Constrained quantum systems as an adiabatic problem

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(Received 12 May 2010; published 23 August 2010)

We derive the effective Hamiltonian for a quantum system constrained to a submanifold (the constraint manifold) of configuration space (the ambient space) in the asymptotic limit, where the restoring forces tend to infinity. In contrast to earlier works, we consider, at the same time, the effects of variations in the constraining potential and the effects of interior and exterior geometry, which appear at different energy scales and, thus, provide a complete picture, which ranges over all interesting energy scales. We show that the leading order contribution to the effective Hamiltonian is the adiabatic potential given by an eigenvalue of the confining potential well known in the context of adiabatic quantum waveguides. At next to leading order, we see effects from the variation of the normal eigenfunctions in the form of a Berry connection. We apply our results to quantum waveguides and provide an example for the occurrence of a topological phase due to the geometry of a quantum wave circuit (i.e., a closed quantum waveguide).

DOI: 10.1103/PhysRevA.82.022112 PACS number(s): 03.65.Ca, 02.40.Ky, 03.65.Vf, 73.63.−b

I. INTRODUCTION

The derivation of effective Hamiltonians for constrained quantum systems has been considered many times in the literature with different motivations and applications in mind [1–8]. Roughly speaking, the available results split into two different categories, which are related to two different energy scales. In the context of adiabatic quantum waveguides, one considers the situation, where the strong forces that restrict the particle to the waveguide change their form along the direction of propagation [1–4]. The eigenvalues of the transverse Hamiltonian, thus, also vary along this direction and produce an effective adiabatic potential for the tangential dynamics (i.e., for the propagation). In this case, the tangential kinetic energy is of the same order of magnitude as the energy in the transversal modes. The geometry of the waveguide plays no role at this level. On the other hand, in the literature concerned primarily with the effects of the geometry of constraint manifolds on the effective Hamiltonian [5–8], it is assumed that the constraining forces are constant along the constraint manifold. This is because the geometric effects are much smaller and would be dominated by the adiabatic potential otherwise. It is, thus, assumed that the tangential kinetic energy is of the same small magnitude as the geometric effects and, thus, much smaller than the transversal energies.

In this paper, we show how these two regimes are related and derive an effective Hamiltonian valid on all interesting energy scales. It contains contributions from the adiabatic potential, from a generalized Berry connection, and from the intrinsic and extrinsic geometry of the constraint manifold. The derivation is based on superadiabatic perturbation theory, and a mathematically rigorous treatment of the problem is given in Ref. [9]. We present our results first on a general and abstract level. However, there are several concrete applications, which have motivated us and the many preceding works, most notably molecular dynamics (see Ref. [10]) and adiabatic quantum waveguides (see Ref. [11]). In Sec. IV, we apply our results to adiabatic quantum waveguides and, in particular, obtain interesting results about global geometric effects in quantum wave circuits (i.e., closed waveguides).

A. Qualitative discussion of the results

Although the mathematical structure of the linear Schrödinger equation,

$$i\partial_t\Psi = -\Delta\Psi + V\Psi =: H\psi, \quad \Psi|_{t=0} \in L^2(\mathcal{A},d\tau), \tag{1}$$

is quite simple, in many cases, the high dimension of the underlying configuration space $\mathcal{A}$ makes even a numerical solution impossible. Therefore, it is important to identify situations, where the dimension can be reduced by approximating the solutions of the original equation Eq. (1) on the high-dimensional configuration space $\mathcal{A}$ by solutions of an *effective equation*,

$$i\partial_t\psi = H_{\text{eff}}\psi, \quad \psi|_{t=0} \in L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M, \tag{2}$$

on a lower-dimensional configuration space $\mathcal{C}$. The factor $\mathbb{C}^M$ allows for the possibility of additional internal degrees of freedom in the effective description.

A famous example for such a reduction is the time-dependent Born-Oppenheimer approximation: Due to the small ratio $\frac{m_{\text{el}}}{m_{\text{nu}}}$ of the mass m_{el} of an electron and the mass m_{nu} of a typical nucleus, the molecular Schrödinger equation,

$$\begin{aligned} i\partial_t\psi &= -\frac{1}{m_{\text{nu}}}\Delta_x\Psi - \frac{1}{m_{\text{el}}}\Delta_y\Psi + V\Psi, \\ \Psi|_{t=0} &\in L^2(\mathbb{R}^{3(n+m)},dx\,dy), \end{aligned} \tag{3}$$

on the full configuration space $\mathbb{R}^{3(n+m)} \hat{=} \mathcal{A}$ of electrons and nuclei, may be approximated by an equation,

$$i\partial_t\psi = -\frac{1}{m_{\text{nu}}}\Delta_x\psi + E_{\text{el}}\psi, \quad \psi|_{t=0} \in L^2(\mathbb{R}^{3n},dx),$$

on the lower-dimensional configuration space $\mathbb{R}^{3n} \hat{=} \mathcal{C}$ of the nuclei only. In this case, the interaction $V(x,y)$ of all particles is replaced by an electronic energy surface $E_{\text{el}}(x)$, which serves as an effective potential for the dynamics of the nuclei. The assumption here is that the electrons remain in an eigenstate of the electronic Hamiltonian $H_{\text{e}}(x) = -\frac{1}{m_{\text{el}}}\Delta_y + V(x,y)$, which corresponds to the eigenvalue $E_{\text{el}}(x)$. This assumption is

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typically satisfied, since the light electrons move fast compared to the heavy nuclei; and, thus, the electronic state adjusts adiabatically to the slow motion of the nuclei. This is an example of *adiabatic decoupling*, where the reduction in the size of the effective configuration space stems from different masses in the system.

A physically different but mathematically similar situation, where such a dimensional reduction is possible is constrained mechanical systems. In these systems, strong forces effectively constrain the system to remain in the vicinity of a submanifold $\mathcal{C}$ of the configuration space $\mathcal{A}$.

For classical Hamiltonian systems on a Riemannian manifold $(\mathcal{A},G)$, there is a straightforward mathematical reduction procedure. One just restricts the Hamilton function to $\mathcal{C}$'s cotangent bundle $T^*\mathcal{C}$ by embedding $T^*\mathcal{C}$ into $T^*\mathcal{A}$ via the metric G and then studies the induced dynamics on $T^*\mathcal{C}$. For quantum systems, Dirac [12] proposed to quantize the restricted classical Hamiltonian system on the submanifold by following an intrinsic quantization procedure. However, for curved submanifolds $\mathcal{C}$, there is no unique quantization procedure. One natural guess would be an effective Hamiltonian H_{eff} in Eq. (2) of the form

$$H_{\text{eff}} = -\Delta_{\mathcal{C}} + V|_{\mathcal{C}}, \tag{4}$$

where $\Delta_{\mathcal{C}}$ is the Laplace-Beltrami operator on $\mathcal{C}$ with respect to the induced metric and $V|_{\mathcal{C}}$ is the restriction of the potential $V : \mathcal{A} \to \mathbb{R}$ to $\mathcal{C}$.

To justify or to invalidate the earlier procedures from first principles, one needs to model the constraining forces within the dynamics Eq. (1) on the full space $\mathcal{A}$. This is done by adding a localizing part to the potential V. Then one analyzes the behavior of solutions of Eq. (1) in the asymptotic limit, where the constraining forces become very strong and try to extract a limiting equation on $\mathcal{C}$. This limit of strong confining forces has been studied in classical mechanics and in quantum mechanics many times in the literature.

The classical case was first investigated by Rubin and Ungar [13], who found that the effective Hamiltonian for the motion on the constrained manifold contains an extra potential that accounts for the energy contained in the normal oscillations. The quantum mechanical analog of this extra potential is the adiabatic potential. The intrinsic geometry of the submanifold only appears in the definition of the kinetic energy $\frac{1}{2}g(p,p)$; its embedding into the ambient space $\mathcal{A}$ plays no role.

On the other hand, for the quantum mechanical case, Marcus [14] and, later on, Jensen and Koppe [15] and Da Costa [16] pointed out that the limiting quantum Hamiltonian contains a potential term, the geometric potential, which depends on the embedding of the submanifold $\mathcal{C}$ into the ambient space $\mathcal{A}$. However, these statements (such as the more refined results by Froese-Herbst [6], Maraner [7], and Mitchell [8]) require that the constraining potential is the same at each point on the constraint manifold. The reason behind this assumption is that, in the limit of strong confinement, the adiabatic potential is much larger (by 2 orders in the adiabatic parameter) than the geometric potential. For the geometric potential to be of leading order, one must, thus, assume that the tangential kinetic energy is of the same small order. Then, one ends up in the situation, where the energy in the transversal modes is much larger than the typical tangential energies and where, by assumption, any transfer of energy between transversal and tangential modes is suppressed. In conclusion, the effective Hamiltonian obtained in this way describes the constrained system only for very small energies and under very restrictive assumptions on the confining potential. Note that, in many important applications, the assumption of a constant confining potential is violated. For example, for the reaction paths of molecular reactions, the valleys vary in shape depending on the configuration of the nuclei.

In this paper, we present a general result that concerns the precise form of the limiting dynamics Eq. (2) on an arbitrary constraint manifold $\mathcal{C}$ starting from Eq. (1) on the ambient space $\mathcal{A}$ with a strongly confining potential V. The most important new aspect of our result is that we allow for confining potentials that vary in shape and for solutions with normal and tangential energies of the same order and, at the same time, capture the effects of geometry. As a consequence, our effective Hamiltonian on the constraint manifold has a richer structure than earlier results and resembles, at leading order, the results from classical mechanics. However, similar to the hierarchic structure of the spectrum of molecules, with electronic, vibrational, and rotational levels, now, different geometric effects appear in the higher-order corrections to the effective Hamiltonian. We note that, in the limit of small tangential energies and under the same restrictive assumptions on the confining potential, we recover the limiting dynamics by Mitchell [8].

The key observation for our analysis is that the problem is an adiabatic limit and has, at least locally, a structure similar to the Born-Oppenheimer approximation in molecular dynamics. In particular, we transfer ideas from adiabatic perturbation theory, which were developed on a rigorous level by Martinez-Sordoni-Nenciu [17–19] and Panati-Spohn-Teufel in [20–22] and independently on a theoretical physics level by Belov *et al.* in Ref. [23], to a nonflat geometry. We note that the adiabatic nature of the problem was observed many times before in the physics literature (e.g., in the context of adiabatic quantum waveguides and thin films [1,2]). However, the only work considering constraint manifolds with general geometries in quantum mechanics from this point of view so far is Ref. [3], where only the leading order dynamics of localized semiclassical wave packets is analyzed and effects of geometry or geometric phases play no role. We, thus, believe that our effective equations have not been derived before, neither on a mathematical nor on a theoretical physics level.

B. The scaling explained in a simple example

Before we describe the general setup, it is instructive to first explain the scaling and the different energy scales within the simple example of a straight quantum waveguide in two dimensions. Let x be the coordinate in the direction of propagation, and let y be the transversal direction. By saying that the potential $V(x,y)$ is (at least partially) confining in the y direction just means, that the normal or transverse Hamiltonian $H_{\text{n}}(x) := -\Delta_y + V(x,y)$ has some eigenvalues $E_j(x)$ with localized eigenfunctions $\varphi_j(x,y)$, the constrained normal modes. For a sketch of such a potential, see Fig. 1(a). Now, we would like to implement the asymptotic limit of strong confinement in such a way, that the eigenfunctions of

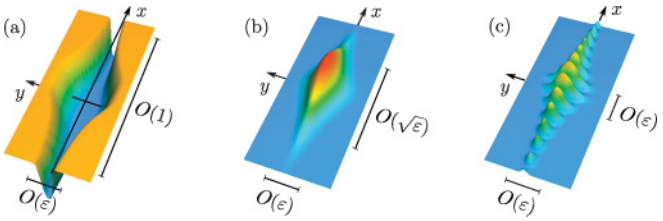

FIG. 1. (Color online) In (a), we plotted a potential for a waveguide, which widens near $x = 0$. The widening lowers the energy of normal modes and, thus, produces an attractive effective potential for the motion in the x direction. In (b), the modulus of the ground state wave function is sketched. Its variation in the x direction is slower than in the y direction, but its tangential derivatives already grow in ε. In (c), the modulus of an excited state with energy of order 1 above the ground state is sketched. Its variation in the x direction is on the same scale as the confinement (i.e., it oscillates on a scale of order ε). Thus, any analysis that assumes bounded tangential derivatives of the solutions will be restricted to confining potentials with a constant profile.

the scaled Hamiltonian $H_{\mathrm{n}}^{\varepsilon}(x)$ become localized on a length scale of order $\varepsilon \ll 1$. This is done by scaling the potential $V^{\varepsilon}(x,y) := V(x,y/\varepsilon)$, which yields restoring forces of order ε^{-1}. However, localization on a scale of order ε leads to kinetic energies of order ε^{-2}. So, in order to see localization, one has to increase not only the forces, but also the potential energies to the same level by putting

$$H_{\mathrm{n}}^{\varepsilon}(x) := -\Delta_y + \varepsilon^{-2} V(x,y/\varepsilon).$$

Then, the normal energies and eigenfunctions are just $E_j^{\varepsilon}(x) = \varepsilon^{-2} E_j(x)$, and $\varphi_j^{\varepsilon}(x,y) = \varepsilon^{-1/2}\varphi_j(x,y/\varepsilon)$. The full Hamiltonian becomes

$$\tilde{H}^{\varepsilon} = -\Delta_x - \Delta_y + \varepsilon^{-2} V(x,y/\varepsilon).$$

In order to understand the asymptotic limit $\varepsilon \to 0$, it is more convenient to rescale units of energy in such a way that the transverse energies are of order 1 again, that is, to look at

$$H^{\varepsilon} := \varepsilon^2 \tilde{H}^{\varepsilon} = -\varepsilon^2 \Delta_x - \varepsilon^2 \Delta_y + V(x,y/\varepsilon). \tag{5}$$

A change in units of length in the transverse direction to $\tilde{y} = y/\varepsilon$ finally leads to the form of the Hamiltonian,

$$H_{\varepsilon} := \varepsilon^2 \tilde{H}^{\varepsilon} = -\varepsilon^2 \Delta_x - \Delta_{\tilde{y}} + V(x,\tilde{y}), \tag{6}$$

for which the normal eigenfunctions φ_j are independent of ε and the physical meaning of the asymptotic $\varepsilon \to 0$ is most apparent. The limit of strong confinement really corresponds to the situation where the transversal modes are quantized with gaps of order 1, while in the tangential direction, the behavior is semiclassical and, in particular, the level spacing is of order ε. Here, it is easy to guess the leading order effective Hamiltonian for the constrained system: On the subspace of wave functions of the form $\Psi^{\varepsilon}(x,\tilde{y}) = \varphi_j(x,\tilde{y})\psi^{\varepsilon}(x)$, the Hamiltonian acts as

$$\begin{aligned} H_{\varepsilon}\Psi^{\varepsilon}(x,\tilde{y}) &= [-\varepsilon^2\Delta_x - \Delta_{\tilde{y}} + V(x,\tilde{y})]\varphi_j(x,\tilde{y})\psi^{\varepsilon}(x) \\ &= \varphi_j(x,\tilde{y})\{[-\varepsilon^2\Delta_x + E_j(x)]\psi^{\varepsilon}(x)\} \\ &\quad - 2[\varepsilon\nabla_x\varphi_j(x,\tilde{y})][\varepsilon\nabla_x\psi^{\varepsilon}(x)] \\ &\quad - \varepsilon^2\Delta_x\varphi_j(x,\tilde{y})\psi^{\varepsilon}(x). \end{aligned} \tag{7}$$

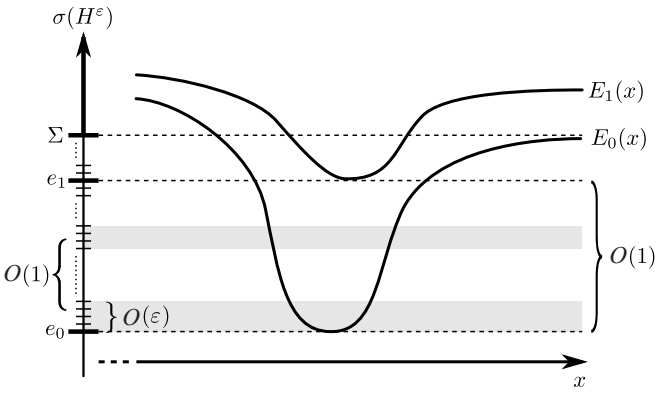

FIG. 2. The curves $E_0(x)$ and $E_1(x)$ are sketches of the lowest normal eigenvalues for a waveguide potential as depicted in Fig. 1(a). On the vertical axis, the spectrum of H^{ε} is drawn: One expects spectral bands, which start at the minima e_0 and e_1 of the effective potentials with level spacing of order ε^2. The continuum edge Σ is determined by the threshold of E_0. Eigenstates in the lower shaded region vary on a $\sqrt{\varepsilon}$ scale in the x direction as indicated in Fig. 1(b). Eigenstates in the upper shaded region with energies of order 1 above e_0 have ε oscillations in the x direction as indicated in Fig. 1(c).

