\phi}\hat{J}_+ + e^{i\phi}\hat{J}_-\right]. \quad (80)$$

Using Eq. (62), we obtain the complex metric for the atomic coherent states,

$$C_2 = \frac{1}{2}\begin{pmatrix} j(j+1) - m^2 & -im\sin\theta \\ im\sin\theta & (j(j+1) - m^2)\sin^2\theta \end{pmatrix}. \quad (81)$$

Taking the determinant results in

$$\mathrm{Det}[C_2] = \tfrac{1}{4}[j(j+1) - m(m+1)][j(j+1) - m(m-1)] \times \sin^2\theta. \quad (82)$$

The PVM together with the BC is recovered by setting $m = -j$ in Eq. (81). We also find that there are four values of m for which the determinant vanishes, $m = -j-1, -j, j, j+1$, but two of these do not contribute, because they are outside the range of m for the representation of the SU(2) group [Eq. (75)]. Hence, for arbitrary values of the coordinates, only the extremal states correspond to a trivial complex quantum metric. For the remaining states the metric is nontrivial, except if $\theta = 0, \pi$, which are the north and south poles of the sphere.

We can consider a mixed quantum-classical system of the type chronicled in Sec. V. A 2×2 inverse mass tensor has the form

$$Q = \begin{pmatrix} Q'_{11} & Q'_{12} \\ Q'_{12} & Q'_{22} \end{pmatrix} - i\begin{pmatrix} 0 & Q''_{12} \\ -Q''_{12} & 0 \end{pmatrix}, \quad (83)$$

leading to a potential term of the form

$$\Phi(\theta) = \left(j(j+1) - m^2\right)(Q'_{11} + Q'_{22}\sin^2\theta) + 2mQ''_{12}\sin\theta. \quad (84)$$

The second term is the contribution due to the imaginary component of the inverse mass tensor.

D. SU(1, 1) coherent states

SU(1, 1) coherent states are generated by the Lie algebra, $\mathfrak{g} = \{\hat{J}_x, \hat{J}_y, \hat{J}_z\}$, whose members obey the relations

$$[\hat{J}_x, \hat{J}_y] = -i\hat{J}_z, [\hat{J}_y, \hat{J}_z] = i\hat{J}_x, [\hat{J}_z, \hat{J}_x] = i\hat{J}_y. \quad (85)$$

The raising and lowering operators are defined according to Eq. (73). A convenient basis is formed by the states $|j, m\rangle$, which satisfy

$$\hat{J}^2|j, m\rangle = j(j+1)|j, m\rangle,$$
$$\hat{J}_z|j, m\rangle = m|j, m\rangle, \quad (86)$$

but here the Casimir operator of the group G, $\hat{J}$, is defined as

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 - \hat{J}_z^2. \quad (87)$$

The algebra of the stability group is $\mathfrak{h} = \{\hat{J}_z\}$, and the coset space of G/H corresponds to a hyperboloid (parametrized below by ρ, ϕ).

The SU(1, 1) group has several possible series of quantum numbers, depending on representation [46]. Using the notation used in Ref. [46], here we list the ones corresponding to the single-valued representations of the group. There are two discrete series, D_j^+ and D_j^-, and two continuous series, C_k^0 and $C_k^{1/2}$. For D_j^+, the quantum number j can take negative integer or half-integer values, while m can start from $-j$ and can increase in integral steps, but unlike the SU(2) series, the m quantum number is not bounded from above. We have

$$j = -\tfrac{1}{2}, -1, -\tfrac{3}{2}, -2, \ldots,$$
$$m = -j, -j+1, -j+2, \ldots. \quad (88)$$

The series of m values is only bounded from below. For the series D_j^-, the quantum number j can take negative integer or half-integer values, while m can start from j and can decrease in integral steps:

$$j = -\frac{1}{2}, -1, -\frac{3}{2}, -2, \ldots,$$
$$m = j, j-1, j-2, \ldots. \quad (89)$$

The series of m values are only bounded from above. For the two continuous series,

$$j = -\tfrac{1}{2} + ik,$$
$$m = 0, \pm 1, \pm 2, \ldots \;\text{ for }\; C_k^0,$$
$$m = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots \;\text{ for }\; C_k^{1/2}, \quad (90)$$

where k is a real number, such that $k > 0$.

