Gauge fields and extrapotentials in constrained quantum systems

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We derive an effective Hamiltonian for a quantum system constrained to a submanifold (the constraint manifold) of configuration space (the ambient space) by an infinite restoring force. We pay special attention to how this Hamiltonian depends on quantities which are external to the constraint manifold, such as the extrinsic curvature of the constraint manifold, the curvature of the ambient space, and the constraining potential. In particular, we find the remarkable fact that the twisting of the constraining potential appears as a gauge potential in the constrained Hamiltonian. This gauge potential is closely related to the geometric phase originally discussed by Berry. The constrained Hamiltonian also contains an effective potential depending on the extrinsic curvature of the constraint manifold, the curvature of the ambient space, and the twisting of the constraining potential. The general nature of our analysis allows applications to a wide variety of problems, such as rigid molecules, the evolution of molecular systems along reaction paths, and quantum strip waveguides.

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I. INTRODUCTION

A. Summary of results

We derive an effective Hamiltonian for a quantum system subject to an infinite restoring force. Though our results are quite general, we are motivated by several specific applications, such as stiff molecular bonds in rigid molecules and clusters of rigid molecules, molecular systems evolving along reaction paths, and electrons confined to quantum strip waveguides.

For comparison, consider first a classical system. We have in mind a system which initially occupies any position in the full configuration space (called the ambient space) but is subsequently confined to a submanifold (called the constraint manifold) by the introduction of a restoring force, which in a certain limit becomes infinite. Here, the Hamiltonian is simply the kinetic energy plus the constraining potential, which we assume is constant along the constraint manifold. Assuming the initial velocity is tangent to the constraint manifold, it is well known that the system's trajectory remains on the constraint manifold and that its motion is determined solely by the form of the kinetic energy tangent to the manifold [1,2]. This kinetic energy, in turn, depends only on the Riemannian metric of the constraint manifold. Thus, the motion of the constrained classical system depends only on the intrinsic metric of the constraint manifold and is independent of the ambient space, the embedding of the constraint manifold within the ambient space, or the details of the constraining potential. It is a remarkable fact, then, that for a quantum system this is no longer true. The constrained quantum Hamiltonian depends on the curvature of the ambient space, the extrinsic curvatures of the constraint manifold, and on properties of the constraining potential.

It has been known for some time that a constrained quantum system ''senses'' the local neighborhood of the constraint manifold [3–11]. As a simple example, consider a quantum system whose motion transverse to the constraint manifold is in the ground state. Due to the conservation of the transverse action, the constrained quantum system sees the transverse zero point energy as an effective potential on the constraint manifold. (We call this the adiabatic potential.) The adiabatic potential also appears classically if the initial velocity of the system has a nonzero component normal to the constraint manifold. Classically, the adiabatic potential can always be eliminated by choosing an initial velocity tangent to the constraint manifold. Quantum mechanically, however, due to the Heisenberg principle, the transverse action and hence the adiabatic potential can never be eliminated.

The present paper focuses on effects of the ambient space and constraining potential other than the adiabatic potential. Following da Costa [6–8,10], we assume that the constraining potential has the same form in the neighborhood of each point of the constraint manifold (in a manner to be made precise later.) The adiabatic potential is thereby forced to be constant along the constraint manifold and can subsequently be ignored. (In Sec. IV C, we discuss briefly how a small amount of variation in the adiabatic potential can be accommodated.) In two noteworthy papers [6,7], da Costa, using this assumption, derived the effective Hamiltonian for a system of n constrained point particles. This Hamiltonian contains two terms. The first is proportional to the Laplacian on the constraint manifold, and therefore depends only on the intrinsic metric of the constraint manifold. The second, however, is an effective potential, called the extrapotential, which depends not only on the intrinsic curvature, but also the extrinsic curvature of the constraint manifold. This extrapotential is of order $\hbar^2$ and therefore vanishes in the classical (and semiclassical) limit. As a simple, yet illustrative, example, consider a system defined on $\mathbb{R}^3$ constrained to lie on a curve. For this system, the extrapotential is $-\hbar^2/(8\rho^2)$, where ρ is the radius of curvature. This result was obtained by da Costa [6]; the same result was obtained earlier by Marcus [3] and Switkes *et al.* [5] for curves in $\mathbb{R}^2$. This extrapotential has been studied by others as well, including Jensen and Koppe [4] and Kaplan, Maitra, and Heller [11]. Since the extrapotential depends on the extrinsic curvature, it can never be derived from a procedure which

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quantizes the constrained classical system (which depends only on the intrinsic curvature), an approach common in the literature of constrained quantum mechanics. (See, for example, the review of DeWitt [12].)

As mentioned above, once the constraining potential is defined at one point of the constraint manifold, the constraining potential at all other points must have the same functional form. However, this requirement does not completely determine the constraining potential since the orientation of the potential is left unspecified. In other words, the equipotentials surrounding the constraint manifold can twist in some unspecified manner as one moves along the manifold. This potential twist is a critical quantity in our theory.

da Costa fixed the twisting ambiguity by imposing what we call a ''no twist'' condition on the potential. Physically, this condition requires the restoring forces in the neighborhood of the constraint manifold to be normal to the manifold. It can be viewed as an extension of the fact that in classical mechanics nondissipative forces are normal to the constraint manifold at the point of the manifold itself. da Costa astutely realized that if the no twist condition were violated, the motion transverse to the constraint manifold would be coupled to the motion tangent to the manifold and the Schrödinger equation would not separate.

For some submanifolds there exist no potentials which satisfy the no twist condition. In Ref. [7] da Costa derived a local geometric criterion on the extrinsic curvature of a submanifold which was necessary and sufficient to determine the existence of a nontwisting potential. Unfortunately, several common examples of constrained systems do not satisfy this criterion. For example, consider a model of a polymer by $n>2$ point particles where the distance between each particle i and its neighbor $i+1$ is fixed. Such systems fail da Costa's criterion [13]. A system of $n>2$ point particles constrained to form a rigid body similarly fails da Costa's criterion. Even for a submanifold which admits a nontwisting constraining potential, the physics may nevertheless dictate a twisting potential. These examples illustrate the need for a theory of constrained quantum mechanics which is not limited to potentials without twist.

The principal objective of this paper is to derive an effective Hamiltonian for a constrained quantum system with arbitrary twisting of the potential. The presence of the potential twist leads to several qualitative changes in the Hamiltonian. First, the Hamiltonian is no longer a scalar operator, but rather a $k\times k$ matrix of operators acting on a k-dimensional vector-valued wave function defined over the constraint manifold. Here, k is the degeneracy of the transverse energy, and each component of the vector wave function represents a different transverse mode. Of course, for a nondegenerate transverse energy, the constrained Hamiltonian is a scalar operator.

The second and perhaps most interesting consequence of dropping the no twist condition is the emergence of a $U(k)$ gauge potential, or connection, in the constrained Hamiltonian. This gauge potential is a coupling between the potential twist and the generalized angular momentum of the transverse modes. Modes with no such angular momentum are unaffected by the potential twist. The gauge potential is closely related to the geometric phase originally introduced by Berry in the context of adiabatic transport of quantum states [14]. It is interesting to note that the gauge potential is of order $\hbar^0$ and therefore, like the adiabatic potential, is essentially of classical origin.

The third and final consequence of the potential twist is the addition of a term to the original extrapotential derived by da Costa. Unlike the extrapotential terms derived by da Costa, the potential twist term is not a scalar function, but a $k\times k$ matrix of such functions with possible off-diagonal terms coupling the degenerate transverse modes.

In some important applications, the ambient space has nonzero curvature. For example, consider the problem of constraining a molecule to lie on a molecular reaction path. The internal space of such a molecule is in general not flat [15], and therefore, the constraint problem requires an analysis which includes the ambient curvature. Because of such examples, we do not assume in this paper that the ambient space is flat. The effects of the ambient curvature are most notable as additional terms in the extrapotential.

This paper has the following organization. In Sec. I B we introduce many of the key concepts through a simple example: that of a particle in $\mathbb{R}^3$ constrained to a curve. This section is purely expository, containing no derivations. Section I C briefly introduces the general problem. In Sec. II we focus on the constraining potential. We take care to precisely define what it means to have the same form at all points of the constraint manifold. We also define a tensor which measures the twisting of the potential. In Sec. II C we specify how the potential is to scale in ϵ, where $\epsilon\rightarrow 0$ represents an infinite constraining force. The main computations of the paper are in Sec. III in which we expand the kinetic energy in ϵ and arrive at a preliminary expression, Eq. (3.31), for the constrained kinetic energy. Section III D is devoted to various expressions for the extrapotential. In Sec. IV we apply first-order perturbation theory to transform to a set of degenerate transverse modes, thereby obtaining Eqs. (4.21)–(4.23), which are the main results of the paper. Section IV C briefly discusses nonconstant constraining potentials. In Sec. V we study the geometric origins of the gauge potential and various related connections. We also compute their curvatures. Section VI contains some special cases, including constraint manifolds of codimensions one and two, rotationally invariant constraining potentials, and harmonic constraining potentials. In Sec. VI E, we show that the gauge potential vanishes for certain systems with reflection symmetry. Conclusions are in Sec. VII. There are four Appendixes. Appendix A contains a very brief review of curves in $\mathbb{R}^3$. Appendix B is a review of the second fundamental form. Appendix C summarizes an expression we will need for the quantum kinetic energy. Appendix D contains some of the more laborious mathematical derivations.

B. A Simple example: A curve in $\mathbb{R}^3$

The ultimate objective of this paper is to constrain a quantum wave function, defined on an arbitrary manifold (the

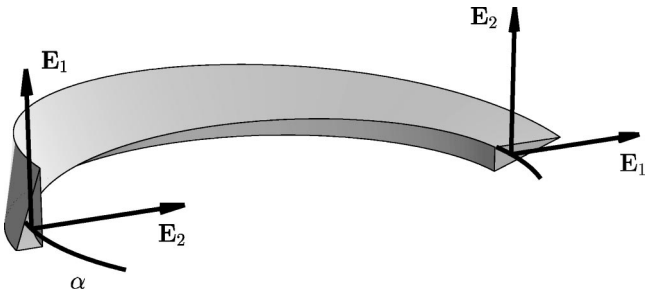

FIG. 1. A twisted quantum waveguide. The cross sectional shape of the tube is constant and is chosen to be a triangle with no reflection symmetry. (Reflection symmetry would force $\langle\Lambda\rangle$ to vanish.) The vectors $\mathbf{E}_1$ and $\mathbf{E}_2$ determine the orientation of the sides of the waveguide, and α measures the distance along the axis.

ambient space), to a (locally) arbitrary submanifold (the constraint manifold) via some general constraining potential. Before solving the full problem, however, it is instructive to consider a simple (though certainly nontrivial), concrete example of the constraining procedure. We present no derivations here; our results will be justified later in Sec. VI B.

We consider a curve embedded in flat three-dimensional space $\mathbb{R}^3$ and parametrized by its arclength α. (See Fig. 1.) Such a curve is characterized by its curvature κ and torsion τ.[1] (See Appendix A.) We take this curve to be the axis of a quantum waveguide. That is, there is a tube enclosing the curve such that the potential is zero inside the tube and infinite outside. We assume the cross section of the tube is constant along the curve. More precisely, if we cut the tube along a plane normal to the curve (called hereafter a normal plane), the cross sectional shape of the tube is independent of where along the curve we cut. Two such cross sections have the same shape if one can be rotated into the other. This rotational freedom permits the cross sectional shape to twist as one moves along the curve, even if the curve itself is straight. The orientation of the cross sectional shape is specified by two orthonormal vectors $\mathbf{E}_1$ and $\mathbf{E}_2$ chosen from each normal plane along the curve. The choice of orthonormal frame $(\mathbf{E}_1,\mathbf{E}_2)$ is such that the cross sectional shape (with respect to this frame) is independent of α. In Fig. 1 the cross section is a triangle with no reflection symmetry. Such symmetry is nongeneric and can cause certain terms to vanish. (See Sec. VI E.)

We assume that the transverse dimensions of the tube are small compared to the radius of curvature $\rho=\kappa^{-1}$ and the inverse torsion τ^{-1}. We can then separate out the ''fast'' transverse degrees of freedom and obtain an effective one-dimensional Hamiltonian in the ''slow'' longitudinal, or tangential, coordinate α. To accomplish this separation, we pick a transverse mode $\chi(u^1,u^2)$ of the waveguide. Here (u^1,u^2) are the Cartesian coordinates in the normal plane taken with respect to the frame $(\mathbf{E}_1,\mathbf{E}_2)$; the quantities (u^1,u^2,α) thus coordinatize the tube. The transverse mode $\chi(u^1,u^2)$ is a normalized eigenfunction of the transverse Hamiltonian $H_\perp=(\pi_1^2+\pi_2^2)/2+V_\perp(u^1,u^2)$, where $\pi_j=-i\hbar\partial/\partial u^j$, $j=1,2$, and $V_\perp(u^1,u^2)$ is the potential energy which defines the tube. The eigenvalue of $H_\perp$ corresponding to χ is called the transverse energy. For simplicity, we assume that the transverse energy is nondegenerate.

To lowest order in the width of the tube, an eigenfunction ψ of the waveguide has the form

$$\psi(u^1,u^2,\alpha)=\chi(u^1,u^2)\phi(\alpha). \tag{1.1}$$

As we take the limit where the transverse dimensions of the waveguide shrink to zero (keeping the quantum numbers of the transverse mode fixed), the transverse energy obviously tends toward infinity. However, due to the constancy of the cross sectional shape, this transverse energy, though very large, is itself constant along the curve. We thus subtract it off, leaving a residual Hamiltonian $H_\parallel$, which we call the constrained Hamiltonian. The constrained Hamiltonian acts only on ϕ, resulting in the Schrödinger equation

$$H_\parallel\phi=E_\parallel\phi. \tag{1.2}$$

The principal objective of this paper is to determine the form of this constrained Hamiltonian.

As we will show later, the constrained Hamiltonian is not simply $\pi_\parallel^2/2$, where $\pi_\parallel=-i\hbar\partial/\partial\alpha$. Rather, there are effects from the curvature κ and the rate at which the cross sectional shape twists along the curve. To make this latter concept more precise, we define the potential twist $S=\mathbf{E}_1\cdot(d\,\mathbf{E}_2/d\alpha)$ which measures the rotation rate of the cross sectional shape. The potential twist admits the following description. Let θ denote the angle between the principal normal $\hat{\mathbf{n}}$ (see Appendix A) and the frame $(\mathbf{E}_1,\mathbf{E}_2)$, specifically $\hat{\mathbf{n}}\cdot\mathbf{E}_1=\cos\theta$, $\hat{\mathbf{n}}\cdot\mathbf{E}_2=-\sin\theta$. Let $\omega=d\theta/d\alpha$ denote the rotation rate of the frame $(\mathbf{E}_1,\mathbf{E}_2)$ with respect to $\hat{\mathbf{n}}$. Then S is related to ω and the torsion τ by $-S=\tau+\omega$. Taking $S=0$, we obtain the case considered by da Costa in Ref. [6]. We next define an angular momentum operator Λ in the tangential direction by $\Lambda=(u^1\pi_2-u^2\pi_1)/2$. The constrained Hamiltonian is then

$$H_\parallel=K_\parallel+V_{ex}, \tag{1.3}$$

where

$$K_\parallel=\frac{1}{2}(\pi_\parallel+2S\langle\Lambda\rangle)^2, \tag{1.4}$$

$$V_{ex}=-\frac{\hbar^2}{8}\kappa^2+2S^2(\langle\Lambda^2\rangle-\langle\Lambda\rangle^2), \tag{1.5}$$

and where the bracket notation $\langle\,\rangle$ denotes the expectation value with respect to the transverse mode χ.

Observe that the tangential kinetic energy $K_\parallel$ departs from $\pi_\parallel^2/2$ due to the inclusion of the term $2S\langle\Lambda\rangle$, which couples the angular momentum of the transverse mode to the potential twist. This term is a gauge coupling, a fact we explore

[1]The term ''torsion'' has two distinct meanings in differential geometry. In this paper, we refer only to the torsion of a curve embedded in $\mathbb{R}^3$ and not the torsion of a connection as typically defined in Riemannian geometry.

further in Sec. V. For now, we simply note that because the curve is one dimensional, the gauge coupling can be removed from Eq. (1.4) by a gauge transformation. In the present context, a gauge transformation consists of changing the phase of the wave function ϕ. This transformation is not without its consequences, however, as it will obviously change the boundary conditions which ϕ must satisfy. Also, we stress that if the constraint manifold has dimension greater than one, it will not in general be possible to remove the gauge coupling by a gauge transformation.

As a final observation on $K_\parallel$, notice that the gauge coupling is of order $\hbar^0$, which indicates that it is essentially a classical quantity. This coupling should therefore appear in a classical theory of constraints which takes into account the potential twist.