By defining the effective Hamiltonian by projecting back onto this subspace via $(P\psi)(x,\tilde{y}) := \varphi_j(x,\tilde{y})\langle\varphi_j|\psi\rangle(x)$ and by integrating out $\tilde{y}$, one finds

$$\begin{aligned} H_{\mathrm{eff}}^{\varepsilon} &= [-i\varepsilon\nabla_x - i\varepsilon\langle\varphi_j(x)|\nabla_x\varphi_j(x)\rangle]^2 + E_j(x) \\ &\quad + \varepsilon^2[\langle\nabla_x\varphi_j(x)|\nabla_x\varphi_j(x)\rangle - |\langle\varphi_j(x)|\nabla_x\varphi_j(x)\rangle|^2]. \end{aligned} \tag{8}$$

Here, we see how the transversal eigenvalue $E_j(x)$ enters as an effective potential, the adiabatic potential, at leading order. For example, the constraining potential sketched in Fig. 1(a) leads to an attractive effective potential sketched in Fig. 2. The two energy scales referred to in Sec. I A now correspond to the following situations: If one assumes small tangential energies [i.e., $\langle\psi^{\varepsilon}| - \varepsilon^2\Delta_x\psi^{\varepsilon}\rangle = O(\varepsilon^2)$], then all terms in Eq. (8) except the term that involves the adiabatic potential $E_j(x)$ are of order ε^2. Thus, the latter must either be constant, or the kinetic energies will also become $O(1)$ under the time evolution. Since it turns out that the geometric potential in the case of nonstraight waveguides is also of order ε^2, this explains why all authors interested in geometric effects up to now assumed $E_j(x) \equiv$ const.

However, the natural scaling is to allow for tangential states ψ^{ε} with kinetic energies of order 1 [i.e., $\langle\psi^{\varepsilon}| - \varepsilon^2\Delta_x\psi^{\varepsilon}\rangle = O(1)$]. Then, all energies in the system are of the same order, and exchange of normal and tangential energies may occur. In particular, the tangential momentum operator $-i\varepsilon\nabla_x$ must be treated as being of order 1 despite the factor ε. This is the situation we will consider in the following.

In Figs. 1 and 2, we sketch the situation for a simple waveguide in a region, where it widens slightly. Wave functions with tangential energies of order ε such as in Fig. 1(b) yield the low-lying part of the spectrum. General states with finite energy above the ground state, which include all states propagating through the waveguide, have tangential energies of order 1 and, thus, ε oscillations in the x direction, as indicated in Fig. 1(c). When the confining potential depends

on x, there are, in general, no solutions with tangential kinetic energies of order ε^2. We also mention an extensive discussion of energy scales from a slightly different point of view in Ref. [1].

Before we explain the general model, it is instructive to mention two important points on the level of this simple model. First of all, one might want to add an external potential $W(x,y)$, which does not contribute to the confinement and, thus, is not scaled. We will allow for such an external potential with $W(x,y) = O(1)$. Note that, in the previous works that focus on geometry [6,8], it was added on the small energy scale [i.e., $W(x,y) = O(\varepsilon^2)$]. The second remark is that the different energy scales correspond also to different time scales. The time scale on which solutions with $\langle\psi^\varepsilon| - \varepsilon^2\Delta_x\psi^\varepsilon\rangle = O(1)$ propagate distances of order 1 are times of order ε^{-1}. This is because kinetic energies of order 1 for particles with mass of order ε^{-2} yield velocities of order ε. The small energy solutions with $\langle\psi^\varepsilon| - \varepsilon^2\Delta_x\psi^\varepsilon\rangle = O(\varepsilon^2)$ propagate even slower, so, here, the natural time scales are times of order ε^{-2}. The best results we can prove hold for even longer times, namely, for times almost up to order ε^{-3}. To control the adiabatic decoupling for such long times, makes the problem highly nontrivial. Roughly speaking, for times of order 1, the problem is just standard time-dependent perturbation theory. For times of order ε^{-1}, one can use the ideas that underlie the standard proof of the adiabatic theorem of quantum mechanics, see Sec. III A. For longer times, however, one has to use superadiabatic (i.e., higher-order adiabatic perturbation theory) see Sec. III C.

II. THE ADIABATIC STRUCTURE

Here, we first discuss, in detail, the model we consider and the assumptions involved. In Sec. II B, we introduce a horizontal momentum operator, the geometric generalization of $-i\varepsilon\nabla_x$ in Sec. I, which will play a crucial role in our results. Then, we reveal the formal similarity with the Born-Oppenheimer approximation, before we explain the resulting adiabatic structure of the problem in Sec. II D.

The reader interested primarily in quantum waveguides may skip the following abstract discussion of the problem and immediately jump to Sec. IV.

A. Description of the model

Let $(\mathcal{A},G)$ be a Riemannian manifold of dimension $d+k$, and let $\mathcal{C}\subset\mathcal{A}$ be a smooth submanifold of dimension d without boundary and equipped with the induced metric $g = G|_{\mathcal{C}}$. We will call $\mathcal{A}$ the ambient manifold, and we will call $\mathcal{C}$ the constraint manifold. We consider the Schrödinger equation on $\mathcal{A}$ with a potential $V_c^\varepsilon : \mathcal{A}\to\mathbb{R}$ that localizes all states from a certain subspace of $L^2(\mathcal{A})$ close to $\mathcal{C}$ for small ε, which will be made precise as follows. By having in mind, for example, a quantum waveguide $\mathcal{C}$ embedded into $\mathcal{A} = \mathbb{R}^3$, we want to start with fixed manifolds $\mathcal{A}$ and $\mathcal{C}$ and to assume that the constraining potential V_c^ε grows fast in the directions normal to $\mathcal{C}$ (strong restoring forces), while the variation along $\mathcal{C}$ is of order 1 (bounded tangential forces). This means we want to assume that

(1) *normal derivatives of* V_c^ε are of order ε^{-1},
(2) *tangential derivatives of* V_c^ε are of order 1,
(3) *all derivatives of the metric* G are of order 1.

As explained in Sec. I B, localization in the normal direction on a scale of order ε produces oscillations of order ε^{-1} in the tangential directions, too.

When we introduce local coordinates $x = (x_i)_{i=1,\dots,d}$ in a neighborhood of $q\in\mathcal{C}$ and coordinates $N = (N_\alpha)_{\alpha=1,\dots,k}$ for the normal directions, the assumptions made previously correspond, by the same reasoning that leads to Eq. (5) in Sec. I B, to the Schrödinger equation,

$$i\partial_t\Psi^\varepsilon = -\varepsilon^2\Delta_G\Psi^\varepsilon + V_c(x,N/\varepsilon)\Psi^\varepsilon + W(y,N)\Psi^\varepsilon, \quad (9)$$

where Δ_G is the Laplace-Beltrami operator associated with $(\mathcal{A},G)$ and the nonconstraining potential W may describe external forces. Here, the upper index ε at Ψ means that we look at solutions with oscillations of order ε^{-1}, and the ε^2 in front of the kinetic energy ensures that these solutions have kinetic energies of order 1. For small ε, at least some solutions of this equation concentrate close to the submanifold $\mathcal{C}$. Therefore, one expects that an effective Schrödinger equation on $\mathcal{C}$ may be derived such that solutions $\psi_\varepsilon(t)$ of the effective equation approximate the solutions $\Psi^\varepsilon(t)$ of the full equation in a suitable way.

The scaling of the potential described in Eq. (9) depends on the choice of coordinates and cannot be implemented globally so naively. It just serves as a motivation for the following. In order to be able to implement a similar scaling globally, we assume that the submanifold $\mathcal{C}$ has a tubular neighborhood $\mathcal{B}$ of fixed diameter $\delta > 0$. Within $\mathcal{B}$, it makes sense to speak of large derivatives of V^ε with respect to the distance to $\mathcal{C}$. More precisely, $\mathcal{B}$ can now be mapped to the δ neighborhood $\mathcal{B}_\delta$ of the zero section in the normal bundle $N\mathcal{C}$. On $N\mathcal{C}$, the scaling of the potential as in Eq. (9) can be realized due to its linear structure. Moreover, for ε much smaller than δ, all solutions below an arbitrary finite energy lie in $\mathcal{B}_{\delta/2}$ up to errors bounded by any power of ε. Therefore, it is possible to work completely on the normal bundle by constructing a diffeomorphism $\Phi : N\mathcal{C}\to\mathcal{B}$ and by choosing a metric $\overline{g}$ on $N\mathcal{C}$ such that Φ is an isometry on $\mathcal{B}_{\delta/2}$.

To avoid all regularity problems, we make the following assumption.

Assumption 1. The injectivity radii of $\mathcal{A}$ and $\mathcal{C}$ are strictly positive, and all curvatures as well as their derivatives of arbitrary order are globally bounded. Furthermore, $V : N\mathcal{C}\to\mathbb{R}$ is smooth and bounded, and arbitrary derivatives of V are also globally bounded.

In particular, this implies that C and $N\mathcal{C}$ may be covered by coordinate neighborhoods such that, for some $K\in\mathbb{N}$, not more than K of them overlap at each point. This allows us to perform all estimates in local coordinates.

Now, our goal is to find approximate solutions of the Schrödinger equation,

$$i\partial_t\Psi^\varepsilon = -\varepsilon^2\Delta_{\overline{g}}\Psi^\varepsilon + V_c(q,N/\varepsilon)\Psi^\varepsilon + W(y,N)\Psi^\varepsilon,$$

on $\mathcal{H} = L^2(N\mathcal{C},d\overline{\mu})$, where $\overline{g}$ is the pullback of G via the diffeomorphism Φ on $\mathcal{B}_{\delta/2}$, suitably extended outside, and $d\overline{\mu}$

denotes the measure associated with $\overline{g}$. As explained in Sec. I, it is helpful to rescale the normal coordinates to $n = N/\varepsilon$. Then, the equation reads

$$i\partial_t \Psi^\varepsilon = -\varepsilon^2 (\Delta_{\overline{g}})^\varepsilon \Psi^\varepsilon + V_c(q,n)\Psi^\varepsilon + W(y,\varepsilon n)\Psi^\varepsilon =: H_\varepsilon \Psi^\varepsilon,$$

where $(\Delta_{\overline{g}})^\varepsilon$ is the accordingly rescaled Laplacian, whose expansion in ε is calculated in Appendix Secs. 2–4.

B. The horizontal connection and the corresponding Laplacian

The basic idea for deriving an effective equation on the submanifold $\mathcal{C}$ is to split the Laplace-Beltrami operator on $N\mathcal{C}$ at leading order into a horizontal and a normal part relative to $\mathcal{C}$, similar to the splitting $-\Delta_x - \Delta_y$ in the simple example of Sec. I B. To make this precise, first, note that, by construction at any point on the zero section of $N\mathcal{C}$ (which we identify with $\mathcal{C}$ in the following), the tangent space splits into two orthogonal subspaces, one tangent to $\mathcal{C}$ and one tangent to the fiber. Hence, the metric tensor $\overline{g}$ and with it also the Laplace-Beltrami operator on $(N\mathcal{C},\overline{g})$ splits into a sum,

$$\Delta_{\overline{g}} = \Delta_g + \Delta_N,$$

where Δ_g is the Laplace-Beltrami operator on $\mathcal{C}$ and Δ_N is the Euclidean Laplacian in the fibers $N_q\mathcal{C} \cong \mathbb{R}^k$ of the normal bundle. We would also like to have a similar splitting away from $\mathcal{C}$. To obtain this, we need a suitable horizontal derivative operator, which we now construct.

Like in the Born-Oppenheimer setting, where one thinks of the wave functions on $\mathbb{R}^{3n+3m}$ as elements of the electronic Hilbert space $L^2(\mathbb{R}^{3m})$, which depend on the nucleonic coordinates from $\mathbb{R}^{3n}$, we will think of the functions on $N\mathcal{C}$ as mappings from $\mathcal{C}$ to the functions on the fibers. Consider the bundle $\mathcal{E}_f := \{(q,\varphi) | q \in \mathcal{C}, \varphi \in L^2(N_q\mathcal{C})\}$ over $\mathcal{C}$, which is obtained when the fibers $N_q\mathcal{C}$ of the normal bundle are replaced with $L^2(N_q\mathcal{C})$ and the bundle structure of $N\mathcal{C}$ is lifted by lifting the action of $\mathrm{SO}(k)$ on the fibers to rotation of functions. We denote the set of all smooth sections of a Hermitian bundle $\mathcal{E}$ by $\Gamma(\mathcal{E})$.

For $\varphi \in \Gamma(\mathcal{E}_f)$, the *horizontal connection* ∇^h is defined by

$$\left(\nabla^h_\tau \varphi\right)(q,n) := \left.\frac{d}{ds}\right|_{s=0} \varphi\big(w(s),v(s)\big), \tag{10}$$

where $\tau \in T_q\mathcal{C}$ and $(w,v) \in C^1\big((-1,1),N\mathcal{C}\big)$ with

$$w(0) = q, \quad \dot{w}(0) = \tau, \quad \text{and} \quad v(0) = n, \quad \nabla^\perp_{\dot{w}} v = 0. \tag{11}$$

Furthermore, Δ_h is the bundle Laplacian associated with ∇^h, that is, defined by

$$\int_{\mathcal{C}} \int_{N_q\mathcal{C}} \psi^* \Delta_h \psi \, dn \, d\mu = -\int_{\mathcal{C}} \int_{N_q\mathcal{C}} g^{ij} \overline{\nabla^h_i \psi} \nabla^h_j \psi \, dn \, d\mu,$$

where g^{ij} is the inverse of the metric tensor g_{ij}. Here, and in the following, we use the abstract index formalism, which includes the convention that one sums over repeated indices. Moreover, we will consistently use latin indices $i,j,\ldots$, which run from 1 to d for coordinates on $\mathcal{C}$, greek indices $\alpha,\beta,\ldots$, which run from $d+1$ to $d+k$ for the normal coordinates, and latin indices $a,b,\ldots$, which run from 1 to $d+k$ for coordinates on the full normal bundle.

To obtain local expressions for these objects, we fix $q \in \mathcal{C}$ and choose geodesic coordinate fields $\{\partial_{x_i}\}_{i=1,\ldots,d}$ on an open neighborhood Ω of q and an orthonormal trivializing frame $\{\nu_\alpha\}_{\alpha=1,\ldots,k}$ of $N\Omega$. We define the connection coefficients $\omega^\gamma_{i\alpha}$ of the normal connection by $\nabla^\perp_i \nu_\alpha = \omega^\gamma_{i\alpha}\nu_\gamma$. Then, the horizontal connection is given by

$$\nabla^h_i \varphi(q,n) = \partial_i \varphi(q,n) - \omega^\gamma_{i\alpha} n^\alpha \partial_\gamma \varphi(q,n), \tag{12}$$

as was already shown by Mitchell [8], and it holds

$$\Delta_h \varphi = \mu^{-1}\big(\partial_i - \omega^\delta_{i\beta} n^\beta \partial_\delta\big)\mu g^{ij}\big(\partial_j - \omega^\gamma_{j\alpha} n^\alpha \partial_\gamma\big)\varphi, \tag{13}$$

with $\mu := \det g_{ij}$. The latter directly follows from the former and the definition of Δ_h. We note that $\Delta_h = \Delta_g$ on functions that are constant on the fibers by Eq. (13). To obtain the former equation, we note that for a normal vector field $v = n^\alpha \nu_\alpha$ over $\mathcal{C}$, it holds

$$(\nabla^\perp_i v)^\gamma = \partial_i n^\gamma + \omega^\gamma_{i\alpha} n^\alpha. \tag{14}$$

Now, let $(w,v) \in C^1\big((-1,1),N\mathcal{C}\big)$ be as in Eq. (11). Then, by definition of ∇^h, we have

$$\begin{aligned}
\nabla^h_i \varphi(q,n) &= \left.\frac{d}{ds}\right|_{s=0} \varphi\big(w(s),v(s)\big) \\
&= \left.\frac{d}{ds}\right|_{s=0} \varphi\big(w(s),n\big) + \left.\frac{d}{ds}\right|_{s=0} \varphi\big(q,v(s)\big) \\
&= \partial_i \varphi(q,n) + (\partial_i n^\gamma)\partial_\gamma \varphi(q,n) \\
&= \partial_i \varphi(q,n) - \omega^\gamma_{i\alpha} n^\alpha \partial_\gamma \varphi(q,n),
\end{aligned}$$

where we used Eq. (14) and the choice of the curve v in the last step.

C. The splitting of the Laplace-Beltrami operator

We recall from Sec. II B that we wanted to generalize the splitting of the Laplace-Beltrami operator on $(N\mathcal{C},\overline{g})$, $\Delta_{\overline{g}} = \Delta_g + \Delta_N$, on $\mathcal{C}$ to $N\mathcal{C}$. Indeed, we will see that also away from $\mathcal{C}$ (i.e., globally on $N\mathcal{C}$), we can approximately split $\Delta_{\overline{g}}$ into a horizontal part, given by Δ_h, and the Laplacian in the fiber Δ_N. The error grows linear with the distance $|N|$ to $\mathcal{C}$. Then, the rescaling of the normal coordinates to $n = N/\varepsilon$ yields

$$H_\varepsilon = -\varepsilon^2 \Delta_h - \Delta_n + V_c(q,n) + W(q,\varepsilon n) + O(\varepsilon|n|). \tag{15}$$

So, the error is small for states that are constrained to an ε neighborhood of $\mathcal{C}$ (i.e., localized on a length scale of order ε). The leading order of Eq. (15) has the same form as the Hamiltonian Eq. (3), which is the starting point for the time-dependent Born-Oppenheimer approximation, or the operator Eq. (6) of our simple waveguide example. This suggests that, also in the general situation considered here, adiabatic decoupling is the mechanism that yields effective Hamiltonians on $\mathcal{C}$.

