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Adiabatic Curvature and the *S*-Matrix

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Abstract: We study the relation of the adiabatic curvature associated to scattering states and the scattering matrix. We show that the curvature of the scattering states is not determined by the scattering data alone. However, for certain tight binding Hamiltonians, the Chern numbers are determined by the *S*-matrix and are given explicitly in terms of integrals of certain odd-dimensional forms constructed from the scattering data. Two examples, which are the natural scattering analogs of Berry's spin 1/2 magnetic Hamiltonian and its quadrupole generalization, serve to motivate the questions and to illustrate the results.

I. Introduction

In this paper we study how the adiabatic curvature and Chern numbers of scattering states are related to the scattering matrix. One motivation comes from the theory of quantum transport where the adiabatic curvature, Chern numbers, and scattering data are all related to notions of conductance. (In the quantum Hall effect, the Hall conductance is related to a Chern number [13, 3]; in mesoscopic networks the charge transport is related to the adiabatic curvature [1]; the Landauer theory of quantum transport expresses the conductance in terms of scattering data [8].) Our aim is to study this chain of relations from a general perspective and without specific reference to quantum transport.

We shall consider local deformations of quantum Hamiltonians that are associated with a scattering situation and have a band of absolutely continuous spectrum. We study the adiabatic curvature associated with this band. We shall not consider deformations that "act at infinity".

As we shall see, the *S*-matrix alone does not determine the adiabatic curvature. This may not be surprising, since even for potential scattering in one dimension the scattering matrix alone does not determine the scattering potential (one needs to know certain norming constants associated with bound states) [9]. On the other hand,

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and this may well be more remarkable, for a class of tight binding Hamiltonians the scattering data *does* determine the Chern numbers. Specifically, we construct a $2k+1$-form s_k from the S-matrix and its first derivatives. Integrating s_k over energy gives a closed $2k$-form whose cohomology class is the k^{th} Chern class of the bundle of scattering states.

The classical studies of vector bundles are concerned with finite dimensional fibers. Scattering situations give rise to bundles with infinite dimensional fibers which arise from the consideration of all the scattering states that lie in a band of energies. The geometry comes about by studying how these infinite dimensional subspaces of a fixed Hilbert space rotate as the Hamiltonian is deformed. Our results can be phrased as stating that the scattering data determine the topology of such bundles, but not their curvature.

In Sect. II we introduce some notation, recall the definition of the adiabatic curvature and some of its elementary properties, and define the forms s_k. In Sect. III we describe two key examples, the natural scattering analog of Berry's spin Hamiltonian, where the scattering bundles have nontrivial curvatures and Chern numbers. In Section IV we give a family of examples that show that the adiabatic curvature cannot be computed from the S-matrix. In Sect. V we state hypotheses on tight binding Hamiltonians under which the forms s_k compute k^{th} Chern numbers. This is the main result of this paper. We also show how these Chern numbers are related to numerical indices associated to level crossings of the S-matrix. Section VI is the proof of the main theorem, as stated in Sect. V. In Sect. VII we consider some exceptional cases. Finally, we include two appendices. The first reviews scattering in tight binding models. The second describes elements of the Chern–Weil theory of characteristic classes for bundles with infinite dimensional fibers.

II. The Adiabatic Curvature

Let X be a space of parameters with local coordinates $y=(y_1,\ldots,y_\ell)$. Let $P(y)$ be a family of orthogonal projections that depends smoothly on $y\in X$. We shall assume throughout that dP is Hilbert–Schmidt, i.e. $Tr\,|\partial_j P|^2<\infty$ for all j. *Range*(P) is a vector bundle over X with a natural connection also known as the adiabatic connection. The resulting curvature, the adiabatic curvature, is the operator valued 2-form:

$$\begin{aligned} F(P) &= -i\,PdP\wedge dPP \\ &= -i\sum_{1\leqq i<j\leqq \ell} P[\partial_i P,\partial_j P]P\,dy_i\wedge dy_j\,. \end{aligned} \tag{2.1}$$

Associated to $F(P)$ are real valued (closed) $2k$-forms $\omega_k(P)$ defined by

$$\omega_k(P)=\frac{1}{(2\pi)^k k!}Tr\,F^k(P)\,. \tag{2.2}$$

We shall denote by $c_k(\Sigma,P)$ the periods of $\omega_k(P)$ associated with a closed $2k$ dimensional manifold $\Sigma\in X$. These are closely related to the k^{th} Chern numbers and are topological invariants.[1] For scattering states we need to consider situations where P is infinite dimensional.