Turning to the quantity V_{ex}, we note that it is a real-valued function of α, containing no differential operators. For this reason, we call V_{ex} an extrapotential. The extrapotential contains two terms, $-\hbar^2\kappa^2/8$ and $2S^2(\langle\Lambda^2\rangle-\langle\Lambda\rangle^2)$. The first of these was derived by da Costa for the case $S=0$ [6]. It has the physical effect of attracting ϕ to regions of high curvature, a fact which may produce curvature-induced bound states in the waveguide. Such bound states are of current interest [16–18] and are reviewed by Duclos and Exner [19]. The term $-\hbar^2\kappa^2/8$ is of order $\hbar^2$ and therefore disappears in the classical (and semiclassical) limit. The second term of V_{ex}, like the gauge coupling in $K_\parallel$, depends on both the potential twist S and the angular momentum Λ. Notice, however, that it is the standard deviation of the angular momentum which appears in V_{ex}. This means, for example, that the second term of V_{ex} vanishes for transverse modes which are angular momentum eigenstates. It is interesting to observe that, in contrast to the first term, the second term of V_{ex} has the physical effect of expelling the wave function ϕ from regions of high twist S. Also, the second term is of order $\hbar^0$, which means that, like the gauge coupling in $K_\parallel$, it survives the classical limit.

C. The general problem

We describe here how the setup in Sec. I B is modified for the general problem. First, the ambient space in Sec. I B was assumed to be $\mathbb{R}^3$. In the general problem, we allow the ambient space to be an arbitrary Riemannian manifold, which we denote by $\mathcal{A}$. The kinetic energy of the wave function ψ, defined over $\mathcal{A}$, is given by $K=-\hbar^2\triangle/2$, where $\triangle$ is the Laplacian on $\mathcal{A}$. Unlike Sec. I B, the ambient space is not assumed to be flat, and, as we will discover, the curvature of the ambient space produces additional terms in V_{ex}.

Next, we constrain the wave function to lie in the vicinity of a (locally) arbitrary (embedded) submanifold $\mathcal{C}$ of $\mathcal{A}$ with dimension m and codimension d. We call $\mathcal{C}$ the constraint manifold. In Sec. I B, the constraint manifold was a one-dimensional curve. The curvature and torsion of this curve played a critical role in the analysis. The appropriate generalization of the curvature and torsion is the second fundamental form T, which is a rank-three tensor. (See Appendix B.)

In Sec. I B, the constraint was imposed by a hard-wall potential that was infinite outside of a tube and zero inside. We then took the limit in which the width of the tube went to 0. In the general problem, we impose the constraint by an arbitrary potential $V_\perp$, subject to a few reasonable conditions. This potential is defined on a set of coordinates transverse to the constraint manifold and, for this reason, is called the transverse (or constraining) potential. The transverse potential depends on a scaling parameter ϵ which is analogous to the width parameter of the tube; the constraint is imposed by taking the limit ϵ goes to 0.

One of the conditions we do still require of $V_\perp$ is that it be independent of the location on the constraint manifold. This condition, as well as a few other minor conditions, are explained fully in the next section.

II. THE TRANSVERSE POTENTIAL

A. Constancy of the transverse potential

In Sec. I B we defined the constraining potential by first specifying the form of the potential on a plane normal to the curve and then specifying the orientation of this potential at all points along the curve. For the general case, we use the same fundamental idea except that now, due to the curvature of the ambient space, we must take care to define how we generalize the concept of the normal plane.

It is useful to consider two separate but related spaces for a given point q on the constraint manifold. The first is the linear space of all vectors normal to the constraint manifold. We call this the normal space at q and denote it by N_q. The second space of interest is the submanifold of the ambient space formed by geodesics emanating from q normal to the constraint manifold. We call this the transverse space at q and denote it by $\mathcal{U}_q$. The spaces N_q and $\mathcal{U}_q$ are related by the exponential map which takes a vector $\mathbf{v}\in N_q$ into the point $\exp\mathbf{v}\in\mathcal{A}$. The point $\exp\mathbf{v}\in\mathcal{A}$ lies on the geodesic emanating from q in the direction of $\mathbf{v}$; it lies at a distance $|\mathbf{v}|=(\langle\mathbf{v},\mathbf{v}\rangle)^{1/2}$ from q along this geodesic. (We use the notation $\langle,\rangle$ for the metric on $\mathcal{A}$.) Thus, we find $\mathcal{U}_q=\exp N_q$. We now slightly modify our definition of $\mathcal{U}_q$. If the geodesics emanating from the constraint manifold $\mathcal{C}$ in the neighborhood of q flow to an arbitrary length, they will in general intersect one another. This can be witnessed even in the simple example of Sec. I B. Thus, in defining $\mathcal{U}_q$, we assume that the geodesics flow for a small enough length to avoid such intersections and that this maximal length is independent of the point q on the constraint manifold. In summary, then, we foliate a neighborhood (which we call the tubular neighborhood) of the constraint manifold $\mathcal{C}$ by the transverse spaces $\mathcal{U}_q$, which we have in turn related to the normal spaces N_q by the exponential map. Using the exponential map to construct tubular neighborhoods in this fashion is a standard technique. For details, see, for example, Lang [20] and Vanhecke [21].

Since we have identified normal vectors with points in the neighborhood of the constraint manifold, we view the transverse potential $V_\perp$ as a function defined on the normal spaces. With this interpretation, we will require that $V_\perp$, as a function of q and the vectors in N_q, be independent of q. By

independent, we really mean independent modulo SO(d) rotations in N_q. Let us make this more precise. As in Sec. I B, we specify the orientation of the transverse potential by an orthonormal basis $\mathbf{E}_\mu$, $\mu=1,\ldots,d$ of the normal space N_q. This basis forms a normal frame for the constraint manifold which we call the potential frame. For a given normal vector field $\mathbf{u}$, we introduce the components u^μ, $\mu=1,\ldots,d$ with respect to $\mathbf{E}_\mu$. The quantities u^μ coordinatize both the normal space N_q and the transverse space $\mathcal{U}_q$, for which they are commonly called Riemannian normal coordinates [22]. We use sans serif for the list of coordinates $\mathsf{u}=(u^1,\ldots,u^d)$, reserving the bold notation $\mathbf{u}$ for the vector field. The neighborhood of $\mathcal{C}$ is therefore conveniently parametrized by (u,q). The heuristic constraint that $V_\perp$ be independent of position on the constraint manifold can now be made precise by the following statement: the transverse potential $V_\perp(\mathsf{u},q)$ as a function of (u,q) is required to be independent of q.

In general, the construction of the parameters u^μ presented here is only possible locally on $\mathcal{C}$. That is, it may be impossible to define u^μ in the neighborhood of the whole constraint manifold simultaneously. The construction can break down in two ways. First, it may be impossible to construct a tubular neighborhood for the entire constraint manifold. One can see this even with the simple example of Sec. I B. If the one-dimensional curve spirals in on itself, then the width of the tubular neighborhood is forced to go to 0. (Recall that the width of the tubular neighborhood must be the same for all points on the constraint manifold.) Assuming that a tubular neighborhood does indeed exist for the manifold, there is still a second way in which the construction may break down. This occurs if there does not exist a potential frame $\mathbf{E}_\mu$ which is globally defined. (This happens when the normal bundle is nontrivial.) For example, let the ambient space be a Möbius strip and let the constraint manifold be a curve which wraps around the Möbius strip once. Clearly, there does not exist a normal frame for $\mathcal{C}$ which is defined globally. It is our viewpoint that these two obstacles (in particular the first) are not common in physical problems. Even if one did encounter a problem in which the u^μ were not definable globally, the results of this paper would still apply locally.

B. The potential twist tensor

In this section we generalize the potential twist S of Sec. I B to a rank three potential twist tensor (also denoted S) defined for any $q\in\mathcal{C}$. For an arbitrary vector $\mathbf{e}\in T_q\mathcal{A}$, $S_\mathbf{e}$ is a linear map on $T_q\mathcal{A}$. [Here, $T_q\mathcal{A}$ is the $(d+m)$-dimensional tangent space of $\mathcal{A}$ at q.] Let $\mathbf{x}\in T_q\mathcal{A}$ be an arbitrary vector tangent to $\mathcal{C}$. Then, we define

$$S_\mathbf{e}\mathbf{x}=\mathbf{0}. \tag{2.1}$$

Now let $\mathbf{v}\in T_q\mathcal{A}$ be an arbitrary vector normal to $\mathcal{C}$. We extend $\mathbf{v}$ to a vector field on $\mathcal{C}$ (defined in the neighborhood of q) by assuming that $\mathbf{v}$ is normal to $\mathcal{C}$ and, furthermore, that its components with respect to $\mathbf{E}_\mu$ are constant. We now complete the definition of $S_\mathbf{e}$ by prescribing

$$S_\mathbf{e}\mathbf{v}=P_\perp\nabla_{P_\parallel\mathbf{e}}\mathbf{v}, \tag{2.2}$$

where ∇ is the Levi-Civita connection [23–25] on $\mathcal{A}$ and $P_\perp$ and $P_\parallel$ are the projection operators onto the normal and tangent spaces of $\mathcal{C}$, respectively. It is straightforward to verify that S defined by Eqs. (2.1) and (2.2) is indeed a tensor.

Like the second fundamental form T (see Appendix B), S satisfies the antisymmetry property

$$\langle\mathbf{d},S_\mathbf{e}\mathbf{f}\rangle=-\langle\mathbf{f},S_\mathbf{e}\mathbf{d}\rangle, \tag{2.3}$$

where $\mathbf{d},\mathbf{e},\mathbf{f}\in T_q\mathcal{A}$ are arbitrary. To prove the above equation, we need only consider the case $\mathbf{d}=\mathbf{v}\in N_q$, $\mathbf{f}=\mathbf{w}\in N_q$, and $\mathbf{e}=\mathbf{x}$ tangent to $\mathcal{C}$, since all other cases vanish. Since S is a tensor, we may assume that $\mathbf{v}$ and $\mathbf{w}$ are vector fields and that their components with respect to $\mathbf{E}_\mu$ are constant. Since the frame $\mathbf{E}_\mu$ is orthonormal, $\langle\mathbf{v},\mathbf{w}\rangle$ is constant, and therefore Eq. (2.2) implies $\langle\mathbf{v},S_\mathbf{x}\mathbf{w}\rangle=\langle\mathbf{v},\nabla_\mathbf{x}\mathbf{w}\rangle=-\langle\nabla_\mathbf{x}\mathbf{v},\mathbf{w}\rangle=-\langle\mathbf{w},S_\mathbf{x}\mathbf{v}\rangle$.

C. Scaling of the transverse potential

In Sec. I B, we imposed constraints on the position of a particle by introducing an infinite square-well potential in the directions transverse to the axis of a quantum waveguide. The width of this well was proportional to a scaling parameter ϵ, which was assumed to be small. In the general problem, we also require the potential $V_\perp$ to depend on a scaling parameter ϵ. [We use the notation $V_\perp(\mathsf{u};\epsilon)$ to emphasize this fact.] As the scaling parameter ϵ tends toward 0, $V_\perp(\mathsf{u};\epsilon)$ grows narrower and deeper. To make this statement precise, we define a rescaled potential $\tilde{V}_\perp$,

$$\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)=\epsilon^2V_\perp(\epsilon\tilde{\mathsf{u}};\epsilon), \tag{2.4}$$

where $\tilde{u}^\mu$ are rescaled transverse coordinates,

$$u^\mu=\epsilon\tilde{u}^\mu. \tag{2.5}$$

We assume that $\tilde{u}^\mu$ has no dependence itself on ϵ. We also make the very reasonable assumptions that $\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)$ is smooth in ϵ at $\epsilon=0$, by which we mean that $\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)$ can be expanded as $\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)=\tilde{V}^0_\perp(\tilde{\mathsf{u}})+\epsilon\tilde{V}^1_\perp(\tilde{\mathsf{u}})+\epsilon^2\tilde{V}^2_\perp(\tilde{\mathsf{u}})+\cdots$, and furthermore that $\tilde{V}^0_\perp(\tilde{\mathsf{u}})$ does not vanish. In Sec. IV B, we will make some further reasonable assumptions on the existence of bound states for the transverse potential and on the smoothness in ϵ of the corresponding eigenenergies.

To understand the consequences of the relation (2.5), consider a concrete example in which $\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)=\tilde{V}_\perp(\tilde{\mathsf{u}})$ is a finite-depth square well with no ϵ dependence itself. Then the physical potential $V_\perp(\mathsf{u};\epsilon)$ is a finite-depth square well whose width scales as ϵ and whose depth scales as $1/\epsilon^2$. Assuming the quantum number of the transverse mode is fixed, this scaling in the potential guarantees that the width of the wave function scales as ϵ. This is exactly the behavior we want from a system which lies closer and closer to the

constraint manifold as ϵ tends toward 0. As another concrete example, we consider a harmonic transverse potential in Sec. VI D.

We should emphasize that ϵ is introduced as a formal scaling parameter. It allows us to rigorously define the limit of an infinite restoring force and thereby rigorously define the constrained Hamiltonian. The constrained Hamiltonian, however, does not depend on ϵ, and from a practical standpoint, one need not worry about the exact definition of ϵ. The most important fact to keep in mind is that the width of the wave function scales as ϵ. If this width is small compared to other relevant length scales in the system (for example, radii of curvature) then the ϵ to 0 limit is justified.

III. EXPANSION OF THE KINETIC ENERGY

The derivation of the constrained Hamiltonian [such as Eqs. (1.3) –(1.5)] proceeds in two steps. The first is to expand the kinetic energy in powers of ϵ. The second is to transform to a basis of transverse modes and to apply a first-order perturbation treatment to the expanded Hamiltonian. This section is devoted to the first step.

A. Definition of the vielbein

We will express the kinetic energy in terms of a vielbein $\mathbf{E}_a$, $a=1,\ldots,d+m$, on $\mathcal{A}$. Appendix C gives the necessary background for this technique. To span the transverse dimensions, we take $\mathbf{E}_\mu=\partial/\partial u^\mu$, $\mu=1,\ldots,d$, where it is understood that, for the purpose of the partial derivative, the position $q\in\mathcal{C}$ is held fixed. In selecting vector fields to span the remaining dimensions, we first choose an arbitrary set of orthonormal vector fields $\mathbf{E}_i$, $i=d+1,\ldots,d+m$, defined over $\mathcal{C}$ and tangent to $\mathcal{C}$. We then use $\mathbf{E}_\mu$ to Lie transport these vector fields into the tubular neighborhood of $\mathcal{C}$. That is, we require the Lie derivatives with respect to $\mathbf{E}_\mu$ to vanish,

$$[\mathbf{E}_\mu,\mathbf{E}_i]=0. \tag{3.1}$$

We use the following notational scheme in this paper. The indices $a,b,c,\ldots$ range from $1,\ldots,d+m$ and label the basis vectors $\mathbf{E}_a$ and any components with respect to this basis. The indices $\mu,\nu,\sigma,\ldots$ range from $1,\ldots,d$ and label the vector fields $\mathbf{E}_\mu=\partial/\partial u^\mu$ and their related components. The indices $i,j,k,\ldots$ range from $d+1,\ldots,d+m$ and label the vector fields $\mathbf{E}_i$ and their related components. Except where otherwise noted, we employ the convention that an index $a,b,c,\ldots,\ \mu,\nu,\sigma,\ldots,$ or $i,j,k,\ldots$ is implicitly summed over when occurring twice in the same expression.

For future reference, we present some facts regarding the structure constants β^c_{ab}, defined by $[\mathbf{E}_a,\mathbf{E}_b]=\beta^c_{ab}\mathbf{E}_c$. First, Eq. (3.1) immediately yields

$$\beta^c_{\mu j}=\beta^c_{j\mu}=0. \tag{3.2}$$

Furthermore, since $\mathbf{E}_\mu=\partial/\partial u^\mu$ is a coordinate basis on the transverse spaces $\mathcal{U}_q$, we find $\beta^c_{\mu\nu}=0$. Combining this with Eq. (3.2), we have

$$\beta^c_{\mu b}=\beta^c_{b\mu}=0. \tag{3.3}$$

Next we note that

$$0=[\mathbf{E}_\mu,[\mathbf{E}_i,\mathbf{E}_j]]=[\mathbf{E}_\mu,\beta^c_{ij}\mathbf{E}_c]=[\partial/\partial u^\mu\beta^c_{ij}]\mathbf{E}_c, \tag{3.4}$$

where the first equality follows from the Jacobi identity and Eq. (3.1) and the third equality follows from Eq. (3.3). We use the bracket notation [ ] in the final equality to emphasize that the differential operator acts only on the quantities inside the bracket. Since the $\mathbf{E}_c$ form a basis, we have

$$\frac{\partial\beta^c_{ij}}{\partial u^\mu}=0. \tag{3.5}$$

Furthermore, since the $\mathbf{E}_i$ are tangent to $\mathcal{C}$ when restricted to $\mathcal{C}$, we have $\beta^\sigma_{ij}=0$ on $\mathcal{C}$. Combining this fact with Eq. (3.5), we find that

$$\beta^\sigma_{ij}=0 \tag{3.6}$$

within the tubular neighborhood. Thus, the distribution of vector fields $\mathbf{E}_i$ is integrable everywhere. (The submanifolds thus defined by Frobenius's Theorem are manifolds of constant $V_\perp$.)

