Intrinsic geometry of quantum adiabatic evolution and quantum phase transitions

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We elucidate the geometry of quantum adiabatic evolution. By minimizing the deviation from adiabaticity, we find a Riemannian metric tensor underlying adiabatic evolution. Equipped with this tensor, we identify a unified geometric description of quantum adiabatic evolution and quantum phase transitions that generalizes previous treatments to allow for degeneracy. The same structure is relevant for applications in quantum information processing, including adiabatic and holonomic quantum computing, where geodesics over the manifold of control parameters correspond to paths which minimize errors. We illustrate this geometric structure with examples, for which we explicitly find adiabatic geodesics. By solving the geodesic equations in the vicinity of a quantum critical point, we identify universal characteristics of optimal adiabatic passage through a quantum phase transition. In particular, we show that in the vicinity of a critical point describing a second-order quantum phase transition, the geodesic exhibits power-law scaling with an exponent given by twice the inverse of the product of the spatial and scaling dimensions.

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I. INTRODUCTION

Geometric and topological concepts have long played useful roles in both classical and quantum physics [1]. Important applications where the use of geometry has led to new insights include quantum evolutions [2], distance measures in quantum information theory [3,4], circuit-based quantum computation [5], and holonomic quantum computation [6], to name a few. More recently, quantum phase transitions (QPTs) [7] and adiabatic quantum computation [8,9] have also been been explored from a geometric perspective [10,11]. While geometry can be seen as an underlying unifying theme in these applications, an explicit geometry-based connection between them is not always apparent. The central theme of this work is to elucidate the geometry of adiabatic evolution. In particular, we describe an all-geometric connection between QPTs and adiabatic quantum evolution. We do this by showing how the Riemannian metric tensor that describes transitions through quantum critical points [10] also arises in adiabatic quantum evolution. More specifically, we explain how the metric which provides an information-geometric framework for QPTs can also provide a geometry for the control manifold arising in adiabatic evolutions. That QPTs and adiabatic quantum evolution should be so intimately related was previously understood in terms of the role of ground-state evolution in adiabatic quantum computation and, in particular, the basic observation that those points where ground-state properties undergo drastic changes—quantum critical points—are bottlenecks for adiabaticity [8,12,13].

The metric tensor we identify is a natural extension of the metric found in Ref. [10] to systems with degenerate ground states. In this sense, we go beyond adiabatic quantum computation, which is typically concerned with nondegenerate ground states, and find results with applications to holonomic quantum computation, where quantum gates are performed as holonomies in the degenerate ground eigensubspace of the system Hamiltonian. We analyze the relevance of the metric tensor for determining paths with minimum computational error, in the sense of deviation from the desired final adiabatic state. In addition, we find a prescription for adiabatic passage through quantum critical regions by solving the corresponding geodesic equations derived from the metric tensor. As a result, we are able to identify universal characteristics of adiabatic passage through a critical point. Namely, we find that in the vicinity of a critical point, the geodesic exhibits power-law scaling with an exponent given by twice the inverse of the product of the spatial and scaling dimensions.

The structure of this article is as follows. In Sec. II, we formulate our geometric picture. Specifically, after defining the model in Sec. II A, in Sec. II B, we introduce the adiabatic error and show how to upper bound it as a sum of two components, one of which encodes the geometric aspects of the evolution. We obtain a Riemannian metric by minimizing this error. Next, in Sec. II C, we demonstrate the emergence of the same geometry from the concept of adiabatic operator fidelity. In Sec. II D, we show how our metric arises from three more (interrelated) natural origins: Grassmannian geometry, Uhlmann parallel transport, and the Bures metric. In Sec. II E, we compare our metric with another related metric for adiabatic evolutions which we proposed in earlier work [11]. We briefly discuss strategies for further making the adiabatic error small in Sec. II F. We make the connection to QPTs in Sec. III. Specifically, in Sec. III A, we establish the relevance of our metric in the sense of QPTs by showing that the same metric is responsible for signaling quantum criticality. Then, in Sec. III B, we derive the quantum critical scaling of the metric tensor. Switching gears, we define the notion of an adiabatic geodesic in Sec. IV. In Sec. IV A, we analyze three examples, namely, the Deutsch-Jozsa algorithm, projective Hamiltonians (including Grover's algorithm), and the transverse-field Ising model, for which we analytically find the adiabatic metric and the corresponding geodesics. In Sec. IV B, we analyze the properties of geodesics when the adiabatic evolution passes through a quantum critical point. It is here that we identify the universal characteristics of such geodesics. We summarize our results and conclude in Sec. V. Several appendices provide detailed proofs omitted from the main text so as not to interrupt the presentation.

II. GEOMETRY OF ADIABATIC QUANTUM EVOLUTION

A. Model

Consider an n-body system with the N-dimensional Hilbert space $\mathcal{H}$. The Hamiltonian family $\{H(\mathbf{x})\}$ for this system, which depends on the (time-dependent) coupling strengths or control knobs $\mathbf{x}$, can be identified by points over the real M-dimensional manifold $\mathcal{M} \ni \mathbf{x}$. Given a total evolution time T and rescaled time $s = t/T$, a path $\mathbf{x} : s \in [0,1] \mapsto \mathcal{M}$ then represents the dynamics in this time interval, starting from $\mathbf{x}_0 \equiv \mathbf{x}(0)$ and ending at $\mathbf{x}_1 \equiv \mathbf{x}(1)$. We shall use the notation $\mathbf{x}_s \equiv \mathbf{x}(s)$ interchangeably or sometimes drop the s dependence entirely to lighten the notation. We allow for a $g_0(\mathbf{x})$-fold degenerate ground-state eigensubspace of $\{H(\mathbf{x})\}$, with eigenstates $\{|\Phi_0^\alpha(\mathbf{x})\rangle\}$. Thus this subspace can be identified by the projector

$$P_0(\mathbf{x}) = \sum_{\alpha=1}^{g_0(\mathbf{x})} \big|\Phi_0^\alpha(\mathbf{x})\big\rangle\big\langle\Phi_0^\alpha(\mathbf{x})\big|, \tag{1}$$

with $\mathrm{Tr}[P_0(\mathbf{x})] = g_0(\mathbf{x}) \geqslant 1$. We assume that for all finite n, the ground-state energy $E_0(\mathbf{x})$ is separated by a nonvanishing gap $\Delta(\mathbf{x})$ from the rest of the spectrum. In the thermodynamic limit $n \to \infty$, we allow the gap to vanish at some finite set of points $\{\mathbf{x}_c \equiv \mathbf{x}(s_c)\}$, or at a bounded segment of the path. These are the critical points where a QPT takes place. Although our results would hold if we were to pick any other eigensubspace satisfying the previous requirements rather than the ground state, for specificity, we shall henceforth consider the ground state and the initialization $|\psi(0)\rangle = \sum_{\alpha=1}^{g_0(\mathbf{x}_0)} a_\alpha |\Phi_0^\alpha(\mathbf{x}_0)\rangle$ (where $|\psi(s)\rangle \equiv |\psi(\mathbf{x}_s)\rangle$), and we similarly drop the explicit dependence on $\mathbf{x}(s)$ hereafter where possible.

B. Adiabatic error

1. Degenerate case

We wish to compare the desired, ideal adiabatic evolution to the actual evolution induced by the Hamiltonian family. To this end, we shall define an appropriate adiabatic error which measures the deviation between the two. The state of the system

$$|\psi(s)\rangle = V(s)|\psi(0)\rangle \tag{2}$$

at any rescaled time s is given in $\hbar = 1$ units (adopted hereinafter) in terms of the propagator $V(s)$, which is the solution to the time-dependent Schrödinger equation

$$i\partial_s V(s) = T H(s) V(s). \tag{3}$$

We can similarly associate an adiabatic propagator $V_{\mathrm{ad}}(s)$ and an adiabatic Hamiltonian $H_{\mathrm{ad}}(s)$ to the ideal adiabatic evolution, where the two are related via the Schrödinger equation:

$$i\partial_s V_{\mathrm{ad}}(s) = T H_{\mathrm{ad}}(s) V_{\mathrm{ad}}(s). \tag{4}$$

What defines the adiabatic propagator is the intertwining property:

$$V_{\mathrm{ad}}(s) P_0(0) V_{\mathrm{ad}}^\dagger(s) = P_0(s), \tag{5}$$

which means that $V_{\mathrm{ad}}(s)$ preserves the band structure of the ground eigensubspace of $H(s)$. By differentiation, the intertwining property is equivalent to $i\partial_s P_0(s) = T[H_{\mathrm{ad}}(s), P_0(s)]$, and when it holds, we have

$$|\psi_{\mathrm{ad}}(s)\rangle = V_{\mathrm{ad}}(s)|\psi(0)\rangle = \sum_{\alpha\alpha'=0}^{g_0} a_\alpha V^{[0]}_{\alpha\alpha'}(s)\big|\Phi_0^{\alpha'}(s)\big\rangle, \tag{6}$$

where $V^{[0]}_{\alpha\alpha'}(s) = \langle\Phi_0^\alpha(s)|V_{\mathrm{ad}}(s)|\Phi_0^{\alpha'}(0)\rangle$ is the (non-Abelian) Wilczek-Zee holonomy [14], usually expressed as the path-ordered exponential

$$V^{[0]}(s) = \mathcal{P}\exp\left[-\int_0^s A(s')\,ds'\right], \tag{7}$$

with the gauge connection

$$A_{\alpha\alpha'} \equiv \big\langle\Phi_0^\alpha\big|\partial_s\big|\Phi_0^{\alpha'}\big\rangle. \tag{8}$$

We prove Eq. (7) in Appendix A (see also Ref. [15]).

The adiabatic Hamiltonian can be expressed in terms of the original Hamiltonian plus a correction term [16,17]:

$$H_{\mathrm{ad}}(s) = H(s) + i[\partial_s P_0(s), P_0(s)]/T. \tag{9}$$

Clearly, the actual state $|\psi(s)\rangle$ need not be the same as the adiabatic state $|\psi_{\mathrm{ad}}(s)\rangle$. Our objective is to find the path $\mathbf{x}_s$ that minimizes the adiabatic error $\||\psi(\mathbf{x}_s)\rangle - |\psi_{\mathrm{ad}}(\mathbf{x}_s)\rangle\| = \|\{V(\mathbf{x}_s) - V_{\mathrm{ad}}(\mathbf{x}_s)\}|\psi(\mathbf{x}_0)\rangle\|$, where the norm is the standard Euclidean norm: $\||\phi\rangle\| \equiv \sqrt{\langle\phi|\phi\rangle}$. However, so as to obtain a result which does not depend on the initial state $|\psi(\mathbf{x}_0)\rangle$, we shall adopt a state-independent error measure and define the adiabatic error to be

$$\delta[\mathbf{x}(s)] \equiv \|V(\mathbf{x}_s) - V_{\mathrm{ad}}(\mathbf{x}_s)\|. \tag{10}$$

Since $\|(V - V_{\mathrm{ad}})|\psi\rangle\| \leqslant \|V - V_{\mathrm{ad}}\|$, where the norm on the right-hand side is the standard sup-operator norm (often denoted $\|\cdot\|_\infty$) [18],

$$\|X\| \equiv \sup_{|v\rangle:\||v\rangle\|=1} \sqrt{\langle v|X^\dagger X|v\rangle} = \max_i \sigma_i(X), \tag{11}$$

where $\{\sigma_i(X)\}$ are the singular values of X (eigenvalues of $\sqrt{X^\dagger X}$), an upper bound on $\delta[\mathbf{x}(s)]$ is then also an upper bound on $\||\psi(\mathbf{x}_s)\rangle - |\psi_{\mathrm{ad}}(\mathbf{x}_s)\rangle\|$.