[1] More precisely, c_k is the k^{th} Chern number plus certain products of lower Chern numbers. We are typically interested in the lowest nonvanishing Chern classes, whose periods are exactly c_k

Now let $S(y)$ be a family of unitary operators, depending on y, acting on a fixed finite-dimensional vector space. Let the α^{th} eigenvalue of S be $\exp(i\theta_\alpha)$, and let P_α be the projection onto the corresponding eigenspace. We define the $2k+1$-form

$$s_k(y) = \frac{1}{2\pi} \sum_\alpha d\theta_\alpha \wedge \omega_k(P_\alpha) . \tag{2.3}$$

In scattering situations, the S-matrix depends on energy and on the parameters governing the system. The form s_k is then a $2k+1$ form on energy $\times$ parameter space. The relation of $\omega_k(P)$ and $c_k(\Sigma, P)$ to the scattering data and s_k, where P is the spectral projection on the scattering states, is the subject of this work.

Although $F(P)$ is not linear in P, it turns out that $\omega_k(P)$ has certain linearity properties in P, which we shall use in studying the curvature of scattering states. What we need is summarized by:

Proposition 1. *Let P be a family of smooth orthogonal projections, with dPP Hilbert–Schmidt, and $P_\perp = 1 - P$, then*

1. *dP and $PdPP_\perp$ are also Hilbert–Schmidt.*
2. *$\omega_k(P)$ and $\omega_k(1-P)$ are well defined and finite for all natural k. Furthermore,*

$$\omega_k(P) = -\omega_k(1-P) . \tag{2.4}$$

3. *Let Q be a second orthogonal projection with dQ Hilbert–Schmidt and with $PQ = QP = 0$. Then*

$$\omega_1(P+Q) = \omega_1(P) + \omega_1(Q) . \tag{2.5}$$

Proof. Since $P = P^2$, $dP = PdP + dPP$ and $PdPP = 2PdPP = 0$. Thus $PdP = PdPP_\perp$ and

$$\partial_j P = P(\partial_j P)P_\perp + P_\perp(\partial_j P)P , \tag{2.6}$$

which implies statement 1. Consequently,

$$(\partial_j P)(\partial_k P) = P(\partial_j P)P_\perp(\partial_k P)P + P_\perp(\partial_j P)P(\partial_k P)P_\perp . \tag{2.7}$$

The product of two Hilbert–Schmidt operators is trace class [12], so $F(P)$ and $F(P_\perp)$ are trace class and $\omega_k(P)$ and $\omega_k(1-P)$ are well-defined. To derive Eq. (2.4) note that

$$\begin{aligned} F(P_\perp) &= -i\, P_\perp dP_\perp \wedge dP_\perp P_\perp \\ &= -i\, P_\perp dP \wedge dPP_\perp \\ &= -i\, dP_\perp P \wedge PdP_\perp \\ &= -i\, dPP \wedge PdP . \end{aligned} \tag{2.8}$$

Now, with $A = dPP$ and $B = PdP$, the commutativity of trace and anticommutativity of forms gives:

$$\begin{aligned} Tr(A \wedge B)^k &= Tr[(A \wedge B)^{k-1}(A \wedge B)] \\ &= -Tr[B \wedge (A \wedge B)^{k-1} \wedge A] \\ &= -Tr(B \wedge A)^k , \end{aligned} \tag{2.9}$$

from which Eq. (2.4) follows. To prove Eq. (2.5), use the algebraic identity

$$F(P+Q) = F(P) + F(Q) - iCC^\dagger - iC^\dagger C , \tag{2.10}$$

where $C = (dQ)P$. Since $Tr\, CC^\dagger = -Tr\, C^\dagger C$ by the commutativity of trace and anticommutativity of forms, Eq. (2.5) follows.