B. Transformation of the kinetic energy

As in Appendix C, the momentum operators are defined to be $\pi_a=-i\hbar\mathbf{E}_a$. They are not in general Hermitian since the Hermitian conjugate is given by Eq. (C4). The kinetic energy is given by $K=\pi_a^\dagger G^{ab}\pi_b/2$, where $G_{ab}=\langle\mathbf{E}_a,\mathbf{E}_b\rangle$ are the components of the metric tensor and G^{ab} is the inverse of G_{ab}.

Appendix C also provides the framework for scaling the quantum wave function by an arbitrary (strictly) positive function $s:\mathcal{A}\to\mathbb{R}$ [see Eq. (C5)] in order to modify the form of the kinetic energy. We apply this scaling formalism here, taking

$$s=G^{1/4}, \tag{3.7}$$

where $G=\det G_{ab}$. As mentioned in Appendix C, this scaling defines a new inner product of wave functions. We observe that the original inner product of two wave functions φ and φ' is given by

$$\langle\varphi|\varphi'\rangle=\int\sqrt{G}\,\nu\,\varphi^*(\mathsf{u},q)\varphi'(\mathsf{u},q), \tag{3.8}$$

where ν is the $(d+m)$-form

$$\begin{aligned}\nu&=E^{*1}\wedge\cdots\wedge E^{*(d+m)}\\&=du^1\wedge\cdots\wedge du^d\wedge E^{*(d+1)}\wedge\cdots\wedge E^{*(d+m)}.\end{aligned} \tag{3.9}$$

Here, E^{*a} is the basis of one-forms dual to the vielbein $\mathbf{E}_a$. We have also used the fact that $E^{*\mu}=du^\mu$. (Be careful not to confuse the notation $\langle|\rangle$ with $\langle,\rangle$, the latter denoting the

Riemannian metric on $\mathcal{A}$.) From Eq. (C6) we therefore find that the scaled inner product of two (scaled) wave functions ψ and ψ' is

$$\langle \psi | \psi' \rangle_s = \int \nu\, \psi^*(\mathsf{u},q)\psi'(\mathsf{u},q). \tag{3.10}$$

This scaled inner product gives rise to a scaled Hermitian conjugate, denoted as a superscript $\dagger(s)$. Using Eqs. (C4), (C8), and (3.3), we find that π_μ is Hermitian with respect to the scaled Hermitian conjugate,

$$\pi_\mu^{\dagger(s)} = \pi_\mu . \tag{3.11}$$

Furthermore, Eqs. (C4), (C8), and (3.2) give the (scaled) Hermitian conjugate of π_j as

$$\pi_j^{\dagger(s)} = \pi_j + i\hbar\beta_{jb}^b = \pi_j + i\hbar\beta_{jk}^k . \tag{3.12}$$

We now restrict the momentum operator π_j to $\mathcal{C}$. We write $\pi_j|_0$ to make this explicit; we use the notation $|_0$ for any quantity restricted to $\mathcal{C}$ since this corresponds to $u^\mu = 0$. For present purposes, we consider the constraint manifold in its own right without being viewed as embedded in the ambient space. With this interpretation, the vector field $\pi_j|_0$ has a well-defined Hermitian conjugate which we denote by $(\pi_j|_0)^\dagger$. This Hermitian conjugate is given by Eq. (C4), where it is understood that the symbol G now refers only to the determinant of the metric G_{ij} on $\mathcal{C}$. However, since the basis $\mathbf{E}_i|_0$ is orthonormal, we have $G=1$, and hence

$$(\pi_j|_0)^\dagger = \pi_j|_0 + i\hbar\gamma_{jk}^k , \tag{3.13}$$

where the functions γ_{ij}^k, defined on $\mathcal{C}$, are the structure constants for $\mathbf{E}_i|_0$. Since $[\mathbf{E}_i|_0, \mathbf{E}_j|_0] = [\mathbf{E}_i, \mathbf{E}_j]|_0$, the structure constants γ_{ij}^k are equal to $\beta_{ij}^k|_0$. Comparing Eq. (3.13) to Eq. (3.12), we now have the following convenient description for $\pi_j^{\dagger(s)}$ when restricted to $\mathcal{C}$:

$$(\pi_j^{\dagger(s)})|_0 = (\pi_j|_0)^\dagger . \tag{3.14}$$

The scaled kinetic energy is given by Eq. (C9). Noting Eq. (3.11), we rewrite this as

$$K_s = \tfrac{1}{2}(\pi_\mu G^{\mu\nu}\pi_\nu + \pi_\mu G^{\mu j}\pi_j + \pi_i^{\dagger(s)} G^{i\nu}\pi_\nu + \pi_i^{\dagger(s)} G^{ij}\pi_j) + V_s , \tag{3.15}$$

where

$$V_s = -\tfrac{1}{8}(\tfrac{1}{4}G^{ab}[\pi_a \ln G][\pi_b \ln G] + [\pi_a^{\dagger(s)} G^{ab}[\pi_b \ln G]]). \tag{3.16}$$

We will henceforth drop the s index on K_s, $\dagger(s)$, and $\langle|\rangle_s$, with the scaling being implicitly understood.

C. Expansion of the kinetic energy

In this section we expand the kinetic energy Eq. (3.15) through order ϵ^0. Recall from Eq. (2.5) that u^μ is of order ϵ^1, and hence the momentum $\pi_\mu = -i\hbar\partial/\partial u^\mu$ is of order ϵ^{-1}. From Eq. (3.1), we see that the momentum π_i is of order ϵ^0. Furthermore, from Eq. (3.5), we see that β_{ij}^k is of order ϵ^0, and combining this fact with Eq. (3.12) we find that $\pi_i^\dagger$ is of order ϵ^0. [Recall that ''(s)'' is now implicit.] These scaling properties imply that to expand Eq. (3.15) to order ϵ^0, we must expand V_s, G^{ij}, $G^{i\mu}$, and $G^{\mu\nu}$ to orders ϵ^0, ϵ^0, ϵ^1, and ϵ^2, respectively.

Since $\mathbf{E}_a$ is an orthonormal frame at $u^\mu = 0$, we have the following identities:

$$G_{ab}|_0 = G^{ab}|_0 = \delta_{ab} , \tag{3.17}$$

$$G^{ab}{}_{,\sigma}|_0 = -G_{ab,\sigma}|_0 , \tag{3.18}$$

where we use the notation ''$,\sigma$'' for the derivative $\partial/\partial u^\sigma$. Equations (3.17) and (3.18) yield the following expansions of G^{ab}:

$$G^{ij}(\mathsf{u}) = \delta_{ij} + O(\epsilon), \tag{3.19}$$

$$G^{\mu j}(\mathsf{u}) = G^{\mu j}{}_{,\sigma}|_0 u^\sigma + O(\epsilon^2) = -G_{\mu j,\sigma}|_0 u^\sigma + O(\epsilon^2), \tag{3.20}$$

$$\begin{aligned} G^{\mu\nu}(\mathsf{u}) &= \delta_{\mu\nu} + G^{\mu\nu}{}_{,\sigma}|_0 u^\sigma + \tfrac{1}{2}G^{\mu\nu}{}_{,\sigma\tau}|_0 u^\sigma u^\tau + O(\epsilon^3) \\ &= \delta_{\mu\nu} - G_{\mu\nu,\sigma}|_0 u^\sigma + \tfrac{1}{2}(-G_{\mu\nu,\sigma\tau} + 2G_{\mu a,\sigma}G_{a\nu,\tau})|_0 \\ &\quad \times u^\sigma u^\tau + O(\epsilon^3). \end{aligned} \tag{3.21}$$

The derivatives of the metric G_{ab} appearing above are conveniently expressed in terms of the potential twist tensor S and the Riemannian curvature R on $\mathcal{A}$. To see this, we first introduce the components of S, T, and R via

$$S_{abc} = \langle \mathbf{E}_a, S_{\mathbf{E}_c}\mathbf{E}_b \rangle, \tag{3.22}$$

$$T_{abc} = \langle \mathbf{E}_a, T_{\mathbf{E}_c}\mathbf{E}_b \rangle, \tag{3.23}$$

$$R_{abcd} = \langle \mathbf{E}_a, R_{\mathbf{E}_c\mathbf{E}_d}\mathbf{E}_b \rangle, \tag{3.24}$$

where T is included for completeness and for future reference. In Appendix D, we derive the identities

$$G_{\mu j,\sigma}|_0 = S_{\mu\sigma j}|_0 , \tag{3.25}$$

$$G_{\mu\nu,\sigma}|_0 = 0, \tag{3.26}$$

$$G_{\mu\nu,\sigma\tau}|_0 = -\tfrac{1}{3}(R_{\mu\sigma\nu\tau} + R_{\nu\sigma\mu\tau})|_0 . \tag{3.27}$$

In actuality, the $|_0$ notation on $S_{\mu\sigma j}$ is redundant since S is only defined on $\mathcal{C}$, but we will make use of this notation as a convenient reminder. Inserting Eqs. (3.25)– (3.27) into Eqs. (3.19)–(3.21), we obtain

$$G^{ij}(\mathsf{u}) = \delta_{ij} + O(\epsilon), \tag{3.28}$$

$$G^{\mu j}(\mathsf{u}) = -S_{\mu\sigma j}|_0 u^\sigma + O(\epsilon^2), \tag{3.29}$$

$$G^{\mu\nu}(\mathsf{u}) = \delta_{\mu\nu} + (\tfrac{1}{3}R_{\mu\sigma\nu\tau} + S_{\mu\sigma k}S_{\nu\tau k})|_0 u^\sigma u^\tau + O(\epsilon^3), \tag{3.30}$$

where we have used the well-known symmetry of the Riemannian curvature $R_{abcd}=R_{cdab}$. We next insert Eqs. (3.28)–(3.30) into Eq. (3.15) to arrive at the main result of this section,

$$K=K_\perp+K_\parallel^p+K_R+V_{ex}^p+O(\epsilon), \tag{3.31}$$

where

$$K_\perp=\tfrac{1}{2}\pi^\mu|_0\pi_\mu, \tag{3.32}$$

$$K_\parallel^p=\tfrac{1}{2}(\pi^i|_0+S^{\mu\nu i}|_0\Lambda_{\mu\nu})^\dagger(\pi_i+S^{\sigma\tau}{}_i|_0\Lambda_{\sigma\tau}), \tag{3.33}$$

$$K_R=\tfrac{1}{6}R^{\mu\nu\sigma\tau}|_0\Lambda_{\mu\nu}\Lambda_{\sigma\tau}, \tag{3.34}$$

$$V_{ex}^p=V_s|_0. \tag{3.35}$$

We have taken advantage of the antisymmetry property Eq. (2.3), $S_{\mu\nu i}=-S_{\nu\mu i}$, and the well-known antisymmetry relations $R_{\mu\nu\sigma\tau}=-R_{\nu\mu\sigma\tau}=-R_{\mu\nu\tau\sigma}$ to introduce the operators

$$\Lambda_{\mu\nu}=\tfrac{1}{2}(u_\mu\pi_\nu-u_\nu\pi_\mu)=\tfrac{1}{2}(\pi_\nu u_\mu-\pi_\mu u_\nu), \tag{3.36}$$

which are generalized angular momentum operators acting on the transverse space. That is, they generate SO(d) rotations in the transverse space. They are the generalization of the angular momentum Λ defined in Sec. I B.

In Eqs. (3.32)–(3.34), we have employed the standard practice of raising tensor indices by contraction with G^{ab}. Thus, $\pi^\mu=G^{\mu a}\pi_a$, $S^{\mu\nu i}=G^{\mu a}G^{\nu b}G^{ic}S_{abc}$, etc. However, since $G^{ab}|_0=\delta_{ab}$, the raised components and lowered components of any tensor evaluated at $u^\mu=0$ are actually equal. One could, therefore, equally well have written Eqs. (3.32)–(3.34) with all components lowered. The purpose of using raised components is simply to express these equations in manifestly covariant form.

We now mention a few facts concerning the Hermitian conjugate which we used to derive Eq. (3.33). First, notice from Eq. (3.11) that $\Lambda_{\mu\nu}^\dagger=\Lambda_{\mu\nu}$. Also notice that since $S^{\mu\nu i}|_0$ has no dependence on u^μ, $S^{\mu\nu i}|_0$ and $\Lambda_{\mu\nu}$ commute. This means in particular that the Hermitian conjugate in Eq. (3.33) may be applied to the $\pi^i|_0$ term alone. Finally, we used Eq. (3.14) to relate $(\pi_i|_0)^\dagger$ to $(\pi_i^\dagger)|_0$. Notice from Eq. (3.13) that if $\mathbf{E}_i|_0$ is a coordinate basis on $\mathcal{C}$ then the Hermitian conjugate may be dispensed with altogether.

We call the terms $K_\perp$, $K_\parallel^p$, and K_R appearing in Eq. (3.31) the transverse kinetic energy, the (preliminary) tangential kinetic energy, and the curvature energy, respectively. The last term V_{ex}^p, being a scalar, nondifferential operator, we call the (preliminary) extrapotential. The three terms $K_\parallel^p$, K_R, and V_{ex}^p are all order ϵ^0. The transverse kinetic energy $K_\perp$ is of order ϵ^{-2} and therefore goes to infinity as ϵ shrinks to 0. The energy associated with this term will therefore be subtracted off with the remaining three terms giving rise to the residual kinetic energy. Notice that each of the four terms in Eq. (3.31) is Hermitian with respect to the (scaled) Hermitian conjugate.

D. Expressions for the extrapotential

In Appendix D 2, we derive the following manifestly covariant form for the extrapotential:

$$V_{ex}^p=-\frac{\hbar^2}{8}\left(2T^{i\mu j}T_{i\mu j}-T^{i\mu}{}_iT^j{}_{\mu j}+2R^{i\mu}{}_{i\mu}+\frac{2}{3}R^{\mu\nu}{}_{\mu\nu}\right)\Bigg|_0. \tag{3.37}$$

Notice that V_{ex}^p is expressed solely in terms of the second fundamental form T of the constraint manifold and the Riemannian curvature R of $\mathcal{A}$ evaluated on $\mathcal{C}$ with no dependence on the potential twist S. Setting $R_{abcd}=0$, Eq. (3.37) agrees with da Costa [Ref. [7], Eq. (33)]. da Costa also assumes that $S=0$. Since we do not make this assumption, Eq. (3.37) is a generalization of da Costa's result to both the case of nonzero Riemannian curvature in the ambient space and nonzero twist of the potential.

There are several other convenient forms for V_{ex}^p. We first introduce the following notation:

$$\mathcal{R}=R^{ab}{}_{ab}|_0, \tag{3.38}$$

$$\mathcal{R}_\perp=R^{\mu\nu}{}_{\mu\nu}|_0, \tag{3.39}$$

$$\mathcal{R}_\parallel=R^{ij}{}_{ij}|_0, \tag{3.40}$$

$$\hat{\mathcal{R}}=\hat{R}^{ij}{}_{ij}, \tag{3.41}$$

$$\mathcal{T}^2=\tfrac{1}{2}T^{abc}T_{abc}=T^{i\mu j}T_{i\mu j}=T^{\mu ij}T_{\mu ij}, \tag{3.42}$$

$$\mathcal{M}^2=T^{ab}{}_aT^c{}_{bc}=T^{i\mu}{}_iT^j{}_{\mu j}=T^{\mu i}{}_iT^j_{\mu j}, \tag{3.43}$$

where we use Eqs. (B4), (B6), and (B7) in Eqs. (3.42) and (3.43). The quantities $\mathcal{R}$ and $\hat{\mathcal{R}}$ are the scalar curvatures on $\mathcal{A}$ and $\mathcal{C}$, respectively. The quantity $\mathcal{M}$ is called the mean curvature. Using the fact that $\mathcal{R}=\mathcal{R}_\parallel+\mathcal{R}_\perp+2R^{i\mu}{}_{i\mu}|_0$, we rewrite Eq. (3.37) as

$$V_{ex}^p=-\frac{\hbar^2}{8}\left(2\mathcal{T}^2-\mathcal{M}^2+\mathcal{R}-\mathcal{R}_\parallel-\frac{1}{3}\mathcal{R}_\perp\right). \tag{3.44}$$

Furthermore, the Gauss Eq. (B10) yields

$$\mathcal{T}^2=\mathcal{M}^2-\hat{\mathcal{R}}+\mathcal{R}_\parallel, \tag{3.45}$$

from which we find

$$V_{ex}^p=-\frac{\hbar^2}{8}\left(\mathcal{T}^2-\hat{\mathcal{R}}+\mathcal{R}-\frac{1}{3}\mathcal{R}_\perp\right) \tag{3.46}$$

$$=-\frac{\hbar^2}{8}\left(\mathcal{M}^2-2\hat{\mathcal{R}}+\mathcal{R}+\mathcal{R}_\parallel-\frac{1}{3}\mathcal{R}_\perp\right). \tag{3.47}$$

Assuming the tensor R is 0, Eq. (3.47) agrees with Ref. [7], Eq. (36).