A generalized SU(1, 1) coherent state ($|\tau\rangle$) is generated by the SU(1, 1) shift operator,

$$D(\tau) = \exp(\tau \hat{J}_+) \exp(\beta \hat{J}_z) \exp(-\tau^* \hat{J}_-), \quad (91)$$

where

$$\tau = -\tanh\frac{\rho}{2}e^{-i\phi},$$
$$\beta = \ln(1-|\tau|^2), \tag{92}$$

by acting on a basis state $|j,m\rangle$,

$$|\tau\rangle = D(\tau)|j,m\rangle. \tag{93}$$

After some algebra it is possible to show that

$$D(\tau)^\dagger\partial_\rho D(\tau) = -\frac{1}{2}[e^{-i\phi}\hat{J}_+ - e^{i\phi}\hat{J}_-],$$
$$D(\tau)^\dagger\partial_\phi D(\tau) = \frac{i}{2}\sinh(\rho)[e^{-i\phi}\hat{J}_+ + e^{i\phi}\hat{J}_-]. \tag{94}$$

Using Eq. (62), we obtain the complex metric for the hyperbolic coherent states,

$$C_2 = \frac{1}{2}\begin{pmatrix}[-j(j+1)+m^2] & -im\sinh\rho \\ im\sinh\rho & [-j(j+1)+m^2]\sinh^2\rho\end{pmatrix}. \tag{95}$$

Taking the determinant results in

$$\mathrm{Det}[C_2] = \tfrac{1}{4}[j(j+1)-m(m+1)][j(j+1)-m(m-1)] \times \sinh^2\rho. \tag{96}$$

This determinant is zero if $\rho = 0$. It is also possible to get zero for particular values of the quantum numbers. The determinant of the complex quantum metric is zero for the extremal states in each of the series D_j^+ ($m=-j$) and D_j^- ($m=j$). For the two continuous series there is no way for the determinant of the complex quantum metric to be zero. We note in passing that there exists [46] also a supplementary series for the SU(1, 1) group. This series does not contribute to the solution of the relevant Laplace equation (defined on a hyperboloid), since the series D_j^+, D_j^-, C_k^0, and $C_k^{1/2}$ together form a complete set in which any function can be expanded. For this supplementary series,

$$-\tfrac{1}{2} < j < 0, \quad m = 0, \pm1, \pm2, \ldots. \tag{97}$$

The determinant of the complex quantum metric is never zero.

We also consider a mixed quantum-classical system with inverse mass tensor of the form given in Eq. (83); the potential term will be of the form

$$\Phi(\rho) = (-j(j+1)+m^2)(Q'_{11}+Q'_{22}\sinh^2\rho) + 2mQ''_{12}\sinh\rho. \tag{98}$$

Again, the second term is the contribution due to the imaginary component of the inverse mass tensor.

E. Projective representations of SU(1, 1) and two coupled oscillators as an example

Group spaces can have single-valued and multivalued representations. The former correspond to the universal covering space of the group, whereas the latter correspond to projective representations. An intuitive example is the case of the one-dimensional translation group, which is single valued, and its group space is the one-dimensional line. The group of uniaxial rotations correspond to a *projective* representation of the one-dimensional translation group, but in this case the representation is no longer single valued, and the group space will be the circle. The one-dimensional translation group is known as the universal covering group of the group of uniaxial rotations. Analogously, the one-dimensional line is the universal covering space of the circle. Exactly this situation occurs for SU(1, 1). In addition to the single-valued representations studied in the previous section, SU(1, 1) also has *projective* representations, which correspond to multivalued group representations.

The Lie algebras are the same [Eq. (85)], because locally the universal covering space and the group space of the multivalued representations are the same. The form of the quantum metric is also the same as that of the single-valued representations, given by Eq. (95); what changes are the series of quantum numbers. We state without proof that the *projective discrete* representation corresponds to the series

$$m = -j, -j+1, \ldots, \tag{99}$$

for $j < 0$, j real. In this case, Det[C_2] is zero for $m = -j$. The projective continuous representation is characterized by two numbers:

$$j = -\tfrac{1}{2} + i\delta, \quad \delta = \text{real} > 0,$$
$$m_0 = \text{real}, \quad 0 \leqslant m_0 < 1. \tag{100}$$