Remark. For $k \neq 1$, $\omega_k(P+Q)$ is not, in general, the sum of $\omega_k(P)$ and $\omega_k(Q)$. For example, for $k = 2$,

$$F^2(P+Q) = F^2(P) - i\{F(P), C^\dagger C\} - C^\dagger C C^\dagger C + (\text{terms with } (Q,C) \leftrightarrow (P,C^\dagger))\,, \tag{2.11}$$

so

$$\omega_2(P+Q) = \omega_2(P) + \omega_2(Q) - \frac{i}{(2\pi)^2} Tr(F(P)C^\dagger C + F(Q)CC^\dagger)\,. \tag{2.12}$$

However, we shall see that $c_k(\Sigma, P+Q)$ does equal $c_k(\Sigma,P) + c_k(\Sigma,Q)$.

It sometimes happens that symmetry, in particular time-reversal symmetry, forces certain periods to equal zero. We recall [2]

Proposition 2. *Suppose P commutes with an antiunitary operator. Then*

$$\omega_{2k+1}(P) = 0\,. \tag{2.13}$$

The example below gives the curvature of certain families of infinite dimensional projections. This example will play a role in Sect. IV.

Example 1. Let $X = \mathbb{R}^2$, let $\Lambda(x)$ be a fixed, smooth real-valued function, and let $U(a,b)$ be a two parameter family of unitary operators on $L^2(\mathbb{R})$ associated with gauge transformations and translations:

$$(U(a,b)\psi)(x) = \exp(i\, b\Lambda(x-a))\,\psi(x-a)\,. \tag{2.14}$$

Consider the projections $P(a,b) = U(a,b)QU^\dagger(a,b)$, with Q a fixed projection such that $Tr\, Q(-\Delta + \Lambda^2)Q < \infty$. We compute

$$\begin{aligned} 2\pi\omega_1(P) &= da \wedge db\, Tr(Q\Lambda' Q + [Q\Lambda Q, Q\nabla Q]) \\ &= da \wedge db\, Tr\, Q\Lambda' Q\,. \end{aligned} \tag{2.15}$$

We have used the fact that $Tr[A,B] = 0$ if A and B are Hilbert–Schmidt. If Λ' is a non-negative function of x then $Tr\, Q\Lambda' Q \geqq 0$. For $\Lambda(x) = x$, the curvature for finite dimensional projections is actually a positive integral multiple of the area form:

$$2\pi\omega_1(P) = da \wedge db\, Tr\, P\,. \tag{2.16}$$

It follows that for $\Lambda' > 0$ and P finite dimensional, the adiabatic curvature is a positive, increasing function of P. If P has finite codimension, then Eq. (2.4) says that the curvature is a negative increasing function of P. This is peculiar. Finite codimensional projections are clearly "larger" than finite dimensional projections, and the adiabatic curvature increases with P, so how can the curvature be positive for finite dimensional projections and negative for finite codimensional projections? A useful analogy, where something similar happens, is negative temperatures in canonical ensembles; energy is an increasing function of temperature, but ensembles with negative temperature have more energy than those with positive temperature.

A key feature of the forms ω_k is that their periods are topological invariants. This is a result of Chern–Weil theory, as discussed in Appendix II. In particular, we have the following

Proposition 3. *Let P be a family of orthogonal projections such that dP is Hilbert–Schmidt, and let Σ be a (smooth) closed $2k$ dimensional surface in parameter space. Then*

$$c_k(\Sigma, P) = \int_\Sigma \omega_k(P) \tag{2.17}$$

is a topological invariant of P. If Q is another orthogonal projection with $PQ = 0$ and with dQ Hilbert–Schmidt, then

$$c_k(\Sigma, P+Q) = c_k(\Sigma, P) + c_k(\Sigma, Q)\,. \tag{2.18}$$

If $k = 1$, or if the first $k-1$ Chern classes of P vanish on Σ, then $c_k(\Sigma, P)$ is an integer, the k^{th} Chern class of P applied to Σ.