IV. THE CONSTRAINED HAMILTONIAN

In Sec. III we expanded the kinetic energy in ϵ, obtaining two terms. One term, the transverse kinetic energy, is of

order ϵ^{-2}; the other term is of order ϵ^0. In this section we apply (degenerate) first-order perturbation theory to derive a constrained Hamiltonian for the eigenenergies. In doing so, we introduce the transverse modes characterizing the wave function away from the constraint manifold.

A. Rescaling by ϵ and the expansion of the Hamiltonian

By adding the potential energy $V_\perp(\mathsf{u})$ to the kinetic energy Eq. (3.31), we have the following Hamiltonian:

$$H = H_\perp + H_\parallel + O(\epsilon), \tag{4.1}$$

where

$$H_\perp = K_\perp + V_\perp, \tag{4.2}$$

$$H_\parallel^p = K_\parallel^p + K_R + V_{ex}^p, \tag{4.3}$$

are called the transverse and (preliminary) tangential Hamiltonians, respectively.

In order to clarify the subsequent perturbation analysis, we explicitly exhibit the ϵ dependence of various quantities by rescaling them in ϵ. To begin, we repeat the previous definition Eq. (2.5) of the rescaled quantities $\tilde{u}^\mu$ and also define rescaled momenta $\tilde{\pi}_\mu$,

$$u^\mu = \epsilon \tilde{u}^\mu, \tag{4.4}$$

$$\pi_\mu = \frac{1}{\epsilon}\tilde{\pi}_\mu. \tag{4.5}$$

Notice that both $\tilde{u}^\mu$ and $\tilde{\pi}_\mu$ scale as ϵ^0. In general, the scaled version of a quantity (denoted with a tilde) is defined such that the lowest order nonvanishing term of its expansion in ϵ is of order ϵ^0. Thus, for a quantity homogeneous in ϵ, the scaled version is independent of ϵ. For convenience, we repeat the definition Eq. (2.4) of the rescaled potential energy $\tilde{V}_\perp$ and also define a rescaled transverse kinetic energy and transverse Hamiltonian

$$\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon) = \epsilon^2 V_\perp(\mathsf{u};\epsilon) = \epsilon^2 V_\perp(\epsilon\tilde{\mathsf{u}};\epsilon), \tag{4.6}$$

$$\tilde{K}_\perp = \epsilon^2 K_\perp = \tfrac{1}{2}\tilde{\pi}_\mu \tilde{\pi}_\mu, \tag{4.7}$$

$$\tilde{H}_\perp(\epsilon) = \epsilon^2 H_\perp(\epsilon) = \tilde{K}_\perp + \tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon). \tag{4.8}$$

By our previous assumptions in Sec. II C, $\tilde{V}_\perp(\tilde{\mathsf{u}};\epsilon)$ is smooth in ϵ and does not vanish at $\epsilon=0$. As for $\tilde{K}_\perp$, it is clearly independent of ϵ. Thus, $\tilde{H}_\perp(\epsilon)$ is smooth in ϵ at $\epsilon=0$; its lowest-order term is order ϵ^0, but depending on $\tilde{V}_\perp$, it may have higher-order terms as well. Recall that $K_\parallel^p$, K_R, V_{ex}^p, and $H_\parallel^p$ are already independent of ϵ and therefore need no further scaling. For notational continuity, however, we nevertheless define

$$\tilde{K}_\parallel^p = K_\parallel^p, \tag{4.9}$$

$$\tilde{K}_R = K_R, \tag{4.10}$$

$$\tilde{V}_{ex}^p = V_{ex}^p, \tag{4.11}$$

$$\tilde{H}_\parallel^p = H_\parallel^p. \tag{4.12}$$

We rescale the full Hamiltonian by defining

$$\tilde{H}(\epsilon) = \epsilon^2 H(\epsilon) = \tilde{H}_\perp(\epsilon) + \epsilon^2 \tilde{H}_\parallel^p + O(\epsilon^3). \tag{4.13}$$

In a typical Taylor-series expansion of $\tilde{H}(\epsilon)$, we would remove the order ϵ term from $\tilde{H}_\perp(\epsilon)$ and leave it as a separate term. We would also combine the order ϵ^2 term of $\tilde{H}_\perp(\epsilon)$ with the tangential Hamiltonian $\epsilon^2\tilde{H}_\parallel^p$. Here, however, we wish to keep the ϵ and ϵ^2 terms together in the transverse Hamiltonian $\tilde{H}_\perp(\epsilon)$. We therefore define a new perturbation parameter $\kappa=\epsilon^2$ and rewrite Eq. (4.13) as

$$\tilde{H}(\epsilon,\kappa) = \tilde{H}_\perp(\epsilon) + \kappa\tilde{H}_\parallel^p + O(\epsilon^3). \tag{4.14}$$

Our objective is to find the eigenvalues of $\tilde{H}$ through order ϵ^2. Viewing ϵ and κ as formally independent in Eq. (4.14), our objective becomes finding the eigenvalues of $\tilde{H}$ through second order in ϵ and first order in κ. Our procedure is to assume that the eigenvalues of $H_\perp(\epsilon)$ can be solved exactly (or at least through order ϵ^2) and then apply first-order perturbation theory in κ. To simplify notation, we drop the ϵ dependence (but not κ dependence) for the duration of the derivation.

B. Transformation to the transverse modes

The zeroth-order term (in κ) of $\tilde{H}(\kappa)$ is the transverse Hamiltonian $\tilde{H}_\perp$, which has the form

$$\tilde{H}_\perp = -\frac{\hbar^2}{2}\frac{\partial}{\partial\tilde{u}^\mu}\frac{\partial}{\partial\tilde{u}^\mu} + \tilde{V}_\perp(\tilde{\mathsf{u}}). \tag{4.15}$$

Since $\tilde{H}_\perp$ depends only on the quantities $\tilde{u}^\mu$, we may restrict its domain to functions of $\tilde{u}^\mu$ alone. For the moment we adopt this understanding for the domain of $\tilde{H}_\perp$. We pick an eigenvalue $\tilde{E}_\perp$ (the transverse energy) of $\tilde{H}_\perp$ with finite multiplicity k and bounded eigenstates. We call these eigenstates the transverse modes (with energy $\tilde{E}_\perp$). We let $\chi_n(\tilde{\mathsf{u}})$, $n=1,\ldots,k$, denote an orthonormal basis of these transverse modes. By orthonormal, we mean

$$\langle\chi_n|\chi_{n'}\rangle_{\mathsf{u}} = \int du^1\wedge\cdots\wedge du^d \chi_n^*(\tilde{\mathsf{u}})\chi_{n'}(\tilde{\mathsf{u}}) = \delta_{nn'}, \tag{4.16}$$

where the u subscript indicates integration only over the variables u^μ as opposed to the full $(d+m)$ form ν in Eq. (3.9).

We now adopt the understanding that $\tilde{H}_\perp$ acts on wave functions of both $\tilde{u}^\mu$ and q. Such an eigenfunction with eigenvalue $\tilde{E}_\perp$ has the general form

$$\psi(\tilde{\mathsf{u}},q)=\sum_{n=1}^{k}\chi_n(\tilde{\mathsf{u}})\phi_n(q), \tag{4.17}$$

where the functions $\phi_n(q)$ are arbitrary. We therefore identify an eigenfunction $\psi(\tilde{\mathsf{u}},q)$, having eigenvalue $\tilde{E}_\perp$, with the k functions $\phi_n(q)$. Notice that with our current understanding for the domain of the operator $\tilde{H}_\perp$, $\tilde{E}_\perp$ is a degenerate eigenvalue, even for $k=1$, because there is an infinite basis of functions $\phi_n(q)$.

Recall the steps involved in first-order degenerate perturbation theory. First, one verifies that the desired eigenvalue and eigenfunction is analytic in the perturbation parameter κ. (Here, we simply assume this fact.) Next, one determines the zeroth-order energy and zeroth-order eigenstates. Then, one considers the operator formed by restricting the first-order term of the Hamiltonian to the space of zeroth-order eigenstates. The first-order corrections to the energy are the eigenvalues of this restricted operator. In the present case, the zeroth-order energy is $\tilde{E}_\perp$, and the zeroth-order eigenstates are given by Eq. (4.17). The first-order correction to the Hamiltonian is $\kappa\tilde{H}_\parallel^p$. Denoting the first-order correction to the energy by $\kappa\tilde{E}_\parallel$, the eigenvalue equation for $\tilde{E}_\parallel$ is

$$\sum_{n'=1}^{k}(\tilde{H}_\parallel)_{nn'}\phi_{n'}=\tilde{E}_\parallel\phi_n, \tag{4.18}$$

where the $(\tilde{H}_\parallel)_{nn'}$ are the differential operators

$$\begin{aligned}(\tilde{H}_\parallel)_{nn'}&=\langle\chi_n|\tilde{H}_\parallel^p\chi_{n'}\rangle_{\mathsf{u}}\\&=\int du^1\wedge\cdots\wedge du^d\chi_n^*(\tilde{\mathsf{u}})(\tilde{H}_\parallel^p\chi_{n'})(\tilde{\mathsf{u}}).\end{aligned} \tag{4.19}$$

We call $(\tilde{H}_\parallel)_{nn'}$ the constrained, or tangential, Hamiltonian.

We now recall that $\kappa=\epsilon^2$ and reintroduce the explicit ϵ dependence. Summarizing our analysis thus far, we have shown that an eigenvalue of $\tilde{H}(\epsilon)$ through order ϵ^2 is given by $\tilde{E}_\perp(\epsilon)+\epsilon^2\tilde{E}_\parallel(\epsilon)$, where $\tilde{E}_\perp(\epsilon)$ and $\tilde{E}_\parallel(\epsilon)$ are eigenvalues of $\tilde{H}_\perp(\epsilon)$ and $(\tilde{H}_\parallel)_{nn'}(\epsilon)$. Of course, assuming smoothness in ϵ, it is sufficient to solve for $\tilde{E}_\perp(\epsilon)$ and $\tilde{E}_\parallel(\epsilon)$ through orders ϵ^2 and ϵ^0 respectively. We will therefore only require $\tilde{E}_\parallel(\epsilon)$ and $(\tilde{H}_\parallel)_{nn'}(\epsilon)$ evaluated at $\epsilon=0$, which we denote by $\tilde{E}_\parallel$ and $(\tilde{H}_\parallel)_{nn'}$, respectively. Also, by virtue of Eq. (4.19), we assume for the remainder of the paper that the transverse modes $\chi_n(\tilde{\mathsf{u}})$ are only order ϵ^0 eigenfunctions of $\tilde{H}_\perp(\epsilon)$.

We view Eq. (4.18) as a k-dimensional vector wave equation for a vector wave function defined over the constraint manifold. We introduce the bold notation $\boldsymbol{\phi}(q)$ for the vector wave function with components $\phi_n(q)$ and the sans serif notation $\tilde{\mathsf{H}}_\parallel$ for the matrix of differential operators with components $(\tilde{H}_\parallel)_{nn'}$. Equation (4.18) can therefore be written more compactly as

$$\mathsf{H}_\parallel\boldsymbol{\phi}=E_\parallel\boldsymbol{\phi}. \tag{4.20}$$

Having completed the perturbation analysis, we have dropped the superfluous tildes from $\mathsf{H}_\parallel$ and its eigenvalue $E_\parallel$. Using Eqs. (4.3), (3.33), and (3.34) and a little algebra, we express $\mathsf{H}_\parallel$ as

$$\mathsf{H}_\parallel=\mathsf{K}_\parallel+\mathsf{V}_{ex}, \tag{4.21}$$

where

$$\mathsf{K}_\parallel=\tfrac{1}{2}(\pi^i|_0\mathsf{I}+S^{\mu\nu i}|_0\underline{\Lambda}_{\mu\nu}{}^\dagger)(\pi_i\mathsf{I}+S^{\sigma\tau}{}_i|_0\underline{\Lambda}_{\sigma\tau}), \tag{4.22}$$

$$\begin{aligned}\mathsf{V}_{ex}&=V_{ex}^p\mathsf{I}+(\tfrac{1}{2}S^{\mu\nu i}S^{\sigma\tau}{}_i+\tfrac{1}{6}R^{\mu\nu\sigma\tau})|_0\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau}\\&\quad-(\tfrac{1}{2}S^{\mu\nu i}S^{\sigma\tau}{}_i)|_0\underline{\Lambda}_{\mu\nu}\underline{\Lambda}_{\sigma\tau}\\&=V_{ex}^p\mathsf{I}+(\tfrac{1}{2}S^{\mu\nu i}S^{\sigma\tau}{}_i)|_0(\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau}-\underline{\Lambda}_{\mu\nu}\underline{\Lambda}_{\sigma\tau})\\&\quad+\tfrac{1}{6}R^{\mu\nu\sigma\tau}|_0\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau},\end{aligned} \tag{4.23}$$

and where I is the $k\times k$ identity matrix and $\underline{\Lambda}_{\mu\nu}$ and $\underline{\Lambda}^2_{\mu\nu\sigma\tau}$ are the $k\times k$ matrices having the following components, respectively,

$$(\Lambda_{\mu\nu})_{nn'}=\langle\chi_n|\Lambda_{\mu\nu}\chi_{n'}\rangle_{\mathsf{u}}, \tag{4.24}$$

$$(\Lambda^{(2)}_{\mu\nu\sigma\tau})_{nn'}=\langle\chi_n|\Lambda_{\mu\nu}\Lambda_{\sigma\tau}\chi_{n'}\rangle_{\mathsf{u}}. \tag{4.25}$$

Equations (4.21)–(4.23) encapsulate the main result of this paper. We make the following observations.

(i) The constrained Hamiltonian $\mathsf{H}_\parallel$ is a $k\times k$ matrix of operators. It is the residual Hamiltonian remaining after the infinite transverse energy $E_\perp$ is subtracted off.

(ii) The kinetic energy $\mathsf{K}_\parallel$, which we call the (final) tangential kinetic energy, differs from the ''standard'' kinetic energy due to the appearance of a gauge potential. Physically, the gauge potential couples the tangential momenta to the generalized angular momentum of the transverse modes.

(iii) The quantity V_{ex}, which we call the (final) extrapotential, is a $k\times k$ matrix of nondifferential operators.

(iv) All off-diagonal coupling in $\mathsf{H}_\parallel$ is due to the generalized angular momentum of the transverse modes.

(v) For a nondegenerate transverse mode ($k=1$), the constrained Hamiltonian is a scalar operator $H_\parallel$ which acts on scalar wave functions. In this case, we see the emergence of Eqs. (1.3)–(1.5) presented in Sec. I B. The exact derivation of these equations from the more general Eqs. (4.21)–(4.23) will be presented in Sec. VI B.

The preliminary tangential kinetic energy $K_\parallel^p$, preliminary extrapotential V_{ex}^p, and preliminary tangential Hamiltonian $H_\parallel^p$ are distinguished from the (final) tangential kinetic energy $\mathsf{K}_\parallel$, (final) extrapotential V_{ex}, and constrained Hamiltonian $\mathsf{H}_\parallel$ by the ''p'' superscript. We often drop the ''pre-

liminary'' and ''final'' modifiers when referring to these terms, relying on their symbols and context to make the precise meaning clear.

C. Nonconstant transverse potentials

Up to now we have assumed that the transverse potential $V_\perp(\mathsf{u})$ is constant [modulo SO(d) rotations] along the constraint manifold $\mathcal{C}$. For some physical systems this assumption holds exactly due to symmetry on the ambient space, such as SO(3) rotations in the case of a rigid body. However, for other systems, this assumption may be only approximately satisfied; the constraining potential may in fact vary along the constraint manifold. This is true, for example, of a molecule evolving along a reaction path; there is no symmetry dictating that the frequencies of the small transverse vibrations be constant. The purpose of this section is to illustrate how small variations in the transverse potential may be easily included within our formalism.

The key idea is to only allow dependence on q at order ϵ^2. Specifically, we assume the transverse potential can be expanded as

$$\tilde{V}_\perp(\tilde{\mathsf{u}},q;\epsilon)=\tilde{V}_\perp^0(\tilde{\mathsf{u}})+\epsilon\tilde{V}_\perp^1(\tilde{\mathsf{u}})+\epsilon^2\tilde{V}_\perp^2(\tilde{\mathsf{u}},q)+O(\epsilon^3). \tag{4.26}$$

Applying this expansion to Eq. (4.8), an eigenvalue $\tilde{E}_\perp$ of $\tilde{H}_\perp$ (assuming analyticity in ϵ) can be expanded as

$$\tilde{E}_\perp(q;\epsilon)=\tilde{E}_\perp^0+\epsilon\tilde{E}_\perp^1+\epsilon^2\tilde{E}_\perp^2(q)+O(\epsilon^3). \tag{4.27}$$

The first two terms of $E_\perp=\tilde{E}_\perp/\epsilon^2$ go to infinity as ϵ goes to 0. However, these two terms are constant in q and may thus be subtracted off. The next-order term $\tilde{E}_\perp^2(q)$ does depend on q and is of the same order in ϵ as $\mathsf{H}_\parallel$. Thus, $\tilde{E}_\perp^2(q)$ may be combined with the extrapotential V_{ex} in $\mathsf{H}_\parallel$ to form the effective potential

$$\mathsf{V}_{ef}(q)=\mathsf{V}_{ex}(q)+\tilde{E}_\perp^2(q)\mathsf{I}. \tag{4.28}$$

This is the only modification which needs to be made to our formalism. Notice that the transverse modes $\chi_n(\mathsf{u})$ need not be modified since they are defined to be only order ϵ^0 eigenfunctions of $H_\perp$ and hence are unaffected by the term $\tilde{E}_\perp^2(q)$.