Using the fact that the sup-operator norm is unitarily invariant ($\|VAW\| = \|A\|$ for any operator A and any pair of unitaries V and W), we can rewrite δ as

$$\delta[\mathbf{x}(s)] = \|I - \Omega(\mathbf{x}_s)\|, \tag{12}$$

where the wave operator

$$\Omega(s) \equiv V_{\mathrm{ad}}^\dagger(s) V(s) \tag{13}$$

satisfies the Volterra equation

$$\Omega(s) = I - \int_0^s K_T(s')\Omega(s')\,ds', \tag{14}$$

with the kernel

$$K_T(s) \equiv V_{\mathrm{ad}}^\dagger(s)[\partial_s P_0(s), P_0(s)] V_{\mathrm{ad}}(s). \tag{15}$$

Considering Eq. (9), $-iK_T(s)/T$ is simply the interaction-picture Hamiltonian, which results from transforming $H(s)$ to the interaction picture with respect to $H_{\rm ad}(s)$, where $i[\partial_s P_0(s), P_0(s)]/T$ plays the role of the perturbation. Therefore, in analogy to the Dyson series of time-dependent perturbation theory, the Volterra equation can be solved by iteration, which yields

$$\Omega(s) = \sum_{l=0}^{\infty} \Omega_l(s), \tag{16}$$

where

$$\Omega_0(s) = I, \tag{17}$$

$$\Omega_{l>0}(s) = -\int_0^s K_T(s')\Omega_{l-1}(s')\,ds'. \tag{18}$$

As shown in Refs. [16,17], $\forall l \in \{2k-1, 2k\}$ ($k \in \mathbb{N}$),

$$\sup_s \|\Omega_l(s)\| = O(1/T^k), \tag{19}$$

$$\sup_s \left\| \Omega(s) - \sum_{j=0}^{l-1} \Omega_j(s) \right\| = O(1/T^k). \tag{20}$$

Using the preceding results, $\|I - \Omega(s)\|$ can be expressed in terms of a $1/T$ series expansion since

$$\|I - \Omega(s)\| = \left\| \Omega_1(s) - \sum_{l\geqslant 2} \int_0^s K_T(s')\Omega_{l-1}(s')ds' \right\|$$
$$\leqslant \|\Omega_1(s)\| + \int_0^s \|K_T(s')\| \sum_{l\geqslant 2} \|\Omega_{l-1}(s')\|ds' \tag{21}$$
$$= \|\Omega_1(s)\| + \widetilde{\epsilon}(s)O(1/T), \tag{22}$$

where

$$\widetilde{\epsilon}(s) \equiv \int_0^s \|[\partial_{s'} P_0(s'), P_0(s')]\|\,ds'. \tag{23}$$

Thus the error δ is upper bounded as

$$\delta[\mathbf{x}(s)] \leqslant \delta_1(s) + \delta_2[\mathbf{x}(s)], \tag{24}$$

where

$$\delta_1(s) \equiv \|\Omega_1(s)\| \sim O(1/T), \tag{25}$$

$$\delta_2[\mathbf{x}(s)] \equiv \widetilde{\epsilon}[\mathbf{x}(s)]O(1/T). \tag{26}$$

Both error components can evidently be made small by choosing a large T, while for a given T, δ_2 can additionally be made small by choosing a path over the control manifold $\mathcal{M}$ with small $\widetilde{\epsilon}$. Note that in addition to $\|\Omega_1(s)\| \sim O(1/T)$, we also have the bound $\|\Omega_1(s)\| \leqslant \int_0^s \|K_T(s')\|\,ds' = \widetilde{\epsilon}[\mathbf{x}(s)]$, but we cannot conclude from Eqs. (19) and (20), as such, that $\|\Omega_1(s)\|$ is upper bounded by $\widetilde{\epsilon}[\mathbf{x}(s)]O(1/T)$. One can see from Ref. [19] how $\delta_1(s)$ depends on T, the gap, and the norm of the Hamiltonian or its derivatives. However, the coefficient of the $1/T$ term of δ_1 does not appear to have a geometric significance in the sense we use in this article, and we shall therefore exclude δ_1 from our study of adiabatic geometry.

In the following, we shall make the upper bound on δ small by finding a path which makes $\widetilde{\epsilon}[\mathbf{x}(s)]$ small. Finding the path which minimizes $\widetilde{\epsilon}$ is, however, beyond the scope of this work. Instead, as we show subsequently, after replacing the sup-operator norm by the Frobenius norm, the problem of minimizing δ_2 has a geometric solution in the sense that a Riemannian metric tensor is encapsulated in $\epsilon[\mathbf{x}(s)]$ [Eq. (23) with the modified norm]. To this end we prove in Appendix B that

$$\|[\partial_s P_0, P_0]\| = \sqrt{\left\| P_0(\partial_s H)\left(\frac{1}{H - E_0}\right)^2 (\partial_s H)P_0 \right\|}, \tag{27}$$

where $[H - E_0]^{-1}$ is shorthand for $(I - P_0)[H - E_0]^{-1}(I - P_0)$ and is called the reduced resolvent.

For a different method of traversing eigenstate paths of Hamiltonians based on the use of evolution randomization and a quantum phase estimation algorithm, see Ref. [20].

2. *Nondegenerate case*

When H has a discrete and nondegenerate spectrum, $P_0 = |\Phi_0\rangle\langle\Phi_0|$ and $I - P_0 = \sum_{n>0} |\Phi_n\rangle\langle\Phi_n|$, where $\{|\Phi_n\rangle\}_{n>0}$ are the excited eigenstates of H with eigenvalues $\{E_n\}_{n>0}$. In this case,

$$\frac{1}{H - E_0} = \sum_{n>0} \frac{1}{E_n - E_0}|\Phi_n\rangle\langle\Phi_n|. \tag{28}$$

Using the chain rule of differentiation to write $\partial_s H = (\partial_i H)\dot{x}^i$, where a dot denotes ∂_s and ∂_i denotes $\partial/\partial x^i$, and using the Einstein summation convention, Eq. (27) is easily simplified in the nondegenerate case to yield

$$\widetilde{\epsilon}[\mathbf{x}(s)] = \int_0^s \sqrt{2\mathbf{g}_{ij}^{(1)}(\mathbf{x})\dot{x}^i\dot{x}^j}\,ds', \tag{29}$$

where

$$\mathbf{g}_{ij}^{(1)} \equiv \mathrm{Re}\left[\sum_{n>0} \frac{\langle\Phi_0|\partial_i H|\Phi_n\rangle\langle\Phi_n|\partial_j H|\Phi_0\rangle}{(E_n - E_0)^2}\right]. \tag{30}$$

The manner in which $\mathbf{g}_{ij}^{(1)}$ appears in Eq. (29) suggests that it plays the role of a metric tensor. This metric tensor is identical to the metric tensor which was identified in the differential-geometric theory of QPTs and is related to the Fubini-Study metric [10]. We also remark that in the nondegenerate case, Ref. [21] reports a different geometric formulation which employs the length of the path of eigenstates for a fixed path. We next consider how to generalize our result to the degenerate case.

3. *Metric tensor for the degenerate case: Moving to the Hilbert-Schmidt norm*

We would like to identify Eq. (27) with a metric tensor. However, the appearance of the sup-operator norm presents a problem since this norm need not be differentiable. Hence we replace the sup-operator norm with the Frobenius (or Hilbert-Schmidt) norm

$$\|X\|_2 \equiv \sqrt{\mathrm{Tr}[X^\dagger X]} = \sqrt{\sum_{i=1}^{\mathrm{rank}(X)} \sigma_i^2(X)}, \tag{31}$$

which satisfies [18]

$$\|X\| \leqslant \|X\|_2 \leqslant \sqrt{\mathrm{rank}(X)}\|X\|. \tag{32}$$

Note that the operator $P_0(\partial_s H)\big(1/(H-E_0)\big)^2(\partial_s H)P_0$ appearing in Eq. (27) has support purely over the ground-state eigensubspace of H because of the projections P_0 to the left and right. Therefore its rank is at most g_0, and as a consequence of Eq. (32), the replacement of the sup-operator norm by the Frobenius norm does not alter $\|[\partial_s P_0, P_0]\|$ (hence $\widetilde{\epsilon}$ or $\mathbf{g}$) for the nondegenerate case ($g_0=1$), while it enables a differential-geometric bound in the degenerate case, which is at most $\sqrt{g_0}$ times greater than the expression obtained with the operator norm. Additionally, and this is our main reason for moving to the Frobenius norm, it guarantees analyticity of the adiabatic error and the metric tensor when H is analytic.

With these considerations in mind, let us now redefine the adiabatic error using the Frobenius norm:

$$\epsilon(s) \equiv \int_0^s \|[\partial_{s'} P_0(s'), P_0(s')]\|_2\, ds'. \tag{33}$$

Then $\widetilde{\epsilon}(s) \leqslant \epsilon(s) \leqslant \sqrt{g_0}\,\widetilde{\epsilon}(s)$, and consequently,

$$\delta_2(s) \leqslant \epsilon(s) O(1/T) \leqslant \sqrt{g_0}\delta_2(s). \tag{34}$$

Minimization of $\epsilon(s)$ thus squeezes the error component δ_2.

We show in Appendix C that

$$\epsilon(s) = \int_0^s \sqrt{2 g_0 \mathbf{g}_{ij}(\mathbf{x})\dot{x}^i\dot{x}^j}\, ds', \tag{35}$$

where the metric tensor is defined as

$$\mathbf{g}_{ij} \equiv \frac{1}{2g_0}\mathrm{Tr}[\partial_i P_0 \partial_j P_0] \tag{36}$$

$$= \frac{1}{2g_0}\mathrm{Tr}\left[P_0(\partial_i H)\left(\frac{1}{H-E_0}\right)^2(\partial_j H)P_0\right] + i \leftrightarrow j. \tag{37}$$

It is simple to verify that $\mathbf{g}_{ij}$ reduces to $\mathbf{g}^{(1)}_{ij}$ in the nondegenerate case, and similarly, $\epsilon(s)$ reduces to $\widetilde{\epsilon}(s)$ in this case.

Standard calculus of variations then tells us that minimization of $\epsilon[\mathbf{x}(s)]$ is tantamount to finding the geodesic path which is the solution to the following Euler-Lagrange equations:

$$\ddot{x}^i + \Gamma^i_{jk}\dot{x}^j\dot{x}^k = 0, \tag{38}$$

where the connection Γ is

$$\Gamma^i_{jk} = \tfrac{1}{2}\mathbf{g}^{il}(\partial_k \mathbf{g}_{lj} + \partial_j \mathbf{g}_{lk} - \partial_l \mathbf{g}_{jk}). \tag{39}$$

We have thus endowed the control manifold $\mathcal{M}$ with a Riemannian structure, given by the metric tensor $\mathbf{g}: T_{\mathcal{M}} \otimes T_{\mathcal{M}} \mapsto \mathbb{R}$. That $\mathbf{g}$ really satisfies all the properties required of a metric is shown in Appendix D. Other geometric functions, such as the curvature tensor $\mathbf{R}$, can be calculated from $\mathbf{g}$ [22].

C. Operator fidelity

Another approach to the adiabatic error is provided by the operator fidelity [23] between V and V_{ad}:

$$f_\varrho[\mathbf{x}(s)] \equiv |\mathrm{Tr}[\Omega(\mathbf{x}_s)\varrho]|, \tag{40}$$

where ϱ is an arbitrary density matrix of the system, which here we take to be the totally mixed state I/N. The operator fidelity derives its name from the fact that it quantifies the fidelity in the entire Hilbert space and, unlike our previous error measures $\widetilde{\epsilon}$ and ϵ, which involve the ground-state projector P_0, is not restricted just to ground states. However, neither is the adiabatic error δ [Eq. (10)] restricted just to ground states, and the two are obviously closely related. In Appendix E, we show that

$$1 - \frac{1}{\sqrt{N}}\epsilon \leqslant f_\varrho \leqslant 1, \tag{41}$$

so that minimizing ϵ maximizes f_ϱ and vice versa.

Let X be an arbitrary observable, and consider it in the rotated bases associated with the actual or adiabatic dynamics:

$$X(s) \equiv V(s) X V^\dagger(s), \tag{42}$$

$$X_{\mathrm{ad}}(s) \equiv V_{\mathrm{ad}}(s) X V^\dagger_{\mathrm{ad}}(s), \tag{43}$$

In addition to the bound of Eq. (41), we show in Appendix E that

$$\|X(s) - X_{\mathrm{ad}}(s)\| \leqslant \|X\|\,\{\delta_1(s) + \delta_2[\mathbf{x}(s)]\}\,[2 + O(1/T)], \tag{44}$$

which is identical to the adiabatic error bound of Eq. (24), apart from the factor $\|X\|[2+O(1/T)]$. Thus our bound of the operator distance $\|X(s) - X_{\mathrm{ad}}(s)\|$ also has the component δ_1 and the component δ_2 with its apparent geometric contribution, which can be squeezed by choosing a geodesic path, as in Sec. II B3.

D. Natural geometric formulation

1. Grassmannian

An alternative, natural way to obtain a geometry for adiabatic evolutions employs the Grassmannian structure of the dynamics [24]. As explained earlier, in the ideally adiabatic case, the eigensubspaces corresponding to the ground state and the rest of the spectrum (P_0 and $I - P_0$, respectively) do not mix; each follows its own unitary dynamics determined by its Wilczek-Zee holonomy, and hence $V_{\mathrm{ad}} = V^{[0]} \oplus V^{[\mathrm{rest}]}$. This implies a Grassmannian manifold

$$\mathcal{G}_{N,g_0} \cong U(N)/U(g_0)U(N-g_0)$$
$$\cong \left\{P_0 \in \mathcal{D}(\mathcal{H}) \middle| P_0^2 = P_0, \mathrm{Tr}[P_0] = g_0\right\}, \tag{45}$$

where $U(k)$ is the group of $k \times k$ unitary matrices and $\mathcal{D}(\mathcal{H})$ is the convex space of all density operators (positive semidefinite, unit trace matrices) defined over $\mathcal{H}$. A natural distance (metric) over this space is given by [25][1]

$$d(P_0, P_0') \equiv \frac{1}{\sqrt{2g_0}}\|P_0 - P_0'\|_2, \tag{46}$$

whence, keeping only the lowest nonvanishing order, we have

$$d^2\big(P_0(\mathbf{x}), P_0(\mathbf{x}+d\mathbf{x})\big) = \frac{1}{2g_0}\big\|P_0(\mathbf{x}+d\mathbf{x}) - P_0(\mathbf{x})\big\|_2^2$$

[1] We insert the prefactor $1/\sqrt{2g_0}$ into the definition in order to ensure $d(P_0, P_0') \leqslant 1$ because the maximum occurs when P_0 and P_0' are orthogonal ($P_0 P_0' = 0$).

$$= \frac{1}{2g_0}\mathrm{Tr}\left\{\left[dP_0(\mathbf{x}) + \frac{1}{2}d^2P_0(\mathbf{x})\right]^2\right\}$$
$$= \frac{1}{2g_0}\mathrm{Tr}[dP_0(\mathbf{x})\,dP_0(\mathbf{x})]$$
$$= \frac{1}{2g_0}\mathrm{Tr}[\partial_i P_0 dx^i \partial_j P_0 dx^j]$$
$$= \mathbf{g}_{ij}dx^i dx^j, \tag{47}$$

with the metric tensor as defined in Eq. (36). Thus the adiabatic metric tensor is precisely the metric over the Grassmannian manifold defined by the ground-state projectors.