We now explain, in more detail, how to achieve the previous splitting of the Laplacian. An important step is to turn the measure on $N\mathcal{C}$ into product form. To do so, we define

$$\begin{aligned}
M_\rho : L^2(N\mathcal{C},d\overline{\mu}) &\to L^2(N\mathcal{C},dN d\mu), \\
\Psi &\mapsto M_\rho \Psi := \rho^{-1/2}\Psi,
\end{aligned}$$

where dN denotes the Lebesgue measure on the fibers $N_q\mathcal{C} \cong \mathbb{R}^k$ and $\rho = \frac{d\overline{\mu}}{d\mu dN}$ is the density of the original measure with respect to the product measure on $N\mathcal{C}$. It is well known that

the unitary transformation of our Hamiltonian with M_ρ leads to the occurrence of a purely geometric extra potential:

$$V_\rho = -\tfrac{1}{4}\overline{g}^{ab}(\partial_a \ln\rho)\partial_b \ln\rho + \tfrac{1}{2}\Delta_{\overline{g}} \ln\rho.$$

More precisely, it holds that

$$M_\rho^*(-\Delta_{\overline{g}})M_\rho = -\Delta_{\mathrm{h}} - \Delta_N + V_\rho(q,N) + O(|N|), \quad (16)$$

which is shown in Appendix Secs. 2–4. Therefore, after application of the unitary transformation M_ρ and a Taylor expansion of W, the rescaled Hamiltonian H_ε is of the following form close to $\mathcal{C}$:

$$H_\varepsilon = -\varepsilon^2\Delta_{\mathrm{h}} - \Delta_n + V_{\mathrm{c}}(q,n) + W(q,0) + \varepsilon^2 V_\rho(q,\varepsilon n) + O(\varepsilon|n|).$$

We note that $-\varepsilon^2\Delta_{\mathrm{h}}$ is of order 1 on functions with oscillations of order ε^{-1}. So, the extra potential does not play a role for the leading order of the horizontal dynamics, unless the tangential kinetic energies are assumed to be small. Finally, it should be kept in mind that the remaining error term is small only when it is applied to functions that decay fast in the normal directions.

D. Adiabatic decoupling

Next, we explain the principle of adiabatic decoupling in detail. Analogously with the electronic Hamiltonian H_{e} in the Born-Oppenheimer setting, we define, for any $q \in \mathcal{C}$, the fiber Hamiltonian,

$$H_{\mathrm{f}}(q) = -\Delta_n + V_{\mathrm{c}}(q,n) + W(q,0),$$

on the Sobolev space $W^{2,2}(N_q\mathcal{C},dn) \subset L^2(N_q\mathcal{C},dn)$. We consider a q-dependent family of eigenvalues $E_{\mathrm{f}}(q)$ of multiplicity M, called an *energy band* in the following, and an associated family of normalized eigenfunctions $(\varphi_{\mathrm{f}}^J(q))_{J=1,\ldots,M}$:

$$H_{\mathrm{f}}(q)\varphi_{\mathrm{f}}^J(q,\cdot) = E_{\mathrm{f}}(q)\varphi_{\mathrm{f}}^J(q,\cdot). \quad (17)$$

Since the variation of the potential along the constraint manifold $\mathcal{C}$ is small compared to the normal variation, the normal profile of a wave function will adiabatically adjust to the nonconstraint degrees of freedom. Therefore, the transitions between different energy bands should be small, at least for times of order 1. This means that the subspace,

$$\mathcal{P}_0 := \left\{\varphi_{\mathrm{f}}^J(q,n)\psi_J(q) | \psi_J \in L^2(\mathcal{C},g)\right\} \subset L^2(N\mathcal{C})$$

is approximately invariant under the dynamics e^{-itH_ε} for times of order 1. This is due to the fact that the associated projector P_0 defined by $P_0(q) := (|\varphi_{\mathrm{f}}^J\rangle\langle\varphi_{\mathrm{f}}^J|)(q)$ is a spectral projection of H_{f}, and so we know that $[H_{\mathrm{f}},P_0]=0$, $[E_{\mathrm{f}},P_0]=0$, and $H_{\mathrm{f}}P_0 = E_{\mathrm{f}}P_0$. Hence,

$$[H_\varepsilon,P_0] = [-\varepsilon^2\Delta_{\mathrm{h}},P_0] + O(\varepsilon) = O(\varepsilon), \quad (18)$$

because, by definition of H_{f}, it holds that $H_\varepsilon = H_{\mathrm{f}} - \varepsilon^2\Delta_{\mathrm{h}} + O(\varepsilon)$ on states that decay fast enough. More precisely, the solution of the full Schrödinger equation with initial value $\Psi^\varepsilon|_{t=0} = \psi_J^\varepsilon\varphi_{\mathrm{f}}^J$ satisfies

$$\Psi^\varepsilon(t,q) = \varphi_{\mathrm{f}}^J(q,n)\psi_J^\varepsilon(t,q) + O(\varepsilon|t|),$$

where $\psi_J^\varepsilon(t,q)$ solves the following effective Schrödinger equation on $\mathcal{C}$:

$$i\partial_t\psi_J^\varepsilon(t,q) = -\varepsilon^2\Delta_g\psi_J^\varepsilon(t,q) + E_{\mathrm{f}}(q)\psi_J^\varepsilon(t,q). \quad (19)$$

It is well known that an equation of the form of Eq. (19) does show interesting behavior only on the semiclassical time scale $s = t/\varepsilon$. The adiabatic principle, however, suggests that $\mathcal{P}_0$ may be expected to be invariant for such and even much longer times, if the energy band $(E_{\mathrm{f}})_q$ is separated by a gap from the rest of the spectrum. Therefore, we also assume the following.

Assumption 2. For all $q \in \mathcal{C}$, the fiber Hamiltonian $H_{\mathrm{f}}(q)$ has an eigenvalue $E_{\mathrm{f}}(q)$ of multiplicity M such that

$$\inf_{q\in\mathcal{C}} \mathrm{dist}\{E_{\mathrm{f}}(q),\mathrm{spec}[H_{\mathrm{f}}(q)\setminus E_{\mathrm{f}}(q)]\} \geqslant c_{\mathrm{gap}} > 0.$$

In addition, there is a family of normalized eigenfunctions $(\varphi_{\mathrm{f}}^J(q))_{J=1,\ldots,M}$, which is globally smooth in q (in particular, the corresponding eigenspace bundle is trivializable) and satisfies

$$\sup_{q\in\mathcal{C}} \left\| e^{\Lambda_0\langle n\rangle}\varphi_{\mathrm{f}}^J \right\| < \infty$$

for $\langle n\rangle := \sqrt{1+|n|^2}$, some $\Lambda_0 > 0$, and all J.

An assumption about the decay is necessary because the error in the splitting $-\Delta_{\overline{g}} = -\varepsilon^2\Delta_{\mathrm{h}} - \Delta_n + O(\varepsilon)$ is only small when applied to functions that decay fast enough, as was explained earlier. However, in many cases, the decay is implied by the gap condition, in particular, for E_{f} below the continuous spectrum of H_{f}. The assumption about triviality is necessary to get an effective equation on $L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M$. If we dropped it, we would end up with an equation on a nontrivial rank-M bundle over $L^2(\mathcal{C},d\mu)$, which would complicate things quite a bit.

III. MAIN RESULTS

By having revealed the adiabatic structure of the constraining Hamiltonian H_ε in Sec. II, we have two different techniques at hand in order to deduce results about effective dynamics.

On one hand, it is possible to derive an analog of the standard adiabatic theorem of quantum mechanics in order to show that the subspace $\mathcal{P}_0$ is invariant under H_ε for times of order ε^{-1} up to errors of order ε. This is analogous to the approach used in Ref. [24] in the context of the Born-Oppenheimer approximation and will be carried out in the first part of this section. It leads to the occurrence of a Berry connection that will be investigated in Sec. III B.

In order to get a better approximation of the spectrum and/or to go to longer time scales for the dynamics, the usual adiabatic technique, which relies on cancellation of errors due to oscillations is no longer practicable. However, the general machinery of adiabatic perturbation theory, developed by Martinez-Sordoni-Nenciu in Refs. [17–19] and Panati-Spohn-Teufel in Refs. [20,21] and reviewed in Ref. [22], allows to construct superadiabatic subspaces that are invariant for times of order ε^{-n_1} up to errors of order ε^{n_2} for arbitrary $n_1,n_2 \in \mathbb{N}$. More precisely, it allows to construct a projector P_ε, which projects to a subspace $\mathcal{P}_\varepsilon$ close to $\mathcal{P}_0$ and satisfies $(H_\varepsilon,P_\varepsilon) = O(\varepsilon^m)$ for any $m > 1$. Adiabatic perturbation theory was

adapted to constrained quantum systems in Ref. [9]. For technical reasons, it could be made rigorous only for $m \leqslant 3$. The case $m = 3$ seems enough for all applications though. Before we discuss the resulting effective Hamiltonian and the approximation of bound states in Secs. III E and IIIF, we explain the construction of P_ε in Sec. III C.

A. Effective dynamics for times of order ε^{-1}

In order to relate wave functions from $\mathcal{P}_0$ to elements of $L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M$, we use an identification operator $U_0 : \mathcal{P}_0 \to L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M$ given by

$$U_0^* : L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M \to \mathcal{P}_0, \quad \psi^\varepsilon(q) \mapsto \varphi_{\mathrm{f}}^J(q,n)\psi_J^\varepsilon(q).$$

This defines a partial unitary operator, that is,

$$U_0^* U_0 = P_0, \quad U_0 U_0^* = 1.$$

Since $\mathcal{P}_0$ is approximately invariant under H_ε, we expect that $P_0 H_\varepsilon P_0$ is a good approximation to H_ε on $\mathcal{P}_0$. On $L^2(\mathcal{C},d\mu)\otimes\mathbb{C}^M$, the former operator corresponds to

$$H_{\mathrm{eff}}^{(1)} := U_0 P_0 H_\varepsilon P_0 U_0^*.$$

We may also use U_0 to compare the unitary group generated by $H_{\mathrm{eff}}^{(1)}$ with the one generated by H_ε. To verify our expectation, we have to show that $(e^{-iH_\varepsilon t} - U_0^* e^{-iH_{\mathrm{eff}}^{(1)}t}U_0)P_0$ is small. The analog of the adiabatic theorem, which achieves this for times of order ε^{-1}, reads as follows:

Theorem 1. Fix $E_{\max} < \infty$, and denote the characteristic function of $(-\infty, E_{\max}]$ by χ. Let the energy band E_{f} and the family of normalized eigenfunctions $(\varphi_f^J)_{J=1,\ldots,M}$ be as in Assumption 2.

Then there is a $C < \infty$ such that for all ε small enough:

$$\left\| \left(e^{-iH_\varepsilon t} - U_0^* e^{-iH_{\mathrm{eff}}^{(1)}t}U_0\right) P_0 \chi(H_\varepsilon) \right\| < C\varepsilon(1+\varepsilon|t|). \quad (20)$$

Up to terms of order ε^2 the first-order effective Hamiltonian $H_{\mathrm{eff}}^{(1)}$ is given by

$$\left\langle \psi^\varepsilon | H_{\mathrm{eff}}^{(1)} \psi^\varepsilon \right\rangle_{\mathcal{C}} = \int_{\mathcal{C}} \left(g_{\mathrm{eff}}^{ijIJ} \overline{p_{\mathrm{eff}\,i}^{IK} \psi_K^\varepsilon} p_{\mathrm{eff}\,j}^{JL} \psi_L^\varepsilon + V_{\mathrm{eff}}^{IJ} \overline{\psi_I^\varepsilon} \psi_J^\varepsilon \right) d\mu,$$

with

$$\begin{aligned} p_{\mathrm{eff}\,j}^{JL} &= -i\varepsilon\delta^{JL}\partial_j - \varepsilon\left\langle \varphi_{\mathrm{f}}^J \middle| i\nabla_j^{\mathrm{h}} \varphi_{\mathrm{f}}^L \right\rangle, \\ g_{\mathrm{eff}}^{ijIJ} &= g^{ij}\delta^{IJ} + \varepsilon 2\Pi_\alpha^{ij}\left\langle \varphi_{\mathrm{f}}^I \middle| n^\alpha \varphi_{\mathrm{f}}^J \right\rangle, \\ V_{\mathrm{eff}}^{IJ} &= E_{\mathrm{f}}\delta^{IJ} + \varepsilon(\partial_\alpha W)_{n=0}\left\langle \varphi_{\mathrm{f}}^I \middle| n^\alpha \varphi_{\mathrm{f}}^J \right\rangle, \end{aligned}$$

where II is the second fundamental form (see Appendix Sec. 1 for the definition), $\langle\cdot|\cdot\rangle_{\mathcal{C}}$ is the scalar product on $L^2(\mathcal{C},d\mu)$, and $\langle\cdot|\cdot\rangle$ is the scalar product on $L^2(\mathbb{R}^k,dN)$.

Via the operator U_0^* it is, hence, possible to obtain approximate solutions of the original equation from the solutions of the effective equation. We point out that $P_0\chi(H_\varepsilon)$ both cuts off high energies and produces initial states in $\mathcal{P}_0$. However, the cutoff energy $E_{\max}$ is arbitrary and, in particular, independent of ε. It is only needed in order to get a uniform error bound, since for larger tangential energies, the adiabatic decoupling becomes worse. Physically, this is expected, since large tangential energies correspond to large tangential velocities, and the separation of time scales for the normal and the tangential motions, which adiabatic decoupling is based on, breaks down for large velocities.

The effective Hamiltonian may be calculated by using standard perturbation theory, which is performed in Appendix Sec. 6. However, to verify that it yields effective dynamics on the relevant time scale $t = s/\varepsilon$ [i.e., to prove Eq. (20)], an additional adiabatic argument is needed. To make this clear, we notice that the usual perturbative argument only yields an error of order 1 for times of order ε^{-1}: By using that $U_0^* U_0 = P_0$ and $U_0 U_0^* = 1$, we have

$$\begin{aligned} &(e^{-iH_\varepsilon t} - U_0^* e^{-iU_0 P_0 H_\varepsilon P_0 U_0^* t} U_0) P_0 \\ &\quad = -e^{-iH_\varepsilon t} \int_0^t \frac{d}{ds} e^{iH_\varepsilon s} U_0^* e^{-iU_0 H_\varepsilon U_0^* s} U_0 \, ds \\ &\quad = -e^{-iH_\varepsilon t} \int_0^t e^{iH_\varepsilon s} i\,(H_\varepsilon, P_0)_0^* \, e^{-iU_0 H_\varepsilon U_0^* s} U_0 \, ds, \end{aligned} \quad (21)$$

which is of order $\varepsilon|t|$ by Eq. (18) but cannot directly be seen to be small for times of order ε^{-1}. However, adaptation of the calculation in the derivation of the standard adiabatic theorem (see, e.g., Ref. [22]) shows that the integrand is, up to errors of order ε^2, the time derivative of

$$e^{iH_\varepsilon s}\left(R_{H_{\mathrm{f}}}[H_\varepsilon, P_0] - [P_0, H_\varepsilon] R_{H_{\mathrm{f}}}\right) U_0^* e^{-iU_0 H_\varepsilon U_0^* s} U_0,$$

where $R_{H_{\mathrm{f}}} = P_0^\perp (H_{\mathrm{f}} - E_{\mathrm{f}})^{-1} P_0^\perp$ is the reduced resolvent. Therefore, the time integral of this term yields an error of order ε independent of t, which shows that the whole error is, indeed, only of order $\varepsilon(1+\varepsilon|t|)$.

For times of order ε^{-1}, the corrections of order ε yield relevant contributions:

(1) The corrected momentum operator $p_{\mathrm{eff}}^\varepsilon$ is a Berry connection on the $\mathbb{C}^M$ bundle over $\mathcal{C}$, where the effective wave function takes its values and, therefore, may give rise to topological and/or geometric phases (see Sec. III B).

(2) In general, all the corrections couple the effective internal degrees of freedom. If they, however, mutually commute, simultaneous diagonalization allows to split the effective $\mathbb{C}^M$ bundle into M effective bundles of rank 1 locally.

(3) If the center of mass of $\overline{\varphi_{\mathrm{f}}^I}\varphi_{\mathrm{f}}^J(q)$ lies on $\mathcal{C}$ for all q, then $\langle\varphi_{\mathrm{f}}^I | n^\alpha \varphi_{\mathrm{f}}^J\rangle = 0$. So, both the corrections to $g_{\mathrm{eff}}^\varepsilon$ and to V_{eff} vanish in this case. In particular, a local splitting into M effective bundles of rank 1 is possible in this case.

B. The effective Berry connection

In this section, we take a closer look at the induced Berry connection $p_{\mathrm{eff}}^{IJ} = -i\varepsilon\partial_x\delta^{IJ} - \varepsilon\langle\varphi_{\mathrm{f}}^I | i\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle$ that occurs in the effective Hamiltonian (see Theorem 1).

For $M = 1$ (i.e., if the energy E_{f} is nondegenerate), it is simply a U(1) connection that effects the dynamics similar to the vector potential of a magnetic field. If its curvature (the analog of the magnetic field) is zero, one can achieve, at least locally, $p_{\mathrm{eff}} = -i\varepsilon\partial_x$ by choosing a proper gauge [i.e., by choosing proper eigenfunctions $\varphi_{\mathrm{f}}(x)$]. However, such a gauge might not exist globally, and effects analogous to the Aharonov-Bohm effect may occur. In Sec. IV B, we give an example for a closed quantum waveguide without any external magnetic fields in which such an effect occurs purely due to the geometry of the waveguide.