V. ANALYSIS OF CONNECTIONS

Both the preliminary and the final tangential kinetic energies $K_\parallel^p$ and $\mathsf{K}_\parallel$ exhibit a gauge potential proportional to S_{abc}. In this section we study the geometric origins of these gauge potentials and compute their curvatures.

We begin by reviewing the connection on normal vector fields over $\mathcal{C}$. We note that many equivalent definitions exist for the general concept of a connection. For the purposes of this paper, a connection is taken to be a covariant derivative operator which acts on some space of vector fields. For more background, see any of a number of standard references [23–25]. For the remainder of this section, $\mathbf{v}$ is an arbitrary normal vector field over $\mathcal{C}$, and $\mathbf{x}$ and $\mathbf{y}$ are arbitrary tangent vector fields over $\mathcal{C}$. The normal connection ∇^N is defined by

$$\nabla^N_{\mathbf{x}}\mathbf{v}=P_\perp\nabla_{\mathbf{x}}\mathbf{v}=P_\perp\nabla_{\mathbf{x}}P_\perp\mathbf{v}, \tag{5.1}$$

where ∇ is the Levi-Civita connection on $\mathcal{A}$. Notice that $\nabla^N_{\mathbf{x}}\mathbf{v}$ is itself a normal vector field. The curvature of ∇^N, denoted B^N, is computed to be

$$\begin{aligned}B^N_{\mathbf{xy}}\mathbf{v}&=(\nabla^N_{\mathbf{x}}\nabla^N_{\mathbf{y}}-\nabla^N_{\mathbf{y}}\nabla^N_{\mathbf{x}}-\nabla^N_{[\mathbf{x},\mathbf{y}]})\mathbf{v}\\&=P_\perp(\nabla_{\mathbf{x}}P_\perp\nabla_{\mathbf{y}}-\nabla_{\mathbf{y}}P_\perp\nabla_{\mathbf{x}}-\nabla_{[\mathbf{x},\mathbf{y}]})P_\perp\mathbf{v}\\&=P_\perp(R_{\mathbf{xy}}-\nabla_{\mathbf{x}}P_\parallel\nabla_{\mathbf{y}}+\nabla_{\mathbf{y}}P_\parallel\nabla_{\mathbf{x}})P_\perp\mathbf{v}\\&=P_\perp(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}})P_\perp\mathbf{v},\end{aligned} \tag{5.2}$$

where the first equality is simply the definition of the curvature, the second follows from Eq. (5.1), the third from noting $P_\perp=I-P_\parallel$ and Eq. (B8), and the forth from Eq. (B1). As expected, the curvature depends only on the nature of the embedding of $\mathcal{C}$ (via the tensor T) and on the curvature of $\mathcal{A}$. If we assume that the tensors B^N and R vanish, then we obtain the class of embeddings considered by da Costa [7]. For such embeddings, one can choose a potential frame with vanishing twist, thus eliminating coupling between the transverse modes. [This follows from Eq. (5.5) below and the fact that for vanishing curvature, one can always find a frame for which the gauge potential vanishes.] Also, for a nontwisting potential frame, the submanifolds of constant potential are orthogonal to the transverse spaces $\mathcal{U}_q$. Hence, at all points the restoring force is directed inward tangent to the $\mathcal{U}_q$.

It is instructive to compute the gauge potential explicitly for the connection ∇^N. For this computation we first choose an arbitrary orthonormal frame (not necessarily the potential frame) $\mathbf{V}_\mu$, $\mu=1,\ldots,d$, for each normal space N_q. We denote the components of an arbitrary normal vector field $\mathbf{v}$ with respect to $\mathbf{V}_\mu$ by v^μ. Then, the components of $\nabla^N_{\mathbf{E}_i}\mathbf{v}$ are given by

$$(\nabla^N_{\mathbf{E}_i}\mathbf{v})^\mu=\mathbf{E}_i v^\mu+(A_i^N)^\mu{}_\nu v^\nu, \tag{5.3}$$

where we have defined the gauge potential

$$(A_i^N)_{\mu\nu}=\langle\mathbf{V}_\mu,\nabla^N_{\mathbf{E}_i}\mathbf{V}_\nu\rangle=\langle\mathbf{V}_\mu,\nabla_{\mathbf{E}_i}\mathbf{V}_\nu\rangle. \tag{5.4}$$

Due to the orthonormality of the $\mathbf{V}_\mu$, $(A_i^N)_{\mu\nu}$ is antisymmetric in μ and ν. The gauge potential can therefore be viewed as a one-form on $\mathcal{C}$ with values in the Lie algebra so(d), which contains all antisymmetric $d\times d$ matrices. If we choose $\mathbf{V}_\mu=\mathbf{E}_\mu$, we recognize from Eq. (2.2) that the gauge potential is related to the potential twist tensor by

$$(A_i^N)_{\mu\nu}=S_{\mu\nu i}. \tag{5.5}$$

This result will be important below for analyzing $K_\parallel^p$ and $\mathsf{K}_\parallel$.

We now consider a function $\psi(\mathbf{v},q)$, such as the quantum wave function, defined in the neighborhood of $\mathcal{C}$. (We use the bold notation $\mathbf{v}$ instead of sans serif used earlier because we wish to emphasize the dependence of ψ on the normal vector and not on its components with respect to a given frame,

such as the potential frame.) The connection ∇^N which acts on normal vector fields gives rise to another connection $\nabla^{\|p}$ which acts on the function $\psi(\mathbf{v},q)$. In order to define $(\nabla^{\|p}_{\mathbf{x}}\psi)(\mathbf{v},q)$, we first choose a path $q'(\alpha)$ such that $q'(0)=q$ and $(dq'/d\alpha)(0)=\mathbf{x}$. We then denote by $\mathbf{v}'(\alpha)$ the unique normal vector at each point $q'(\alpha)$ satisfying $\mathbf{v}'(0)=\mathbf{v}$ and $(\nabla^N_{d/d\alpha}\mathbf{v}')(\alpha)=0$. Then, the connection $\nabla^{\|p}$ is defined by

$$(\nabla^{\|p}_{\mathbf{x}}\psi)(\mathbf{v},q)=\frac{d}{d\alpha}\bigg|_{\alpha=0}\psi(\mathbf{v}'(\alpha),q'(\alpha)). \tag{5.6}$$

The transverse kinetic energy $K^p_{\|}$ can be directly related to the covariant derivative $\nabla^{\|p}$. To do this, it is useful to compute the gauge potential of $\nabla^{\|p}$ explicitly. As before, we consider an orthonormal frame $\mathbf{V}_\mu$ and denote the components of $\mathbf{v}$ by v^μ. Then, the function $\psi(\mathbf{v},q)$ can also be interpreted as a function of (v,q), where $\mathsf{v}=(v^1,\ldots,v^d)$ is the collection of components. We therefore have

$$\begin{aligned}(\nabla^{\|p}_{\mathbf{E}_i}\psi)(\mathbf{v},q)&=\frac{d}{d\alpha}\bigg|_{\alpha=0}\psi(\mathsf{v}'(\alpha),q'(\alpha))\\&=\frac{d}{d\alpha}\bigg|_{\alpha=0}\psi(\mathsf{v}'(\alpha),q)+\frac{d}{d\alpha}\bigg|_{\alpha=0}\psi(\mathsf{v},q'(\alpha))\\&=(\mathbf{E}_i v'^{\mu})(q)\frac{\partial\psi}{\partial v^\mu}(\mathbf{v},q)+(\mathbf{E}_i\psi)(\mathbf{v},q),\end{aligned} \tag{5.7}$$

where in the third equality, the derivatives $\partial/\partial v^\mu$ and $\mathbf{E}_i$ are understood to have q and v^ν held fixed, respectively. From Eq. (5.3) and the condition $\nabla^N_{\mathbf{E}_i}\mathbf{v}'=0$, we find

$$\mathbf{E}_i v'^{\mu}=-(A^N_i)^\mu{}_\nu v'^{\nu}. \tag{5.8}$$

Inserting this result into Eq. (5.7) yields

$$(\nabla^{\|p}_{\mathbf{E}_i}\psi)(\mathbf{v},q)=[(\mathbf{E}_i+A^{\|p}_i)\psi](\mathbf{v},q), \tag{5.9}$$

where

$$A^{\|p}_i=(A^N_i)^{\mu\nu}\Omega_{\mu\nu}, \tag{5.10}$$

and where we have used the antisymmetry of $(A^N_i)_{\mu\nu}$ to introduce the operator

$$\Omega_{\mu\nu}=\frac{1}{2}\left(v_\mu\frac{\partial}{\partial v^\nu}-v_\nu\frac{\partial}{\partial v^\mu}\right). \tag{5.11}$$

Obviously if $\mathbf{V}_\mu=\mathbf{E}_\mu$, then $\Lambda_{\mu\nu}=-i\hbar\Omega_{\mu\nu}$. The relevance of $\nabla^{\|p}$ for $K^p_{\|}$ is now clear. By choosing $\mathbf{V}_\mu=\mathbf{E}_\mu$ and applying Eqs. (5.5), (5.9), and (5.10) to Eq. (3.33), we see that

$$K^p_{\|}=\frac{\hbar^2}{2}(\nabla^{\|p}_{\mathbf{E}_i})^\dagger\nabla^{\|p}_{\mathbf{E}_i}. \tag{5.12}$$

Thus the preliminary tangential kinetic energy is just proportional to the Laplacian defined in terms of the connection $\nabla^{\|p}$. [Compare Eq. (5.12) to Eq. (C2).]

Considering Eq. (5.10), we see that the two gauge potentials $(A^N_i)_{\mu\nu}$ and $A^{\|p}_i$ differ only in their representation of so(d). For $(A^N_i)_{\mu\nu}$, we use a representation by $d\times d$ antisymmetric matrices, whereas for $A^{\|p}_i$ we use a representation by the operators $\Omega_{\mu\nu}$. Therefore, the curvature of the connections ∇^N and $\nabla^{\|p}$ are also related by simply switching the representation of so(d). Hence the curvature $B^{\|p}$ of $\nabla^{\|p}$ is

$$\begin{aligned}B^{\|p}_{\mathbf{xy}}\psi&=(\nabla^{\|p}_{\mathbf{x}}\nabla^{\|p}_{\mathbf{y}}-\nabla^{\|p}_{\mathbf{y}}\nabla^{\|p}_{\mathbf{x}}-\nabla^{\|p}_{[\mathbf{x},\mathbf{y}]})\psi\\&=(B^N_{\mathbf{xy}})^{\mu\nu}\Omega_{\mu\nu}\psi\\&=(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}})^{\mu\nu}\Omega_{\mu\nu}\psi.\end{aligned} \tag{5.13}$$

We now consider a k-dimensional vector-valued function $\boldsymbol{\phi}(q)$ with components $\phi_n(q)$. The connection $\nabla^{\|p}$ induces a connection $\nabla^{\|}$ on $\boldsymbol{\phi}$ by the formula

$$(\nabla^{\|}_{\mathbf{x}}\boldsymbol{\phi})_n=\left\langle\chi_n\middle|\nabla^{\|p}_{\mathbf{x}}\sum_{n'=1}^{k}\chi_{n'}\phi_{n'}\right\rangle_{\mathsf{u}}. \tag{5.14}$$

The tangential kinetic energy $\mathsf{K}_{\|}$ is closely related to the connection $\nabla^{\|}$ as we now show. We take the orthonormal frame $\mathbf{V}_\mu$ to be $\mathbf{E}_\mu$, and we recall that $\chi_n(\mathsf{u})$ is a function of u^μ alone and $\boldsymbol{\phi}(q)$ is a function of q alone. Then applying Eqs. (5.5), (5.9), and (5.10), we find

$$\nabla^{\|p}_{\mathbf{x}}\chi_n=(S_{\mathbf{x}})^{\mu\nu}\Omega_{\mu\nu}\chi_n, \tag{5.15}$$

$$\nabla^{\|p}_{\mathbf{x}}\phi_n=\mathbf{x}\phi_n, \tag{5.16}$$

where $(S_{\mathbf{x}})_{\mu\nu}=\langle\mathbf{E}_\mu,S_{\mathbf{x}}\mathbf{E}_\nu\rangle$. Then Eq. (5.14) yields

$$\nabla^{\|}_{\mathbf{x}}=\mathbf{x}\mathsf{I}+\mathsf{A}^{\|}_{\mathbf{x}}, \tag{5.17}$$

$$\mathsf{A}^{\|}_{\mathbf{x}}=(S_{\mathbf{x}})^{\mu\nu}\underline{\Omega}_{\mu\nu}, \tag{5.18}$$

where $\underline{\Omega}_{\mu\nu}$ is the $k\times k$ matrix with components

$$(\Omega_{\mu\nu})_{nn'}=\langle\chi_n|\Omega_{\mu\nu}\chi_{n'}\rangle_{\mathsf{u}}. \tag{5.19}$$

From Eq. (5.15), we note that the components of $\mathsf{A}^{\|}_{\mathbf{x}}$ can also be written as

$$(A^{\|}_{\mathbf{x}})_{nn'}=\langle\chi_n|\nabla^{\|p}_{\mathbf{x}}\chi_{n'}\rangle_{\mathsf{u}}. \tag{5.20}$$

Equations (5.17) and (5.18) show that the tangential kinetic energy $\mathsf{K}_{\|}$, Eq. (4.22), is given by

$$\mathsf{K}_{\|}=\frac{\hbar^2}{2}(\nabla^{\|}_{\mathbf{E}_i})^\dagger\nabla^{\|}_{\mathbf{E}_i}, \tag{5.21}$$

analogous to Eq. (5.12) for $K^p_{\|}$.

The connection $\nabla^{\|}$ is closely related to the adiabatic transport of quantum states and the associated geometric phase due to Berry [14]. If a set of k degenerate quantum states $\xi_n(\eta)$, $n=1,\ldots,k$, depending smoothly on a set of m external parameters $\eta=(\eta_1,\ldots,\eta_m)$, is subject to an adiabatic variation $\eta(\alpha)$ of these parameters, then the $\xi_n(\alpha)$

$=\xi_n(\eta(\alpha))$ satisfy $\langle\xi_n|d\xi_{n'}/d\alpha\rangle=\Sigma_i\langle\xi_n|\partial\xi_{n'}/\partial\eta_i\rangle\times(d\eta_i/d\alpha)=0$. Simon [26] recognized that this condition defines a connection

$$\nabla^B_{\partial/\partial\eta_i}=\frac{\partial}{\partial\eta_i}\mathsf{I}+\mathsf{A}^B_i \tag{5.22}$$

acting on the vector-valued wave function $\boldsymbol{\xi}=(\xi_1,\ldots,\xi_k)$ parametrized by η. The gauge potential A^B_i is a $k\times k$ matrix with components

$$(A^B_i)_{nn'}=\left\langle\xi_n\left|\frac{\partial\xi_{n'}}{\partial\eta_i}\right\rangle\right. . \tag{5.23}$$

If the parameters η_i are themselves quantized, then the momentum conjugate to η_i is not simply $-i\hbar(\partial/\partial\eta_i)\mathsf{I}$, but rather $-i\hbar\nabla^B_{\partial/\partial\eta_i}=-i\hbar(\partial/\partial\eta_i\mathsf{I}+\mathsf{A}^B_i)$. This situation applies, for example, to the Born-Oppenheimer theory of molecules, wherein the parameters η_i describe the positions of the nuclei and the ξ_n represent the quantum state of the electrons [27]. For the constrained quantum systems considered in this paper, the ordering in ϵ adiabatically separates the transverse modes χ_n (analogous to the ξ_n) from the motion along the constraint manifold (analogous to the space of η_i). Therefore, the gauge potential $\mathsf{A}^\parallel_{\mathbf{x}}$ occurring in Eq. (5.17) is essentially the same as Berry's gauge potential A^B_i occurring in Eq. (5.22). We say ''essentially the same'' because the coordinate derivative $\partial/\partial\eta_i$ of Eq. (5.23) has been replaced by the covariant derivative $\nabla^{\parallel p}$ of Eq. (5.20), this covariant derivative being the geometrically natural connection for the transverse modes.