2. Adiabatic parallel transport

In this section, we wish to define a notion of adiabatic parallel transport. We start with the standard purification [26,27]

$$W = P_0U \tag{48}$$

of P_0, where U is an arbitrary unitary acting on $\mathcal{H}$ so that $P_0 = WW^\dagger$. Here W is considered a vector in a larger (extended) Hilbert space $\mathcal{H}_{\mathrm{ext}}$, that is, a pure state whose reduction yields (the unnormalized density matrix) P_0. The Hilbert space $\mathcal{H}_{\mathrm{ext}}$ is equipped with the the Hilbert-Schmidt inner product

$$\langle A,B\rangle := \mathrm{Tr}[A^\dagger B]. \tag{49}$$

Given P_0, the fiber of all purifications sitting on the unit sphere $\mathcal{S}(\mathcal{H}_{\mathrm{ext}}) := \{W \in \mathcal{H}_{\mathrm{ext}} : \langle W,W\rangle = 1\}$ of $\mathcal{H}_{\mathrm{ext}}$ is the Stiefel manifold of orthonormal g_0 frames of $\mathcal{H}_{\mathrm{ext}}$, where $\mathrm{Tr}[P_0] = g_0$ (i.e., the set of ordered g_0 tuples of orthonormal vectors in $\mathcal{H}_{\mathrm{ext}}$). The gauge transformation (48) means that the fiber admits the unitaries of $\mathcal{H}$ as right multipliers. Informally, the Us act as arbitrary phases associated with P_0.

Starting with a curve of (unnormalized) density operators $s \mapsto P_0(s)$ and one of its purifications,

$$s \mapsto W(s), \quad P_0(s) = W(s)W^\dagger(s), \tag{50}$$

the length $\ell_U[s] = \int_0^s \sqrt{\langle \dot W(s'), \dot W(s')\rangle}ds'$ of the curve in $\mathcal{H}_{\mathrm{ext}}$ is not invariant against gauge transformations (48). The Euler equations for the variational problem $\ell[s] := \inf_U \ell_U[s]$, that is, for the geodesic, are [26,27]

$$W^\dagger dW = dW^\dagger W, \tag{51}$$

also known as the Uhlmann parallel transport condition. Substituting $W^\dagger = U^\dagger P_0$ and $dW = (dP_0)U + P_0dU$ yields the condition

$$U^\dagger P_0\big((dP_0)U + P_0dU\big) = [U^\dagger dP_0 + (dU^\dagger)P_0]P_0U, \tag{52}$$

which, using $UdU^\dagger = -(dU)U^\dagger$, reduces to

$$P_0(dU)U^\dagger + (dU)U^\dagger P_0 = [dP_0, P_0] \tag{53}$$

on the vector bundle over the Grassmannian $\mathcal{G}_{N,g_0}$. Here $U = U(s)$ is a general unitary undergoing parallel transport as $s \mapsto P_0(s)$. We now seek those unitaries U which, in addition to parallel transport, also satisfy adiabaticity.

To this end, let $J(s)$ be the infinitesimal generator of $U(s)$, that is,

$$i\partial_s U(s) = TJ(s)U(s). \tag{54}$$

Substituting this expression into Eq. (53), we obtain

$$P_0J + JP_0 = i[\partial_s P_0, P_0]/T \tag{55}$$
$$= H_{\mathrm{ad}} - H, \tag{56}$$

where in the second line, we used Eq. (9). Thus U satisfies adiabatic parallel transport if in addition to being a solution to the parallel transport condition of Eq. (53), its generator also satisfies the adiabaticity condition

$$P_0J + JP_0 = 0. \tag{57}$$

What is the generator J which satisfies this last condition? Using Eqs. (B10) and (B12) for the nondegenerate case, we obtain

$$-iT(P_0J + JP_0) = [\dot P_0, P_0]$$
$$= -\frac{1}{H-E_0}\dot H P_0 + P_0\dot H\frac{1}{H-E_0}$$
$$= \sum_{n>0}\frac{P_0\dot H|\Phi_n\rangle\langle\Phi_n| - |\Phi_n\rangle\langle\Phi_n|\dot H P_0}{E_n - E_0}. \tag{58}$$

Taking matrix elements, we find $\langle\Phi_0|J|\Phi_0\rangle = 0$ and $-iT\langle\Phi_0|J|\Phi_k\rangle = \frac{1}{E_k-E_0}\langle\Phi_0|\dot H|\Phi_k\rangle$, while the matrix elements of J between the excited states are unspecified so that

$$J = \frac{i}{T}\sum_{n>0}\frac{\langle\Phi_0|\partial_s H|\Phi_n\rangle}{E_n - E_0}|\Phi_0\rangle\langle\Phi_n| + \mathrm{H.c.} + J_\perp, \tag{59}$$

where $J_\perp$ is an arbitrary operator satisfying $J_\perp = Q_0J_\perp Q_0$.

Instead of trying to obtain perfect adiabaticity ($H_{\mathrm{ad}} = H$), we can settle for an approximation. Noting that Eqs. (33) and (55) imply

$$\epsilon(s) = T\int_0^s \|P_0(s')J(s') + J(s')P_0(s')\|_2\,ds',$$
$$= \int_0^s \sqrt{2g_0\mathbf{g}_{ij}(\mathbf{x})\dot x^i\dot x^j}ds', \tag{60}$$

it follows that minimizing ϵ, or equivalently, finding the adiabatic geodesic, endows the phase U of P_0 with an adiabatic characteristic which is compatible with the Uhlmann parallel transport condition. Thus we have shown that the metric tensor $\mathbf{g}$ emerges naturally also from the notion of adiabatic parallel transport.

3. Bures metric

There is also a straightforward connection between our metric and the Bures metric [28]. For two arbitrary density matrices ρ_1 and ρ_2, the Bures distance is defined as

$$d^2_{\text{Bures}}(\rho_1,\rho_2) \equiv 1 - F(\rho_1,\rho_2), \tag{61}$$

where $F(\rho_1,\rho_2) \equiv \text{Tr}[(\rho_1^{1/2}\rho_2\rho_1^{1/2})^{1/2}]$ is the fidelity between these two states [29].[2] When the density matrices depend on a parameter $\mathbf{x}$, the infinitesimal distance $d^2_{\text{Bures}}(\rho(\mathbf{x}),\rho(\mathbf{x}+d\mathbf{x}))$ can be shown to be [4]

$$d^2_{\text{Bures}}(\rho(\mathbf{x}),\rho(\mathbf{x}+d\mathbf{x})) = \text{Tr}[\rho(\mathbf{x})\mathcal{L}^2(\mathbf{x})], \tag{62}$$

where $\mathcal{L}(\mathbf{x})$ is the symmetric logarithmic derivative (SLD), defined via

$$d\rho(\mathbf{x}) = \tfrac{1}{2}[\mathcal{L}(\mathbf{x})\rho(\mathbf{x}) + \rho(\mathbf{x})\mathcal{L}(\mathbf{x})]. \tag{63}$$

From the property $P_0^2 = P_0$, we obtain

$$dP_0(\mathbf{x}) = dP_0(\mathbf{x})P_0(\mathbf{x}) + P_0(\mathbf{x})\,dP_0(\mathbf{x}), \tag{64}$$

and hence [see Eq. (A2)]

$$dg_0 = \text{Tr}[dP_0] = 2\text{Tr}[P_0 dP_0] = 2\text{Tr}[P_0 dP_0 P_0] = 0, \tag{65}$$

that is, the degeneracy is constant. Thus, if $\rho(\mathbf{x}) \equiv P_0(\mathbf{x})/g_0$, then $d[P_0(\mathbf{x})/g_0] = (P_0(\mathbf{x})/g_0)dP_0 + dP_0 P_0(\mathbf{x})/g_0$, and the definition of the SLD [Eq. (63)] yields

$$\mathcal{L}(\mathbf{x}) = 2dP_0(\mathbf{x}). \tag{66}$$

Inserting this back into Eq. (62) results in

$$\begin{aligned} d^2_{\text{Bures}}(P_0(\mathbf{x}),P_0(\mathbf{x}+d\mathbf{x})) &= \frac{4}{g_0}\text{Tr}\{P_0(\mathbf{x})[dP_0(\mathbf{x})]^2\} \\ &\equiv \mathbf{g}^{\text{Bures}}_{ij}(\mathbf{x})\,dx^i dx^j, \end{aligned} \tag{67}$$

where

$$\mathbf{g}^{\text{Bures}}_{ij}(\mathbf{x}) = \frac{4}{g_0}\text{Tr}[\partial_i P_0(\mathbf{x})\partial_j P_0(\mathbf{x})]. \tag{68}$$

By comparison with Eq. (36), we obtain

$$\mathbf{g}^{\text{Bures}}_{ij} = 8\mathbf{g}_{ij}. \tag{69}$$

We note that the Bures metric is also connected to the quantum Fisher information tensor, which plays a principal role in quantum estimation theory [4,28,30,31]. In fact, the Bures metric is (up to an unimportant constant multiplicative factor) equal to the Fisher tensor. Therefore the adiabatic metric is the quantum Fisher metric, and the metric $\mathbf{g}$ obtains a natural role in quantum estimation theory.

[2] Some authors define the Bures distance as $d^2_{\text{Bures}}(\rho_1,\rho_2) \equiv 2[1 - \sqrt{F(\rho_1,\rho_2)}]$ and the fidelity as $F(\rho_1,\rho_2) \equiv \{\text{Tr}[(\rho_1^{1/2}\rho_2\rho_1^{1/2})^{1/2}]\}^2$.

E. Comparison of adiabatic metrics

In adiabatic evolution (as well as in adiabatic quantum computation), δ and T are the primary objects of interest. Our method for obtaining the metric $\mathbf{g}$ here is based on minimizing an upper bound on the adiabatic error δ for a given evolution time T. In Ref. [11], we pursued a complementary route and proposed a different metric:

$$\widetilde{\mathbf{g}}_{ij}(\mathbf{x}) = \text{Tr}[\partial_i H(\mathbf{x})\partial_j H(\mathbf{x})]/\Delta^4(\mathbf{x}), \tag{70}$$

derived from minimizing a time functional inspired by the traditional adiabatic condition. We called this the quantum adiabatic brachistochrone.

The major difference between these two metrics is in their distinct gap dependence. This can be understood, for example, by noting that

$$|\mathbf{g}_{ij}| \leqslant \frac{\|\partial_i H\partial_j H\|_1}{\min_s \Delta^2}, \tag{71}$$

whereas

$$|\widetilde{\mathbf{g}}_{ij}| \leqslant \frac{\|\partial_i H\partial_j H\|_1}{\min_s \Delta^4}, \tag{72}$$

where $\|X\|_1 \equiv \text{Tr}[\sqrt{X^\dagger X}] = \sum_i \sigma_i(X)$ is the trace norm [18] (see Appendix F for the proof). Thus the metric $\mathbf{g}$ has a quadratically smaller dependence on the inverse gap. It is furthermore dimensionless, while the metric $\widetilde{\mathbf{g}}$ is not. These differences show that the two metrics are essentially distinct.

F. Strategies for reducing the adiabatic error and their effect on geometry

Considering that $\mathbf{g}$ is related to minimizing the upper bound on δ, it is useful to briefly recall how δ scales with T and how this scaling may be improved.

Rigorous proofs of the adiabatic theorem—based on successive integration by parts of Ω—state that if $\{H(s)\}$ is a family of C^k (k times continuously differentiable) interpolations/paths with bounded $\|\partial_s^l H\|$ ($l \in \{1,\ldots,k\}$) and compactly supported $\partial_s H$ over $s \in (0,1)$, then $\delta = O(1/T^{2(k-1)})$ [16,17,19]. If these assumptions are supplemented with that of analyticity of $H(s \in \mathbb{C})$ in a small strip around the real-time axis, and if, in addition,

$$\partial_s^l H(0) = \partial_s^l H(1) = 0\,\forall l \leqslant k, \tag{73}$$

the result is an exponentially smaller error:

$$\delta = O(e^{-cT}), \tag{74}$$

where $c \equiv \min_s \Delta^3/\max_s \|\partial_s H\|^2$ (up to an $O(1)$ prefactor) [32].

Our path—as the solution to the second-order differential equation [Eq. (38)]—minimizes ϵ rather than δ, which is not necessarily compatible with the boundary conditions $\partial_s^l H(\{0,1\}) = 0$. Thus, in principle, there remains room for further optimization of the path for δ beyond what is captured by simply minimizing its upper bound $\epsilon(s)O(1/T)$ [16,17,33]. Such finer optimizations, however, may not always result in a Riemannian geometry because the corresponding functionals and Euler-Lagrange equations would depend on higher derivatives of H.