III. Examples–Scattering of Spinning Particles

In this section we describe two fairly natural scattering problems where the bundles of scattering states have nontrivial curvatures and Chern numbers. The question of recovering the curvature and Chern numbers from the scattering data is therefore not an empty question. It turns out that the two examples of this section also fall into the wider class that we shall introduce in Sect. V, for which we show that the Chern numbers can be recovered from the scattering data. We use these two examples to illustrate how this procedure works.

Consider an electron with spin 1/2 on a semi-infinite chain with the site at the origin coupled to an adiabatically rotating magnetic field $\vec{B}$. In this example the S-matrix turns out to be essentially the Hilbert transform of Berry's spin Hamiltonian, so it may be viewed as playing the analogous role in scattering situations.

Let $h(\vec{B}) = \vec{B} \cdot \vec{\sigma} + |B|$, with $\vec{\sigma}$ the triplet of Pauli matrices. Consider the tight binding Hamiltonian $H(\vec{B})$ on the non-negative integers:

$$(H(\vec{B})\psi)(n) = \psi(n+1) + \psi(n-1) + \delta_{n0}\, h(\vec{B})\psi(n)\,, \tag{3.1}$$

where $\psi(n) \in \mathbb{C}^2$ and $\psi(-1) = 0$.

The spectrum is an interval if $|B| \leqq 1/2$ (and is absolutely continuous) and it is an interval and a point if $|B| > 1/2$. Namely,

$$Spec(H(\vec{B})) = \begin{cases} [-2,2] & \text{if } |B| \leqq 1/2 \\ [-2,2] \cup \{2|B| + \frac{1}{2|B|}\} & \text{if } |\vec{B}| > 1/2\,. \end{cases} \tag{3.2}$$

The bound state for $|\vec{B}| > 1/2$ has an exponentially localized wave function

$$\psi_0(\vec{B}, n) = (2|B|)^{-n} u\,, \tag{3.3}$$

where $u \in \mathbb{C}^2$ is an eigenvector of $\vec{B} \cdot \vec{\sigma}$ with eigenvalue $|B|$. Let P be the projection onto the scattering states; $Tr(P) = \infty$. $P_\perp = 1 - P$ is the projection onto the bound state with $Tr(P_\perp) \leqq 1$. $P_\perp$ is smooth away from $|B| = 1/2$ and we can use Eq. (2.4)

to compute the adiabatic curvature of P. The parameter space in this example is three dimensional, so only $\omega_1(P)$ may be different from zero. Using for example the explicit computation in [3] for a single spin 1/2 electron in a magnetic field, one finds:

$$2\pi\omega_1(P) = -2\pi\omega_1(P_\perp) = \begin{cases} 0 & \text{if } |\vec{B}| \leqq 1/2\,; \\ -(1/2)dArea & \text{if } |\vec{B}| > 1/2\,, \end{cases} \tag{3.4}$$

where $dArea$ is the area form on the unit sphere $|B| = 1$. Integrating the curvature on a 2-sphere S^2 enclosing the origin in the 3-dimensional space of magnetic fields gives the first Chern number for the bundle of scattering states P:

$$c_1(S^2, P) = \begin{cases} 0, & \text{if } |B| \leqq 1/2\,; \\ -1 & \text{if } |B| > 1/2\,. \end{cases} \tag{3.5}$$