We next compute the curvature of the connection $\nabla^\parallel$. In terms of the gauge potential $\mathsf{A}^\parallel=(S_{\mathbf{x}})^{\mu\nu}\underline{\Omega}_{\mu\nu}$, we have

$$\begin{aligned}\mathsf{B}^\parallel_{\mathbf{xy}}&=(d\mathsf{A}^\parallel)(\mathbf{x},\mathbf{y})+[\mathsf{A}^\parallel_{\mathbf{x}},\mathsf{A}^\parallel_{\mathbf{y}}]\\&=(dS^{\mu\nu})(\mathbf{x},\mathbf{y})\underline{\Omega}_{\mu\nu}+(S_{\mathbf{x}})^{\mu\nu}(S_{\mathbf{y}})^{\sigma\tau}[\underline{\Omega}_{\mu\nu},\underline{\Omega}_{\sigma\tau}],\end{aligned} \tag{5.24}$$

where $dS^{\mu\nu}$ is the exterior derivative of $S^{\mu\nu}$, viewed as a one-form over $\mathcal{C}$. We determine $dS^{\mu\nu}$ from the formula Eq. (5.13) for the curvature $B^{\parallel p}$. We first note

$$\begin{aligned}B^{\parallel p}_{\mathbf{xy}}&=(dA^{\parallel p})(\mathbf{x},\mathbf{y})+[A^{\parallel p}_{\mathbf{x}},A^{\parallel p}_{\mathbf{y}}]\\&=(dS^{\mu\nu})(\mathbf{x},\mathbf{y})\Omega_{\mu\nu}+(S_{\mathbf{x}})^{\mu\nu}(S_{\mathbf{y}})^{\sigma\tau}[\Omega_{\mu\nu},\Omega_{\sigma\tau}],\end{aligned} \tag{5.25}$$

where we have used Eqs. (5.5) and (5.10). It is straightforward to verify that the $\Omega_{\mu\nu}$ satisfy the following commutation relations:

$$[\Omega_{\mu\nu},\Omega_{\sigma\tau}]=\tfrac{1}{2}(\delta_{\mu\sigma}\Omega_{\tau\nu}+\delta_{\nu\tau}\Omega_{\sigma\mu}+\delta_{\mu\tau}\Omega_{\nu\sigma}+\delta_{\nu\sigma}\Omega_{\mu\tau}), \tag{5.26}$$

and hence Eq. (5.25) reduces to

$$B^{\parallel p}_{\mathbf{xy}}=[(dS^{\mu\nu})(\mathbf{x},\mathbf{y})+(S_{\mathbf{x}}S_{\mathbf{y}}-S_{\mathbf{y}}S_{\mathbf{x}})^{\mu\nu}]\Omega_{\mu\nu}. \tag{5.27}$$

Combining this equation with Eq. (5.13) produces

$$(dS^{\mu\nu})(\mathbf{x},\mathbf{y})=(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}}-S_{\mathbf{x}}S_{\mathbf{y}}+S_{\mathbf{y}}S_{\mathbf{x}})^{\mu\nu}. \tag{5.28}$$

Combining Eq. (5.28) in turn with Eq. (5.24), we arrive at the following useful formula for the curvature of $\nabla^\parallel$:

$$\begin{aligned}\mathsf{B}^\parallel_{\mathbf{xy}}&=(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}}-S_{\mathbf{x}}S_{\mathbf{y}}+S_{\mathbf{y}}S_{\mathbf{x}})^{\mu\nu}\underline{\Omega}_{\mu\nu}\\&\quad+(S_{\mathbf{x}})^{\mu\nu}(S_{\mathbf{y}})^{\sigma\tau}[\underline{\Omega}_{\mu\nu},\underline{\Omega}_{\sigma\tau}].\end{aligned} \tag{5.29}$$

Using the commutation relations Eq. (5.26) the above equation can be recast as

$$\begin{aligned}\mathsf{B}^\parallel_{\mathbf{xy}}&=(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}})^{\mu\nu}\underline{\Omega}_{\mu\nu}\\&\quad+[(S_{\mathbf{x}})^{\mu\nu}(S_{\mathbf{y}})^{\sigma\tau}-(S_{\mathbf{y}})^{\mu\nu}(S_{\mathbf{x}})^{\sigma\tau}](\underline{\Omega}_{\mu\nu}\underline{\Omega}_{\sigma\tau}-\underline{\Omega}^{(2)}_{\mu\nu\sigma\tau}),\end{aligned} \tag{5.30}$$

where $\underline{\Omega}^{(2)}_{\mu\nu\sigma\tau}$ is the $k\times k$ matrix with components

$$(\Omega^{(2)}_{\mu\nu\sigma\tau})_{nn'}=\langle\chi_n|\Omega_{\mu\nu}\Omega_{\sigma\tau}\chi_{n'}\rangle. \tag{5.31}$$

VI. SPECIFIC CASES AND EXAMPLES

We consider several concrete examples to help clarify the general theory.

A. Codimension-one case

We assume here that the codimension of the constraint manifold is $d=1$. Since there is only one normal direction, we expect the potential twist to vanish. Indeed, this follows from the antisymmetry property $S_{\mu\nu i}=-S_{\nu\mu i}$ [Eq. (2.3)] and the fact that $\mu=\nu=1$. Similarly, the normal components of the Riemannian curvature $R_{\mu\nu\sigma\tau}$ also vanish due to the well-known antisymmetry property $R_{abcd}=-R_{bacd}=-R_{abdc}$. From this fact follows $\mathcal{R}_\perp=R^{11}{}_{11}|_0=0$ and $\mathcal{R}=\mathcal{R}_\parallel$. The expressions for $\mathcal{T}^2$ and $\mathcal{M}^2$ can also be simplified by introducing the rank two symmetric tensor W defined on vectors tangent to $\mathcal{C}$ and with components $W^i{}_j=T^i{}_{1j}$. (This tensor is often called the Weingarten map.) Then $\mathcal{T}^2=\mathrm{Tr}\,(W^2)$ and $\mathcal{M}^2=(\mathrm{Tr}\,W)^2$. Hence, the tangential Hamiltonian Eq. (4.21) becomes

$$\mathsf{H}_\parallel=\mathsf{K}_\parallel+\mathsf{V}_{ex}, \tag{6.1}$$

$$\mathsf{K}_\parallel=\tfrac{1}{2}\pi^i|_0{}^\dagger\pi_i\mathsf{I}, \tag{6.2}$$

$$\begin{aligned}\mathsf{V}_{ex}=V^p_{ex}\mathsf{I}&=-\frac{\hbar^2}{8}(\mathcal{T}^2-\hat{\mathcal{R}}+\mathcal{R}_\parallel)\mathsf{I}\\&=-\frac{\hbar^2}{8}(\mathcal{M}^2-2\hat{\mathcal{R}}+2\mathcal{R}_\parallel)\mathsf{I}\\&=-\frac{\hbar^2}{8}(2\mathcal{T}^2-\mathcal{M}^2)\mathsf{I},\end{aligned} \tag{6.3}$$

where we have used Eqs. (3.44), (3.46), and (3.47). Notice that the tangential kinetic energy is proportional to the standard Laplacian on $\mathcal{C}$. All reference to $\Lambda_{\mu\nu}$ has vanished, and hence all coupling between the degenerate transverse modes

has been eliminated. The k-dimensional Schrödinger equation therefore separates into k independent scalar Schrödinger equations.

We consider the case where the ambient space $\mathcal{A}$ is a flat two-dimensional space and the constraint manifold $\mathcal{C}$ is a curve in that space. Then, we note that $\hat{\mathcal{R}}=\mathcal{R}=\mathcal{R}_{\|}=0$. Furthermore, the second fundamental form, or equivalently the Weingarten map, has only one nonzero component. We denote this component by $W=W_{ii}=\kappa=1/\rho$, where κ is the extrinsic curvature and ρ is the radius of curvature. Then, the extrapotential is

$$V_{ex}^{p}=-\frac{\hbar^2}{8}\frac{1}{\rho^2}=-\frac{\hbar^2}{8}\kappa^2. \tag{6.4}$$

As in Sec. I B the sign on V_{ex}^{p} is such that ϕ is attracted to regions of high curvature. This extrapotential was derived earlier by Marcus [3] and Switkes, Russell, and Skinner [5].

We next consider the case where $\mathcal{A}$ is a flat three-dimensional space and $\mathcal{C}$ is a two-dimensional surface. We still have that $\mathcal{R}=\mathcal{R}_{\|}=0$. Furthermore, the eigenvalues of the second rank two-dimensional tensor W_{ij} are $\kappa_1=1/\rho_1$ and $\kappa_2=1/\rho_2$, where ρ_1 and ρ_2 are the two extrinsic radii of curvature. Then the extrapotential V_{ex}^{p} is conveniently written

$$\begin{aligned}V_{ex}^{p}&=-\frac{\hbar^2}{8}[2\,\mathrm{Tr}(W^2)-(\mathrm{Tr}\,W)^2]\\&=-\frac{\hbar^2}{8}\left(\frac{1}{\rho_1}-\frac{1}{\rho_2}\right)^2\\&=-\frac{\hbar^2}{8}(\kappa_1-\kappa_2)^2.\end{aligned} \tag{6.5}$$

This result was previously derived by Jensen and Koppe [4] as well as da Costa [6].

B. Codimension-two case

We assume here that the codimension of the constraint manifold is $d=2$. This allows us to define quantities S_i, $\underline{\Lambda}$, and $\underline{\Lambda}^{(2)}$ by

$$S_{\mu\nu i}=S_i\epsilon_{\mu\nu}, \tag{6.6}$$

$$\underline{\Lambda}_{\mu\nu}=\underline{\Lambda}\,\epsilon_{\mu\nu}, \tag{6.7}$$

$$\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau}=\underline{\Lambda}^{(2)}\epsilon_{\mu\nu}\epsilon_{\sigma\tau}, \tag{6.8}$$

where $\epsilon_{\mu\nu}$ is the 2×2 antisymmetric tensor with $\epsilon_{12}=-\epsilon_{21}=1$. Furthermore, we have

$$R_{\mu\nu\sigma\tau}=\tfrac{1}{2}\mathcal{R}_{\perp}\epsilon_{\mu\nu}\epsilon_{\sigma\tau}. \tag{6.9}$$

We express the tangential Hamiltonian Eq. (4.21) as

$$\mathsf{H}_{\|}=\mathsf{K}_{\|}+\mathsf{V}_{ex}, \tag{6.10}$$

$$\mathsf{K}_{\|}=\tfrac{1}{2}(\pi^i|_0\mathsf{I}+2S^i|_0\underline{\Lambda})^{\dagger}(\pi_i\mathsf{I}+2S_i\underline{\Lambda}), \tag{6.11}$$

$$\mathsf{V}_{ex}=V_{ex}^{p}\mathsf{I}+(2S^iS_i)|_0(\underline{\Lambda}^{(2)}-\underline{\Lambda}^2)+\tfrac{1}{3}\mathcal{R}_{\perp}|_0\underline{\Lambda}^2. \tag{6.12}$$

We consider the case of Sec. I B where $\mathcal{A}$ is a flat three-dimensional space and $\mathcal{C}$ is a one-dimensional curve. First, we note $\hat{\mathcal{R}}=\mathcal{R}=\mathcal{R}_{\perp}=\mathcal{R}_{\|}=0$. Next, we denote the single component of tangential momentum by $\pi_{\|}=\pi_i$. Since $\mathcal{C}$ is one dimensional, $\pi_{\|}=-i\hbar\partial/\partial\alpha=\pi_{\|}^{\dagger}$, where α is the geodesic length. Furthermore, the potential twist is determined by the sole component $\mathcal{S}=S_i$. The second fundamental form can be identified with a normal vector $T^{\mu}=T^{i\mu i}$ of magnitude $\kappa=1/\rho$. Hence, $\mathcal{M}^2=T^{i\mu}{}_iT^j{}_{\mu j}=T^{\mu}T_{\mu}=\kappa^2=1/\rho^2$. Using Eq. (3.47), Eqs. (6.11) and (6.12) therefore simplify to

$$\mathsf{K}_{\|}=\tfrac{1}{2}(\pi_{\|}\mathsf{I}+2\mathcal{S}\underline{\Lambda})^2, \tag{6.13}$$

$$\mathsf{V}_{ex}=-\frac{\hbar^2}{8}\kappa^2\mathsf{I}+(2\mathcal{S}^2)(\underline{\Lambda}^{(2)}-\underline{\Lambda}^2). \tag{6.14}$$

Assuming a single nondegenerate transverse mode, Eqs. (6.13) and (6.14) yield Eqs. (1.4) and (1.5).

C. Rotationally invariant transverse potential

In this section, we assume the transverse potential $V_{\perp}(\mathsf{u})$ is rotationally invariant, depending only on the radius $u=(u^{\mu}u^{\mu})^{1/2}$ in the normal space. The potential frame $\mathbf{E}_{\mu}$ can therefore be any orthonormal frame we like. This freedom in the choice of potential frame produces a large range of possible potential twist tensors S, with the actual choice of S being simply a matter of convention. The Hamiltonian $\mathsf{H}_{\|}$ in Eq. (4.21), however, should be independent (up to a rescaling of the wave function $\boldsymbol{\phi}$) of any such conventions. In the remainder of this section, we show explicitly how the dependence on S drops out of $\mathsf{H}_{\|}$ under the assumption of rotational invariance.

First, we observe that the transverse Hamiltonian Eq. (4.2) has the form

$$H_{\perp}=-\frac{\hbar^2}{2}\frac{1}{u^{d-1}}\frac{\partial}{\partial u}u^{d-1}\frac{\partial}{\partial u}+\frac{\Lambda^2}{2u^2}+V_{\perp}(u), \tag{6.15}$$

where Λ^2 is the Casimir operator

$$\Lambda^2=\Lambda_{\mu\nu}\Lambda^{\mu\nu}. \tag{6.16}$$

Therefore, an eigenfunction χ_n of $H_{\perp}$ is necessarily an eigenfunction of Λ^2. We denote by χ_n^{λ} such an eigenfunction whose Λ^2 eigenvalue is λ. A basic fact concerning the eigenspaces of the Casimir Λ^2 is that they block diagonalize the generators $\Lambda_{\mu\nu}$. That is, $\langle\chi_n^{\lambda}|\Lambda_{\mu\nu}\chi_{n'}^{\lambda'}\rangle_{\mathsf{u}}=0$ if $\lambda\neq\lambda'$.[2] Based on the definitions Eqs. (4.24) and (4.25) for $\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau}$ and $\underline{\Lambda}_{\mu\nu}$, this fact implies that for the space of transverse

[2]This follows quickly from $[\Lambda^2,\Lambda_{\mu\nu}]=0$. Note, $(\lambda-\lambda')\langle\chi_n^{\lambda}|\Lambda_{\mu\nu}\chi_{n'}^{\lambda'}\rangle_u=\langle\chi_n^{\lambda}|[\Lambda^2,\Lambda_{\mu\nu}]\chi_{n'}^{\lambda'}\rangle_u=0$.

modes for a given $E_\perp$, $\underline{\Lambda}^{(2)}_{\mu\nu\sigma\tau}=\underline{\Lambda}\mu\nu\underline{\Lambda}_{\sigma\tau}$. Similarly, $\underline{\Omega}^{(2)}_{\mu\nu\sigma\tau}=\underline{\Omega}_{\mu\nu}\underline{\Omega}_{\sigma\tau}$. We therefore see from Eq. (4.23) that all S dependence drops out of V_{ex},

$$\mathsf{V}_{ex}=V^p_{ex}\mathsf{I}+\tfrac{1}{6}R^{\mu\nu\sigma\tau}|_0\underline{\Lambda}_{\mu\nu}\underline{\Lambda}_{\sigma\tau}. \tag{6.17}$$

Considering $\mathsf{K}_\parallel$, even though Eq. (4.22) is written in terms of the potential twist S, we showed in Sec. V [specifically Eq. (5.21)] that $\mathsf{K}_\parallel$ can be expressed in terms of the Laplacian associated with the connection $\nabla^\parallel$. From Eq. (5.30) and the results above, we see that the curvature $\mathsf{B}^\parallel$ of this connection is independent of S,

$$\mathsf{B}^\parallel_{\mathbf{xy}}=(R_{\mathbf{xy}}-T_{\mathbf{x}}T_{\mathbf{y}}+T_{\mathbf{y}}T_{\mathbf{x}})^{\mu\nu}\underline{\Omega}_{\mu\nu}. \tag{6.18}$$

Now if two connections $\nabla^\parallel$ and $\nabla^{\parallel\prime}$ have the same curvature, then their associated Laplacians can only differ by a rescaling of the wave function. Hence, the Hamiltonian $\mathsf{H}_\parallel$ for different choices of the potential twist S can at most differ by such a rescaling.