III. CONNECTION TO QUANTUM PHASE TRANSITIONS

The other physically important aspect of our geometric formulation emerges from the observation that the metric $\mathbf{g}$ also arises naturally as the underlying geometry of QPTs. QPTs take place at zero temperature [7], where the system is, in principle, in its ground state. Such phase transitions are radically different from their thermal counterparts. In particular, in contrast to thermal phase transitions, the standard paradigm of the Landau-Ginzburg symmetry-breaking mechanism [7,34] fails to explain the underlying physics of some QPTs. In fact, defining an appropriate local order parameter—an essential ingredient of the Landau-Ginzburg theory—is not straightforward for a quantum critical system; some QPTs, such as those involving topological order, provably do not admit any local order parameter [35,36]. Additionally, tracking singularities of the ground-state energy cannot always foreshadow QPTs; quantum systems with matrix-product states may elude this test [37].

Notwithstanding the preceding subtleties with identifying QPTs, it has recently been shown that the simple notion of the ground-state fidelity is remarkably successful in signaling QPTs [10,38]. This can be understood by noting that since QPTs take place at zero temperature, in which the system is in its ground state, quantum criticality should be identifiable by ground-state properties. Specifically, the ground states right before and right after a quantum critical point are expected to have very little overlap. In this manner, ground-state fidelity may be considered as a natural, fairly general order parameter for quantum critical systems, irrespective of their internal symmetries [10]. We shall discuss this feature in more detail later.

A. Metric tensor for QPTs

Here we derive the metric attributed to QPTs for the case of degenerate ground states as a natural extension of the similar metric proposed for the nondegenerate case [10].

In the degenerate case, we should work with the ground-state projector $P_0(\mathbf{x})$. A variation in the properties of $P_0(\mathbf{x})$, caused by the change $\mathbf{x} \to \mathbf{x} + d\mathbf{x}$ in the Hamiltonian parameters, can be captured by the order parameter chosen to be the operator fidelity of $P_0(\mathbf{x})$ and $P_0(\mathbf{x}+d\mathbf{x})$ relative to, for example, $\varrho = I_{g_0}/g_0$ (I_{g_0} is the $g_0 \times g_0$ identity matrix):

$$\begin{aligned} f_\varrho\big(P_0(\mathbf{x}), P_0(\mathbf{x}+d\mathbf{x})\big) &= \langle P_0(\mathbf{x}), P_0(\mathbf{x}+d\mathbf{x})\rangle_\varrho \\ &= 1 - \mathbf{G}_{ij}(\mathbf{x})\, dx^i dx^j, \end{aligned} \tag{75}$$

in which the Hermitian matrix

$$\mathbf{G}_{ij} \equiv \frac{1}{g_0}\mathrm{Tr}[P_0(\partial_i P_0)(\partial_j P_0)P_0] \tag{76}$$

is the geometric tensor for the degenerate case (see Appendix G for the proof). Thus the information about the criticality of the quantum system is contained in the $\mathbf{G}$ tensor. Note that in the nondegenerate case ($g_0 = 1$), $\mathbf{G}_{ij}$ reduces to

$$\mathbf{G}_{ij} = \langle \partial_i \Phi_0 | \partial_j \Phi_j\rangle - \langle \partial_i \Phi_i | \Phi_0\rangle\langle \Phi_0 | \partial_j \Phi_0\rangle. \tag{77}$$

Accordingly, a Riemannian QPT metric tensor can be defined through

$$\mathbf{g}^{\mathrm{QPT}}_{ij}(\mathbf{x}) \equiv \mathrm{Re}[\mathbf{G}_{ij}(\mathbf{x})] = \frac{1}{2g_0}\mathrm{Tr}[\partial_i P_0 \partial_j P_0] = \mathbf{g}_{ij}, \tag{78}$$

where we used the same trick as that used in arriving at Eq. (C2). Therefore the QPT metric tensor $\mathbf{g}^{\mathrm{QPT}}$ is the same as the adiabatic quantum evolution metric $\mathbf{g}$ defined in Eq. (36).

B. Quantum critical scaling of the QPT metric tensor

The critical behavior of a quantum system with a degenerate ground state can be characterized by the metric tensor $\mathbf{g}$. This is already evident from the fact that the divergence of $\mathbf{g}^{\mathrm{QPT}}$ is a sufficient condition for signaling quantum criticality. To further elaborate on this connection, we follow Ref. [39] and obtain the scaling of the geometric tensor [Eq. (76)]:

$$\begin{aligned} \mathbf{G}_{ij} &= \frac{1}{g_0}\mathrm{Tr}\left[P_0(\partial_i H)\left(\frac{1}{H-E_0}\right)^2(\partial_j H)P_0\right] &(79)\\ &= \frac{1}{g_0}\sum_{n>0}\sum_{\alpha,\eta=1}^{g_0,g_n}\frac{\langle \Phi_0^\alpha|\partial_i H|\Phi_n^\eta\rangle\langle\Phi_n^\eta|\partial_j H|\Phi_0^\alpha\rangle}{(E_n-E_0)^2}, &(80)\end{aligned}$$

and via Eq. (78), also for $\mathbf{g}_{ij}$. For simplicity, we restrict ourselves only to gapped quantum systems with second-order QPTs. Thus, in a critical region $\mathbf{x} \approx \mathbf{x}_c$, the correlation length ξ and the gap Δ exhibit the following scalings:

$$\xi \sim \|\mathbf{x}-\mathbf{x}_c\|^{-\nu}, \quad \Delta \sim \|\mathbf{x}-\mathbf{x}_c\|^{z\nu}, \tag{81}$$

with the critical exponents $\nu > 0$ and $z\nu$, where $z > 0$ is the dynamical exponent [7]. The geometric tensor $\mathbf{G}$ has an integral representation which not only facilitates the derivation of the scaling relation for $\mathbf{G}$ but also enables an interpretation for $\mathbf{G}$ in terms of correlation (or response) functions. Indeed, as shown in Appendix H, Eq. (80) can be expressed as

$$\begin{aligned} \mathbf{G}_{ij} = \frac{1}{g_0}\int_0^\infty d\tau\, \tau e^{-p\tau}\Big(&\mathrm{Tr}[P_0\partial_i H_\tau \partial_j H] \\ &-\frac{1}{g_0}\mathrm{Tr}[P_0\partial_i H]\mathrm{Tr}[P_0\partial_j H]\Big)\Big|_{p=0}, \end{aligned} \tag{82}$$

with $\partial_i H_\tau \equiv e^{\tau H}\partial_i H e^{-\tau H}$.

Now we make some generic assumptions about the Hamiltonian H. First, let $\partial_i H$ be a local operator; that is, one can write

$$\partial_i H = \sum_y h_i(y), \tag{83}$$

in which y labels the spatial region over which the local operator $h_i(y)$ has support. Second, the $h_i(y)$ operators have well-defined scaling dimensions α_i near the quantum critical point $\mathbf{x}_c$ such that if

$$y \to ay, \quad \tau \to a^z\tau, \tag{84}$$

for $a > 0$, we obtain

$$h_i(y) \to a^{-\alpha_i} h_i(y). \tag{85}$$

Under these transformations, Eq. (82) yields the following scaling for the rescaled geometric tensor in the thermodynamic limit:

$$\frac{1}{L^d}\mathbf{G}_{ij} \to a^{-\kappa_{ij}} \frac{1}{L^d}\mathbf{G}_{ij}, \tag{86}$$

where

$$\kappa_{ij} \equiv \alpha_i + \alpha_j - 2z - d. \tag{87}$$

Here L is the linear size of the system and d is its spatial dimension. From Eq. (81), we obtain $\|\mathbf{x}-\mathbf{x}_c\| \sim \xi^{-1/\nu}$; that is, the scaling dimension of the Hamiltonian parameter $\mathbf{x}$ is $1/\nu$. Following standard scaling analysis arguments, the scaling behavior of the metric tensor (recall that $\mathbf{g} = \mathrm{Re}[\mathbf{G}]$) in the off-critical limit $\xi \ll L$ is

$$\mathbf{g}_{ij}(\mathbf{x} \approx \mathbf{x}_c) \approx L^d \|\mathbf{x}-\mathbf{x}_c\|^{\nu\kappa_{ij}}. \tag{88}$$

Moreover, in the critical region, where $\xi \gg L \gg$ the spacing between adjacent particles on the system lattice, in addition to the regular extensive scaling L^d, the finite-size scaling of the metric is $\mathbf{g}_{ij} \sim L^{d-\kappa_{ij}}$, which could be extensive, subextensive, or superextensive ($\kappa = 0$, positive, or negative, respectively). We also remark that there exist models, exhibiting quantum topological order, in which the critical $\mathbf{g}$ scales logarithmically, for example, $\mathbf{g} \sim \ln\|\mathbf{x}-\mathbf{x}_c\|$ [40–42].

IV. ADIABATIC GEODESICS

In this section, we solve the geodesic equation [Eq. (38)] analytically for some specific examples. Note that since the eigenprojections do not depend on $\mathrm{Tr}[H]$, Eq. (38) corresponds to an underdetermined system of coupled second-order differential equations. This can be seen more clearly by adopting a new parametrization (i.e., coordinate system) $\mathbf{y}(\mathbf{x})$ for the Hamiltonian such that $H(\mathbf{y}(\mathbf{x})) = y^1(\mathbf{x})I + H'(y^2(\mathbf{x}),\ldots,y^M(\mathbf{x}))$, in which $y^1 = \mathrm{Tr}[H]/N$ and $H' = H - \mathrm{Tr}[H]1/N$. Since $P_0(\mathbf{y})$ does not depend on y^1, the metric $\mathbf{g}(\mathbf{y})$ does not depend on this parameter either. Independence from y^1 translates in terms of $\mathbf{x}$ into the fact that only $M-1$ equations in the system (38) are independent.

A. Examples

1. Deutsch-Jozsa algorithm

In the Deutsch-Jozsa algorithm [43], one is given an oracle that calculates a function $f:\{0,1\}^n \mapsto \{0,1\}$. The promise is that f is either constant or balanced, meaning, respectively, that $f(\mathbf{i}) = f(\mathbf{i}')\forall \mathbf{i},\mathbf{i}'$ or $f(\text{half of all } \mathbf{i}\text{s}) = 0$, where $\mathbf{i}$ is the length-n binary representation of the decimal number $i \in \{0,\ldots,2^n-1\}$ [29]. The objective is to conclude whether f is constant or balanced. The Deutsch-Jozsa algorithm finds the answer by querying the oracle only once, while classical deterministic algorithms require a number of queries that is exponential in n.

An adiabatic version of this algorithm was introduced in Ref. [44]. We consider the unitary interpolation Hamiltonian [45]

$$H(x(s)) = \widetilde{V}(x(s))H_0\widetilde{V}^\dagger(x(s)), \tag{89}$$

where $\widetilde{V}(x(s)) = e^{i\frac{\pi}{2}x(s)G}$, in which the Hermitian-unitary G operator is defined by $G|\mathbf{i}\rangle = (-1)^{f(\mathbf{i})}|\mathbf{i}\rangle$. Here H_0 is chosen such that $|\Phi_0(0)\rangle = |+\rangle^{\otimes n} = 2^{-n/2}\sum_{i=0}^{2^n-1}|\mathbf{i}\rangle$ is its ground state, for example,

$$H_0 = h_0\sum_{k=1}^{n}|-\rangle_k\langle -|, \tag{90}$$

where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$, $\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$ is a Pauli matrix, and $h_0 > 0$ is an energy scale. The boundary conditions are chosen as $(x_0,x_1) = (0,1)$, so that $H(0) = H_0$ and $H(1) = GH_0G^\dagger$; the latter guarantees that $|\Phi_0(1)\rangle = G|\Phi_0(0)\rangle$ is the ground state of $H(1)$.

From Eq. (89), it is seen that $|\Phi_0(s)\rangle = \widetilde{V}(s)|\Phi_0(0)\rangle$, whence we obtain

$$P_0(x(s)) = 2^{-n}\sum_{i,i'=0}^{2^n-1} e^{i\frac{\pi}{2}x(s)[(-1)^{f(\mathbf{i})}-(-1)^{f(\mathbf{i}')}]}|\mathbf{i}\rangle\langle\mathbf{i}'|,$$
$$\partial_x P_0(x(s)) = i\frac{\pi}{2}[G,P_0(x(s))]. \tag{91}$$

A straightforward calculation then yields

$$\begin{aligned}\mathbf{g} &= \mathrm{Tr}\{[\partial_x P_0(x)]^2\}\\ &= \frac{\pi^2}{2}\{\mathrm{Tr}[P_0(x)G^2] - \mathrm{Tr}[(P_0(x)G)^2]\}\\ &= \frac{\pi^2}{2}\left\{1 - 2^{-2n}\left[\sum_{i=0}^{2^n-1} e^{i\pi f(\mathbf{i})}\right]^2\right\}.\end{aligned} \tag{92}$$

Since $\mathbf{g}$ is independent of $x(s)$, the geodesic equation [Eq. (38)] reduces to $\ddot{x} = 0$, whence the geodesic is simply

$$x(s) = s, \tag{93}$$

which corresponds to a rotation of the initial Hamiltonian H_0 at a constant rate.