If the curvature of p_{eff} is nonzero, it does even locally change the dynamics at order ε. In Ref. [10], Maraner identified the curvature as the origin of rotovibrational couplings in simple molecular models. Moreover, further important effects are to be expected, which are known for Berry connections from different areas: On one hand, the anomalous velocity term in the semiclassical model for electrons in crystalline solids also stems from the curvature of a Berry connection, see Refs. [25,26]. On the other hand, in the Born-Oppenheimer approximation, the Berry connection term in the effective dynamics exactly cancels the effect of an external magnetic field on the nuclei, see, for example, Ref. [24]. To neglect the Berry term would lead to wrong physics: In the Born-Oppenheimer approximation, a neutral molecule would suddenly react to the Lorentz force.

To state a formula for the curvature of the Berry connection, we fix $q \in \mathcal{C}$ and again choose normal coordinate fields $\{\partial_i\}_{i=1,\dots,d}$ on an open neighborhood Ω of q. Then, it holds that $(\partial_i, \partial_j) = 0$.

Proposition 1. $\nabla^{\text{eff}} := ip_{\text{eff}}$ is a metric connection on the rank-M bundle over $\mathcal{C}$, where the effective wave function takes its values. Its curvature vanishes for $M = 1$ and, otherwise, is given by

$$\begin{aligned} R^{\nabla^{\text{eff}}}_{IJij} &:= \left(\nabla^{\text{eff}}_i \nabla^{\text{eff}}_j - \nabla^{\text{eff}}_j \nabla^{\text{eff}}_i - \nabla^{\text{eff}}_{(\partial_i,\partial_j)}\right)_{IJ} \\ &= \left(\nabla^{\text{eff}}_i \nabla^{\text{eff}}_j - \nabla^{\text{eff}}_j \nabla^{\text{eff}}_i\right)_{IJ} \\ &= -\varepsilon^2 \langle \varphi^I_{\text{f}} \,|\, R^{\perp\gamma}_{\alpha ij} n^\alpha \partial_\gamma \varphi^J_{\text{f}} \rangle(q) \\ &\quad + \varepsilon^2 \left(\langle \nabla^{\text{h}}_i \varphi^I_{\text{f}} \,|\, \nabla^{\text{h}}_j \varphi^J_{\text{f}} \rangle - \langle \nabla^{\text{h}}_j \varphi^I_{\text{f}} \,|\, \nabla^{\text{h}}_i \varphi^J_{\text{f}} \rangle \right)(q) \\ &\quad + \varepsilon^2 \left(\langle \varphi^I_{\text{f}} \,|\, \nabla^{\text{h}}_i \varphi^K_{\text{f}} \rangle \langle \varphi^K_{\text{f}} \,|\, \nabla^{\text{h}}_j \varphi^J_{\text{f}} \rangle \right. \\ &\quad \left. - \langle \varphi^I_{\text{f}} \,|\, \nabla^{\text{h}}_j \varphi^K_{\text{f}} \rangle \langle \varphi^K_{\text{f}} \,|\, \nabla^{\text{h}}_i \varphi^J_{\text{f}} \rangle \right)(q), \end{aligned}$$

where $R^\perp$ is the curvature of the normal connection (defined in Appendix Sec. 1) and $\langle \cdot | \cdot \rangle$ is the scalar product on $L^2(\mathbb{R}^k, dN)$.

This is deduced in Appendix Sec. 6. An analogous expression was derived by Mitchell in Ref. [8] in the special case where φ^J_{f} is independent of q up to twisting. It was not realized that it always vanishes for $M = 1$ though.

C. Construction of the superadiabatic subspace

There are several motivations and ways for further improving the result formulated in Theorem 1. First of all, one can aim at a better approximation (i.e., smaller error estimates). Next, one can try to cover even longer time scales (i.e., times of order ε^{-2} and beyond). These long time scales become relevant (e.g., when considering the propagation of states with tangential energies of order ε^2 in waveguides, where the energy band E_{f} is constant on all of $\mathcal{C}$), (i.e., in the situation considered in earlier papers on geometric effects on constrained systems [6–8,10]). Last but not least, one also expects the eigenvalues of the effective Hamiltonian to be close to those of the full Hamiltonian and that one can recover, at least in a certain energy range, all eigenvalues of the full Hamiltonian in this way.

In order to achieve all three additional goals, we show how to construct an effective Hamiltonian that is unitarily equivalent to the full Hamiltonian on a certain subspace of the full Hilbert space up to errors of order ε^3. To this end, we use adiabatic perturbation theory [20]. The strategy is to first associate a so-called superadiabatic subspace $\mathcal{P}_\varepsilon$ with any energy band E_{f} that satisfies Assumption 2. The associated projector P_ε turns out to be uniquely fixed (up to terms of order ε^3) by the requirement that it projects on $\mathcal{P}_0$ to leading order and that the commutator $(H_\varepsilon, P_\varepsilon)$ is of order $O(\varepsilon^3)$. In a second step, we construct a unitary U_ε mapping the range of P_ε to the Hilbert space of the constrained system $L^2(\mathcal{C}, d\mu) \otimes \mathbb{C}^M$.

Then, on the superadiabatic subspace $H_\varepsilon|_{\mathcal{P}_\varepsilon} = P_\varepsilon H_\varepsilon P_\varepsilon$, up to terms of order ε^3. The effective Hamiltonian on $L^2(\mathcal{C}, d\mu) \otimes \mathbb{C}^M$ is now given by $H^{(2)}_{\text{eff}} = U_\varepsilon P_\varepsilon H_\varepsilon P_\varepsilon U^*_\varepsilon$ and solves all three problems mentioned previously.

We now explain this construction in detail. For the superadiabatic projection, we search for a bounded operator P_ε with

(i) $P_\varepsilon P_\varepsilon = P_\varepsilon$,
(ii) $P_\varepsilon - P_0 = O(\varepsilon)$,
(iii) $[H_\varepsilon, P_\varepsilon]\chi(H_\varepsilon) = O(\varepsilon^3)$.

Property (i) simply means that P_ε is an orthogonal projection, property (ii) is the requirement to be close to the adiabatic projection P_0, and (iii) says that $P_\varepsilon \chi(H_\varepsilon)\mathcal{H}$ is invariant under the Hamiltonian H_ε up to errors of order ε^3.

Since we saw in Eq. (18) that $(H_\varepsilon, P_0) = O(\varepsilon)$, it is consistent to make the ansatz for P_ε as an expansion in ε that starts with P_0:

$$P_\varepsilon = P_0 + \varepsilon P_1 + \varepsilon^2 P_2 + O(\varepsilon^3).$$

We first construct P_ε in a formal way by ignoring problems of boundedness. Afterward, we will explain how to obtain a well-defined projector and the associated unitary U_ε. We make the ansatz $P_1 := T_1^* P_0 + P_0 T_1$ with $T_1 : \mathcal{H} \to \mathcal{H}$ to be determined. By using the expansion of $H_\varepsilon = H_0 + \varepsilon H_1 + O(\varepsilon^2)$ from Appendix Sec. 4 and by assuming that $[P_1, -\varepsilon^2 \Delta_{\text{h}} + E_{\text{f}}] = O(\varepsilon)$, we have

$$\begin{aligned} [H_\varepsilon, P_\varepsilon]/\varepsilon &= [H_0/\varepsilon + H_1, P_0 + \varepsilon P_1] + O(\varepsilon) \\ &= [H_0/\varepsilon + H_1, P_0] + [H_0, P_1] + O(\varepsilon) \\ &= [-\varepsilon\Delta_{\text{h}} + H_1, P_0] + [H_{\text{f}} - E_{\text{f}}, P_1] + O(\varepsilon) \\ &= (-\varepsilon\Delta_{\text{h}} + H_1)P_0 - P_0(-\varepsilon\Delta_{\text{h}} + H_1) \\ &\quad + (H_{\text{f}} - E_{\text{f}})T_1^* P_0 - P_0 T_1 (H_{\text{f}} - E_{\text{f}}) + O(\varepsilon). \end{aligned}$$

We have to choose T_1 such that the first term is canceled. By observing that the right-hand side is off diagonal with respect to P_0, we may multiply with P_0 from the right and $P_0^\perp := 1 - P_0$ from the left and vice versa to determine P_1. This leads to

$$-(H_{\text{f}} - E_{\text{f}})^{-1} P_0^\perp ([-\varepsilon\Delta_{\text{h}}, P_0] + H_1) P_0 = P_0^\perp T_1^* P_0, \quad (22)$$

and

$$-P_0([P_0, -\varepsilon\Delta_{\text{h}}] + H_1) P_0^\perp (H_{\text{f}} - E_{\text{f}})^{-1} = P_0 T_1 P_0^\perp, \quad (23)$$

where we have used that the operator $H_{\text{f}} - E_{\text{f}}$ is invertible on $P_0^\perp \mathcal{H}_{\text{f}}$. In view of Eqs. (22) and (23), we define T_1 by

$$\begin{aligned} T_1 := &-P_0([P_0, -\varepsilon\Delta_{\text{h}}] + H_1) R_{H_{\text{f}}} \\ &+ R_{H_{\text{f}}}([-\varepsilon\Delta_{\text{h}}, P_0] + H_1) P_0, \end{aligned} \quad (24)$$

with $R_{H_\mathrm{f}} = P_0^\perp (H_\mathrm{f} - E_\mathrm{f})^{-1} P_0^\perp$. T_1 is antisymmetric so that $P^{(1)} := P_0 + \varepsilon P_1 = P_0 + \varepsilon(T_1^* P_0 + P_0 T_1)$ automatically satisfies condition (i) for P_ε up to first order. Due to $P_0^2 = P_0$:

$$\begin{aligned} P^{(1)} P^{(1)} &= P^{(1)} + \varepsilon P_0 (T_1^* + T_1) P_0 + O(\varepsilon^2) \\ &= P^{(1)} + O(\varepsilon^2). \end{aligned}$$

Moreover, it turns out that P_1 satisfies the assumption $(P_1, -\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) = O(\varepsilon)$ made earlier, too.

In order to derive the form of the second-order correction, we make the ansatz $P_2 = T_1^* P_0 T_1 + T_2^* P_0 + P_0 T_2$ with some $T_2 : \mathcal{H} \to \mathcal{H}$. The antisymmetric part of T_2 is determined analogously with T_1 just by calculating the commutator $[P_\varepsilon, H_\varepsilon]$ up to second order and by inverting $H_\mathrm{f} - E_\mathrm{f}$. One ends up with

$$\begin{aligned} (T_2 - T_2^*)/2 = &-P_0([P^{(1)}, H^{(2)}]/\varepsilon^2) R_{H_\mathrm{f}} \\ &+ R_{H_\mathrm{f}}([H^{(2)}, P^{(1)}]/\varepsilon^2) P_0, \end{aligned}$$

with $H^{(2)} := H_0 + \varepsilon H_1 + \varepsilon^2 H_2$. Note that $[H^{(2)}, P^{(1)}]/\varepsilon^2 = O(1)$ due to the construction of $P^{(1)}$. The symmetric part is again determined by the first condition for P_ε. By setting $P^{(2)} := P^{(1)} + \varepsilon^2 P_2$, we have

$$P^{(2)} P^{(2)} = P^{(2)} + \varepsilon^2 P_0 (T_1 T_1^* + T_2^* + T_2) P_0 + O(\varepsilon^3),$$

which forces $T_2^* + T_2 = -T_1 T_1^*$ in order to satisfy condition (i) up to second order.

We note that T_1 is quadratic in the momentum (and T_2 even quartic) and will, therefore, not be bounded on the full Hilbert space and, thus, neither P_ε. This is related to the well-known fact that, for a quadratic dispersion relation, adiabatic decoupling breaks down for momenta that tend to infinity. The problem can be circumvented by cutting off high energies in the right place, which was carried out by Sordoni for the Born-Oppenheimer setting in Ref. [18] and by Tenuta and Teufel for a model of nonrelativistic QED in Ref. [27].

To do so, we fix $E_\mathrm{max} < \infty$. Since H_ε is bounded from below, $E_- := \inf \sigma(H_\varepsilon)$ is finite. We choose $\tilde{\chi} \in C_0^\infty[\mathbb{R}, (0,1)]$ with $\tilde{\chi}|_{(E_- - 1, E+1]} \equiv 1$ and $\mathrm{supp}\tilde{\chi} \subset (E_- - 2, E + 2]$. Then, we define

$$\begin{aligned} P_\varepsilon^{\tilde{\chi}} := &P_0 + (P^{(2)} - P_0)\tilde{\chi}(H_\varepsilon) \\ &+ \tilde{\chi}(H_\varepsilon)(P^{(2)} - P_0)[1 - \tilde{\chi}(H_\varepsilon)], \end{aligned} \tag{25}$$

with $\tilde{\chi}(H_\varepsilon)$ defined via the spectral theorem. We emphasize that $P_\varepsilon^{\tilde{\chi}}$ is symmetric.

It holds that $P_\varepsilon^{\tilde{\chi}} - P_0 = O(\varepsilon)$ in the sense of bounded operators. That is why, for ε small enough, a projector is obtained via the formula,

$$P_\varepsilon := \frac{i}{2\pi} \oint_\Gamma \left(P_\varepsilon^{\tilde{\chi}} - z\right)^{-1} dz, \tag{26}$$

where $\Gamma = \{z \in \mathbb{C} \,||z - 1| = 1/2\}$ is the positively oriented circle around 1 (see, e.g., Ref. [28]). By denoting the associated subspace by $\mathcal{P}_\varepsilon$, we define a unitary mapping $\tilde{U}_\varepsilon : \mathcal{P}_\varepsilon \to \mathcal{P}_0$ by the so-called Sz.-Nagy formula:

$$\tilde{U}_\varepsilon := [P_0 P_\varepsilon + (1 - P_0)(1 - P_\varepsilon)][1 - (P_\varepsilon - P_0)^2]^{-1/2}. \tag{27}$$

Then, $U_\varepsilon := U_0 \tilde{U}_\varepsilon$ yields an isometry between $\mathcal{P}_\varepsilon$ and $L^2(\mathcal{C}, d\mu) \otimes \mathbb{C}^M$. In Ref. [9], it is shown that P_ε, indeed, satisfies (i)–(iii):

Proposition 2. Fix $E_\mathrm{max} < \infty$. For all ε small enough, P_ε is an orthogonal projection, and $\tilde{U}_\varepsilon$ is unitary. There are constants C_i such that

$$\begin{aligned} &\|P_\varepsilon - P_0\|_{\mathcal{L}(\mathcal{H})} \leqslant C_1 \varepsilon, \\ &\|[H_\varepsilon, P_\varepsilon]\chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))} \leqslant C_2 \varepsilon^3, \\ &\|\langle n \rangle^l P_\varepsilon \langle n \rangle^j\|_{\mathcal{L}(\mathcal{H})} \leqslant C_3, \quad \forall j,l \in \mathbb{N}_0, \end{aligned} \tag{28}$$

with χ as the characteristic function of $(-\infty, E]$.

The last estimate guarantees that the range of P_ε consists of states that decay faster than any polynomial, which is necessary to use the expansion of H_ε obtained in Appendix Sec. 4.

D. Effective dynamics for times of order ε^{-2}

By combining the results of Sec. III C with the standard perturbation theory, we can conclude that, for $H_\mathrm{eff}^{(2)} := U_\varepsilon P_\varepsilon H_\varepsilon P_\varepsilon U_\varepsilon^*$, we have

$$\left\| \left(e^{-iH_\varepsilon t/} - U_\varepsilon^* e^{-iH_\mathrm{eff}^{(2)} t} U_\varepsilon\right) P_\varepsilon \chi(H_\varepsilon) \right\| < C\varepsilon^3 |t|.$$

In the superadiabatic setting, no further adiabatic averaging is needed. This clearly improves Eq. (20) in the two ways anticipated: We get a better approximation and longer times. To get a simpler expression, we can approximate P_ε and U_ε by P_0 and U_0 and find

$$\left\| \left(e^{-iH_\varepsilon t} - U_0^* e^{-iH_\mathrm{eff}^{(2)} t} U_0\right) P_0 \chi(H_\varepsilon) \right\| < C\varepsilon(1 + \varepsilon^2 |t|)$$

(i.e., still a good approximation for long times on the adiabatic subspace $\mathcal{P}_0$). However, we cannot replace $H_\mathrm{eff}^{(2)}$ by $H_\mathrm{eff}^{(1)} = U_0 P_0 H_\varepsilon P_0 U_0^*$ without losing a factor ε in front of $|t|$ in the error. This is because the order ε^2 terms in the effective Hamiltonian are relevant for times of order ε^{-2}, and the expansion of the naive adiabatic Hamiltonian $H_\mathrm{eff}^{(1)}$ yields incorrect second-order terms.

So, we still have to provide the correct second-order expansion of the effective Hamiltonian $H_\mathrm{eff}^{(2)}$. Since the expression becomes quite complex and since we do not want to overburden the result, we restrict ourselves to a nondegenerate energy band (i.e., with one-dimensional eigenspaces).

Theorem 2. In addition to Assumptions 1 and 2, assume that E_f is nondegenerate and that arbitrary derivatives of the corresponding family of eigenfunctions φ_f are globally bounded.