The spectrum of J_z in this case is

$$m = m_0, m_0 \pm 1, m_0 \pm 2, \ldots. \tag{101}$$

As an example we can consider the case of a pair of coupled oscillators, a system which has been studied in Refs. [47–50]. We define

$$\hat{J}_+ = \frac{1}{2}\hat{a}^\dagger\hat{a}^\dagger, \quad \hat{J}_- = \frac{1}{2}\hat{a}\hat{a}, \quad \hat{J}_z = \frac{1}{2}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{102}$$

where $\hat{a}^\dagger$ ($\hat{a}$) are bosonic creation (annihilation) operators. It can easily be shown that the operators $\hat{J}_+, \hat{J}_-$, and $\hat{J}_z$ satisfy the SU(1, 1) commutation rules, showing that the Lie algebra is the same as before. The Casimir operator is also unchanged, meaning that Eq. (86) is still valid. After some algebra we find, though, that the Casimir operator, using the definitions in Eq. (102), becomes

$$\hat{J}^2 = -\tfrac{3}{16}\hat{I}, \tag{103}$$

where $\hat{I}$ denotes the identity. Solving Eq. (86) results in two possible j values,

$$j = -\frac{1}{4}, -\frac{3}{4}. \tag{104}$$

The essential point is that Eq. (103) does not fit into any of the sequences given in Sec. VIII D (D_j^+, D_j^-, C_k^0, and $C_k^{1/2}$) even though the Lie algebra of the generators is unchanged. However, it can be accommodated by the sequence given in Eq. (99):

$$m = \frac{1}{4}, \frac{5}{4}, \ldots, \quad m = \frac{3}{4}, \frac{7}{4}, \ldots. \tag{105}$$

The two series are each distinct projective discrete representations, and their direct sum is the representation of the two-oscillator system. The series corresponding to $j = -\frac{1}{4}$

($j = -\frac{3}{4}$) are the odd (even) photon squeezed vacuum states [48] (see also Refs. [47–50]). In such a system, characterized by a direct sum, there are two instances where the geometry becomes trivial, $m = \frac{1}{4}$ and $m = \frac{3}{4}$.

IX. CONCLUSION

In this paper we investigated the complex geometric tensor of quantum state manifolds. We showed that the imaginary part of this tensor, the Berry curvature, gives rise to a potential term in mixed quantum-classical systems obeying the Born-Oppenheimer approximation, if the inverse mass tensor has an imaginary component.

From the scalar product of two quantum states a generating function can be written, which generates, in principle, all orders of quantum fluctuations. The second cumulant (variance) corresponds to the complex quantum metric, higher-order cumulants correspond to higher-order geometric quantities, the skew is related to the affine connection, and the kurtosis gives the complex analog of the four-index Riemann curvature tensor. Requiring the determinant of the complex quantum metric to be positive definite gives generalized uncertainty relations. Our calculations for Lie group coherent states led to trivial geometries for the usual coherent states, when they are generated from an extremal state; however, for other cases, the determinant of the complex metric can be nontrivial. Of particular interest is the representation of the SU(1, 1) group formed by coupling a pair of harmonic oscillator creation and annihilation operators, whose representation consists of the direct sum of two projective representations of the group. In this case the extremal states of both direct sums give zero for the determinant of the complex quantum metric, meaning the geometry is trivial. Again, for other states the geometry is nontrivial.

We envision a variety of interesting further studies based on the formalism we presented. In quantum optics, the properties of squeezed coherent states are measured via various correlation functions of the number operator [47–49], which are four operator products of creation and annihilation operators. Another interesting direction would be to study time-dependent coherent states to connect the underlying geometry with the dynamics.

ACKNOWLEDGMENTS

B.H. was supported by the National Research, Development and Innovation Fund of Hungary within the Quantum Technology National Excellence Program (Project No. 2017-1.2.1-NKP-2017-00001), K142179, and by the BME-Nanotechnology FIKP grant (BME FIKP-NAT). P.L. was supported by the Ministry of Culture and Innovation and the National Research, Development and Innovation Office within the Quantum Information National Laboratory of Hungary (Grant No. 2022-2.1.1-NL-2022-00004).

APPENDIX: MOMENTS AND CUMULANTS

In this Appendix, we derive the moments and cumulants from the scalar product of two quantum states and compare them to relations known for ordinary moments and cumulants used in statistics. First we review the definition of ordinary moments and cumulants.