2. Projective Hamiltonians

Consider the following Hamiltonian:

$$H(\mathbf{x}(s)) = x^1(s)P_{\mathbf{a}}^\perp + x^2(s)P_{\mathbf{b}}^\perp, \tag{94}$$

where $P_{\mathbf{a}}^\perp = I - |\mathbf{a}\rangle\langle\mathbf{a}|$ for a given $|\mathbf{a}\rangle \in \mathcal{H}$ (similarly for $P_{\mathbf{b}}^\perp$), $\langle\mathbf{a}|\mathbf{b}\rangle$ is a given function of N, and the boundary conditions are $\mathbf{x}_0 = (1,0)$ and $\mathbf{x}_1 = (0,1)$. This Hamiltonian may represent the adiabatic preparation of an unknown (hard to find) state $|\mathbf{b}\rangle$ from the supposedly known (simple to prepare) initialization $|\mathbf{a}\rangle$, provided that one has access to the oracle $P_{\mathbf{b}}^\perp$ [11]. An important instance of this class is Grover's Hamiltonian for search of a marked item among N unsorted items [46] (generalized to arbitrary initial amplitude distributions in Refs. [47,48]), where $|\mathbf{a}\rangle = \sum_{k=0}^{N-1}|k\rangle/\sqrt{N}$ and $|\mathbf{b}\rangle = |m\rangle$, for $m \in \{0,\ldots,N-1\}$. A successful adiabatic version of this algorithm was first described in Ref. [49].

Since the Hamiltonian [Eq. (94)] is effectively two-dimensional over the span of the vectors $|\mathbf{a}\rangle$ and $|\mathbf{b}\rangle$, it can be diagonalized analytically. Indeed, given $|\mathbf{a}\rangle$, we have the freedom to choose $N-1$ vectors $\{|\mathbf{a}_i^\perp\rangle\}_{i=1}^{N-1}$ such that together with $|\mathbf{a}\rangle$, they constitute an orthonormal basis for $\mathcal{H}$, that is, $\langle\mathbf{a}|\mathbf{a}_i^\perp\rangle = 0$ and $\langle\mathbf{a}_i^\perp|\mathbf{a}_j^\perp\rangle = \delta_{ij}$. Thus we can decompose

$|\mathbf{b}\rangle = \alpha_0|\mathbf{a}\rangle + \sum_{i=1}^{N-1}\alpha_i|\mathbf{a}_i^\perp\rangle$. Utilizing the freedom in choosing $\{|\mathbf{a}_i^\perp\rangle\}$ (up to the orthonormality condition), we can always rotate them such that $\alpha_{i>1} = 0$. In this case, we have

$$|\mathbf{b}\rangle = \alpha_0|\mathbf{a}\rangle + \alpha_1|\mathbf{a}_1^\perp\rangle, \tag{95}$$

where $\alpha_0 = \langle\mathbf{a}|\mathbf{b}\rangle$ and $\alpha_1 = \langle\mathbf{a}_1^\perp|\mathbf{b}\rangle$ [or more explicitly, $\alpha_1 = e^{i\phi_1}\sqrt{1-|\langle\mathbf{a}|\mathbf{b}\rangle|^2}$ for some arbitrary $\phi_1 \in [0,2\pi)$].

Expanding Eq. (94) in the $\{|\mathbf{a}\rangle,|\mathbf{a}_i^\perp\rangle\}_{i=1}^{N-1}$ basis and using Eq. (95) yields

$$\begin{aligned}H(\mathbf{x}) &= \begin{bmatrix} x^2(1-|\alpha_0|^2) & -x^2\alpha_0\bar{\alpha}_1 \\ -x^2\bar{\alpha}_0\alpha_1 & x^1 + x^2|\alpha_0|^2\end{bmatrix}\\ &\quad \oplus (x^1+x^2)I_{\{2,\ldots,N-1\}},\end{aligned} \tag{96}$$

where we have used the completeness of the basis to write $I = |\mathbf{a}\rangle\langle\mathbf{a}| + \sum_{i=1}^{N-1}|\mathbf{a}_i^\perp\rangle\langle\mathbf{a}_i^\perp|$, $I_{\{2,\ldots,N-1\}} \equiv \sum_{i=2}^{N-1}|\mathbf{a}_i^\perp\rangle\langle\mathbf{a}_i^\perp|$, and the matrix on the right-hand side is written in the $\{|\mathbf{a}\rangle,|\mathbf{a}_1^\perp\rangle\}$ (sub-) basis. It then follows from Eq. (96) that the spectrum of H consists of the two nondegenerate eigenvalues

$$E_\pm = \tfrac{1}{2}(x^1 + x^2 \pm \sqrt{(x^1)^2 + (x^2)^2 + 2(2|\langle\mathbf{a}|\mathbf{b}\rangle|^2 - 1)x^1x^2} \tag{97}$$

and the $(N-2)$-fold degenerate eigenvalue

$$E_> = x^1 + x^2. \tag{98}$$

Thus the gap between the ground state (E_-) and the first excited state (E_+) becomes

$$\Delta(\mathbf{x}) = \sqrt{(x^1)^2 + (x^2)^2 + 2(2|\langle\mathbf{a}|\mathbf{b}\rangle|^2 - 1)x^1x^2}. \tag{99}$$

The Hamiltonian [Eq. (96)] can be diagonalized by noting that one can rewrite

$$H(\mathbf{x}) = \tfrac{1}{2}A(\mathbf{x})[\Delta(\mathbf{x})\Sigma_z - (x^1+x^2)I_{\{0,1\}}]A^\dagger(\mathbf{x}) + (x^1+x^2)I, \tag{100}$$

where Σ_z is the Pauli matrix $\sigma_z = \mathrm{diag}(1,-1) \equiv |0\rangle\langle 0| - |1\rangle\langle 1|$ padded with zeros to embed it trivially into the N-dimensional representation [i.e., $\Sigma_z = \mathrm{diag}(\sigma_z,0,\ldots,0)$], $I_{\{0,1\}} \equiv \mathrm{diag}(1,1,0,\ldots,0)$, and the 2×2 unitary matrix $A(\mathbf{x})$ is defined as

$$A(\mathbf{x}) = e^{-i\theta(\mathbf{x})\sigma_y} \tag{101}$$

(the extension to N dimensions is similar to that of Σ_z by padding with sufficiently many zeros), with

$$\begin{aligned}\cos\theta &= 2x^2|\langle\mathbf{a}|\mathbf{b}\rangle|\sqrt{1-|\langle\mathbf{a}|\mathbf{b}\rangle|^2}\{4|\langle\mathbf{a}|\mathbf{b}\rangle|^2(1-|\langle\mathbf{a}|\mathbf{b}\rangle|^2)\\ &\quad\times (x^2)^2 + [x^1 - (1-2|\langle\mathbf{a}|\mathbf{b}\rangle|^2)x^2 - \Delta]^2\}^{-1/2}.\end{aligned} \tag{102}$$

After removing the energy shift $(x^1+x^2)I$ from Eq. (100), it is evident that the ground-state projection is

$$P_0(\mathbf{x}) = A(\mathbf{x})|1\rangle\langle 1|A^\dagger(\mathbf{x}) \tag{103}$$

(padded with zeros). This yields

$$\begin{aligned}\mathbf{g}_{ij} &= \mathrm{Tr}[\partial_i P_0 \partial_j P_0]\\ &= -\partial_i\theta\partial_j\theta\,\mathrm{Tr}([\sigma_y,P_0]^2)\\ &= \partial_i\theta\partial_j\theta.\end{aligned} \tag{104}$$

Obtaining the geodesic for the one-dimensional case $\mathbf{x} = (1-x,x)$ turns out to be simple and can be performed analytically, yielding

$$x(s) = \frac{1}{2} - \frac{|\langle\mathbf{a}|\mathbf{b}\rangle|}{2\sqrt{1-|\langle\mathbf{a}|\mathbf{b}\rangle|^2}}\tan[(1-2s)\arccos|\langle\mathbf{a}|\mathbf{b}\rangle|]. \tag{105}$$

It is interesting to note that this is exactly the solution obtained in Ref. [11] from the different metric $\widetilde{\mathbf{g}}$ [Eq. (70)].

3. One-dimensional transverse-field Ising chain

Consider a one-dimensional chain of spin-1/2 particles interacting according to the following Hamiltonian:

$$H(\mathbf{x}(s)) = -\sum_{\ell=-m}^{m} x^1(s)\sigma_z^{(\ell)} + x^2(s)\,\sigma_x^{(\ell)}\sigma_x^{(\ell+1)}, \tag{106}$$

with the boundary conditions $\mathbf{x}_0 = (1,0)$, $\mathbf{x}_1 = (0,1)$, and $\boldsymbol{\sigma}^{(m+1)} \equiv \boldsymbol{\sigma}^{(1)}$ [50]. Exact diagonalization by the Jordan-Wigner transformation [7] yields

$$|\Phi_0(\mathbf{x})\rangle = \otimes_{\ell=1}^m[\cos\theta_\ell(\mathbf{x})|0\rangle_{-\ell}|0\rangle_\ell + i\sin\theta_\ell(\mathbf{x})|1\rangle_{-\ell}|1\rangle_\ell], \tag{107}$$

where (cf. Ref. [10])

$$\sin 2\theta_\ell = \frac{x^2\sin\left(\frac{2\pi\ell}{2m+1}\right)}{\sqrt{\left(x^2\cos\frac{2\pi\ell}{2m+1} - x^1\right)^2 + (x^2)^2\sin^2\frac{2\pi\ell}{2m+1}}}. \tag{108}$$

It is evident from Eq. (107) that

$$\begin{aligned}|\dot{\Phi}_0\rangle &= \sum_{i=1}^2 \dot{x}^i\partial_i|\Phi_0\rangle\\ &= \sum_{i=1}^2\dot{x}^i\sum_{\ell=1}^m\partial_i\theta_\ell(-\sin\theta_\ell|0\rangle_{-\ell}|0\rangle_\ell + i\cos\theta_\ell|1\rangle_{-\ell}|1\rangle_\ell)\\ &\quad\otimes|\Phi_{\bar{\ell}}\rangle,\end{aligned}$$

where $|\Phi_{\bar{\ell}}\rangle$ is the same as $|\Phi_0\rangle$ [Eq. (107)], except that the term with the label ℓ is absent. In addition, it is easily verified that $\langle\Phi_0|\dot{\Phi}_0\rangle = 0$. Thus we obtain

$$\langle\dot{\Phi}_0|\dot{\Phi}_0\rangle = \sum_{i,j=1}^2\dot{x}^i\dot{x}^j\sum_\ell^m\partial_i\theta_\ell\partial_j\theta_\ell. \tag{109}$$

After inserting these results into Eq. (36), we have

$$\mathbf{g}_{ij}(\mathbf{x}) = \sum_{\ell=1}^m\partial_i\theta_\ell(\mathbf{x})\partial_j\theta_\ell(\mathbf{x}). \tag{110}$$

This is the geometric tensor for the transverse-field Ising model.

To make further progress, we focus on the one-parameter cases (1) $\mathbf{x} = (1-x,x)$, (2) $\mathbf{x} = (x,1)$, and (3) $\mathbf{x} = (1,x)$, all subject to the boundary conditions $x(0) = 1 - x(1) = 0$.

Let

$$p(x) = \frac{1}{4}\sum_{\ell=1}^m\frac{\sin^2\left(\frac{2\pi\ell}{2m+1}\right)}{\left[1-2\left(1+\cos\frac{2\pi\ell}{2m+1}\right)(1-x)x\right]^2}. \tag{111}$$

For a given finite lattice size m, the geodesic equation for case 1 reads

$$2p(x)\ddot{x} + \partial_x p(x)(\dot{x})^2 = 0. \tag{112}$$

This equation can be integrated to yield

$$2s = \int_0^{x(s)} \sqrt{p(x')}dx' \Big/ \int_0^{1/2} \sqrt{p(x')}\,dx'. \tag{113}$$

We next consider the thermodynamic limit $m \to \infty$, where we can obtain a simple closed-form formula for the geodesic. The expression in this limit follows from substituting $\sum_\ell \to (2m+1)/(2\pi)\int_0^\pi dz$ [with $z_\ell = 2\pi\ell/(2m+1)$] and taking into account that the model exhibits a QPT at $x_c = 1/2$ corresponding to $s_c = 1/2$. This yields

$$x(s) = \begin{cases} \frac{1}{2}1 - \tan^2\left[\frac{\pi}{4}(1-2s)\right], & 0 \leqslant s \leqslant \frac{1}{2}, \\ \frac{1}{2}1 + \tan^2\left[\frac{\pi}{4}(1-2s)\right], & \frac{1}{2} \leqslant s \leqslant 1. \end{cases} \tag{114}$$

For details of the derivation, see Appendix I.

Similarly, for both cases 2 and 3, we obtain the geodesic for a given finite m as

$$s = \int_0^{x(s)} \sqrt{q(x')}\,dx' \Big/ \int_0^{1} \sqrt{q(x')}\,dx', \tag{115}$$

where

$$q(x) = \frac{1}{4}\sum_{\ell=1}^{m} \frac{\sin^2\left(\frac{2\pi\ell}{2m+1}\right)}{\left[1 - 2\cos\frac{2\pi\ell}{2m+1}\right]^2}. \tag{116}$$

In the thermodynamic limit, a quantum critical point emerges at $x_c = 1$ ($s_c = 1$), and a similar approach as in case 1 yields the geodesic

$$x(s) = \sin(\pi s/2). \tag{117}$$

For details of the derivation, again, see Appendix I. Figure 1 illustrates the geodesics obtained for the transverse-field Ising model subject to the three parametrizations we have discussed.

B. Geodesic for passage through a quantum critical point

A limitation of our formalism is that in principle, exact knowledge of the ground state is required in order to obtain the geodesic. Unfortunately, such knowledge is rarely available, the exceptions being certain exactly solvable models such as those we treated in the previous section. With partial knowledge or an approximation for the gap, one should solve Eq. (38) on a case-by-case basis, possibly numerically.