The on-shell scattering matrix at wave number k is the 2×2 matrix (see Appendix I)

$$S(k, \vec{B}) = -\frac{h(\vec{B}) - z}{h(\vec{B}) - 1/z}\,, \tag{3.6}$$

where $z = \exp ik$, $0 \leqq k \leqq \pi$. Let $P^S_{0,1}$ denote the two spectral projections for the S matrix. The corresponding eigenvalues (related to the phase shifts) and adiabatic curvatures are:

$$\exp i\theta_0(k, \vec{B}) = -z^2, \qquad \exp i\theta_1(k, \vec{B}) = -(2|\vec{B}| - z)/(2|\vec{B}| - 1/z)\,, \tag{3.7}$$

$$2\pi\omega_1(P^S_0) = -2\pi\omega_1(P^S_1) = -(1/2)dArea\,. \tag{3.8}$$

We now consider the 3-form s_1 defined in Eq. (2.3). In this example,

$$\begin{aligned} s_1(k, \vec{B}) &= \frac{1}{2\pi}(d\theta_0 \wedge \omega_1(P^S_0) + d\theta_1 \wedge \omega_1(P^S_1)) \\ &= \frac{1}{8\pi^2}(d\theta_1 - d\theta_0) \wedge dArea\,. \end{aligned} \tag{3.9}$$

Now let $\ell_i = (\theta_i(k = \pi) - \theta_i(k = 0))/2\pi$. We refer to ℓ_i as the *winding* of θ. From Eq. (3.7) we compute

$$\ell_0 = 1, \qquad \ell_1 = \begin{cases} 1 & \text{for } |\vec{B}| < 1/2\,; \\ 0 & \text{for } |\vec{B}| > 1/2\,. \end{cases} \tag{3.10}$$

For $|B| \neq 1/2$, by integrating the 3-form s_1 over k we recover $\omega_1(P)$, as given in Eq. (3.4). By integrating s_1 over energy $\times S^2$ we recover the Chern numbers.

The spin 1/2 example is a basic paradigm for adiabatic curvature of scattering states in situations where time reversal invariance is broken. In systems with time reversal invariance, the abelian curvature $\omega_1(P)$ vanishes identically, by Proposition 2, and only the even forms $\omega_{2n}(P)$ are interesting. A basic paradigm for a non-abelian adiabatic curvature is a spin 3/2 particle interacting with an adiabatically varying quadrupole field (for details, see [2]).

Consider a spin-3/2 particle on a semi-infinite chain interacting with a quadrupole at the origin. That is, let

$$(H(B)\psi)(n) = \psi(n+1) + \psi(n-1) + \delta_{n0}\, h(Q)\psi(n)\,, \tag{3.11}$$

where $\psi(n) \in \mathbb{C}^4$, $\psi(-1) = 0$ and

$$h(Q) = |Q| + \sum_{i,j=1}^{3} Q_{ij} J_i J_j\,. \tag{3.12}$$

Q is a real, symmetric, traceless 3×3 matrices and $\{J_i\}$ are the usual angular momentum operators and $|Q|^2 = \frac{3}{2}\, Tr(Q^2)$. The parameter space associated with unit quadrupoles is a 4-sphere of the form $|Q| = 1$.

The spectral analysis of $H(Q)$ shows that the spectrum is an interval if $|Q| \leqq 1/2$ and an interval and a point if $|Q| > 1/2$. More precisely

$$Spec(H(Q)) = \begin{cases} [-2,2] & \text{if } |Q| \leqq 1/2 \\ [-2,2] \cup \{2|Q| + \frac{1}{2|Q|}\} & \text{if } |Q| > 1/2\,. \end{cases} \tag{3.13}$$

The main difference with the spin 1/2 example is that the multiplicity of the continuous spectrum is now 4, rather than 2.

The bound state, with spectral projection $P_\perp$, is doubly degenerate and has curvature $\omega_2(P_\perp)$ which is $3/(8\pi^2)$ the area form on the 4-sphere [2]. The scattering states, with spectral projection P, have the complementary curvature by Eq. (2.4). Consequently

$$\omega_2(P) = -\,\omega_2(P_\perp) = \begin{cases} 0 & \text{if } |Q| < 1/2\,; \\ -(3/8\pi^2) dVol & \text{if } |Q| > 1/2\,, \end{cases} \tag{3.14}$$

where $dVol$ is the volume form of the unit 4-sphere. For the Chern numbers, which are now integrals of the curvature on the 4-sphere one has

$$c_2(S^4, P) = \begin{cases} 0, & \text{if } |Q| \leqq 1/2\,; \\ -1 & \text{if } |Q| > 1/2\,. \end{cases} \tag{3.15}$$