Up to terms of order ε^3, the second-order effective Hamiltonian $H_\mathrm{eff}^{(2)}$ is given by

$$\begin{aligned} \left\langle \psi^\varepsilon \middle| H_\mathrm{eff}^{(2)} \psi^\varepsilon \right\rangle_{\mathcal{C}} = \int_{\mathcal{C}} \Big(&g_\mathrm{eff}^{ij} \overline{p_i^\mathrm{eff} \psi^\varepsilon} p_j^\mathrm{eff} \psi^\varepsilon + V_\mathrm{eff} |\psi^\varepsilon|^2 \\ &- \varepsilon^2 \overline{\psi^\varepsilon} U_1^* R_{H_\mathrm{f}} U_1 \psi^\varepsilon \Big) d\mu, \end{aligned}$$

where

$$\begin{aligned} g_\mathrm{eff}^{ij} = &\, g^{ij} + \varepsilon 2 \Pi_\alpha^{ij} \langle \varphi_\mathrm{f} | n^\alpha \varphi_\mathrm{f} \rangle + \varepsilon^2 \overline{\mathcal{R}}_{\alpha\ \beta}^{i\ j} \langle \varphi_\mathrm{f} | n^\alpha n^\beta \varphi_\mathrm{f} \rangle \\ &+ \varepsilon^2 \mathcal{W}_{\alpha l}^i g^{lm} \mathcal{W}_{\beta m}^j \langle \varphi_\mathrm{f} | 3 n^\alpha n^\beta \varphi_\mathrm{f} \rangle, \end{aligned}$$

$$
\begin{aligned}
p_j^{\mathrm{eff}} &= -i\varepsilon\partial_j - \varepsilon\langle\varphi_{\mathrm{f}}|i\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle - \varepsilon^2\overline{\mathcal{R}}_{j\alpha\ \beta}^{\ \gamma}\langle\varphi_{\mathrm{f}}|\tfrac{2}{3}n^\alpha n^\beta i\partial_\gamma\varphi_{\mathrm{f}}\rangle \\
&\quad + \varepsilon^2\mathcal{W}_\alpha^{ji}\langle\varphi_{\mathrm{f}}|2\big(n^\alpha - \langle\varphi_{\mathrm{f}}|n^\alpha\varphi_{\mathrm{f}}\rangle\big)i\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle, \\
V_{\mathrm{eff}} &= E_{\mathrm{f}} + \varepsilon(\partial_\alpha W)_{n=0}\langle\varphi_{\mathrm{f}}|n^\alpha\varphi_{\mathrm{f}}\rangle \\
&\quad + \varepsilon^2(V_{\mathrm{geom}} + V_{\mathrm{BH}} + V_{\mathrm{amb}} + W_2), \\
U_1 &= 2g^{ij}\overline{\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}}\partial_j + n^\alpha\varphi_{\mathrm{f}}\mathcal{W}_\alpha^{ij}\partial_{ij}^2 - n^\alpha\varphi_{\mathrm{f}}(\partial_\alpha W)_{n=0},
\end{aligned}
$$

and

$$
\begin{aligned}
V_{\mathrm{geom}} &= -\tfrac{1}{4}\eta^\alpha\eta_\alpha + \tfrac{1}{2}\mathcal{R}^{ij}{}_{ij} - \tfrac{1}{6}\big(\overline{\mathcal{R}}^{ab}{}_{ab} + \overline{\mathcal{R}}^{aj}{}_{aj} + \overline{\mathcal{R}}^{ij}{}_{ij}\big), \\
V_{\mathrm{BH}} &= g^{ij}\langle\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}|(1-|\varphi_{\mathrm{f}}\rangle\langle\varphi_{\mathrm{f}}|)\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle, \\
V_{\mathrm{amb}} &= \overline{\mathcal{R}}_{\alpha\ \beta}^{\ \gamma\ \ \delta}\langle\partial_\gamma\varphi_{\mathrm{f}}|\tfrac{1}{3}n^\alpha n^\beta\partial_\delta\varphi_{\mathrm{f}}\rangle, \\
W_2 &= \big(\partial_{\alpha\beta}^2 W\big)_{n=0}\langle\varphi_{\mathrm{f}}|n^\alpha n^\beta\varphi_{\mathrm{f}}\rangle,
\end{aligned}
$$

with $\mathcal{W}$ as the Weingarten mapping, η as the mean curvature vector, and $\mathcal{R}$ and $\overline{\mathcal{R}}$ as the Riemann tensors of $\mathcal{C}$ and $\mathcal{A}$ (see Appendix Sec. 1 for the definitions).

This effective Hamiltonian is derived in Ref. [9]. One might wonder whether the complicated form of the effective Hamiltonian renders the result useless for practical purposes. However, as explained in Sec. I, the possibly much lower dimension of $\mathcal{C}$ compared to that of $\mathcal{A}$ outweighs the more complicated form of the Hamiltonian. Moreover, the effective Hamiltonian is of a form that allows the use of semiclassical techniques for a further analysis. Finally, in practical applications, typically only some of the terms that appear in the effective Hamiltonian are relevant. As an example, we discuss the case of a quantum waveguide in Sec. IV. At this point, we only add some general remarks that concern the numerous terms in $H_{\mathrm{eff}}^{(2)}$ and their consequences.

(1) The off-band coupling $U_1^* R_{H_{\mathrm{f}}} U_1$ can easily be checked to be gauge invariant (i.e., not by depending on the choice of φ_{f} but only on P_0). Due to the replacement of U_0 by U_ε, it occurs and, thus, is missed when one expands the naive adiabatic Hamiltonian $H_{\mathrm{eff}}^{(1)} = U_0 P_0 H_\varepsilon P_0 U_0^*$. Even if one, in addition, uses standard perturbation theory in the fibers, still the first term in U_1, which originates from $(-\varepsilon^2\Delta_{\mathrm{h}}, P_0)$, would be missing.

(2) Both V_{BH}, an analog of the so-called Born-Huang potential, and V_{amb}, already found in Ref. [8], are also easily checked to be gauge invariant, which justifies calling them extra potentials.

(3) The occurrence of the geometric potential V_{geom} has been stressed in the literature, in particular, as the origin of curvature-induced bound states in quantum waveguides (reviewed by Duclos and Exner in Ref. [29]); see Sec. IV.

E. Approximation of bound states up to order ε^3

The unitary equivalence of H_ε and $H_{\mathrm{eff}}^{(2)}$ up to errors of order ε^3 allows us to deduce that the lower parts of their spectra coincide up to errors of order ε^3 when E_{f} is the ground-state band. The following result, which is proved in Ref. [9], shows how to obtain quasimodes of H^ε from the bound states of $H_{\mathrm{eff}}^{(2)}$ and vice versa.

Theorem 3. Let E_{f} be a nondegenerate constraint energy band, and let $U^\varepsilon, H_{\mathrm{eff}}^{(2)}$ be the operators associated with E_{f} in Sec. III D.

(a) Let $E \in \mathbb{R}$. Then, there is a $C < \infty$ such that for any family (E_ε) with $\limsup_{\varepsilon\to 0} E_\varepsilon < E$ and all ε small enough, the following implications hold:

$$
\begin{aligned}
H_{\mathrm{eff}}^{(2)}\psi_\varepsilon = E_\varepsilon\psi_\varepsilon \implies \|(H_\varepsilon - E_\varepsilon)U_\varepsilon^*\psi_\varepsilon\| \leqslant C\varepsilon^3\|U_\varepsilon^*\psi_\varepsilon\|, \\
H_\varepsilon\psi^\varepsilon = E_\varepsilon\psi^\varepsilon \implies \big\|\big(H_{\mathrm{eff}}^{(2)} - E_\varepsilon\big)U_\varepsilon\psi^\varepsilon\big\| \leqslant C\varepsilon^3\|\psi^\varepsilon\|.
\end{aligned}
$$

(b) Let $E_{\mathrm{f}}(q) = \inf\sigma\big(H_{\mathrm{f}}(q)\big)$ for some (and, thus, for all) $q \in \mathcal{C}$, and define $E_1(q) := \inf[\sigma\big(H_{\mathrm{f}}(q)\big) \setminus E_{\mathrm{f}}(q)]$. Let (ψ^ε) be a family with

$$
\limsup_{\varepsilon\to 0}\langle\psi^\varepsilon|H_{\mathrm{f}}\psi^\varepsilon\rangle < \inf_{q\in\mathcal{C}} E_1. \tag{29}
$$

Then, there is $c > 0$ such that $\|U_\varepsilon\psi^\varepsilon\| \geqslant c\|\psi^\varepsilon\|$ for all ε small enough.

We recall that, for any self-adjoint operator H, the bound $\|(H-\lambda)\psi\| < \delta\|\psi\|$ for $\lambda \in \mathbb{R}$ implies that H has a spectrum in the interval $(\lambda-\delta, \lambda+\delta)$. So, (a), (i) entails that H^ε has an eigenvalue in an interval of length $2C\varepsilon^3$ around E_ε, if one knows *a priori* that the spectrum of H^ε is discrete below the energy E. The statement (b) ensures that (a), (ii) really yields a quasimode for normal energies below $\inf_{q\in\mathcal{C}} E_1$, that is, that

$$
H_\varepsilon\psi^\varepsilon = E_\varepsilon\psi^\varepsilon \implies \big\|\big(H_{\mathrm{eff}}^{(2)} - E_\varepsilon\big)U_\varepsilon\psi^\varepsilon\big\| \leqslant \frac{C}{c}\varepsilon^3\|U_\varepsilon\psi^\varepsilon\|.
$$

If the ambient manifold $\mathcal{A}$ is flat, then Eq. (29) follows from:

$$
\limsup_{\varepsilon\to 0}\langle\psi^\varepsilon|H_\varepsilon\psi^\varepsilon\rangle < \inf_{q\in\mathcal{C}} E_1 - \sup_{(q,n)}(W_{n=0} - W) =: E_*. \tag{30}
$$

Therefore, Theorem 3, in particular, implies that at least for flat $\mathcal{A}$, there is a one-to-one correspondence between the spectra of H_ε and $H_{\mathrm{eff}}^{(2)}$ below E_*. In the example of Sec. I B depicted in Fig. 2, this implies that all eigenvalues of H_ε in the interval $[e_0, e_1)$ and the corresponding eigenfunctions are determined by the effective Hamiltonian of the ground-state band E_0 modulo terms of order ε^3.

The bound states of $H_{\mathrm{eff}}^{(2)}$ can be approximated by the standard WKB construction. In the simplest case, one obtains:

Corollary 1. Assume that $\mathcal{A}$ is flat and that E_{f} is a nondegenerate constraint energy band with $\inf E_{\mathrm{f}} < E_*$ and $E_{\mathrm{f}}(q) = \inf\sigma\big(H_{\mathrm{f}}(q)\big)$ for all $q \in \mathcal{C}$. Let there be $q_0 \in \mathcal{C}$ such that $E_{\mathrm{f}}(q_0) < E_{\mathrm{f}}(q)$ for all $q \neq q_0$, and $(\nabla_{i,j}^2 E_{\mathrm{f}})(q_0)$ is positive definite.

Denote by $E_\ell(A)$ the ℓth eigenvalue of a semibounded operator A, counted from the bottom of the spectrum. Then, for any $\ell \in \mathbb{N}$,

$$
E_\ell(H^\varepsilon) = E_{\mathrm{f}}(q_0) + \varepsilon E_\ell(H_{\mathrm{HO}}) + O(\varepsilon^2),
$$

where $H_{\mathrm{HO}} := -\Delta_{\mathbb{R}^d} + \frac{1}{2}(\nabla^2_{\partial_{x^i},\partial_{x^j}} E_{\mathrm{f}})(q_0)x^i x^j$ is a harmonic oscillator on $\mathbb{R}^d$.

IV. QUANTUM WAVEGUIDES

In this section, we look at the special case of a curve $\mathcal{C}$ in $\mathcal{A} = \mathbb{R}^3$ equipped with the Euclidean metric. Such curves may model quantum waveguides, which have been discussed theoretically for a long time (see, e.g., the review in Ref. [29]) but are nowadays also investigated experimentally (see, e.g., the review in Ref. [11]).

In the Sec. IV A, we provide the expression for our effective Hamiltonian when applied to waveguides and make some general remarks about trapping and splitting of wave packets. In Sec. IV B, we explain how to produce topological phases in closed waveguides. The effects on the spectrum of such waveguides are discussed in Sec. IV C.

A. Trapping and splitting in quantum waveguides

We first look at spatially infinite quantum waveguides. So, let the curve $\mathcal{C}$ be given as a smooth injective $c : \mathbb{R} \to \mathbb{R}^3$ that is parametrized by arc length ($|\dot{c}| = 1$). The mean curvature vector of c is $\eta = \ddot{c}$, and its (exterior) curvature is $|\eta|$. By denoting the usual scalar product in $\mathbb{R}^3$ by $\cdot$, we define $y(n) := n \cdot \eta/|\eta|$, where $\eta \neq 0$ and $y(n) := 0$ elsewhere. By the Frenet formulas, the Weingarten mapping satisfies $\mathcal{W}(\eta) = |\eta|^2$ (see, e.g., Ref. [30]) and $\mathcal{W} \equiv 0$ on the orthogonal complement of η [which is $N_q\mathcal{C}$ if $\eta(q) = 0$].

A normalized section of the tangent bundle $T\mathcal{C}$ is given by $\tau := \dot{c}$. We extend this to an orthonormal frame of $T\mathcal{C} \times N\mathcal{C}$, where $N\mathcal{C}$ is the normal bundle, in the following way: We fix $q \in \mathcal{C}$, choose an arbitrary orthonormal basis of $N_q\mathcal{C}$, and take ν_1, ν_2 to be the parallel transport of this basis with respect to the normal connection $\nabla^\perp$ (defined in Appendix Sec. 1) along the whole curve. This yields an orthonormal frame of $N\mathcal{C}$. Together with τ, we obtain an orthonormal frame of $T\mathcal{C} \times N\mathcal{C}$, which is sometimes called the Tang frame. We denote the coordinates with respect to τ, ν_1, and ν_2 by x, n_1, and n_2 respectively. In these coordinates, it holds $\nabla^h = \partial_x$ [as can be seen from the coordinate formula of Eq. (12) and the definition of the connection coefficients ω in Appendix Sec. 1].

Now, let E_f and $(\varphi_f^J)_J$ be as in Assumption 2. We start by spelling out the formula for $H_{\text{eff}}^{(1)}$ from Theorem 1. Since $\mathcal{C}$ is one dimensional and contractible, the families of φ_f^J can be chosen such that $p_{\text{eff}}^{\varepsilon} \equiv -i\varepsilon\partial_x$ globally. Then, the first-order effective Hamiltonian is

$$H_{\text{qwg}}^{(1)} = -i\varepsilon\partial_x\big(1 + \varepsilon|\eta|\langle\varphi_f^I|y\varphi_f^J\rangle\big)i\varepsilon\partial_x + E_f + \varepsilon(\partial_\alpha W)_{n=0}\langle\varphi_f^I|n^\alpha\varphi_f^J\rangle, \tag{31}$$

with $\langle\phi|\psi\rangle := \int_{\mathbb{R}^2}\phi^*\psi dn_1 dn_2$.

For highly oscillating states ψ (i.e., with $\langle\psi|-\varepsilon^2\partial_{xx}^2\psi\rangle \sim 1$), the only term of order 1 besides $-\varepsilon^2\partial_{xx}^2$ is E_f. So, if E_f is constant, in particular, if the waveguide has a constant cross section, the dynamics is free at leading order and, even more, the potential terms are of order ε^2. So, they only become relevant for times of order ε^{-2}. However, a semiclassical wave packet ψ covers distances of order ε^{-1} on this time scale. Hence, for such ψ, noteworthy trapping occurs only for very long waveguides!

If we consider a straight waveguide (i.e., $\eta \equiv 0$), the formula we end up with is the expected adiabatic approximation:

$$H_{\text{qwg}}^{(1)}\big|_{\eta\equiv 0} = -\varepsilon^2\partial_{xx}^2 + E_f + \varepsilon(\partial_\alpha W)_{n=0}\langle\varphi_f^I|n^\alpha\varphi_f^J\rangle.$$

We note that, although $\eta \equiv 0$, the x dependence of the constraining potential still allows us to model interesting situations. For example, a beam splitter may be realized by fading a single-well into a double-well potential (see, e.g., Ref. [4]).

B. Topological phases in quantum wave circuits

Up to now, we have considered a spatially infinite waveguide, which, of course, has the topology of a line. The only possible nontrivial topology for a curve $\mathcal{C}$ is that of a circle. We refer to a waveguide modeled over such a $\mathcal{C}$ as a *quantum wave circuit*. In order to keep formulas simple and transparent, we look at a so-called round circle, that is, with constant η. Then, the Tang frame from Sec. IV A is still globally smooth. However, because of the nontrivial topology, our choices of the families φ_f^J made earlier are only possible locally but, in general, not globally. Therefore, we rewrite Eq. (31) without those choices. For the sake of brevity, we assume that W, the nonconstraining part of the potential, is identically zero in the following:

$$H_{\text{qwc}}^{(1)} = p_{\text{eff}}^*\big(1 + \varepsilon|\eta|\langle\varphi_f^I|y\varphi_f^J\rangle\big)p_{\text{eff}} + E_f, \tag{32}$$

with $p_{\text{eff}} = -i\varepsilon\partial_x + \varepsilon\langle\varphi_f^I|i\partial_x\varphi_f^J\rangle$. Although the curvature of the connection ip_{eff} always vanishes, it may lead to a topological phase, which we will discuss next.