However, while these observations apply in a setting where one wishes to obtain the geodesic over the entire parameter manifold, the situation in the vicinity of a quantum critical point is rather different. Indeed, the most interesting physics often happens in the vicinity of quantum criticality. In addition, the behavior of a quantum adiabatic algorithm is essentially governed by how the system approaches and/or passes through a quantum critical region. These considerations suggest that knowledge of the geodesic around quantum critical regions should suffice for most algorithmic or physically relevant applications, thus obviating the need for knowing P_0 everywhere.

Computation of the critical behavior of other geometric functions, such as Γ and $\mathbf{R}$, is straightforward. For example, in the one-parameter case, where $\mathbf{x} = (x)$, the Euler-Lagrange (geodesic) equation [Eq. (38)] in the critical region, slightly before and after the critical point, reduces to $\ddot{x} + \nu\kappa\dot{x}^2/2x = 0$, whence

$$x(s \approx s_c) \approx x_c + A(s - s_c)^\chi. \tag{118}$$

After using $\alpha = d + z - 1/\nu$ [51,52], where α is the scaling dimension [recall Eq. (85)], we obtain

$$\chi = 2/(2 + \nu\kappa) = 2/d\nu > 0, \tag{119}$$

with A constant (derivation details are given in Appendix I). This is a remarkable result as it characterizes the optimal adiabatic passage through a quantum critical point in terms of the universality class of the system. Moreover, this result confirms that the critical geodesic has a power-law dependence on s (as first reported in Ref. [53]), although away from the critical region, the dependence can be different. References [52–55] report critical behaviors of the metric tensor and related parameters obtained using different methods, such as minimizing exact expressions for the transition probability in thermodynamic limit. In contrast to the result of Ref. [53], in our analysis, the exponent χ of the critical geodesic depends on the dimensionality d, whereas it is independent of the total time T. In adiabatic evolution, the dependence on T is, of course, expected; however, note that our scaling result depends only upon the geometry of the control manifold, which does not depend on T.

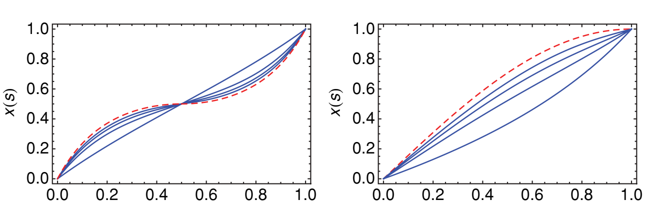

FIG. 1. (Color online) Optimal adiabatic paths for the one-dimensional transverse-field Ising model, corresponding to the parametrizations (left) $\mathbf{x} = (1 - x, x)$ and (right) $\mathbf{x} = (x, 1)$ and $\mathbf{x} = (1, x)$. The red dashed lines represent the thermodynamic limit, while the solid blue lines correspond to $m = 1, 4, 10, 30, 100$, approaching the dashed line as m increases.

V. SUMMARY AND CONCLUSIONS

In this work, we set out to elucidate the role of geometry in adiabatic quantum evolution. By splitting the adiabatic error, that is, the norm of the difference between the ideal adiabatic evolution operator and the actual propagator, into two components, one of which is endowed with a geometric meaning, we were able to derive a Riemannian metric tensor which encodes the geometry of adiabatic evolution. This metric is capable of describing evolution over both nondegenerate and degenerate subspaces. We then showed that this same metric tensor arises naturally from a number of different but complementary viewpoints, including a minimization of the operator fidelity and a focus on the Grassmannian structure of the dynamics.

Our second major goal in this work was to establish a firm connection between adiabatic evolution and quantum phase transitions. By analyzing the infinitesimal variation in the operator fidelity, we showed that in fact, the same metric tensor arises in both cases. We further derived the quantum critical scaling of this metric tensor.

Having established a unified geometric framework for adiabatic quantum evolution and quantum phase transitions, we proceeded to find the geodesics on the manifold described by the unifying Riemannian metric tensor. Such geodesics are of particular interest in adiabatic quantum computing, where they correspond to paths which minimize the geometric component of the deviation between the actual and desired final states. We analytically determined the geodesics in three examples of interest: the Deutsch-Jozsa algorithm, a generalization of Grover's algorithm, and a model described by the transverse-field Ising model. While such examples are important as proofs of principle, one cannot in general hope to analytically find the geodesics. For this reason, we focused on the passage through the quantum critical point and showed that in general, for second-order QPTs, the geodesic in this case obeys a universal scaling relation.

Among other applications, we expect that the formalism we have developed will lead to further developments in adiabatic quantum computing, where the role of criticality is well appreciated. We expect additional applications in holonomic quantum computing, where degeneracy plays an essential role and where a differential geometric analysis of gate error minimization has not yet been carried out.

Note Added. Recently, a related manuscript appeared [56], which similarly proposes a generalized quantum geometric tensor related to adiabatic evolution of quantum many-body systems.

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APPENDIX A: PROOF OF THE WILCZEK-ZEE HOLONOMY FORMULA

Notice that from the fact that P_0 is a projector, that is, $P_0 = P_0^2$, we obtain

$$\dot{P}_0 = \dot{P}_0 P_0 + P_0 \dot{P}_0 \tag{A1}$$

[where $\dot{P}_0 \equiv \partial_s P_0$] so that

$$P_0 \dot{P}_0 P_0 = 0, \tag{A2}$$

$$[\dot{P}_0, P_0] = 2\dot{P}_0 P_0 - \dot{P}_0. \tag{A3}$$

Let Q_0 denote the projector orthogonal to P_0, that is, $P_0 + Q_0 = I$. Then we have

$$P_0 Q_0 = Q_0 P_0 = 0. \tag{A4}$$

The differential equation for $V^{[0]}_{\alpha\alpha'}$ [Eq. (7)] can be obtained as follows:

$$\partial_s V^{[0]}_{\alpha\alpha'} = \langle \dot{\Phi}^{\alpha}_0 | V_{\text{ad}} | \Phi^{\alpha'}_0(0)\rangle + \langle \Phi^{\alpha}_0 | \dot{V}_{\text{ad}}(s) | \Phi^{\alpha'}_0(0)\rangle. \tag{A5}$$

In addition, consider the action of $H_{\text{ad}}(s)$ [Eq. (9)] on $|\Phi^{\alpha}_0(s)\rangle$:

$$\begin{aligned} &H_{\text{ad}}(s)|\Phi^{\alpha}_0(s)\rangle \\ &\quad = [H(s) + 2i\dot{P}_0(s)P_0(s)/T - i\dot{P}_0(s)/T]|\Phi^{\alpha}_0(s)\rangle \\ &\quad = E_0(s)|\Phi^{\alpha}_0(s)\rangle + i\dot{P}_0(s)|\Phi^{\alpha}_0(s)\rangle/T. \end{aligned} \tag{A6}$$

Since $\dot{P}_0(s) = \sum_{\beta=1}^{g_0} |\dot{\Phi}^{\beta}_0(s)\rangle\langle\Phi^{\beta}_0(s)| + |\Phi^{\beta}_0(s)\rangle\langle\dot{\Phi}^{\beta}_0(s)|$, we have

$$\dot{P}_0(s)|\Phi^{\alpha}_0(s)\rangle = |\dot{\Phi}^{\alpha}_0(s)\rangle + \sum_{\beta=1}^{g_0}\langle\dot{\Phi}^{\beta}_0(s)|\Phi^{\alpha}_0(s)\rangle|\Phi^{\beta}_0(s)\rangle. \tag{A7}$$

Using Eqs. (A6) and (A7), we can rewrite Eq. (A5) as

$$\begin{aligned} &\partial_s V^{[0]}_{\alpha\alpha'}(s) \\ &\quad = \langle\dot{\Phi}^{\alpha}_0(s)|V_{\text{ad}}(s)|\Phi^{\alpha'}_0(0)\rangle - iT\langle\Phi^{\alpha}_0(s)|H_{\text{ad}}(s)V_{\text{ad}}(s)|\Phi^{\alpha'}_0(0)\rangle \\ &\quad = -iTE_0(s)\langle\Phi^{\alpha}_0(s)|V_{\text{ad}}(s)|\Phi^{\alpha'}_0(0)\rangle - \sum_{\beta=1}^{g_0}\langle\Phi^{\alpha}_0(s)|\dot{\Phi}^{\beta}_0(s)\rangle \\ &\qquad \times\langle\Phi^{\beta}_0(s)|V_{\text{ad}}(s)|\Phi^{\alpha'}_0(0)\rangle. \end{aligned} \tag{A8}$$

Without loss of generality, after setting $E_0(s) = 0$, we obtain the following differential equation for $V^{[0]}_{\alpha\alpha'}(s)$:

$$\begin{aligned} \partial_s V^{[0]}_{\alpha\alpha'}(s) &= -\sum_{\beta=1}^{g_0}\langle\Phi^{\alpha}_0(s)|\dot{\Phi}^{\beta}_0(s)\rangle\langle\Phi^{\beta}_0(s)|V_{\text{ad}}(s)|\Phi^{\alpha'}_0(0)\rangle \\ &= -\sum_{\beta=1}^{g_0} A_{\alpha\beta}(s)V^{[0]}_{\beta\alpha'}(s), \end{aligned} \tag{A9}$$

whose solution is

$$V^{[0]}(s) = \mathcal{P}\exp\left[-\int_0^s A(s')\,ds'\right], \tag{A10}$$

with

$$A_{\alpha\beta} \equiv \langle\Phi^{\alpha}_0|\partial_s|\Phi^{\beta}_0\rangle. \tag{A11}$$

APPENDIX B: PROOF OF EQ. (27)

Equation (A2) yields

$$[\dot{P}_0, P_0]^2 = -(\dot{P}_0 P_0 \dot{P}_0 + P_0 \dot{P}_0^2 P_0). \tag{B1}$$

Using Eq. (A1) to write $P_0\dot{P}_0 = \dot{P}_0 - \dot{P}_0 P_0$ and substituting this into the first term of Eq. (B1), we then have

$$\begin{aligned} [\dot{P}_0, P_0]^2 &= -(\dot{P}_0^2 - \dot{P}_0^2 P_0 + P_0\dot{P}_0^2 P_0) \\ &= -\dot{P}_0^2 + Q_0\dot{P}_0^2 P_0. \end{aligned} \tag{B2}$$

The second term vanishes, as can be seen by using Eq. (A1) to write $\dot{P}_0^2 = (\dot{P}_0 P_0 + P_0 \dot{P}_0)^2$:

$$\begin{aligned} Q_0\dot{P}_0^2 P_0 = Q_0(&\dot{P}_0 P_0 \dot{P}_0 P_0 + \dot{P}_0 P_0 P_0 \dot{P}_0 + P_0\dot{P}_0^2 P_0 \\ &+ P_0\dot{P}_0 P_0 \dot{P}_0)P_0 = 0, \end{aligned}$$

where we used Eq. (A2) on the first two summands and Eq. (A4) on the last two. Thus we conclude that

$$[\dot{P}_0, P_0]^2 = -\dot{P}_0^2. \tag{B3}$$

Note that $\dot{P}_0 = \sum_{\alpha=1}^{g_0} |\dot{\Phi}_0^\alpha\rangle\langle\Phi_0^\alpha| + |\Phi_0^\alpha\rangle\langle\dot{\Phi}_0^\alpha|$ is Hermitian and that therefore $[\dot{P}_0, P_0]$ is anti-Hermitian. Thus both $\dot{P}_0$ and $[\dot{P}_0, P_0]$ are unitarily diagonalizable: $-\dot{P}_0 = VDV^\dagger$, $[\dot{P}_0, P_0] = WEW^\dagger$, where V and W are unitary, while D and E are the diagonal matrices of eigenvalues. Therefore it follows from Eq. (B2) that $\|VD^2V^\dagger\| = \|WE^2W^\dagger\|$ and from the unitary invariance of the operator norm that $\|D^2\| = \|E^2\|$. From here we conclude that the maximum absolute values of their eigenvalues are equal, that is,

$$\|[\dot{P}_0, P_0]\| = \|\dot{P}_0\|. \tag{B4}$$

It also follows that $\|\dot{P}_0^2\| = \|[\dot{P}_0, P_0]^2\| = \|D^2\| = \|D\|^2 = \|[\dot{P}_0, P_0]\|^2$, that is,

$$\|[\dot{P}_0, P_0]\| = \sqrt{\|\dot{P}_0^2\|}. \tag{B5}$$

Next we wish to show that

$$\dot{P}_0 = -\left(P_0\dot{H}\frac{1}{H - E_0} + \frac{1}{H - E_0}\dot{H}P_0\right). \tag{B6}$$

To prove this, note first that the Hamiltonian can be decomposed as

$$H = E_0P_0 + Q_0HQ_0. \tag{B7}$$

Then

$$\dot{H} = \dot{E}_0P_0 + E_0\dot{P}_0 - \dot{P}_0HQ_0 + Q_0\dot{H}Q_0 - Q_0H\dot{P}_0, \tag{B8}$$

and multiplying this equation by P_0 from the right, while using Eqs. (A2) and (A4) and the fact that H commutes with P_0, yields

$$\begin{aligned}\dot{H}P_0 &= \dot{E}_0P_0 + E_0\dot{P}_0P_0 - (I - P_0)H\dot{P}_0P_0 \\ &= \dot{E}_0P_0 + E_0\dot{P}_0P_0 - H\dot{P}_0P_0.\end{aligned} \tag{B9}$$

The operator $H - E_0$ is invertible when its domain excludes the spectrum of H (and is then called the reduced resolvent; see, e.g., Ref. [33]); that is, the inverse is defined as $Q_0[H - E_0]^{-1}Q_0$ (but for brevity and when there is no risk of confusion, we simply write $[H - E_0]^{-1}$ henceforth). With this restriction in mind, we then have

$$\dot{P}_0P_0 = -\frac{1}{H - E_0}(\dot{H} - \dot{E}_0)\quad P_0 = -\frac{1}{H - E_0}\dot{H}P_0, \tag{B10}$$

where in the last step, we used

$$\frac{1}{H - E_0}P_0 = P_0\frac{1}{H - E_0} = 0, \tag{B11}$$

which is due to the fact that the range of $[H - E_0]^{-1}$ is the range of Q_0 [recall also Eq. (28)]. Similarly, by multiplying Eq. (B8) from the left by P_0, we obtain

$$P_0\dot{P}_0 = -P_0\dot{H}\frac{1}{H - E_0}. \tag{B12}$$

Adding Eqs. (B10) and (B12), and using Eq. (A1) again, then yields Eq. (B6).