The on-shell scattering matrix at wave number k is now the 4×4 matrix (see Appendix I)

$$S(k, Q) = -\frac{h(Q) - z}{h(Q) - 1/z}\,, \tag{3.16}$$

where, as before, $z = \exp ik$, $0 \leqq k \leqq \pi$. It has two eigenvalues

$$\exp i\theta_0(k, Q) = -z^2, \qquad \exp i\theta_1(k, Q) = -\,(2|Q| - z)/(2|Q| - 1/z)\,, \tag{3.17}$$

each of which is two-fold degenerate. Let $P^S_{0,1}$ denote the two spectral projections for the S matrix. The corresponding adiabatic curvatures are:

$$\omega_2(P^S_0) = -\,\omega_2(P^S_1) = -\frac{3}{8\pi^2} dVol\,. \tag{3.18}$$

Consider now the 5-form $s_2(k, Q)$, defined in Eq. (2.3). By integrating s_2 over k we recover ω_2 of the scattering states, and by integrating s_2 over energy $\times\, S^4$ we recover c_2.

At this stage, the fact that in both examples the adiabatic curvatures ω_i have been recovered from the scattering data might appear to be a coincidence. We shall see in Sect. V that the dependence of Chern numbers on scattering data (by integrating forms such as s_1 and s_2) is a general phenomenon. However, the recovery of the forms ω_i pointwise is indeed a coincidence and is a consequence of the rotational symmetry of these examples.

IV. Curvature is not Computable from Scattering Data

Here we construct examples that show that ω_1 of the scattering states need not be computable from the S-matrix. In these examples ω_1 of the scattering states is nonzero, but the on-shell S-matrix is independent of one of the parameters, so s_1 is identically zero.

Let V be any reasonable perturbation of the Laplacian in one dimension such that there is a good scattering theory and one or more bound states. For example, let V be a short range potential on the line. Consider the family of Hamiltonians

$$H(a,b) = U(a,b)\left(-\frac{d^2}{dx^2} + V\right)U^\dagger(a,b) = \left(-i\frac{d}{dx} - b\Lambda'(x-a)\right)^2 + V(x-a)\,, \tag{4.1}$$

where U is as in Eq. (2.14). Let $y = (k,a,b)$ and let ψ_y be a solution of the differential equation $(H(a,b) - k^2)\psi_y = 0$. Since $\psi_y = U(a,b)\psi_{k,0,0}$ we have, in the limit $|x| \to \infty$,

$$\psi_y(x) = e^{ib\Lambda(\pm\infty)}\psi_{k,0,0}(x-a)\,. \tag{4.2}$$

From this and the definition of the on-shell S-matrix (see appendix I), we see that

$$S(k,a,b) = \begin{pmatrix} r_R(k)e^{2ika} & t_L(k)e^{ib\Delta\Lambda} \\ t_R(k)e^{-ib\Delta\Lambda} & r_L(k)e^{-2ika} \end{pmatrix}, \tag{4.3}$$

where $\Delta\Lambda = \Lambda(\infty) - \Lambda(-\infty)$. In particular, if $\Lambda(\infty) = \Lambda(-\infty)$, the S-matrix is independent of b. Since curvature is a property of pairs of variables and only one parameter affects S, S cannot see any curvature.

Now let Q be the projection on the (finite dimensional) subspace of bound states of H, and suppose that $Tr\,Q(-\Delta + \Lambda^2)Q < \infty$. Let $P = 1 - Q$. P is the projection on the (positive energy) scattering states. From Proposition 1 and Example 1 we have that

$$2\pi\omega_1(P) = -2\pi\omega_1(Q) = -da \wedge db\, Tr\, Q\Lambda' Q\,. \tag{4.4}$$

Since Λ can be chosen independently of V, and hence of Q, we can easily arrange for $Tr\,Q\Lambda'Q$ to be nonzero. For example, we can take

$$\Lambda'(x) = \begin{cases} 1 & |x| < L\,; \\ -1 & |x-2L| < L\,; \\ 0 & \text{otherwise}\,, \end{cases} \tag{4.5}$$

for a large value of L. $\Delta\Lambda = 0$, so S sees no curvature, but $Tr\,Q\Lambda'Q \to rank(Q) \neq 0$ as $L \to \infty$.