D. Harmonic transverse potentials

We assume that the transverse potential is quadratic in the u^μ

$$V_\perp(\mathsf{u};\epsilon)=\sum_\mu \frac{1}{2}(\omega_\mu(\epsilon))^2u^\mu u^\mu \tag{6.19}$$

and that the oscillation frequencies depend on ϵ via $\omega_\mu(\epsilon)=\tilde{\omega}_\mu/\epsilon^2$, with $\tilde{\omega}_\mu$ being independent of ϵ. (For clarity, we make summation over the indices μ, ν, σ, . . . explicit in this section.) We introduce the standard machinery of raising, lowering, and number operators for each degree of freedom,

$$a_\mu=\frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega_\mu}u_\mu+i\frac{\pi_\mu}{\sqrt{\omega_\mu}}\right), \tag{6.20}$$

$$u^\mu=\sqrt{\frac{\hbar}{2\omega_\mu}}(a_\mu+a^\dagger_\mu), \tag{6.21}$$

$$\pi_\mu=-i\sqrt{\frac{\hbar\omega_\mu}{2}}(a_\mu-a^\dagger_\mu), \tag{6.22}$$

$$N_\mu=a^\dagger_\mu a_\mu, \tag{6.23}$$

$$[a_\mu,a^\dagger_\nu]=\delta_{\mu\nu}. \tag{6.24}$$

Notice that a_μ and N_μ scale as ϵ^0. The transverse Hamiltonians $H_\perp$ and $\tilde{H}_\perp$ have the usual form

$$H_\perp(\epsilon)=\sum_\mu \hbar\omega_\mu(\epsilon)\left(N_\mu+\frac{1}{2}\right), \tag{6.25}$$

$$\tilde{H}_\perp=\sum_\mu \hbar\tilde{\omega}_\mu\left(N_\mu+\frac{1}{2}\right), \tag{6.26}$$

and the transverse modes can therefore be labeled by the number of quanta n_μ in each degree of freedom μ. We denote such a mode by χ_{n} where $\mathsf{n}=(n_1,\ldots,n_d)$. Inserting Eqs. (6.21) and (6.22) into Eq. (3.36) yields

$$\Lambda_{\mu\nu}=\frac{i\hbar}{4\sqrt{\omega_\mu\omega_\nu}}[(\omega_\mu-\omega_\nu)(a_\mu a_\nu-a^\dagger_\mu a^\dagger_\nu) +(\omega_\mu+\omega_\nu)(a^\dagger_\nu a_\mu-a^\dagger_\mu a_\nu)], \tag{6.27}$$

from which one quickly sees

$$\langle\chi_{\mathsf{n}}|\Lambda_{\mu\nu}\chi_{\mathsf{n}}\rangle_{\mathsf{u}}=0. \tag{6.28}$$

A significantly more involved computation yields

$$\langle\chi_{\mathsf{n}}|\Lambda_{\mu\nu}\Lambda_{\sigma\tau}\chi_{\mathsf{n}}\rangle_{\mathsf{u}}=-\frac{\hbar^2}{8}\left[2\left(n_\mu+\frac{1}{2}\right)\left(n_\nu+\frac{1}{2}\right)\frac{\omega_\mu^2+\omega_\nu^2}{\omega_\mu\omega_\nu}-1\right] \times(\delta_{\mu\tau}\delta_{\nu\sigma}-\delta_{\mu\sigma}\delta_{\nu\tau}). \tag{6.29}$$

We now assume that $\chi=\chi_{\mathsf{n}}$ is a nondegenerate transverse mode. The tangential Hamiltonian Eq. (4.21) is therefore a scalar operator. Using Eqs. (6.28) and (6.29), $H_\parallel$ is

$$H_\parallel=K_\parallel+V_{ex}, \tag{6.30}$$

$$K_\parallel=\frac{1}{2}\pi^i|_0{}^\dagger\pi_i, \tag{6.31}$$

$$V_{ex}=V^p_{ex}-\frac{\hbar^2}{8}\sum_{\mu\nu}\left(S^{\mu\nu i}S_{\mu\nu i}+\frac{1}{3}R^{\mu\nu}{}_{\mu\nu}\right)\Big|_0 \times\left[1-2\left(n_\mu+\frac{1}{2}\right)\left(n_\nu+\frac{1}{2}\right)\frac{\omega_\mu^2+\omega_\nu^2}{\omega_\mu\omega_\nu}\right]. \tag{6.32}$$

The most striking aspect of the above equations is that, due to the vanishing of $\langle\chi|\Lambda_{\mu\nu}\chi\rangle_{\mathsf{u}}$, the tangential kinetic energy $K_\parallel$ is proportional to the standard Laplacian on the constraint manifold. Thus, all of the effects of extrinsic curvature and potential twist are contained in the extrapotential V_{ex}.

E. Potentials with reflection symmetry

The vanishing of $\langle\chi|\Lambda_{\mu\nu}\chi\rangle_{\mathsf{u}}$ (and hence the potential twist as well) from $K_\parallel$ in Eq. (6.31) follows from general considerations of reflection symmetry, and therefore occurs for a large class of symmetric potentials.

Let $\mathsf{Q}\in O(d)$ be a reflection acting on the transverse coordinates $\mathsf{u}=(u^1,\ldots,u^d)$ and assume that, for a given σ, u^σ is mapped to $-u^\sigma$ and all other coordinates remain fixed. Thus, $\mathsf{Q}=\mathsf{Q}^{-1}=\mathsf{Q}^\dagger$. Furthermore, assume that $V_\perp(\mathsf{u})$ is invariant under the action of Q, that is $V_\perp(\mathsf{Qu})=V_\perp(\mathsf{u})$. The reflection Q also has an induced action on the transverse modes, which we denote by Q and which is given by $(Q\chi_n)(\mathsf{u})=\chi_n(\mathsf{Q}^{-1}\mathsf{u})$. Due to the symmetry of $V_\perp$, Q commutes with $H_\perp$,

$$[Q,H_\perp]=0. \tag{6.33}$$

Furthermore, the following are easily verified:

$$Qu^{\sigma}Q^{\dagger}=-u^{\sigma}, \tag{6.34}$$

$$Q\pi_{\sigma}Q^{\dagger}=-\pi_{\sigma}, \tag{6.35}$$

$$Q\Lambda_{\sigma\mu}Q^{\dagger}=-\Lambda_{\sigma\mu} \quad \text{for all } \mu. \tag{6.36}$$

We now consider a single nondegenerate transverse mode, denoted simply by χ. Due to Eq. (6.33), χ must also be an eigenfunction of Q with eigenvalue either $+1$ or -1 (since $Q^2=I$). Combining these facts with Eq. (6.36) and recalling $Q=Q^{\dagger}$, we have

$$\begin{aligned}\langle\chi|\Lambda_{\sigma\mu}\chi\rangle_{\mathsf{u}}&=\langle Q\chi|\Lambda_{\sigma\mu}Q\chi\rangle_{\mathsf{u}}\\&=\langle\chi_n|Q\Lambda_{\sigma\mu}Q^{\dagger}\chi_n\rangle_{\mathsf{u}}\\&=-\langle\chi|\Lambda_{\sigma\mu}\chi\rangle_{\mathsf{u}},\end{aligned} \tag{6.37}$$

and hence

$$\langle\chi|\Lambda_{\sigma\mu}\chi\rangle_{\mathsf{u}}=0 \quad \text{for all } \mu. \tag{6.38}$$

If the potential $V_{\perp}(\mathsf{u})$ is symmetric with respect to at least $d-1$ such Q reflections, possessing $d-1$ distinct and orthogonal reflection axes u^{σ}, then $\langle\chi|\Lambda_{\sigma\mu}\chi\rangle_{\mathsf{u}}$ vanishes for all $\mu,\nu=1,\ldots,d$. For such highly symmetric potentials, $K_{\parallel}$ is again given by Eq. (6.31) and the only effect of the potential twist is to be found in V_{ex}. This is the case for such common potentials as the simple harmonic oscillator, analyzed in the preceding section, as well as the d-dimensional square well. Note that this analysis says nothing about the off-diagonal terms of $(\Lambda_{\mu\nu})_{nn'}$ for a system with degenerate transverse modes; for such systems, there may indeed be a nonvanishing gauge potential.

VII. CONCLUSIONS

We have rigorously derived the effective Hamiltonian of a constrained quantum system by considering the limit as the restoring force becomes infinite. In doing so, we have been careful to avoid unnecessary assumptions on the curvature of the ambient space, the form of the constraint manifold, and the manner of the constraining potential. This general approach yields important new terms in the effective potential V_{ex}, as outlined in Secs. III D and IV B, as well as a gauge potential in the tangential kinetic energy $\mathsf{K}_{\parallel}$, as outlined in Secs. IV B and V. Furthermore, this general approach allows our theory to be applied to several examples of physical importance. These examples include reaction paths for molecular reaction and scattering problems, twisted quantum waveguides, the double pendulum, and models of polymers by rigid constraints.

Perhaps the most important example of a constrained quantum system is the quantum rigid body. Physically, we have in mind systems such as semirigid molecules. Though we lack the space to include the analysis here, we have applied our theory to such molecules. Assuming that the standard Born-Oppenheimer ordering is valid, our constrained Hamiltonian reproduces the standard results for the rotation-vibration energy levels of such molecules (through the lowest three orders in the Born-Oppenheimer ordering parameter. See, for example, Papoušek and Aliev [28].) For semirigid molecules, the constraining potential (resulting from the semirigid bonds) is well approximated by a harmonic potential. Hence the gauge potential in $K_{\parallel}$ vanishes. (We assume a nondegenerate vibrational state; see Sec. VI D.) For this reason, a semirigid molecule is a poor example for viewing the effects of the gauge potential (at least for nondegenerate modes.) A more interesting example might be a cluster of rigid molecules held together by weak van der Waals forces. The potentials between such molecules can be quite anharmonic and unsymmetric, meaning the gauge potential is not forced to vanish. Such systems might therefore provide a fruitful context in which to observe the physical consequences of this gauge potential.

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APPENDIX A: A BRIEF REVIEW OF CURVES IN $\mathbb{R}^3$

We cite a few important facts about curves in $\mathbb{R}^3$ which we need in the body of the paper. For greater depth, see, for example, Spivak [24]. Consider a curve $\mathbf{x}(\alpha)$ in $\mathbb{R}^3$. The parametrization of the curve is given by α which measures the arclength along the curve. Hence the tangent vector $\hat{\mathbf{t}}=d\mathbf{x}/d\alpha$ is of unit length. We denote the principal normal and the binormal by $\hat{\mathbf{n}}$ and $\hat{\mathbf{b}}$, respectively. They are given by

$$\hat{\mathbf{n}}=\frac{d\hat{\mathbf{t}}/d\alpha}{|d\hat{\mathbf{t}}/d\alpha|}, \tag{A1}$$

$$\hat{\mathbf{b}}=\hat{\mathbf{t}}\times\hat{\mathbf{n}}. \tag{A2}$$

The vectors $(\hat{\mathbf{t}},\hat{\mathbf{n}},\hat{\mathbf{b}})$ form an orthonormal right-handed frame. The derivatives of this frame are given by the famous Serret-Frenet formulas which may be summarized as

$$\frac{d}{d\alpha}\begin{bmatrix}\hat{\mathbf{t}}\\ \hat{\mathbf{n}}\\ \hat{\mathbf{b}}\end{bmatrix}=\begin{bmatrix}0 & \kappa & 0\\ -\kappa & 0 & \tau\\ 0 & -\tau & 0\end{bmatrix}\begin{bmatrix}\hat{\mathbf{t}}\\ \hat{\mathbf{n}}\\ \hat{\mathbf{b}}\end{bmatrix}, \tag{A3}$$

where $\kappa(\alpha)$ and $\tau(\alpha)$ are called the curvature and torsion, respectively. The curvature and torsion have units of reciprocal length. The reciprocal of κ is the radius of curvature $\rho=\kappa^{-1}$.

APPENDIX B: THE SECOND FUNDAMENTAL FORM

The extrinsic curvature of a submanifold $\mathcal{C}$ embedded in a manifold $\mathcal{A}$ is conveniently specified by a rank-three tensor T called the second fundamental form. Since the second fundamental form is of critical importance in the body of this paper, we briefly review a few of its relevant properties. For greater detail, see Refs. [29,30].

Throughout this appendix, **d**, **e**, **f** denote arbitrary vector fields tangent to $\mathcal{A}$ and defined over $\mathcal{C}$; **w**, **x**, **y**, **z** denote vector fields tangent to $\mathcal{C}$; and **v** denotes a vector field normal to $\mathcal{C}$. The second fundamental form applied to **e** and **f**, denoted $T_{\mathbf{e}}\mathbf{f}$, is a vector field defined by

$$T_{\mathbf{e}}\mathbf{f}=P_{\perp}\nabla_{P_{\parallel}\mathbf{e}}P_{\parallel}\mathbf{f}+P_{\parallel}\nabla_{P_{\parallel}\mathbf{e}}P_{\perp}\mathbf{f}, \tag{B1}$$

where ∇ is the Levi-Civita connection on $\mathcal{A}$ and $P_{\parallel}$ and $P_{\perp}$ are, respectively, the tangent and normal projection operators of $\mathcal{C}$.[3] It is straightforward to verify that T is in fact a tensor. Furthermore, the second fundamental form satisfies the identities

$$\langle \mathbf{d}, T_{\mathbf{e}}\mathbf{f}\rangle = -\langle \mathbf{f}, T_{\mathbf{e}}\mathbf{d}\rangle, \tag{B2}$$

$$T_{\mathbf{x}}\mathbf{y}=T_{\mathbf{y}}\mathbf{x}, \tag{B3}$$

where $\langle,\rangle$ denotes the Riemannian metric on $\mathcal{A}$. In terms of the components $T_{abc}=\langle \mathbf{E}_a, T_{\mathbf{E}_c}\mathbf{E}_b\rangle$ introduced in Sec. III C, we have

$$T_{abc}=-T_{bac}, \tag{B4}$$

$$T_{aij}=T_{aji}, \tag{B5}$$

$$T_{ab\mu}=0, \tag{B6}$$

$$T_{\mu\nu a}=T_{ija}=0, \tag{B7}$$

where the first two equations are simply component forms for Eqs. (B2) and (B3) and the last two follow easily from Eq. (B1).

In Secs. D I and III D, we need the Gauss equation, a well-known identity relating the second fundamental form T, the Riemannian curvature $\hat{R}$ of $\mathcal{C}$, and the Riemannian curvature R of $\mathcal{A}$. The Riemannian curvatures are defined by

$$R_{\mathbf{de}}\mathbf{f}=(\nabla_{\mathbf{d}}\nabla_{\mathbf{e}}-\nabla_{\mathbf{e}}\nabla_{\mathbf{d}}-\nabla_{[\mathbf{d},\mathbf{e}]})\mathbf{f}, \tag{B8}$$

$$\hat{R}_{\mathbf{xy}}\mathbf{z}=(\hat{\nabla}_{\mathbf{x}}\hat{\nabla}_{\mathbf{y}}-\hat{\nabla}_{\mathbf{y}}\hat{\nabla}_{\mathbf{x}}-\hat{\nabla}_{[\mathbf{x},\mathbf{y}]})\mathbf{z}, \tag{B9}$$

where $\hat{\nabla}$ denotes the Levi-Civita connection on $\mathcal{C}$. The Gauss equation is then [29]

$$\langle \mathbf{w}, R_{\mathbf{xy}}\mathbf{z}\rangle = \langle \mathbf{w}, \hat{R}_{\mathbf{xy}}\mathbf{z}\rangle + \langle T_{\mathbf{x}}\mathbf{z}, T_{\mathbf{y}}\mathbf{w}\rangle - \langle T_{\mathbf{y}}\mathbf{z}, T_{\mathbf{x}}\mathbf{w}\rangle. \tag{B10}$$

[3]Our definition of the second fundamental form differs in the choice of domain and range from that in Ref. [29]. We follow the definition of Ref. [30].

APPENDIX C: THE QUANTUM KINETIC ENERGY WITH RESPECT TO A VIELBEIN

We present two expressions for the kinetic energy of a quantum system on a Riemannian manifold of dimension n. These expressions differ in the scaling of the quantum wave function. We refer the reader to earlier related analyses [31–33] for derivations and discussion.

We express the kinetic energy in terms of a vielbein. By a vielbein on a Riemannian manifold, we mean a set of vector fields $\mathbf{E}_a$, $a=1,\ldots,n$, forming a basis of each tangent space. The structure constants β^c_{ab} of the vielbein are defined by

$$[\mathbf{E}_a,\mathbf{E}_b]=\beta^c_{ab}\mathbf{E}_c, \tag{C1}$$

where $[,]$ denotes the Lie bracket. The structure constants vanish if and only if the vielbein is a coordinate basis, that is if and only if there exists a set of coordinates x^a such that $\mathbf{E}_a=\partial/\partial x^a$. We denote the components of the Riemannian metric with respect to the vielbein by G_{ab} and the inverse of G_{ab} by G^{ab}.

We define the kinetic energy of the quantum system by $K=-\hbar^2\triangle/2$, where $\triangle$ is the Laplacian. In terms of the vielbein, the kinetic energy is [31],

$$K=\frac{\hbar^2}{2}\mathbf{E}_a^{\dagger}G^{ab}\mathbf{E}_b=\frac{1}{2}\pi_a^{\dagger}G^{ab}\pi_b, \tag{C2}$$

where

$$\pi_a=-i\hbar\mathbf{E}_a, \tag{C3}$$

are the momentum operators. In the above † denotes the Hermitian conjugate. In general, the momenta π_a are not Hermitian. They do, however, satisfy the following useful identity

$$\pi_a^{\dagger}=\pi_a+[\pi_a\ln\sqrt{G}]+i\hbar\beta^b_{ab}, \tag{C4}$$

where $G=\det G_{ab}$. The bracket notation in Eq. (C4) indicates that the quantity inside the brackets is a scalar; that is, π_a acts only on $\ln\sqrt{G}$.