As a corollary, we can also calculate $\dot{E}_0(s)$ from Eq. (B9):

$$\dot{E}_0(s) = \mathrm{Tr}[\dot{H}P_0]/g_0. \tag{B13}$$

Calculation of $\ddot{P}_0$ or higher-order derivatives of P_0 follows similar logic (see, e.g., Ref. [33]). For example, we obtain

$$\begin{aligned}\ddot{P}_0 = -\Bigg(&\dot{P}_0\dot{H}\frac{1}{H - E_0} + P_0\ddot{H}\frac{1}{H - E_0} + P_0\dot{H}\partial_s\left[\frac{1}{H - E_0}\right] \\ &+ \partial_s\left[\frac{1}{H - E_0}\right]\dot{H}P_0 + \frac{1}{H - E_0}\ddot{H}P_0 + \frac{1}{H - E_0}\dot{H}\dot{P}_0\Bigg).\end{aligned} \tag{B14}$$

This relation can be simplified further after replacing $\dot{P}_0$ [Eq. (B6)], using the identity

$$\partial_s\left[\frac{1}{H - E_0}\right] = -\frac{1}{H - E_0}(\dot{H} - \dot{E}_0)\frac{1}{H - E_0} \tag{B15}$$

and inserting $\dot{E}_0$ [Eq. (B13)]. However, we do not need the final explicit form here.

We are now ready to prove Eq. (27). Let

$$A \equiv \frac{1}{H - E_0}\dot{H}P_0, \quad B \equiv P_0\dot{H}\frac{1}{H - E_0}. \tag{B16}$$

Then, using Eqs. (B5), (B6), and (B11) yields

$$\|[\dot{P}_0, P_0]\| = \sqrt{\|A^\dagger A + B^\dagger B\|}. \tag{B17}$$

Note that $A^\dagger A$ and $B^\dagger B$ are both positive operators and that they have orthogonal support. Therefore $\|A^\dagger A + B^\dagger B\| = \max\{\|A^\dagger A\|, \|B^\dagger B\|\}$. Moreover, we have $A^\dagger A = BB^\dagger$, and it is a basic property of the operator norm that $\|BB^\dagger\| = \|B^\dagger B\|$ for any operator B. Thus $\sqrt{\|A^\dagger A + B^\dagger B\|} = \sqrt{\|A^\dagger A\|}$, which is Eq. (27).

APPENDIX C: PROOF OF THE ERROR FORMULA IN THE FROBENIUS NORM

Starting from the definition of the adiabatic error [Eq. (33)], we have, by using Eq. (A2) together with $P_0^2 = P_0$ and cyclic invariance of the trace,

$$\begin{aligned}\epsilon(s) &= \int_0^s \sqrt{\mathrm{Tr}[(P_0\dot{P}_0 - \dot{P}_0P_0)(\dot{P}_0P_0 - P_0\dot{P}_0)]}\,ds' \\ &= \int_0^s \sqrt{\mathrm{Tr}[P_0\dot{P}_0\dot{P}_0 + \dot{P}_0P_0\dot{P}_0]}\,ds' \\ &= \int_0^s \sqrt{\mathrm{Tr}[P_0(\partial_iP_0)(\partial_jP_0) + (\partial_iP_0)P_0(\partial_jP_0)]\dot{x}^i\dot{x}^j}\,ds',\end{aligned} \tag{C1}$$

where $\dot{P}_0 = \partial_iP_0\dot{x}^i$. Using $P_0^2 = P_0$ once more to obtain $P_0(\partial_iP_0) + (\partial_iP_0)P_0 = \partial_iP_0$, we have

$$\epsilon(s) = \int_0^s \sqrt{\mathrm{Tr}\{[\partial_iP_0 - (\partial_iP_0)P_0](\partial_jP_0) + (\partial_iP_0)P_0(\partial_jP_0)\}\dot{x}^i\dot{x}^j}\,ds' \tag{C2}$$

$$= \int_0^s \sqrt{2g_0\mathbf{g}_{ij}(\mathbf{x})\dot{x}^i\dot{x}^j}\,ds', \tag{C3}$$

where the metric tensor is defined as $\mathbf{g}_{ij} \equiv \mathrm{Tr}[\partial_iP_0\partial_jP_0]/(2g_0)$, which is Eq. (36).

Next let us derive Eq. (37). From Eq. (B6), we have

$$\partial_iP_0 = -\left[P_0(\partial_iH)\frac{1}{H - E_0} + \frac{1}{H - E_0}(\partial_iH)P_0\right]. \tag{C4}$$

Inserting this into $\mathrm{Tr}[\partial_i P_0 \partial_j P_0]$ and expanding the product while using Eq. (B11), we obtain

$$\begin{aligned}
&\mathrm{Tr}[\partial_i P_0 \partial_j P_0] \\
&= \mathrm{Tr}\left\{\left[P_0(\partial_i H)\frac{1}{H-E_0} + \frac{1}{H-E_0}(\partial_i H)P_0\right]\right. \\
&\quad \times \left.\left[P_0(\partial_j H)\frac{1}{H-E_0} + \frac{1}{H-E_0}(\partial_j H)P_0\right]\right\} \\
&= \mathrm{Tr}\left[P_0(\partial_i H)\left(\frac{1}{H-E_0}\right)\left(\frac{1}{H-E_0}\right)(\partial_j H)P_0\right. \\
&\quad + \left.\frac{1}{H-E_0}(\partial_i H)P_0 P_0(\partial_j H)\frac{1}{H-E_0}\right] \\
&= \mathrm{Tr}\left[P_0(\partial_i H)\left(\frac{1}{H-E_0}\right)^2(\partial_j H)P_0\right] \\
&\quad + \mathrm{Tr}\left[P_0(\partial_j H)\left(\frac{1}{H-E_0}\right)^2(\partial_i H)P_0\right], \qquad \text{(C5)}
\end{aligned}$$

as desired.

APPENDIX D: PROOF THAT g IS A METRIC

By definition, a metric must satisfy three properties [1]: It must be positive, real, and symmetric.

1. Positive: For any nonzero $\alpha(\mathbf{x}) \in T_{\mathcal{M}}(\mathbf{x})$, we have

$$\begin{aligned}
&\alpha(\mathbf{x})\cdot \mathbf{g}(\mathbf{x})\cdot \alpha(\mathbf{x}) \\
&= \mathbf{g}_{ij}(\mathbf{x})\alpha^i(\mathbf{x})\alpha^j(\mathbf{x}) \\
&= \frac{1}{2g_0}\mathrm{Tr}\{[\partial_i P_0(\mathbf{x})][\partial_j P_0(\mathbf{x})]\}\alpha^i(\mathbf{x})\alpha^j(\mathbf{x}) \\
&= \mathrm{Tr}\left\{\left[\frac{1}{\sqrt{2g_0}}\alpha^i(\mathbf{x})\partial_i P(\mathbf{x})\right]_{lk}\left[\frac{1}{\sqrt{2g_0}}\alpha^j(\mathbf{x})\partial_j P(\mathbf{x})\right]_{kl}\right\} \\
&\equiv \mathrm{Tr}[C^\dagger(\alpha,\mathbf{x})C(\alpha,\mathbf{x})] \geqslant 0, \qquad \text{(D1)}
\end{aligned}$$

where

$$C(\alpha,\mathbf{x}) \equiv \frac{1}{\sqrt{2g_0}}\alpha^i(\mathbf{x})\partial_i P(\mathbf{x}). \qquad \text{(D2)}$$

Note that although $\mathrm{Tr}[(dP_0)^2]$ is always positive, when we move to a coordinate $\mathbf{x}$, the resulting pull-back metric $\mathbf{g}(\mathbf{x})$ might become singular (noninvertible) at some points or even identically zero. In this strict sense, $\mathbf{g}(\mathbf{x})$ is not a metric.

2. Real: This is obvious from the very construction of $\mathbf{g} = \mathrm{Re}[\mathbf{G}]$.

3. Symmetric: This is obvious from the definition and cyclic invariance of the trace: $\mathbf{g}_{ij} \equiv \mathrm{Tr}[\partial_i P_0 \partial_j P_0]/(2g_0) = \mathrm{Tr}[\partial_j P_0 \partial_i P_0]/(2g_0) = \mathbf{g}_{ji}$.

APPENDIX E: PROOF OF THE OPERATOR FIDELITY INEQUALITIES

We start by proving Eq. (41). From the definition of the operator fidelity [Eq. (40)] with $\varrho = I/N$, we have, using Eq. (14),

$$\begin{aligned}
f(s) &= \left|\mathrm{Tr}\left[\frac{I}{N}\Omega(s)\right]\right| = \left|\mathrm{Tr}\left[\frac{I}{N} - \frac{1}{N}\int_0^s K_T(s')\Omega(s')\,ds'\right]\right| \\
&= \left|1 - \frac{1}{N}\int_0^s \mathrm{Tr}[K_T\Omega]\,ds'\right| \\
&\geqslant 1 - \frac{1}{N}\int_0^s |\mathrm{Tr}[K_T\Omega]|\,ds' \\
&= 1 - \frac{1}{N}\int_0^s |\mathrm{Tr}([\partial_{s'}P_0, P_0]VV_{\mathrm{ad}}^\dagger)|\,ds', \qquad \text{(E1)}
\end{aligned}$$

where in the last line, we used the definitions of $\Omega(s)$ [Eq. (13)] and $K_T(s)$ [Eq. (15)] and cyclic invariance of the trace. Now recall the Cauchy-Schwartz inequality for operators [18]:

$$\|A\|_2\|B\|_2 \geqslant |\langle A,B\rangle| := |\mathrm{Tr}[A^\dagger B]|. \qquad \text{(E2)}$$

Applying this with $A := [\partial_{s'}P_0, P_0]$ and $B := VV_{\mathrm{ad}}^\dagger$ and noting that $\|VV_{\mathrm{ad}}^\dagger\|_2 = \sqrt{\mathrm{Tr}[V_{\mathrm{ad}}V^\dagger VV_{\mathrm{ad}}^\dagger]} = \sqrt{N}$, we obtain

$$f(s) \geqslant 1 - \frac{1}{\sqrt{N}}\int_0^s \|[\partial_{s'}P_0, P_0]\|_2\,ds' = 1 - \frac{1}{\sqrt{N}}\epsilon(s), \qquad \text{(E3)}$$

as we set out to prove. The inequality $f(s) \leqslant 1$ follows from the fact that $\Omega(s)$ is unitary: Diagonalizing $\Omega(s)$ and taking the absolute values of all N of its diagonal elements, which are roots of unity, gives $|\mathrm{Tr}[\Omega(s)]| \leqslant N$.

Next we prove Eq. (44). Using Eq. (14) along with submultiplicativity and the triangle inequality, we have

$$\begin{aligned}
&\|X(s) - X_{\mathrm{ad}}(s)\| \\
&= \|X - \Omega(s)^\dagger X\Omega(s)\| \\
&= \left\|X - \left[I - \sum_{l=1}^{\infty}\Omega_l^\dagger(s)\right]X\left[I - \sum_{l'=1}^{\infty}\Omega_{l'}(s)\right]\right\| \\
&= \left\|\sum_{l=1}^{\infty}\Omega_l^\dagger(s)X + X\sum_{l=1}^{\infty}\Omega_l(s) - \sum_{l,l'=1}^{\infty}\Omega_l^\dagger(s)X\Omega_{l'}(s)\right\| \\
&\leqslant \|X\|\sum_{l=1}^{\infty}\|\Omega_l(s)\|\left[2 + \sum_{l'=1}^{\infty}\|\Omega_{l'}(s)\|\right] \\
&= \|X\|\left[\|\Omega_1(s)\| + \sum_{l=2}^{\infty}\left\|\int_0^s ds' K_T(s')\Omega_{l-1}(s')\right\|\right] \\
&\quad \times \left[2 + \sum_{l'=1}^{\infty}\|\Omega_{l'}(s)\|\right]. \qquad \text{(E4)}
\end{aligned}$$

The term in the first square brackets is identical to that in Eq. (21) and hence is bounded by Eq. (22). The summand $\sum_{l=1}^{\infty}\|\Omega_l(s)\|$ in the second term is $O(1/T)$ according to Eq. (19). We thus have

$$\|X(s) - X_{\mathrm{ad}}(s)\| \leqslant \|X\|[\delta_1(s) + \tilde{\epsilon}(s)O(1/T)][2 + O(1/T)], \qquad \text{(E5)}$$

where δ_1 is defined in Eq. (25), and the last line follows from Eq. (19).