Here, and in Sec. IV C, we again restrict ourselves to the case of a nondegenerate energy band E_f. We note that, even for degenerate energy bands, only Abelian phases will occur because the fundamental group of the circle is generated by only one element. Let x be a 2π-periodic coordinate on the circle. The eigenfunction $\varphi_f(x)$ associated with E_f can be chosen as real valued for each fixed x because H_f is real. This associates a real line bundle with E_f. From the topological point of view, there are exactly two real line bundles over the circle: the trivial one and the nontrivializable Möbius band. In the former case, the global section φ_f can be chosen real everywhere. This implies

$$\langle\varphi_f|\partial_x\varphi_f\rangle = \frac{1}{2}(\langle\varphi_f|\partial_x\varphi_f\rangle + \langle\partial_x\varphi_f|\varphi_f\rangle) = \frac{\partial_x\langle\varphi_f|\varphi_f\rangle}{2} \equiv 0,$$

which results in $ip_{\text{eff}} = \varepsilon\partial_x$. Thus, there will be no topological phase in this case. We will now provide an example for the realization of the Möbius band by a suitable constraining potential and show that, indeed, a topological phase occurs!

Let $\tilde{V}_c \in C_b^\infty(\mathbb{R}^2)$ have two orthogonal axes of reflection symmetry, that is, in suitable coordinates:

$$\tilde{V}_c(-\tilde{n}_1,\tilde{n}_2) = \tilde{V}_c(\tilde{n}_1,\tilde{n}_2) = \tilde{V}_c(\tilde{n}_1,-\tilde{n}_2). \tag{33}$$

Then, the real ground state Φ_0 of $-\Delta_{\mathbb{R}^2} + \tilde{V}_c$ with energy E_0 is symmetric with respect to both reflections,

$$\Phi_0(\tilde{n}_1,\tilde{n}_2) = \Phi_0(-\tilde{n}_1,\tilde{n}_2) = \Phi_0(\tilde{n}_1,-\tilde{n}_2),$$

while the first excited state Φ_1, also taken as real valued, with energy E_1 is typically only symmetric with respect to one

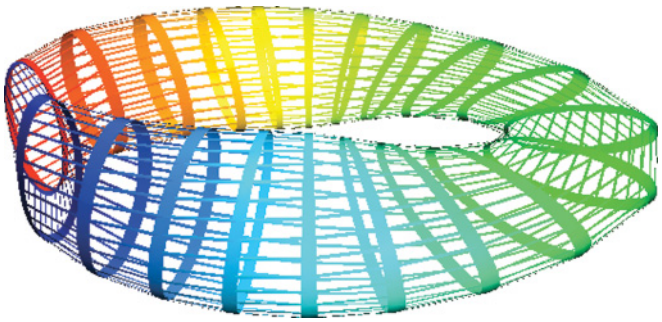

FIG. 3. (Color online) Level set of a potential such as $V_c^{x/2}$, which describes a Möbius wave circuit.

reflection and antisymmetric with respect to the other one, for example,

$$\Phi_1(\tilde{n}_1,\tilde{n}_2) = -\Phi_1(-\tilde{n}_1,\tilde{n}_2) = \Phi_1(\tilde{n}_1,-\tilde{n}_2). \tag{34}$$

This is true, in particular, for a harmonic oscillator with different frequencies. As the potential, which constrains to the circle, we let $\tilde{V}_c$ perform half a twist along the circle, that is,

$$[V_c^{x/2}(x)](n_1,n_2) := \tilde{V}_c[\cos(x/2)n_1 - \sin(x/2)n_2, \sin(x/2)n_1 + \cos(x/2)n_2].$$

We note that due to Eq. (33), this defines a smooth $V_c^{x/2}$. (See Fig. 3.) Then,

$$[\tilde{\varphi}_j(x)](n_1,n_2) := \Phi_j[\cos(x/2)n_1 - \sin(x/2)n_2, \sin(x/2)n_1 + \cos(x/2)n_2]$$

is an eigenfunction of $H_f(x) := -\Delta_v + V_c(x)$ with eigenvalue E_j for every x and $j \in \{0,1\}$. However, while $\tilde{\varphi}_0$ is a smooth section of the corresponding eigenspace bundle, $\tilde{\varphi}_1$ is not. For, by Eq. (34), it holds $\tilde{\varphi}_1(x) = -\tilde{\varphi}_1(x+2\pi)$ (see Fig. 4). Still, the complex eigenspace bundle admits a smooth nonvanishing section. A possible choice is $\varphi_1(x) := e^{ix/2}\tilde{\varphi}_1(x)$. By using Eq. (34), we obtain that, for the first excited band, the effective Hamiltonian Eq. (32) reduces to

$$H_{\mathrm{qwc},1} = (-i\varepsilon\partial_x + \varepsilon/2)^2 + E_1,$$

while for the ground-state band it is

$$H_{\mathrm{qwc},0} = -\varepsilon^2\partial_{xx}^2 + E_0.$$

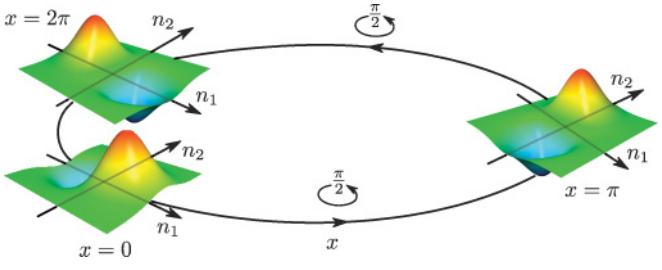

FIG. 4. (Color online) First excited transverse eigenfunction in a Möbius wave circuit: n_1 and n_2 are the normal elements of a global Tang frame; and, with respect to this frame, the confining potential $V_c^{x/2}$ twists by an angle of π when going around the circuit once. Due to its symmetry, $V_c^{x/2}$ is still globally smooth; see Fig. 3. However, since the first excited state Φ_1 does not have the full symmetry of the potential, it changes sign after a twist by π.

This shows that by depending on the symmetry of the normal eigenfunction, the twist by an angle of π has different effects on the effective momentum operator in the effective Hamiltonian. With respect to the connection that appears in $H_{\mathrm{qwc},1}^{\varepsilon}$, the holonomy of a closed loop γ that winds around the circle once is $h(\gamma) = e^{i\int_0^{2\pi} 1/2dx} = -1$. Hence, the $1/2$ cannot be gauged away. Furthermore, a wave packet that travels around the circuit once accumulates a topological phase equal to π.

C. Effects of twisting and bending on the spectrum

At second order, in ε, the effect of the topological phase in quantum wave circuits can also be seen in the level spacing of $H_{\mathrm{qwc},j}$ and, thus, with Theorem 3, also in the spectrum of H_ε. So, we add the corrections of second order from Theorem 2 to Eq. (32). Of course, all terms that contain the inner curvature of $\mathcal{C}$ and $\mathcal{A} = \mathbb{R}^3$ vanish due to the flatness of $\mathcal{C}$ and $\mathcal{A}$ with the Euclidean metric,

$$\begin{aligned} H_{\mathrm{qwc}}^{(2)} = {} & p_{\mathrm{eff}}^*(1 + \varepsilon|\eta|\langle\varphi_f|y\varphi_f\rangle + 3\varepsilon^2|\eta|^2\langle\varphi_f|y^2\varphi_f\rangle)p_{\mathrm{eff}} \\ & + E_f + \varepsilon^2(\langle\partial_x\varphi_f|\partial_x\varphi_f\rangle - |\langle\varphi_f|\partial_x\varphi_f\rangle|^2) \\ & - \varepsilon^2\frac{|\eta|^2}{4} + \varepsilon^2\big(4\varepsilon\partial_x\langle\partial_x\varphi_f|R_{H_f}\partial_x\varphi_f\rangle\varepsilon\partial_x \\ & + 4\mathrm{Re}|\eta|\varepsilon\partial_x\langle\partial_x\varphi_f|R_{H_f}y\varphi_f\rangle\varepsilon^2\partial_{xx}^2 \\ & + |\eta|^2\varepsilon^2\partial_{xx}^2\langle y\varphi_f|R_{H_f}y\varphi_f\rangle\varepsilon^2\partial_{xx}^2\big), \end{aligned} \tag{35}$$

with p_{eff} given by

$$-i\varepsilon\partial_x + \varepsilon\langle\varphi_f|i\partial_x\varphi_f\rangle + \varepsilon^2|\eta|\langle\varphi_f|2(y - \langle\varphi_f|y\varphi_f\rangle)\partial_x\varphi_f\rangle.$$

If V_c does not change its shape but only twists, E_f is constant and, thus, may be removed by redefining zero energy. Furthermore, since the remaining potential terms are of order ε^2, the kinetic energy operator $-\varepsilon^2\partial_{xx}^2$ will also be of order ε^2 at the bottom of the spectrum. So, $H_{\mathrm{qwc}}^{\varepsilon}$ may be divided by ε^2. By keeping only the leading order terms, we arrive at

$$H_{\mathrm{qwc},j} = \tilde{p}_{\mathrm{eff}}^*\tilde{p}_{\mathrm{eff}} - \frac{|\eta|^2}{4} + \langle\partial_x\varphi_j|\partial_x\varphi_j\rangle - |\langle\varphi_j|\partial_x\varphi_j\rangle|^2, \tag{36}$$

with $\tilde{p}_{\mathrm{eff}} := -i\partial_x + \langle\varphi_j|i\partial_x\varphi_j\rangle$. A simple calculation yields

$$\begin{aligned} & \langle\partial_x\varphi_j|\partial_x\varphi_j\rangle - |\langle\varphi_j|\partial_x\varphi_j\rangle|^2 \\ & = \frac{1}{4}\int_{\mathbb{R}^2} |n_1\partial_{n_2}\Phi_j - n_2\partial_{n_1}\Phi_j|^2 dn_1 dn_2 =: L^2(\Phi_j)/4. \end{aligned}$$

We note that the integral is the expectation value of the squared angular momentum of Φ_f and, thus, vanishes for a rotation-invariant Φ_f. So, Eq. (36) shows that bending is attractive, while twisting is repulsive.

Since $|\eta|$ is constant, for $\ell \in \mathbb{N}_0$ the ℓth eigenvalue of $H_{\mathrm{qwc},1}$ is

$$E_\ell(H_{\mathrm{qwc},1}) = E_1 + \varepsilon^2\left[\left(\ell + \frac{1}{2}\right)^2 + \frac{L^2(\Phi_1) - |\eta|^2}{4}\right] + O(\varepsilon^3),$$

while, for $H_{\mathrm{qwc},0}$, we find

$$E_\ell(H_{\mathrm{qwc},0}) = E_0 + \varepsilon^2\left(\ell^2 + \frac{L^2(\Phi_0) - |\eta|^2}{4}\right) + O(\varepsilon^3).$$

We note that, although a constraining potential that twists along a circle was investigated by Maraner in detail in Ref. [7] and

by Mitchell in Ref. [8], the effect discussed previously was not found in both treatments. The reason for this is that they only allowed for whole rotations and not for half ones to avoid the nonsmoothness of $\tilde{\varphi}_1$.

There is a great amount of literature on the spectrum of a quantum waveguide, which is arbitrarily bent and twisted (see the review in Ref. [31] by Krejčiřík). In general, the twisting assumption means that there is $\theta \in C_b^\infty(\mathbb{R})$ and $\tilde{V}_c \in C_b^\infty(\mathbb{R}^2)$ such that the constraining potential has the form

$$\big[V_c^\theta(x)\big](n_1,n_2) := \tilde{V}_c[n_1\cos\theta(x) - n_2\sin\theta(x), \\ n_1\sin\theta(x) + n_2\cos\theta(x)].$$

Then, the family of eigenfunctions φ_f may be chosen as

$$[\varphi_f(x)](n_1,n_2) := \Phi_f[n_1\cos\theta(x) - n_2\sin\theta(x), \\ n_1\sin\theta(x) + n_2\cos\theta(x)]$$

for an eigenfunction Φ_f of $-\Delta_{\mathbb{R}^2} + \tilde{V}_c(x)$ with eigenvalue E_f. It is easy to generalize the preceding discussion to a wave circuit whose curvature and potential twist are nonconstant. Then, the ℓth eigenvalue of H_ε is given by

$$E_\ell(H_\varepsilon) = E_f + \varepsilon^2 E_\ell\big(H_{\text{twist}}^\theta\big) + O(\varepsilon^3),$$

where $E_\ell(H_{\text{twist}}^\theta)$ is the ℓth eigenvalue of the following operator:

$$H_{\text{twist}}^\theta := \tilde{p}_{\text{eff}}^* \tilde{p}_{\text{eff}} - |\eta|^2/4 + L^2(\Phi_f)\dot{\theta}^2/4.$$

with $\tilde{p}_{\text{eff}} := -i\partial_x + \langle\varphi_f|i[\partial_x + (\nu_\alpha\partial_x\nu_\beta)n^\alpha\partial_\beta]\varphi_f\rangle$. This generalizes results by Bouchitté *et al.* [5] and by Borisov and Cardone [32] for waveguides to wave circuits. We note that, for the Tang frame $\nu_\alpha\partial_x\nu_\beta \equiv 0$ but for an arbitrarily curved wave circuit, the Tang frame is, in general, not globally smooth anymore. Anyway, the normal bundle is still trivializable because it inherits the orientation of $\mathbb{R}^3$, and every orientable vector bundle over a curve is trivializable.

V. CONCLUSIONS

While earlier results on constrained quantum systems had to focus either on a certain energy regime or on special geometries, here, we have presented results, both on the dynamics and on the spectrum, that cover all relevant energy regimes in general geometries (recall Fig. 2).

We point out that our results on dynamics (Theorems 1 and 2) are true for all bound states and scattering energies, as long as oscillations faster than ε^{-1} are excluded. The same is true for the quasimodes of the full Hamiltonian H^ε constructed from those of the effective Hamiltonian (Theorem 3).

Furthermore, we have applied our results to quantum waveguides and have obtained the complete second-order effective Hamiltonian Eq. (35). In contrast to earlier theoretical results, it also applies to wave circuits (i.e., closed waveguides). Here, the effect of an Abelian topological phase is observable both in the spectrum and in the dynamics. We believe that, as a next step, it would be interesting to apply our results to simple examples from molecular dynamics, such as those that were treated for small kinetic energies by Maraner in Ref. [10]. Here, also the curvature of the effective Berry connection, calculated in Proposition 1, should play a role. Note that it did not show up for quantum waveguides because of the one-dimensional constraint manifold.

ACKNOWLEDGMENTS

We thank Daniel Grieser, Stefan Keppeler, David Krejčiřík, Christian Loeschcke, Frank Loose, Olaf Post, Hans-Michael Stiepan, Luca Tenuta, Olaf Wittich, and Claus Zimmermann for helpful remarks and inspiring discussions about the topic of this paper. We acknowledge that this work was supported by the DFG within the SFB/Transregio 71.

APPENDIX

1. Geometry of submanifolds

Here, we recall some standard concepts from Riemannian geometry. For further information, see, for example, Ref. [33]. As before, we use the abstract index formalism that includes the convention that one sums over repeated indices. Moreover, we will consistently use latin indices $a,b,\ldots$, which run from 1 to $d+k$ for coordinates on a general manifold, latin indices $i,j,\ldots$, which run from 1 to d for coordinates on a submanifold, and greek indices $\alpha,\beta,\ldots$, which run from $d+1$ to $d+k$ for coordinates in the normal spaces of a submanifold.

First, we give the definition of the Riemann tensor we use (the order of the indices varies in the literature!).

Definition 1. Let $(\mathcal{M},g)$ be a Riemannian manifold with Levi-Civita connection ∇. Let $(\tau_a)_a$ be a set of local coordinate vector fields.

(i) The Christoffel symbols Γ of ∇ are defined by

$$\nabla_a\tau_b = \Gamma_{ab}^c\tau_c.$$

(ii) The Riemann tensor $\mathcal{R}$ is given by

$$\mathcal{R}_{bcd}^a := (\nabla_c\nabla_d\tau_b - \nabla_d\nabla_c\tau_b)^a.$$

As usual, by raising and lowering indices, we mean to shift covariant to contravariant coordinates and vice versa.

Now, we turn to the basic objects related to the exterior curvature of a submanifold of arbitrary codimension.

Definition 2. Let $(\mathcal{A},\overline{g})$ be a Riemannian manifold with Levi-Civita connection $\overline{\nabla}$. Let $\mathcal{C}\subset\mathcal{A}$ be a submanifold equipped with the induced metric $g = \overline{g}|_{\mathcal{C}}$. Denote by $N\mathcal{C}$ the normal bundle of $\mathcal{C}$. Let $(\tau_i)_i$ be a set of local coordinate vector fields of $\mathcal{C}$, and let $(\nu_\alpha)_\alpha$ be a local orthonormal frame of $N\mathcal{C}$.

(i) The Weingarten mapping $\mathcal{W}$ is given by

$$\mathcal{W}_{\alpha j}^i := \big(-\overline{\nabla}_j\nu_\alpha\big)^i.$$

(ii) The second fundamental form II is defined by

$$\mathrm{II}_{ij}^\alpha := (\overline{\nabla}_j\tau_i)^\alpha.$$

(iii) The mean curvature normal η is defined by

$$\eta_\alpha = \mathcal{W}_{\alpha j}^j.$$

The relations and symmetry properties of $\mathcal{W}$ and II for hypersurfaces also hold when the codimension is greater than 1:

$$\mathrm{II}^i_{\alpha j} = \mathcal{W}^i_{\alpha j} = \mathcal{W}^j_{\alpha i} = \mathrm{II}^j_{\alpha i}. \tag{A1}$$

Finally, we provide the definitions of the objects that characterize the geometry of the normal bundle.

Definition 3. (i) We define the normal connection $\nabla^\perp$ to be the bundle connection on the normal bundle given via

$$(\nabla^\perp_j \nu_\alpha)^a = (\overline{\nabla}_j \nu_\alpha)^a,$$

for $a = d+1,\ldots,d+k$ and $(\nabla^\perp_j \nu_\alpha)^a = 0$ for $a = 1,\ldots,d$.