Given a multivariate normalized probability distribution:

$$P(x_1, \ldots, x_N) \geqslant 0, \forall x_i,$$
$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 \cdots dx_N P(x_1, \ldots, x_N) = 1. \quad \text{(A1)}$$

The generating (or characteristic) function is defined as

$$f(k_1, \ldots, k_N) = \int dx_1 \cdots \, dx_N e^{i \sum_{j=1}^{N} k_j x_j} P(x_1, \ldots, x_N). \quad \text{(A2)}$$

Moments are obtained by taking derivatives of $f(k_1, \ldots, k_N)$. The first three moments can be written

$$\begin{aligned}
\mathcal{M}_1(l) &= \frac{1}{i} \frac{\partial}{\partial k_l} f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}} \\
&= \langle x_l \rangle, \\
\mathcal{M}_2(l, m) &= \frac{1}{i^2} \frac{\partial^2}{\partial k_l \partial k_m} f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}} \\
&= \langle x_l x_m \rangle, \\
\mathcal{M}_3(l, m, n) &= \frac{1}{i^3} \frac{\partial^3}{\partial k_l \partial k_m \partial k_n} f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}} \\
&= \langle x_l x_m x_n \rangle. \quad \text{(A3)}
\end{aligned}$$

Cumulants are logarithmic derivatives of the characteristic function. The first three cumulants are defined as

$$\begin{aligned}
\mathcal{C}_1(l) &= \frac{1}{i} \frac{\partial}{\partial k_l} \ln f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}}, \\
\mathcal{C}_2(l, m) &= \frac{1}{i^2} \frac{\partial^2}{\partial k_l \partial k_m} \ln f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}}, \\
\mathcal{C}_3(l, m, n) &= \frac{1}{i^3} \frac{\partial^3}{\partial k_l \partial k_m \partial k_n} \ln f(k_1, \ldots, k_N)|_{\mathbf{k}=\mathbf{0}}, \quad \text{(A4)}
\end{aligned}$$

or, in terms of moments, they can be written

$$\begin{aligned}
\mathcal{C}_1(l) &= \mathcal{M}_1(l), \\
\mathcal{C}_2(l, m) &= \mathcal{M}_2(l, m) - \mathcal{M}_1(l)\mathcal{M}_1(m), \\
\mathcal{C}_3(l, m, n) &= \mathcal{M}_3(l, m, n) - \mathcal{M}_2(l, m)\mathcal{M}_1(n) \\
&\quad - \mathcal{M}_2(l, n)\mathcal{M}_1(m) - \mathcal{M}_2(m, n)\mathcal{M}_1(l) \\
&\quad + 2\mathcal{M}_1(l)\mathcal{M}_1(m)\mathcal{M}_1(n). \quad \text{(A5)}
\end{aligned}$$

In the formalism used in our work the role of the characteristic function is played by the scalar product $S(s', s) = \langle \Psi(s') | \Psi(s) \rangle$ [Eq. (31)]. There are two sets of variables, the primed ones, $s' = s'_1, \ldots, s'_n$, associated with the bra vector of the scalar product, and the unprimed ones, $s = s_1, \ldots, s_n$, associated with the ket. Derivatives of either one can be used to define the analog of a moment. There are two types of first moments, for which we introduce the following notation:

$$\begin{aligned}
\mathcal{M}_1(_; l) &= (i\partial_l) S(s', s)|_{s'=s}, \\
\mathcal{M}_1(l; _) &= (-i\partial'_l) S(s', s)|_{s'=s}. \quad \text{(A6)}
\end{aligned}$$

The underscore is used when no derivatives are taken for a particular set of variables. For the first moments, it holds that

$$\mathcal{M}_1(\_; l) = \mathcal{M}_1(l; \_) = \mathcal{M}_1(l) = -\beta_l. \quad \text{(A7)}$$

See Eq. (37) for the definition of β_l. Depending on whether derivatives are applied to the primed or unprimed variables, there are three different types of second moments. We write them as

$$\begin{aligned}\mathcal{M}_2(\_;kl) &= (i\partial_k)(i\partial_l)S(s',s)|_{s'=s},\\ \mathcal{M}_2(k;l) &= (-i\partial'_k)(i\partial_l)S(s',s)|_{s'=s},\\ \mathcal{M}_2(kl;\_) &= (-i\partial'_k)(-i\partial'_l)S(s',s)|_{s'=s}.\end{aligned} \tag{A8}$$