APPENDIX F: PROOF OF EQS. (71) AND (72)

To prove Eq. (71), we invoke the following inequality:

$$|\mathrm{Tr}[XY]| \leqslant \|X\|_1 \|Y\|, \tag{F1}$$

valid for any pair of arbitrary operators X and Y [57]. In addition, note that by definition, the operator norm of the reduced resolvent $[H(s) - E_0(s)]^{-1}$ satisfies

$$\left\| \frac{1}{H(s) - E_0(s)} \right\| = \frac{1}{\mathrm{dist}\{\{E_0(s)\},\mathrm{spec}[H(s)]\backslash\{E_0(s)\}\}} \leqslant \frac{1}{\min_s \Delta(s)}, \tag{F2}$$

where spec$(H(s))$ is the spectrum of $H(s)$ and the distance between two sets $\mathcal{A}$ and $\mathcal{B}$ is defined as follows:

$$\mathrm{dist}(\mathcal{A},\mathcal{B}) \equiv \inf_{a\in\mathcal{A},b\in\mathcal{B}} |a-b|. \tag{F3}$$

Equation (37) now yields

$$\begin{aligned}
\mathbf{g}_{ij} &\leqslant |\mathbf{g}_{ij}| \\
&\leqslant \frac{1}{g_0}\left|\mathrm{Tr}\left[(\partial_j H)P_0(\partial_i H)\left(\frac{1}{H-E_0}\right)^2\right]\right| \\
&\overset{\text{Eq. (F2)}}{\leqslant} \frac{1}{g_0}\|(\partial_j H)P_0(\partial_i H)\|_1 \left\|\frac{1}{H-E_0}\right\|^2 \\
&\overset{\text{Eq. (F2), submultiplicativity}}{\leqslant} \frac{1}{g_0 \min_s \Delta^2}\|P_0\|_1 \|\partial_i H \partial_j H\|_1 \\
&\overset{\|P_0\|_1 = g_0}{\leqslant} \frac{\|\partial_i H\partial_j H\|_1}{\min_s \Delta^2}.
\end{aligned} \tag{F4}$$

The proof of Eq. (72) is immediate from $|\mathrm{Tr}[X]| \leqslant \sum_i \sigma_i(X) = \|X\|_1$.

APPENDIX G: PROOF OF EQ. (75)

The operator fidelity of two positive operators X and Y relative to a density matrix ϱ is defined as

$$f_\varrho(X,Y) = \mathrm{Tr}[XY\varrho], \tag{G1}$$

which is always nonnegative because the trace of the product of positive operators is nonnegative. When $X,Y \in \mathcal{G}_{N,g_0}$ (Sec. II D1) and when ϱ is fully supported on the ground eigensubspace, one can conclude from the inequality $0 \leqslant \mathrm{Tr}[XY] \leqslant \mathrm{Tr}[Y]$ [18] that $f_\varrho(X,Y) \leqslant 1$.

Now we compute the fidelity of the ground-state projections $P_0(\mathbf{x})$ and $P_0(\mathbf{x}+d\mathbf{x})$ relative to $\varrho = I_{g_0}/g_0$ up to the first nonvanishing order:

$$\begin{aligned}
&f_\varrho(P_0(\mathbf{x}),P_0(\mathbf{x}+d\mathbf{x})) \\
&= \langle P_0(\mathbf{x}),P_0(\mathbf{x}+d\mathbf{x})\rangle_\varrho \\
&= \frac{1}{g_0}\mathrm{Tr}[P_0(\mathbf{x})P_0(\mathbf{x}+d\mathbf{x})] \\
&= \frac{1}{g_0}\mathrm{Tr}\left\{P_0(\mathbf{x})\left[P_0(\mathbf{x}) + dP_0(\mathbf{x}) + \frac{1}{2}d^2P_0(\mathbf{x})\right]\right\} \\
&= 1 + \frac{1}{2g_0}\mathrm{Tr}[P_0(\mathbf{x})d^2P_0(\mathbf{x})P_0(\mathbf{x})],
\end{aligned} \tag{G2}$$

where in the last two lines, we used Eqs. (A1) and (A2). Equation (A1) also yields

$$d^2P_0 = d^2P_0P_0 + 2dP_0dP_0 + P_0d^2P_0, \tag{G3}$$

whence

$$P_0d^2P_0P_0 = -2P_0(dP_0)^2P_0. \tag{G4}$$

Thus Eq. (G2) is simplified as follows:

$$f_\varrho(P_0(\mathbf{x}),P_0(\mathbf{x}+d\mathbf{x})) = 1 - \frac{1}{g_0}\mathrm{Tr}[P_0(dP_0)^2P_0]. \tag{G5}$$

APPENDIX H: PROOF OF EQ. (82)

Note the following identity for the reduced resolvent:

$$\begin{aligned}
Q_0\frac{1}{H-E_0}Q_0 &= Q_0\frac{1}{p+H-E_0}\bigg|_{p=0}Q_0 \\
&= \int_0^\infty Q_0 e^{(-p+H-E_0)\tau}Q_0\,d\tau\bigg|_{p=0}.
\end{aligned} \tag{H1}$$

Therefore

$$\begin{aligned}
\left(Q_0\frac{1}{H-E_0}Q_0\right)^2 &= -\frac{d}{dp}Q_0\frac{1}{p+H-E_0}\bigg|_{p=0}Q_0 \\
&= -\frac{d}{dp}\int_0^\infty Q_0e^{(-p+H-E_0)\tau}Q_0 d\tau|_{p=0}.
\end{aligned} \tag{H2}$$

Substituting Eq. (H2) into Eq. (79), while recalling that in Eq. (79), the inverse $[H-E_0]^{-1}$ is really shorthand for $Q_0[H-E_0]^{-1}Q_0$, yields

$$\begin{aligned}
&\mathbf{G}_{ij} \\
&= -\frac{1}{g_0}\frac{d}{dp}\int_0^\infty d\tau \mathrm{Tr}[P_0(\partial_i H)Q_0e^{-(p+H-E_0)\tau}Q_0(\partial_j H)]|_{p=0} \\
&= -\frac{1}{g_0}\frac{d}{dp}\int_0^\infty d\tau e^{-p\tau}\mathrm{Tr}[P_0(\partial_i H_\tau)Q_0(\partial_j H)]|_{p=0} \\
&= -\frac{1}{g_0}\frac{d}{dp}\int_0^\infty d\tau e^{-p\tau}\{\mathrm{Tr}[P_0(\partial_i H_\tau)(\partial_j H)] \\
&\quad - \mathrm{Tr}[P_0(\partial_i H)P_0(\partial_j H)]\}|_{p=0},
\end{aligned} \tag{H3}$$

with $\partial_i H_\tau \equiv e^{\tau H}\partial_i He^{-\tau H}$. Note that from Eqs. (B8) and (B13), and the property $P_0\dot{P}_0P_0 = 0$, we obtain

$$\begin{aligned}
\mathrm{Tr}[P_0(\partial_i H)P_0(\partial_j H)] &= \partial_i E_0\mathrm{Tr}[P_0(\partial_j H)] \\
&= \frac{1}{g_0}\mathrm{Tr}[P_0(\partial_i H)]\mathrm{Tr}[P_0(\partial_j H)].
\end{aligned} \tag{H4}$$

Substituting Eq. (H4) into Eq. (H3) and taking the derivative with respect to p yields

$$\begin{aligned}
\mathbf{G}_{ij} = \frac{1}{g_0}\int_0^\infty d\tau\tau e^{-p\tau}\bigg\{&\mathrm{Tr}[P_0(\partial_i H_\tau)(\partial_j H)] \\
&- \frac{1}{g_0}\mathrm{Tr}[P_0(\partial_i H)]\mathrm{Tr}[P_0(\partial_j H)]\bigg\}\bigg|_{p=0},
\end{aligned} \tag{H5}$$

as desired.

APPENDIX I: DETAILED DERIVATIONS OF RESULTS REPORTED IN SEC. IV A3

A. Derivation of Eq. (114)

In the thermodynamic limit, we replace $\sum_\ell$ by $(2m+1)/(2\pi)\int_0^\pi dz$, where the prefactor is due to a change of variables. Then Eq. (111) yields

$$\begin{aligned} p(x) &= \frac{1}{4}\sum_{\ell=1}^{m} \frac{\sin^2\left(\frac{2\pi\ell}{2m+1}\right)}{\left[1-2\left(1+\cos\frac{2\pi\ell}{2m+1}\right)(1-x)x\right]^2} \\ &\to \int_0^\pi dz \frac{\sin^2 z}{[1-2(1+\cos z)(1-x)x]^2} \\ &= \frac{\pi}{2(1-x)^2(1-2x)}. \end{aligned} \tag{I1}$$

Hence, for $0 \leqslant x' < 1/2$,

$$\begin{aligned} \int_0^{x(s)} \sqrt{p(x')}\,dx' &= \sqrt{\frac{\pi}{2}}\int_0^{x(s)} \frac{dx'}{(1-x')\sqrt{1-2x'}} \\ &= \frac{1}{2}\sqrt{\frac{\pi}{2}}[\pi - 4\arctan\sqrt{1-2x(s)}], \\ \int_0^{1/2} \sqrt{p(x')}\,dx' &= \frac{\pi}{2}\sqrt{\frac{\pi}{2}}. \end{aligned} \tag{I2}$$

Now, from Eq. (113), we obtain

$$\begin{aligned} 2s &= \int_0^{x(s)} \sqrt{p(x')}\,dx' \Big/ \int_0^{1/2} \sqrt{p(x')}\,dx' \\ &= \frac{1}{\pi}[\pi - 4\arctan\sqrt{1-2x(s)}]. \end{aligned} \tag{I3}$$

The last equation yields the first case in Eq. (114):

$$x(s) = \frac{1}{2}\left\{1 - \tan^2\left[\frac{\pi}{2}\left(s - \frac{1}{2}\right)\right]\right\}. \tag{I4}$$

The second case in Eq. (114) is obtained similarly.

B. Derivation of Eq. (117)

In the thermodynamic limit, using $\sum_\ell \to (2m+1)/(2\pi)\int_0^\pi dz$ again,

$$\begin{aligned} q(x) &= \frac{1}{4}\sum_{\ell=1}^{m} \frac{\sin^2\left(\frac{2\pi\ell}{2m+1}\right)}{\left[1-2\cos\frac{2\pi\ell}{2m+1}\right]^2} \\ &\to \int_0^\pi dz \frac{\sin^2 z}{[1-2x\cos z + x^2]^2} \\ &= \frac{\pi}{2(1-x^2)}. \end{aligned} \tag{I5}$$

Hence, for $0 \leqslant x' \leqslant 1$,

$$\begin{aligned} \int_0^{x(s)} \sqrt{q(x')}\,dx' &= \sqrt{\frac{\pi}{2}}\arcsin x(s), \\ \int_0^{1} \sqrt{q(x')}\,dx' &= \frac{\pi}{2}\sqrt{\frac{\pi}{2}}. \end{aligned} \tag{I6}$$

Now, from Eq. (115), we obtain

$$\begin{aligned} s &= \int_0^{x(s)} \sqrt{q(x')}\,dx' \Big/ \int_0^{1} \sqrt{q(x')}\,dx' \\ &= \frac{2}{\pi}\arcsin x(s). \end{aligned} \tag{I7}$$

Thus we obtain Eq. (117):

$$x(s) = \sin(\pi s/2). \tag{I8}$$

C. Derivation of Eqs. (118) and (119)

To solve

$$\ddot{X} + \nu\kappa\dot{X}^2/2X = 0 \tag{I9}$$

(where $X \equiv x - x_c$), we use the following identity:

$$\ddot{X} = \dot{X}\frac{d\dot{X}}{dX} = \frac{1}{2}\frac{d}{dX}(\dot{X})^2. \tag{I10}$$

Hence

$$\begin{aligned} \frac{d\dot{X}^2}{\dot{X}^2} &= -\nu\kappa\frac{dX}{X} \overset{\int}{\Rightarrow} \dot{X}^2 = KX^{-\nu\kappa} \Rightarrow X^{\nu\kappa/2}dX = K\,ds \\ &\overset{\int}{\Rightarrow} \frac{X^{\nu\kappa+1}}{\nu\kappa/2+1} = K(s-s_c) \\ &\Rightarrow X(s) = [K(\nu\kappa/2+1)(s-s_c)]^{\frac{1}{\nu\kappa/2+1}} \\ &\equiv A(s-s_c)^{\frac{2}{2+\nu\kappa}}. \end{aligned} \tag{I11}$$

Therefore

$$x(s) - x_c = A(s-s_c)^{\frac{2}{2+\nu\kappa}}. \tag{I12}$$

The derivation of Eq. (119) is

$$\begin{aligned} \chi &= \frac{2}{2+\nu\kappa} \\ &\overset{\text{Eq. (87)}}{=} \frac{2}{2+\nu(2\alpha-2z-d)} \\ &\overset{\alpha=d+z-1/\nu}{=} \frac{2}{2+\nu(2d+2z-2/\nu-2z-d)} \\ &= \frac{2}{d\nu}. \end{aligned} \tag{I13}$$

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