(ii) The connection coefficients ω of $\nabla^\perp$ are defined by

$$\nabla^\perp_i \nu_\alpha = \omega^\beta_{i\alpha} \nu_\beta.$$

(iii) The normal curvature tensor $\mathrm{R}^\perp$ is defined by

$$\mathcal{R}^{\perp\alpha}_{\beta ij} := (\nabla^\perp_i \nabla^\perp_j \nu_\beta - \nabla^\perp_j \nabla^\perp_i \nu_\beta)^\alpha.$$

Due to the antisymmetries of any curvature tensor, the normal curvature tensor $\mathrm{R}^\perp$ is identically zero, when the dimension or the codimension of $\mathcal{C}$ is smaller than 2.

When we set $\mathcal{W}^a_{\alpha j} = 0$ for $a = d+1,\ldots,d+k$, the Weingarten equation,

$$(\nabla^\perp_j \nu_\alpha)^a = (\overline{\nabla}_j \nu_\alpha)^a + \mathcal{W}^a_{\alpha j} \tag{A2}$$

is a direct consequence of the definitions.

2. Expansion of the metric tensor

In order to expand the Hamiltonian H_ε in powers of ε, it is crucial to expand the metric $\overline{g}$ on the normal bundle $N\mathcal{C}$ around $\mathcal{C}$ because the Laplace-Beltrami operator depends on it. Such expansions were carried out in almost any work on constrained quantum systems, however, in various generalities and up to varying orders. Here, we provide a simple derivation for an arbitrary submanifold of a curved ambient manifold but only up to first order. However, this is enough in order to obtain Theorem 1.

Fix $q \in \mathcal{C}$. Let $(\tau_i)_i$ be a set of local coordinate vector fields of $\mathcal{C}$, and let $(\nu_\alpha)_\alpha$ be a local orthonormal frame of $N\mathcal{C}$. Furthermore, let $\phi(q) := \big(\phi^1(q),\ldots,\phi^{d+k}(q)\big)$ be the local expression for the isometric embedding of $\mathcal{C}$ into $N\mathcal{C}$, and let $\Phi(q,N)$ be the exponential map in each fiber. Then, by definition of the exponential map $\Phi(q,N) = \gamma(1)$, where $\gamma(s)$ is the geodesic on $N\mathcal{C}$, which starts at $\phi(q)$ with $\dot\gamma(0) = N^\alpha \nu_\alpha$.

Let $(y^a)_{a=1,\ldots,d+k}$ be Riemannian normal coordinates on $(N\mathcal{C},\overline{g})$ around $\phi(q)$, and let Γ^a_{bc} be the associated Christoffel symbols of the Levi-Civita connection. Due to the geodesic equation $\ddot\gamma^a(s) = -\Gamma^a_{bc}\big(\gamma(s)\big)\dot\gamma^b(s)\dot\gamma^c(s)$, a Taylor expansion around $s = 0$ yields

$$\gamma^a(s) = \phi^a(q) + sN^\alpha \nu^a_\alpha(q) - \frac{s^2}{2} N^\alpha N^\beta \Gamma^a_{bc}\big(\phi(q)\big)\nu^b_\alpha(q)\nu^c_\beta(q) + O(s^3).$$

By evaluating at $s = 1$, we obtain that

$$\Phi^a(q,N) = \phi^a(q) + N^\alpha \nu^a_\alpha(q) - \tfrac{1}{2} N^\alpha N^\beta \Gamma^a_{bc}\big(\phi(q)\big)\nu^b_\alpha(q)\nu^c_\beta(q) + O(|N|^3).$$

Therefore,

$$\begin{aligned}
\partial_i \Phi^a(q,N) &= \partial_i \phi^a(q) + N^\alpha \partial_i \nu^a_\alpha(q) + O(|N|^2),\\
\partial_\alpha \Phi^a(q,N) &= \big[\nu^a_\alpha - \tfrac{1}{2} N^\beta \Gamma^a_{bc}\big(\phi(\cdot)\big)\nu^b_\alpha \nu^c_\beta\big](q) + O(|N|^2)\\
&= \nu^a_\alpha(q) + O(|N|^2),
\end{aligned}$$

where we used that $\Gamma^a_{bc}\big(\phi(q)\big) = 0$ in Riemannian normal coordinates. The latter also implies that $(\overline{\nabla}_i \nu_\alpha)^a[\phi(q)] = \partial_i \nu^a_\alpha(q)$. Then, the Weingarten equation Eq. (A2) yields that

$$\partial_i \nu_\alpha(q) = \omega^\gamma_{i\alpha}(q)\nu_\gamma(q) - \mathcal{W}^l_{\alpha i}(q)\partial_l \phi(q).$$

By using that $\partial_i \phi$ and $\mathcal{W}^l_{\alpha i}\partial_l \phi$ are tangent vectors and, thus, orthogonal to ν_β for any i and β, we obtain that

$$\begin{aligned}
\overline{g}_{ij}(q,N) &= (\overline{g}_{ab}\partial_i \Phi^a \partial_j \Phi^b)(q,N)\\
&= \big(\overline{g}_{ab}\partial_i \phi^a \partial_j \phi^b - \overline{g}_{ab}\partial_i \phi^a N^\alpha \mathcal{W}^l_{\alpha j}\partial_l \phi^b\\
&\quad - \overline{g}_{ab} N^\alpha \mathcal{W}^l_{\alpha i}\partial_l \phi^a \partial_j \phi^b\big)(q) + O(|N|^2),\\
\overline{g}_{i\beta}(q,N) &= (\overline{g}_{ab}\partial_i \Phi^a \partial_\beta \Phi^b)(q,N)\\
&= (\overline{g}_{ab} N^\alpha \omega^\gamma_{i\alpha} \nu^a_\gamma \nu^b_\beta)(q) + O(|N|^2) = \overline{g}_{\beta i}(q,N),\\
\overline{g}_{\alpha\beta}(q,N) &= (\overline{g}_{ab}\partial_\alpha \Phi^a \partial_\beta \Phi^b)(q,N)\\
&= \big(\overline{g}_{ab}\nu^a_\alpha \nu^b_\beta\big)(q) + O(|N|^2).
\end{aligned}$$

Since ϕ is an isometric embedding, it holds that $\overline{g}_{ab}\partial_i \phi^a \partial_j \phi^b = g_{ij}$. The orthonormality of the normal frame yields $\overline{g}_{ab}\nu^a_\alpha \nu^b_\beta = \delta_{\alpha\beta}$. Thus,

$$\begin{aligned}
\overline{g}_{ij}(q,N) &\overset{(A1)}{=} g_{ij}(q) - 2N^\alpha \mathrm{II}_{\alpha ij}(q) + O(|N|^2),\\
\overline{g}_{i\beta}(q,n) &= N^\alpha \omega_{i\alpha\beta}(q) + O(|N|^2) = \overline{g}_{\beta i}(q,N),\\
\overline{g}_{\alpha\beta}(q,N) &= \delta_{\alpha\beta} + O(|N|^2).
\end{aligned}$$

By inverting this matrix, we end up with this proposition:

Proposition 3. The inverse metric tensor $\overline{g}^{ab}$ has the following form for all $q \in \mathcal{C}$:

$$\overline{g}(q,\varepsilon n) = \begin{pmatrix} 1 & 0 \\ C^T & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} 1 & C \\ 0 & 1 \end{pmatrix} (q,\varepsilon n),$$

where for $i,j,l,m = 1,\ldots,d$ and $\alpha,\beta,\gamma,\delta = d+1,\ldots,d+k$:

$$\begin{aligned}
A^{ij}(q,\varepsilon n) &= g^{ij}(q) + \varepsilon 2n^\alpha \mathrm{II}^{ij}_\alpha(q) + O(\varepsilon^2|n|^2),\\
B^{\gamma\delta}(q,\varepsilon n) &= \delta_{\gamma\delta} + O(\varepsilon^2|n|^2),\\
C^\gamma_i(q,\varepsilon n) &= -\varepsilon n^\alpha \omega^\gamma_{i\alpha}(q) + O(\varepsilon^2|n|^2).
\end{aligned}$$

Here, II is the second fundamental form, and ω are the coefficients of the connection on the normal bundle (see Appendix Sec. 1 for the definitions).

We note that the error is of order $\varepsilon^2|n|^2$, not only for small $|n|$, but also globally, when the metric $\overline{g}$ is chosen properly outside a tubular neighborhood of $\mathcal{C}$ (see Sec. II A and Ref. [9]). Then, the use of the expansion is justified by the fast decay of functions from the subspaces P_0 and P_ε in the fibers.

3. Transformation of measures

Let σ_1 be the density of the measure $d\overline{\mu}$ on $N\mathcal{C}$, and let σ_2 be the density of the product of the measure $d\mu$ on $\mathcal{C}$ and

the Lebesgue measure dN on the fibers $N_q\mathcal{C} \cong \mathbb{R}^k$. Define $\rho := \frac{\sigma_1}{\sigma_2}$ and

$$M_\rho : L^2(N\mathcal{C}, d\overline{\mu}) \to L^2(N\mathcal{C}, d\mu \otimes dN), \quad \Psi \mapsto \rho^{-1/2}\Psi.$$

M_ρ is an isometry because, for all $\Psi, \tilde{\Psi} \in L^2(N\mathcal{C}, d\mu \otimes dN)$:

$$\int_{N\mathcal{C}} \overline{M_\rho \Psi} M_\rho \tilde{\Psi} d\overline{\mu} = \int_{N\mathcal{C}} \overline{\Psi}\tilde{\Psi}\rho^{-1} d\overline{\mu} = \int_{N\mathcal{C}} \overline{\Psi}\tilde{\Psi} d\mu \otimes dN.$$

Therefore, it is clear that

$$M_\rho^* \Psi = \rho^{1/2}\Psi.$$

One immediately concludes

$$M_\rho M_\rho^* = 1 = M_\rho^* M_\rho,$$

and, thus, M_ρ is unitary. Now, we note that $(\partial_b, \rho^{-1/2}) = -\frac{1}{2}\rho^{-1/2}\partial_b \ln \rho$. So, for $\Delta_{d\sigma_i} := -\sigma_i^{-1}\partial_a \sigma_i g^{ab}\partial_b$, we have

$$\begin{aligned} &M_\rho^*(-\Delta_{d\sigma_1})M_\rho \\ &= -\rho^{1/2}\sigma_1^{-1}\partial_a\sigma_1 g^{ab}\partial_b \rho^{-1/2} \\ &= -\rho^{1/2}\sigma_1^{-1}\partial_a\sigma_1\rho^{-1/2}\big[g^{ab}\partial_b - \tfrac{1}{2}g^{ab}(\partial_b \ln\rho)\big]. \end{aligned}$$

On one hand,

$$\begin{aligned} &\rho^{1/2}\sigma_1^{-1}\partial_a\sigma_1\rho^{-1/2}g^{ab}\partial_b \\ &= \rho\sigma_1^{-1}\partial_a\sigma_1\rho^{-1}g^{ab}\partial_b + \tfrac{1}{2}g^{ab}(\partial_a \ln\rho)\partial_b \\ &= \sigma_2^{-1}\partial_a\sigma_2 g^{ab}\partial_b + \tfrac{1}{2}g^{ab}(\partial_b \ln\rho)\partial_a, \end{aligned}$$

and, on the other hand,

$$\begin{aligned} &\rho^{1/2}\sigma_1^{-1}\partial_a\sigma_1\rho^{-1/2}\tfrac{1}{2}g^{ab}\partial_b \ln\rho \\ &= -\tfrac{1}{4}g^{ab}(\partial_a \ln\rho)(\partial_b \ln\rho) \\ &\quad + \tfrac{1}{2}\big(\sigma_1^{-1}\partial_a\sigma_1 g^{ab}\partial_b \ln\rho\big) + \tfrac{1}{2}g^{ab}(\partial_b \ln\rho)\partial_a. \end{aligned}$$

Together, we obtain

$$\begin{aligned} &M_\rho^*(-\Delta_{d\sigma_1})M_\rho \\ &= -\sigma_2^{-1}\partial_a\sigma_2 g^{ab}\partial_b \\ &\quad -\tfrac{1}{4}g^{ab}(\partial_a \ln\rho)(\partial_b \ln\rho) + \tfrac{1}{2}\big(\sigma_1^{-1}\partial_a\sigma_1 g^{ab}\partial_b \ln\rho\big) \\ &= -\Delta_{d\sigma_2}\psi - \tfrac{1}{4}g^{ab}(\partial_a \ln\rho)(\partial_b \ln\rho) + \tfrac{1}{2}(\Delta_{d\sigma_1}\ln\rho). \end{aligned}$$

Because of $\Delta_{d\sigma_1} = \Delta_{\overline{g}}$, we have shown that

$$M_\rho^*(-\Delta_{\overline{g}})M_\rho = -\Delta_{d\sigma_2} + V_\rho, \tag{A3}$$

with $V_\rho := -\frac{1}{4}g^{ab}(\partial_a \ln\rho)(\partial_b \ln\rho) + \frac{1}{2}(\Delta_{d\sigma_1}\ln\rho)$. This formula was established many times before, and we have provided its derivation for the sake of completeness, as it is the origin of the geometric potential.

4. Expansion of the Hamiltonian

In order to deduce the formula for the effective Hamiltonian, we need that $H_\varepsilon = -\varepsilon^2(\Delta_{\overline{g}})^\varepsilon + V_c(q,n) + W(q,\varepsilon n)$ can be expanded with respect to the normal directions when operating on functions that decay fast enough. For this purpose, we split up the integral over $N\mathcal{C}$ into an integral over the fibers $N_q\mathcal{C}$, isomorphic to $\mathbb{R}^k$, followed by an integration over $\mathcal{C}$.

The following expansion is also the justification for the splitting of H_ε in Eq. (16).

Proposition 4. If an operator A satisfies

$$\|A\langle n\rangle^l\|_{\mathcal{L}(\mathcal{H})} \leqslant C_l, \quad \|\langle n\rangle^l A\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \leqslant C_l$$

for every $l \in \mathbb{N}$, then the operators $H_\varepsilon A$ and AH_ε can be expanded in powers of ε on $\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})$:

$$\begin{aligned} H_\varepsilon A &= (H_0 + \varepsilon H_1)A + O(\varepsilon^2), \\ AH_\varepsilon &= A(H_0 + \varepsilon H_1) + O(\varepsilon^2), \end{aligned}$$

where H_0 and H_1 are the operators associated with

$$\begin{aligned} \langle\Psi|H_0\Psi\rangle &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} g^{ij}\big(\overline{\varepsilon\nabla_i^{\mathrm{h}}\Psi}\big)\varepsilon\nabla_j^{\mathrm{h}}\Psi dn\, d\mu + \langle\Psi|H_{\mathrm{f}}\Psi\rangle, \\ \langle\Psi|H_1\Psi\rangle &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} 2n^\alpha \Pi_\alpha^{ij}\big(\overline{\varepsilon\nabla_i^{\mathrm{h}}\Psi}\big)\varepsilon\nabla_j^{\mathrm{h}}\Psi \\ &\quad + n^\alpha(\partial_\alpha W)_{n=0}|\Psi|^2 dn\, d\mu, \end{aligned} \tag{A4}$$

where ∇^{h} is the horizontal connection (see Sec. II B for the definition).

To derive this, let P with $\|\langle n\rangle^l P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \leqslant C_l$ for $l \in \mathbb{N}_0$ be given. The similar case of a P with $\|P\langle n\rangle^l\|_{\mathcal{L}(\mathcal{H})} \leqslant C_l$ for all $l \in \mathbb{N}_0$ will be omitted.