$\mathcal{M}_2(k;l)$ corresponds to γ_{kl} in Eq. (37). As for third moments, there are four distinct types, but we will only write the two that are useful in establishing the third-order Christoffel symbol (Sec. VI):

$$\begin{aligned}\mathcal{M}_3(j;kl) &= (-i\partial'_j)(i\partial_k)(i\partial_l)S(s',s)|_{s'=s},\\ \mathcal{M}_3(jk;l) &= (-i\partial'_j)(-i\partial'_k)(i\partial_l)S(s',s)|_{s'=s}.\end{aligned} \tag{A9}$$

Cumulants are obtained in a similar way, by applying derivatives to $\ln S(s',s)$. The first-order cumulants can be written

$$\begin{aligned}\mathcal{C}_1(\_;l) &= (i\partial_l)\ln S(s',s)|_{s'=s},\\ \mathcal{C}_1(l;\_) &= (-i\partial'_l)\ln S(s',s)|_{s'=s},\end{aligned} \tag{A10}$$

the second ones as

$$\begin{aligned}\mathcal{C}_2(\_;kl) &= (i\partial_k)(i\partial_l)\ln S(s',s)|_{s'=s},\\ \mathcal{C}_2(k;l) &= (-i\partial'_k)(i\partial_l)\ln S(s',s)|_{s'=s},\\ \mathcal{C}_2(kl;\_) &= (-i\partial'_k)(-i\partial'_l)\ln S(s',s)|_{s'=s},\end{aligned} \tag{A11}$$

and the third-order ones we use here as

$$\begin{aligned}\mathcal{C}_3(j;kl) &= (-i\partial'_j)(i\partial_k)(i\partial_l)\ln S(s',s)|_{s'=s},\\ \mathcal{C}_3(jk;l) &= (-i\partial'_j)(-i\partial'_k)(i\partial_l)\ln S(s',s)|_{s'=s}.\end{aligned} \tag{A12}$$

In the text it was shown that cumulants which have at least one derivative as a function of each set of parameters (the primed and unprimed) are gauge invariant. Moments are not gauge invariant. It can also be shown that cumulants can be expressed in terms of moments, and the expressions look similar to Eq. (A5), with appropriate modifications. For first-order cumulants, it holds that

$$\mathcal{C}_1(\_;l) = \mathcal{C}_1(l;\_) = \mathcal{M}_1(l). \tag{A13}$$

For the second-order cumulants, we have

$$\begin{aligned}\mathcal{C}_2(\_;kl) &= \mathcal{M}_2(\_;kl) - \mathcal{M}_1(\_;k)\mathcal{M}_1(\_;l),\\ \mathcal{C}_2(k;l) &= \mathcal{M}_2(k;l) - \mathcal{M}_1(k;\_)\mathcal{M}_1(\_;l),\\ \mathcal{C}_2(kl;\_) &= \mathcal{M}_2(kl;\_) - \mathcal{M}_1(k;\_)\mathcal{M}_1(l;\_).\end{aligned} \tag{A14}$$

The indices on both sides of the equation "keep their sides of the semicolon," otherwise the second cumulants obey the same relation as for ordinary statistical cumulants [Eq. (A5)]. For the third-order cumulants, we have

$$\begin{aligned}\mathcal{C}_3(j;kl) &= \mathcal{M}_3(j;kl) - \mathcal{M}_2(j;k)\mathcal{M}_1(\_;l)\\ &\quad -\mathcal{M}_2(j;l)\mathcal{M}_1(\_;k) - \mathcal{M}_1(j;\_)\mathcal{M}_2(\_;kl)\\ &\quad +2\mathcal{M}_1(j;\_)\mathcal{M}_1(\_;k)\mathcal{M}_1(\_;l),\\ \mathcal{C}_3(jk;l) &= \mathcal{M}_3(jk;l) - \mathcal{M}_1(j;\_)\mathcal{M}_2(k;l)\\ &\quad -\mathcal{M}_1(k;\_)\mathcal{M}_2(j;l) - \mathcal{M}_2(jk;\_)\mathcal{M}_1(\_;l)\\ &\quad +2\mathcal{M}_1(j;\_)\mathcal{M}_1(k;\_)\mathcal{M}_1(\_;l).\end{aligned} \tag{A15}$$

Again, the indices maintain "their sides of the semicolon." Further simplifications can be made, by using $\mathcal{M}_1(l)$, but we wanted to emphasize the pattern of the placement of indices.

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