V. Chern Numbers are Computable from Scattering Data

In this section we describe the main result of this paper. We give sufficient conditions for the scattering data to determine the Chern numbers of the scattering states. When these conditions hold, the Chern numbers are given by explicit integrals of odd-dimensional forms s_k. The proof is deferred to Sect. VI.

We shall consider a class of scattering problems which we describe below. We shall assume various properties, some of explicit nature, and some about spectral and scattering properties. The scattering problems discussed in Sect. III can be seen to satisfy all the assumptions.

Let X be a manifold with coordinates $\{y_j\}$. Consider the family of (self-adjoint) Hamiltonians on the positive integers

$$(H(\{y\})\psi)(n) = \psi(n+1) + \psi(n-1) + \sum_m h_{nm}(\{y\})\psi(m)\,, \tag{5.1}$$

where $\psi(n) \in \mathbb{C}^N$, $\psi(-1) = 0$, $h_{mn} = h_{nm}^\dagger$, and $h_{nm} = 0$ if either $n > M$ or $m > M$. Such models can be thought of as describing a spin $(N-1)/2$ particle on a half line reflected and scattered by h. Alternatively, one may consider a spinless particle moving on N semi-infinite chains with cross links in a finite ball. In either picture there are precisely N scattering channels. We shall assume that h depends smoothly on y.

We first recall some elementary facts about the spectral properties of such Hamiltonians. The band of scattering states (i.e. the absolutely continuous spectrum) is the interval $[-2,2]$ and has multiplicity N. The rest of the spectrum is made of a finite number of eigenvalues. Those outside the interval $[-2,2]$ have exponentially localized eigenfunctions, while embedded eigenvalues have eigenfunctions of compact support. We shall denote by P the spectral projection on the scattering states. Clearly $Tr(P) = \infty$.

It is convenient to parameterize the energies by the wave vector k with $k \in I = [0,\pi]$. For notational convenience, we let $y_0 = k$. We set $Y = I \times X$.

In order to even begin to ask geometric questions about the bundle of scattering states we need to assume certain spectral properties. In particular, the bundle P is smooth on X if its complement, $P_\perp$ is. This is the case if no eigenvalues dissolve or get absorbed into the continuum as y changes.

In addition, in order to discuss geometric issues associated with the scattering data we need to assume certain things about the on-shell S-matrix. The on-shell S-matrix $S(y)$ is an $N \times N$ matrix which, we assume, is unitary and depends smoothly on all variables y. The phase shifts, $\theta_\alpha(y)$, are the arguments of the eigenvalues of S and $\alpha \in 1,\ldots,N$. A priori the determination of the phase shifts involves two ambiguities. One is that phases are determined modulo 2π and a second is associated with the assignment of the index α. In order to fix a determination we need to discuss eigenvalue crossings.

We assume that $S(y)$ has, at most, level crossings on a set Z of codimension $2k+1, k \geqq 1$. This implies that Y/Z has the same fundamental group as X, so, once we fix a determination of phases and indices at a single surface $k_0 \times X$, there is a unique continuation to all points of X/Z. We shall, in fact, determine the phase shifts and the labels α at one energy k_0.

In ordinary potential scattering theory it is customary to determine the phase shifts by the condition that the phase shifts are zero at infinite energy. In tight-binding models there are no infinite energies, and the natural analog is to fix the

phase shifts at the thresholds of the absolutely continuous spectrum. In order to do that we assume that the S-matrix approaches -1 at the bottom of the (absolutely continuous) spectrum, and set

$$\theta_\alpha(y_0 = 0, \{y_i\}) = -\pi\,. \tag{5.2}$$

To assign indices α near the bottom of the spectrum we assume

$$S(y_0, \{y_i\}) + 1 = iy_0 A(\{y_i\}) + O(y_0^2)\,, \tag{5.3a}$$

with $A(\{y_i\})$ smooth, Hermitian, matrix-valued function that has no level crossings in X. (Compare also [7] which discusses threshold behavior in potential scattering). This allows us to fix a determination by assigning α to the phase shift according to the order of the eigenvalue of A. By continuity (using standard facts from analytic perturbation theory) we have a unique determination of the phases and their labels throughout X/Z.