Often it is useful to scale the original wave function φ by some real positive function s to form a new wave function ψ,

$$\psi=s\varphi. \tag{C5}$$

Such a scaling produces a new kinetic energy operator acting on the new wave function ψ. By conveniently choosing the scale factor s, the new kinetic energy may acquire a more convenient form than the old kinetic energy. To demonstrate how the kinetic energy transforms, we first observe that the scaled wave functions have a different inner product than the unscaled wave functions. Denoting the unscaled inner product by $\langle|\rangle$, the scaled inner product $\langle|\rangle_s$ is defined by

$$\langle\psi|\psi'\rangle_s=\left\langle\frac{1}{s}\psi\middle|\frac{1}{s}\psi'\right\rangle, \tag{C6}$$

for arbitrary wave functions ψ and ψ'. This scaled inner product in turn defines a scaled Hermitian conjugate $A^{\dagger(s)}$ of an operator A. Specifically,

$$A^{\dagger(s)} = s^2 A^\dagger \frac{1}{s^2}. \tag{C7}$$

Applying Eq. (C7) to Eq. (C4), we find

$$\pi_a^{\dagger(s)} = \pi_a^\dagger - 2[\pi_a \ln s]. \tag{C8}$$

The scaling of the wave function transforms the kinetic energy operator K into $K_s = sK(1/s)$. It can be shown [31] that K_s reduces to

$$K_s = \frac{1}{2}\pi_a^{\dagger(s)} G^{ab} \pi_b + V_s, \tag{C9}$$

where

$$\begin{aligned} V_s &= -\tfrac{1}{2}(G^{ab}[\pi_a \ln s][\pi_b \ln s] + [\pi_a^{\dagger(s)} G^{ab}[\pi_b \ln s]]) \\ &= \tfrac{1}{2}(G^{ab}[\pi_a \ln s][\pi_b \ln s] - [\pi_a^\dagger G^{ab}[\pi_b \ln s]]). \end{aligned} \tag{C10}$$

APPENDIX D: MATHEMATICAL DETAILS

1. Proof of identities (3.25)–(3.27)

To prove Eq. (3.25), we first note

$$\begin{aligned} G_{\mu j,\sigma}|_0 &= (\nabla_{\mathbf{E}_\sigma} G_{\mu j})|_0 \\ &= (\nabla_{\mathbf{E}_\sigma} \langle \mathbf{E}_\mu, \mathbf{E}_j \rangle)|_0 \\ &= \langle \nabla_{\mathbf{E}_\sigma} \mathbf{E}_\mu, \mathbf{E}_j \rangle|_0 + \langle \mathbf{E}_\mu, \nabla_{\mathbf{E}_\sigma} \mathbf{E}_j \rangle|_0, \end{aligned} \tag{D1}$$

where in the first equality, we replaced the coordinate derivative by the covariant derivative, treating $G_{\mu j}$ as a scalar function. The second equality is the definition of $G_{\mu j}$, and the third equality follows from the Leibniz rule and the vanishing of the metric tensor under covariant differentiation. We next define the vector

$$\mathbf{M}_{\sigma\mu} = \nabla_{\mathbf{E}_\sigma} \mathbf{E}_\mu, \tag{D2}$$

which we now demonstrate vanishes on $\mathcal{C}$. To prove this, we first show that it is everywhere symmetric in μ and σ by using the general formula

$$\nabla_{\mathbf{d}} \mathbf{e} - \nabla_{\mathbf{e}} \mathbf{d} = [\mathbf{d}, \mathbf{e}], \tag{D3}$$

where $\mathbf{d}$ and $\mathbf{e}$ are arbitrary vector fields on $\mathcal{A}$. By substituting $\mathbf{d} = \mathbf{E}_\sigma$ and $\mathbf{e} = \mathbf{E}_\mu$ and recalling that $[\mathbf{E}_\mu, \mathbf{E}_\sigma] = 0$, we find that $\mathbf{M}_{\sigma\mu} = \mathbf{M}_{\mu\sigma}$. Since $\mathbf{M}_{\sigma\mu}$ is symmetric, it vanishes if and only if $v^\sigma v^\mu \mathbf{M}_{\sigma\mu} = 0$ for an arbitrary list of (constant) real numbers v^σ. For such an arbitrary list, we define the vector field $\mathbf{v} = v^\sigma \mathbf{E}_\sigma$ over $\mathcal{A}$. Since $\partial v^\mu / \partial u^\sigma = 0$, we see from Eq. (D2) that $v^\sigma v^\mu \mathbf{M}_{\sigma\mu} = \nabla_{\mathbf{v}} \mathbf{v}$. Since the quantities u^μ are defined via geodesic flow away from $\mathcal{C}$, an integral curve of $\mathbf{v}$ which passes through $\mathcal{C}$ is itself a geodesic. By the geodesic equation, $(\nabla_{\mathbf{v}} \mathbf{v})|_0 = 0$. Thus, $v^\sigma v^\mu \mathbf{M}_{\sigma\mu}|_0 = 0$ and hence

$$(\nabla_{\mathbf{E}_\sigma} \mathbf{E}_\mu)|_0 = 0. \tag{D4}$$

We return to Eq. (D1) and write

$$G_{\mu j,\sigma}|_0 = \langle \mathbf{E}_\mu, \nabla_{\mathbf{E}_\sigma} \mathbf{E}_j \rangle|_0 = \langle \mathbf{E}_\mu, \nabla_{\mathbf{E}_j} \mathbf{E}_\sigma \rangle|_0 = S_{\mu\sigma j}|_0, \tag{D5}$$

where the first equality follows from Eq. (D4), the second from Eqs. (D3) and (3.1), and the third from Eqs. (3.22) and (2.2). This completes the derivation of Eq. (3.25).

To prove Eqs. (3.26) and (3.27), we fix a point q on the constraint manifold and restrict our attention to a single transverse space $\mathcal{U}_q$ which we temporarily forget is embedded in $\mathcal{A}$. Recall that the vectors $\mathbf{E}_\mu$ are tangent to $\mathcal{U}_q$ and $G_{\mu\nu} = \langle \mathbf{E}_\mu, \mathbf{E}_\nu \rangle$ is the metric tensor on $\mathcal{U}_q$. Furthermore, the coordinates u^μ are Riemannian normal coordinates on $\mathcal{U}_q$, and it is well known that the expansion of the metric to second order in the Riemannian normal coordinates is [22]

$$G_{\mu\nu}(\mathsf{u}) = \delta_{\mu\nu} - \tfrac{1}{3}\overline{R}_{\mu\sigma\nu\tau}|_0 u^\sigma u^\tau + \cdots, \tag{D6}$$

where $\overline{R}$ is the Riemannian curvature of the transverse space $\mathcal{U}_q$. The vanishing in Eq. (D6) of the term linear in u proves Eq. (3.26).

The quadratic term in Eq. (D6) yields

$$G_{\mu\nu,\sigma\tau}|_0 = -\tfrac{1}{3}(\overline{R}_{\mu\sigma\nu\tau} + \overline{R}_{\nu\sigma\mu\tau})|_0. \tag{D7}$$

To complete the proof of Eq. (3.27), we must prove that the components $\overline{R}_{\mu\sigma\nu\tau}|_0$ of the Riemannian curvature on $\mathcal{U}_q$ agree with the components $R_{\mu\sigma\nu\tau}|_0$ of the Riemannian curvature on $\mathcal{A}$. To prove this, we use the Gauss relation given by Eq. (B10) and which we reexpress here in component form

$$R_{\mu\sigma\nu\tau} = \overline{R}_{\mu\sigma\nu\tau} + \overline{T}^a{}_{\sigma\nu}\overline{T}_{a\mu\tau} - \overline{T}^a{}_{\sigma\tau}\overline{T}_{a\mu\nu}. \tag{D8}$$

Since we are applying the Gauss equation to the submanifold $\mathcal{U}_q$ instead of $\mathcal{C}$, we place an overbar on the symbols for the second fundamental form and the Riemannian curvature. Here, $\overline{T}$ is the second fundamental form of $\mathcal{U}_q$. Recall that $P_\parallel$ and $P_\perp$ were defined to be, respectively, the tangent and normal projection operators onto $\mathcal{C}$. We extend the definition of these operators for u^μ not equal to 0 by defining $P_\parallel$ and $P_\perp$ to be the normal and tangent projection operators, respectively, onto $\mathcal{U}_q$. With this definition, the second fundamental form $\overline{T}$ is given by [see Eq. (B1)]

$$\overline{T}_{\mathbf{e}}\mathbf{f} = P_\parallel \nabla_{P_\perp \mathbf{e}} P_\perp \mathbf{f} + P_\perp \nabla_{P_\perp \mathbf{e}} P_\parallel \mathbf{f}, \tag{D9}$$

where $\mathbf{e}$ and $\mathbf{f}$ are arbitrary vector fields over $\mathcal{U}_q$ which are tangent to $\mathcal{A}$. Since $\mathbf{E}_\mu$ is tangent to $\mathcal{U}_q$ everywhere, we have

$$\overline{T}_{\sigma\mu\nu} = \langle \mathbf{E}_\sigma, \overline{T}_{\mathbf{E}_\nu} \mathbf{E}_\mu \rangle = 0. \tag{D10}$$

Furthermore, since $\mathbf{E}_i$ is normal to $\mathcal{U}_q$ at $u^\mu = 0$, we have

$$\overline{T}_{i\mu\nu}|_0 = \langle \mathbf{E}_i, \overline{T}_{\mathbf{E}_\nu} \mathbf{E}_\mu \rangle|_0 = \langle \mathbf{E}_i, \nabla_{\mathbf{E}_\nu} \mathbf{E}_\mu \rangle|_0 = 0, \tag{D11}$$

where the last equality follows from Eq. (D4). Combining Eqs. (D10) and (D11) yields $\overline{T^a}_{\mu\nu}|_0=\overline{T}_{a\mu\nu}|_0=0$ from which follows, using Eq. (D8), $\overline{R}_{\mu\sigma\nu\tau}|_0=R_{\mu\sigma\nu\tau}|_0$. This concludes the proof of Eq. (3.27).

2. Proof of identity (3.37)

Considering the first term of Eq. (3.16), we observe that since $G_{ab}|_0=\delta_{ab}$,

$$[\pi_i \ln G]|_0=0, \tag{D12}$$

$$\begin{aligned}[\pi_\mu \ln G]|_0&=-i\hbar(G^{ab}G_{ba,\mu})|_0\\&=-i\hbar G_{aa,\mu}|_0\\&=-i\hbar G_{jj,\mu}|_0,\end{aligned} \tag{D13}$$

where we have used Eq. (3.26) in the last step of Eq. (D13). Equations (D12) and (D13) yield

$$\frac{1}{4}(G^{ab}[\pi_a \ln G][\pi_b \ln G])|_0=-\frac{\hbar^2}{4}(G_{ii,\mu}G_{jj,\mu})|_0. \tag{D14}$$

Considering the second term of Eq. (3.16), we note

$$\begin{aligned}[\pi_a^\dagger G^{ab}[\pi_b \ln G]]|_0=&([\pi_a^\dagger, G^{ab}][\pi_b \ln G]\\&+G^{ab}[\pi_a^\dagger[\pi_b \ln G]])|_0.\end{aligned} \tag{D15}$$

The first term of Eq. (D15) vanishes from Eqs. (3.11), (3.12), (3.29), (3.30), and (D12). The second term evaluates to

$$\begin{aligned}&(G^{ab}[\pi_a^\dagger[\pi_b \ln G]])|_0\\&\quad=[\pi_\mu[\pi_\mu \ln G]]|_0\\&\quad=\hbar^2(G_{ab,\mu}G_{ab,\mu}-G_{aa,\mu\mu})|_0\\&\quad=\hbar^2\left(2S_{\mu\nu i}S_{\mu\nu i}+G_{ij,\mu}G_{ij,\mu}+\frac{2}{3}R_{\mu\nu\mu\nu}-G_{ii,\mu\mu}\right)\Bigg|_0,\end{aligned} \tag{D16}$$

where the first equality follows from Eqs. (3.11), (3.12), (3.17), and (D12), the second equality is a straightforward computation, and the third equality results from Eqs. (3.25)–(3.27). Collecting the preceding results, we find

$$\begin{aligned}V_{ex}^p=-\frac{\hbar^2}{8}\Bigg(&-\frac{1}{4}G_{ii,\mu}G_{jj,\mu}+G_{ij,\mu}G_{ij,\mu}-G_{ii,\mu\mu}\\&+2S_{\mu\nu i}S_{\mu\nu i}+\frac{2}{3}R_{\mu\nu\mu\nu}\Bigg)\Bigg|_0.\end{aligned} \tag{D17}$$

The various derivatives of G_{ij} appearing in the above may be reexpressed using the following identities, to be derived momentarily,

$$G_{ij,\mu}|_0=2T_{i\mu j}|_0, \tag{D18}$$

$$\begin{aligned}G_{ij,\mu\nu}|_0=&(T_{a\mu i}T_{a\nu j}+T_{a\mu j}T_{a\nu i}+S_{a\mu i}S_{a\nu j}\\&+S_{a\mu j}S_{a\nu i}-R_{i\mu j\nu}-R_{j\mu i\nu})|_0.\end{aligned} \tag{D19}$$

Upon inserting Eqs. (D18) and (D19) into Eq. (D17) one obtains Eq. (3.37).

Returning to Eq. (D18), it is derived via

$$\begin{aligned}G_{ij,\mu}|_0&=(\nabla_{\mathbf{E}_\mu}\langle\mathbf{E}_i,\mathbf{E}_j\rangle)|_0\\&=\langle\nabla_{\mathbf{E}_i}\mathbf{E}_\mu,\mathbf{E}_j\rangle|_0+\langle\mathbf{E}_i,\nabla_{\mathbf{E}_j}\mathbf{E}_\mu\rangle|_0\\&=2T_{i\mu j}|_0,\end{aligned} \tag{D20}$$

where in the second equality we used the Leibniz rule and interchanged the derivatives by virtue of Eqs. (D3) and (3.1). The final equality follows from the definition of the second fundamental form Eq. (B1) and Eqs. (B2) and (B3).

Considering Eq. (D19), we have

$$\begin{aligned}G_{ij,\mu\nu}|_0=&(\nabla_{\mathbf{E}_\nu}\nabla_{\mathbf{E}_\mu}\langle\mathbf{E}_i,\mathbf{E}_j\rangle)|_0\\&=\langle\nabla_{\mathbf{E}_i}\mathbf{E}_\mu,\nabla_{\mathbf{E}_j}\mathbf{E}_\nu\rangle|_0+\langle\nabla_{\mathbf{E}_i}\mathbf{E}_\nu,\nabla_{\mathbf{E}_j}\mathbf{E}_\mu\rangle|_0\\&\quad+\langle\nabla_{\mathbf{E}_\nu}\nabla_{\mathbf{E}_i}\mathbf{E}_\mu,\mathbf{E}_j\rangle|_0+\langle\mathbf{E}_i,\nabla_{\mathbf{E}_\nu}\nabla_{\mathbf{E}_j}\mathbf{E}_\mu\rangle|_0.\end{aligned} \tag{D21}$$

In the second equality, we again applied the Leibniz rule and interchanged derivatives by virtue of Eqs. (D3) and (3.1). We next note that the covariant derivative of $\mathbf{E}_\mu$ by $\mathbf{E}_i$ is given by

$$(\nabla_{\mathbf{E}_i}\mathbf{E}_\mu)|_0=(P_\parallel\nabla_{\mathbf{E}_i}\mathbf{E}_\mu+P_\perp\nabla_{\mathbf{E}_i}\mathbf{E}_\mu)|_0=(T_{\mathbf{E}_i}\mathbf{E}_\mu+S_{\mathbf{E}_i}\mathbf{E}_\mu)|_0, \tag{D22}$$

where the first equality follows from the fact that $P_\parallel+P_\perp$ is the identity and the second from the definitions Eqs. (B1) and (2.2) and the fact that $\mathbf{E}_\mu$ is normal to $\mathcal{C}$. We also observe from Eq. (D4) that $(\nabla_{\mathbf{E}_i}\nabla_{\mathbf{E}_\nu}\mathbf{E}_\mu)|_0=0$, and therefore

$$(\nabla_{\mathbf{E}_\nu}\nabla_{\mathbf{E}_i}\mathbf{E}_\mu)|_0=(R_{\mathbf{E}_\nu\mathbf{E}_i}\mathbf{E}_\mu)|_0, \tag{D23}$$

where we have used Eqs. (3.1) and (B8). Inserting Eqs. (D22) and (D23) into Eq. (D21) yields the desired result Eq. (D19).

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