We set $\Psi_P := P\Psi$. By definition of H_ε, it holds that

$$\begin{aligned} \langle\Psi|H_\varepsilon\Psi_P\rangle &= \langle\Psi| - \varepsilon^2(\Delta_{\overline{g}})^\varepsilon\Psi_P\rangle \\ &\quad + \langle\Psi|[V_c(q,n) + W(q,\varepsilon n)]\Psi_P\rangle. \end{aligned} \tag{A5}$$

The formula Eq. (A3) implies that

$$\begin{aligned} &\langle\Psi| - \varepsilon^2\Delta_{\overline{g}}\Psi_P\rangle \\ &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} \varepsilon^2\overline{g}^{ab}\overline{\partial_a\Psi}\partial_b\Psi_P + \varepsilon^2 V_\rho\overline{\Psi}\Psi_P dN d\mu \\ &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} \varepsilon^2\overline{g}^{ab}\overline{\partial_a\Psi}\partial_b\Psi_P dN d\mu + O(\varepsilon^2). \end{aligned}$$

We emphasize once again that the remaining term may be of order 1 for a Ψ with energy of order 1. To calculate $-\varepsilon^2(\Delta_{\overline{g}})^\varepsilon$, we have to replace N by εn in the preceding formula. Then, we may exploit $\|\langle n\rangle^2 P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \leqslant C_2$ to insert the expansion for $\overline{g}$ from Proposition 3 into Eq. (A6). By noting that the rescaling $n = N/\varepsilon$ does not change ∂_i and replaces ∂_α by $\varepsilon^{-1}\partial_\alpha$, we obtain that

$$\begin{aligned} &\langle\Psi| - \varepsilon^2(\Delta_{\overline{g}})^\varepsilon\Psi_P\rangle \\ &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} \overline{\big[\varepsilon\partial_i + C_i^\alpha(q,\varepsilon n)\partial_\alpha\big]\Psi}A^{ij}(q,\varepsilon n) \\ &\quad \times\big[\varepsilon\partial_j + C_j^\beta(q,\varepsilon n)\partial_\beta\big]\Psi_P \\ &\quad + \overline{(\partial_\alpha\Psi)}B^{\alpha\beta}(q,\varepsilon n)\partial_\beta\Psi_P dn\, d\mu + O(\varepsilon^2) \\ &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} \big\{\varepsilon\overline{\big[\partial_i - n^\gamma\omega_{i\gamma}^\alpha(q)\partial_\alpha\big]\Psi}\big\}\big(g^{ij} + \varepsilon 2n^\alpha\Pi_\alpha^{ij}\big) \\ &\quad \times\varepsilon\big[\partial_i - n^\gamma\omega_{i\gamma}^\beta(q)\partial_\beta\big]\Psi_P \\ &\quad + \overline{(\partial_\alpha\Psi)}\delta^{\alpha\beta}\partial_\beta\Psi_P dn\, d\mu + O(\varepsilon^2) \\ &= \int_{\mathcal{C}}\int_{\mathbb{R}^k} \big(\overline{\varepsilon\nabla_i^{\mathrm{h}}\Psi}\big)\big(g^{ij} + \varepsilon 2n^\alpha\Pi_\alpha^{ij}\big)\varepsilon\nabla_j^{\mathrm{h}}\Psi_P \\ &\quad + \overline{\Psi}(-\Delta_n)\Psi_P dn\, d\mu + O(\varepsilon^2), \end{aligned} \tag{A6}$$

where we used Eq. (12) and $\Delta_n = \delta^{\alpha\beta}\partial_\alpha\partial_\beta$. Due to $\|\langle n\rangle^2 P\| \leqslant C_2$, a Taylor expansion of $W(q,\varepsilon n)$ in the fiber yields

$$W(q,\varepsilon n)P = [W(q,0) + \varepsilon n^\alpha (\partial_\alpha W)(q,0)]P + O(\varepsilon^2).$$

By plugging this and Eq. (A6) into Eq. (A5), we obtain the claim when we recall the definition $H_\mathrm{f} := -\Delta_n + V_\mathrm{c}(q,n) + W(q,0)$.

5. Derivation of the effective Hamiltonian

Here, we derive the formula for $H^{(1)}_\mathrm{eff} = U_0 H_\varepsilon U_0^*$ stated in Theorem 1. By plugging in the expansion of H_ε from Appendix Sec. 4, we have that

$$\begin{aligned} H^{(1)}_\mathrm{eff} &= U_0(H_0 + \varepsilon H_1)U_0^*\psi + O(\varepsilon^2) \\ &= U_0 H_0 U_0^*\psi + \varepsilon U_0 H_1 U_0^*\psi + O(\varepsilon^2). \end{aligned}$$

In the following, we write $\langle\cdot|\cdot\rangle_{N\mathcal{C}}$ for the scalar product on $L^2(N\mathcal{C}, dNd\mu)$. By definition of U_0 in Theorem 1, we have

$$\langle\psi^\varepsilon|U_0 A U_0^*\psi^\varepsilon\rangle_\mathcal{C} = \big\langle\varphi_\mathrm{f}^I\psi_I^\varepsilon\big|A\varphi_\mathrm{f}^J\psi_J^\varepsilon\big\rangle_{N\mathcal{C}} \tag{A7}$$

for any operator A. In view of the definition of ∇^h in Sec. II B, ∇^h satisfies the usual product formula for connections:

$$\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}^I\psi_I^\varepsilon = \varphi_\mathrm{f}^I\varepsilon\partial_i\psi_I^\varepsilon + \varepsilon\psi_I^\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}^I. \tag{A8}$$

We note that $\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}$ is really of order ε, while $\varepsilon\partial_i\psi_I^\varepsilon$ is, in general, of order 1 due to the possibly fast oscillations of ψ^ε. Furthermore, the exponential decay of the φ_f^I, which implies the exponential decay of their derivatives (see Ref. [9]), guarantees that, in the following, all the fiber integrals are bounded in spite of the terms growing polynomially in n. The product formula Eq. (A8) implies that

$$\begin{aligned} &\big\langle\varphi_\mathrm{f}^I\psi_I^\varepsilon\big|H_0\varphi_\mathrm{f}^J\psi_J^\varepsilon\big\rangle_{N\mathcal{C}} \\ &\overset{(A4)}{=} \int_\mathcal{C}\int_{\mathbb{R}^k} g^{ij}\big(\overline{\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}^I\psi_I^\varepsilon}\big)\varepsilon\nabla_j^\mathrm{h}\varphi_\mathrm{f}^J\psi_J^\varepsilon dn\,d\mu \\ &\quad + \big\langle\varphi_\mathrm{f}^I\psi_I^\varepsilon\big|H_\mathrm{f}\varphi_\mathrm{f}^J\psi_J^\varepsilon\big\rangle_{N\mathcal{C}} \\ &= \int_\mathcal{C}\int_{\mathbb{R}^k} g^{ij}\big[\big(\overline{\varphi_\mathrm{f}^I\varepsilon\partial_i\psi_I^\varepsilon}\big)\varphi_\mathrm{f}^J\varepsilon\partial_j\psi_J^\varepsilon + \varepsilon\big(\overline{\varphi_\mathrm{f}^I\varepsilon\partial_i\psi_I^\varepsilon}\big)\psi_J^\varepsilon\nabla_j^\mathrm{h}\varphi_\mathrm{f}^J \\ &\quad + \varepsilon\big(\overline{\psi_I^\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}^I}\big)\varphi_\mathrm{f}^J\varepsilon\partial_j\psi_J^\varepsilon\big]dn\,d\mu \\ &\quad + \int_\mathcal{C}\langle\varphi_\mathrm{f}^I|H_\mathrm{f}\varphi_\mathrm{f}^J\rangle\overline{\psi_I^\varepsilon}\psi_J^\varepsilon d\mu + O(\varepsilon^2) \\ &= \int_\mathcal{C} g^{ij}\delta_{IJ}\overline{p^{IK}_{\mathrm{eff}i}\psi_K^\varepsilon}\,p^{JL}_{\mathrm{eff}j}\psi_L^\varepsilon + E_\mathrm{f}\delta^{IJ}\overline{\psi_I^\varepsilon}\psi_J^\varepsilon dn\,d\mu + O(\varepsilon^2), \end{aligned}$$

with

$$p^{JK}_{\mathrm{eff}j} = -i\varepsilon\delta^{JK}\partial_j - \varepsilon\langle\varphi_\mathrm{f}^J|i\nabla_j^\mathrm{h}\varphi_\mathrm{f}^K\rangle.$$

Furthermore,

$$\begin{aligned} &\big\langle\varphi_\mathrm{f}^I\psi_I^\varepsilon\big|H_1\varphi_\mathrm{f}^J\psi_J^\varepsilon\big\rangle_{N\mathcal{C}} \\ &\overset{(A4)}{=} \int_\mathcal{C}\int_{\mathbb{R}^k} 2n^\alpha\Pi_\alpha^{ij}\big(\overline{\varepsilon\nabla_i^\mathrm{h}\varphi_\mathrm{f}^I\psi_I^\varepsilon}\big)\varepsilon\nabla_j^\mathrm{h}\varphi_\mathrm{f}^J\psi_J^\varepsilon dn\,d\mu \\ &\quad + \int_\mathcal{C}\int_{\mathbb{R}^k} n^\alpha(\partial_\alpha W)_{n=0}\overline{\varphi_\mathrm{f}^I\psi_I^\varepsilon}\varphi_\mathrm{f}^J\psi_J^\varepsilon dn\,d\mu \\ &= \int_\mathcal{C}\int_{\mathbb{R}^k} 2n^\alpha\Pi_\alpha^{ij}\big(\overline{\varphi_\mathrm{f}^I\varepsilon\partial_i\psi_I^\varepsilon}\big)\varphi_\mathrm{f}^J\varepsilon\partial_j\psi_J^\varepsilon dn\,d\mu \\ &\quad + \int_\mathcal{C}(\partial_\alpha W)_{n=0}\langle\varphi_\mathrm{f}^I|n^\alpha\varphi_\mathrm{f}^J\rangle\overline{\psi_I^\varepsilon}\psi_J^\varepsilon d\mu + O(\varepsilon) \\ &= \int_\mathcal{C} 2\Pi_\alpha^{ij}\langle\varphi_\mathrm{f}^I|n^\alpha\varphi_\mathrm{f}^J\rangle\overline{p^{IK}_{\mathrm{eff}}\psi_K^\varepsilon}\,p^{JL}_{\mathrm{eff}j}\psi_L^\varepsilon \\ &\quad + (\partial_\alpha W)_{n=0}\langle\varphi_\mathrm{f}^I|n^\alpha\varphi_\mathrm{f}^J\rangle\overline{\psi_I^\varepsilon}\psi_J^\varepsilon d\mu + O(\varepsilon), \end{aligned}$$

where we used that $p^{JK}_{\mathrm{eff}j} = -i\varepsilon\delta^{JK}\partial_j + O(\varepsilon)$. So we, indeed, obtain that

$$\begin{aligned} \big\langle\psi^\varepsilon\big|H^{(1)}_\mathrm{eff}\psi^\varepsilon\big\rangle_\mathcal{C} = \int_\mathcal{C} &g^{ijIJ}_\mathrm{eff}\overline{p^{IK}_{\mathrm{eff}i}\psi_K^\varepsilon}\,p^{JL}_{\mathrm{eff}j}\psi_L^\varepsilon \\ &+\big[E_\mathrm{f}\delta^{IJ} + \varepsilon(\partial_\alpha W)_{n=0}\langle\varphi_\mathrm{f}^I|n^\alpha\varphi_\mathrm{f}^J\rangle\big]\overline{\psi_I^\varepsilon}\psi_J^\varepsilon d\mu, \end{aligned}$$

with

$$g^{ijIJ}_\mathrm{eff} = g^{ij}\delta^{IJ} + \varepsilon\Pi_\alpha^{ij}\langle\varphi_\mathrm{f}^I|n^\alpha\varphi_\mathrm{f}^J\rangle.$$

6. The curvature of the Berry connection

In this section, we deduce the formula for the curvature of the effective Berry connection provided in Proposition 1.

We will need that the connection ∇^h, which the normal connection induces on the bundle of functions over the normal fibers, is metric (i.e., $\partial_j\langle\varphi_1|\varphi_2\rangle_{\mathcal{H}_\mathrm{f}} = \langle\nabla_j^\mathrm{h}\varphi_1|\varphi_2\rangle_{\mathcal{H}_\mathrm{f}} + \langle\varphi_1|\nabla_j^\mathrm{h}\varphi_2\rangle_{\mathcal{H}_\mathrm{f}}$) and that its curvature is given by

$$R^\mathrm{h}_{ij} := \nabla_i^\mathrm{h}\nabla_j^\mathrm{h} - \nabla_j^\mathrm{h}\nabla_i^\mathrm{h} - \nabla^\mathrm{h}_{(\partial_i,\partial_j)} = R^{\perp\gamma}_{\alpha ij}n^\alpha\partial_\gamma. \tag{A9}$$

Since the normal connection is metric, its connection coefficients $\omega_{i\alpha}^\beta$ are antisymmetric in α and β. So, integration by parts yields

$$\langle\omega^\gamma_{i\alpha}n^\alpha\partial_\gamma\varphi_1|\varphi_2\rangle(q) + \langle\varphi_1|\omega^\gamma_{i\alpha}n^\alpha\partial_\gamma\varphi_2\rangle(q) = 0.$$

Therefore, we have

$$\begin{aligned} \partial_j\langle\varphi_1|\varphi_2\rangle &= \langle\partial_j\varphi_1|\varphi_2\rangle + \langle\varphi_1|\partial_j\varphi_2\rangle \\ &= \big\langle\big(\partial_j - \omega^\gamma_{i\alpha}n^\alpha\partial_\gamma\big)\varphi_1\big|\varphi_2\big\rangle \\ &\quad + \big\langle\varphi_1\big|\big(\partial_j - \omega^\gamma_{i\alpha}n^\alpha\partial_\gamma\big)\varphi_2\big\rangle \\ &\overset{(12)}{=} \big\langle\nabla_j^\mathrm{h}\varphi_1\big|\varphi_2\big\rangle + \big\langle\varphi_1\big|\nabla_j^\mathrm{h}\varphi_2\big\rangle. \end{aligned}$$

To compute the curvature of ∇^h, we notice that a simple calculation yields

$$R^\mathrm{h}_{ij} = \big(\partial_i\omega^\gamma_{j\alpha} - \partial_j\omega^\gamma_{i\alpha}\big)n^\alpha\partial_\gamma + \big(\omega^\delta_{i\alpha}n^\alpha\partial_\delta, \omega^\gamma_{j\beta}n^\beta\partial_\gamma\big).$$

By using the commutator identity,

$$\big(\omega^\delta_{i\alpha}n^\alpha\partial_\delta, \omega^\gamma_{j\beta}n^\beta\partial_\gamma\big) = -\big(\omega^\beta_{i\alpha}\omega^\gamma_{j\beta} - \omega^\beta_{j\alpha}\omega^\gamma_{i\beta}\big)n^\alpha\partial_\gamma,$$

we obtain that

$$\begin{aligned} R^\mathrm{h}_{ij} &= -\big(\partial_{x_i}\omega^\gamma_{j\alpha} - \partial_{x_j}\omega^\gamma_{i\alpha} + \omega^\beta_{i\alpha}\omega^\gamma_{j\beta} - \omega^\beta_{j\alpha}\omega^\gamma_{i\beta}\big)n^\alpha\partial_{n^\gamma} \\ &= -R^{\perp\gamma}_{\alpha ij}n^\alpha\partial_\gamma, \end{aligned}$$

which was the claim. With this, we can compute the curvature of the effective Berry connection. It is not difficult to verify that ∇^eff is indeed a connection. Since ∇^h is metric, we have that

$$\begin{aligned} &\big\langle\varphi_\mathrm{f}^I\big|\nabla_j^\mathrm{h}\varphi_\mathrm{f}^J\big\rangle + \overline{\big\langle\varphi_\mathrm{f}^J\big|\nabla_j^\mathrm{h}\varphi_\mathrm{f}^I\big\rangle} \\ &= \big\langle\varphi_\mathrm{f}^I\big|\nabla_j^\mathrm{h}\varphi_\mathrm{f}^J\big\rangle + \big\langle\nabla_j^\mathrm{h}\varphi_\mathrm{f}^I\big|\varphi_\mathrm{f}^J\big\rangle = \partial_j\big\langle\varphi_\mathrm{f}^I\big|\varphi_\mathrm{f}^J\big\rangle = 0. \end{aligned}$$

Thus, the correction in ∇^{eff} is anti-Hermitian. Hence, for all $\psi_1, \psi_2 : \mathcal{C} \to \mathbb{C}^M$,

$$\begin{aligned}\varepsilon\partial_j(\overline{\psi_1}\cdot\psi_2) &= (\overline{\varepsilon\partial_j\psi_1})\cdot\psi_2 + \overline{\psi_1}\cdot(\varepsilon\partial_j\psi_2)\\ &= (\overline{\nabla_j^{\mathrm{eff}}\psi_1})\cdot\psi_2 + \overline{\psi_1}\cdot\big(\nabla_j^{\mathrm{eff}}\psi_2\big),\end{aligned}$$

which means that ∇^{eff} is metric. Furthermore, this entails that the correction in ∇^{eff} is purely imaginary for $M = 1$. Since φ_{f} can be chosen real valued for every $q \in \mathcal{C}$, which follows from H_{f} being real, we may gauge away the correction in an open neighborhood of any q. This implies that the curvature vanishes for $M = 1$.

To compute the curvature of ∇^{eff} for $M > 1$, we calculate

$$\begin{aligned}R^{\nabla^{\mathrm{eff}}}_{IJij} &= \varepsilon^2\big(\nabla_i^{\mathrm{eff}}\nabla_j^{\mathrm{eff}} - \nabla_j^{\mathrm{eff}}\nabla_i^{\mathrm{eff}}\big)_{IJ}\\ &= \varepsilon^2\big(\partial_i\langle\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle - \partial_j\langle\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big)\\ &\quad+\varepsilon^2\big(\langle\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\\ &\quad-\langle\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big).\end{aligned}$$

By using that ∇^{h} is metric, we obtain

$$\begin{aligned}R^{\nabla^{\mathrm{eff}}}_{IJij} &= \varepsilon^2\langle\varphi_{\mathrm{f}}^I|\mathrm{R}_{ij}^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\\ &\quad+\varepsilon^2\big(\langle\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle - \langle\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big)\\ &\quad+\varepsilon^2\big(\langle\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\\ &\quad-\langle\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big).\end{aligned}$$

Then, Eq. (A9) yields

$$\begin{aligned}R^{\nabla^{\mathrm{eff}}}_{IJij} &= -\varepsilon^2\langle\varphi_{\mathrm{f}}^I|\mathrm{R}_{\alpha ij}^{\perp\gamma}n^\alpha\partial_\gamma\varphi_{\mathrm{f}}^J\rangle\\ &\quad+\varepsilon^2\big(\langle\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle - \langle\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big)\\ &\quad+\varepsilon^2\big(\langle\varphi_{\mathrm{f}}^I|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\\ &\quad-\langle\varphi_{\mathrm{f}}^I|\nabla_j^{\mathrm{h}}\varphi_{\mathrm{f}}^K\rangle\langle\varphi_{\mathrm{f}}^K|\nabla_i^{\mathrm{h}}\varphi_{\mathrm{f}}^J\rangle\big),\end{aligned}$$

which was to be shown.

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