In tight-binding models the bottom and top of the continuous spectrum play similar roles, and therefore together with Eq. (5.3a) we assume also

$$S(y_0, \{y_i\}) + 1 = i(y_0 - \pi)T(\{y_i\}) + O((y_0 - \pi)^2)\,, \tag{5.3b}$$

with $T(\{y_i\})$ smooth, Hermitian, matrix-valued function that has no level crossings in X. Other limiting values for the S-matrix occur when threshold states exist at $y_0 = 0$ or $y_0 = \pi$. In Sect. VII we shall discuss an extension of Theorem 1 below to situations where Eq. (5.3a) and Eq. (5.3b) fail.

Theorem 1. *Let P be the infinite dimensional spectral projection on the scattering states for the Hamiltonian* (5.1), *where X is a closed and smooth $2k$ manifold, with $k \geqq 1$. Suppose that the on-shell S-matrix is smooth and has eigenvalue crossings on a set Z of codimension $2k+1$ and near threshold has the form* (5.3a) *and* (5.3b). *Let*

$$s_k(y) = \frac{1}{2\pi} \sum_\alpha d\theta_\alpha(y) \wedge \omega_k(P_\alpha^S)\,, \tag{5.4}$$

where $\omega_n(P_\alpha^S)$ is the adiabatic curvature associated with the α^{th} spectral projection of the on-shell S-matrix. Suppose $s_k(y) = O(|\text{dist}(y, Z)|^{-2k})$, $y \in Y = I \times X$. Then $c_k(X, P)$ is determined by scattering data:

$$c_k(X, P) = \int_X \omega_k(P) = \int_Y s_k(y)\,. \tag{5.5}$$

The proof of this theorem is based on a one-to-one correspondence between scattering states and eigenstates of the on-shell S-matrix. This correspondence is enough to recover topological information such as Chern numbers. It is not sufficient to recover local geometric information such as curvature. The proof of Theorem 1 is deferred to the next section.

Remark. In general, only unitary invariant properties of the on-shell S-matrix have physical significance [4]. Equation (5.5) implies that the adiabatic curvature for the scattering states is given by

$$\omega_k(P) = (1/2\pi) \int_I s_k(y) + \chi\,, \tag{5.6}$$

where χ is an undetermined exact form. The form $\omega_k(P)$ is physically significant, yet $\int_I s_k$ is not invariant under unitary transformations of S. The phase shifts θ_α are unitary invariants, but the curvatures of projections for the S-matrix, $\omega_k(P_\alpha^S)$, are not. For example, under the transformation $S \to U^\dagger S U$, $P_\alpha^S \to U^\dagger P_\alpha^S U$ and

$$\omega_1(P_\alpha^S) \to \omega_1(P_\alpha^S) + d\, Tr(P_\alpha^S U^\dagger dU)\,. \tag{5.7}$$

It follows that $\int_I s_k(y)$ is not invariant under y-dependent unitary transformations, and requires a basis-dependent correction χ. The cohomology class of $\int_I s_k$, however, is defined independent of basis.

When X is 2-dimensional (or when we are studying a 2-dimensional surface Σ in X) the generic level crossings occur at isolated points in Y. We associate numerical indices to these level crossings, as follows:

Index. Let z_j be a crossing point for the α and β eigenvalues of the S-matrix with $0 < y_0 < \pi$. Let $2\pi n(z_j) = \theta_\alpha(z_j) - \theta_\beta(z_j)$. The index is defined to be

$$Index(z_j) = n(z_j) c_1(S^2(z_j), P_\alpha^S)\,, \tag{5.8}$$

where $S^2(z_j)$ is a small sphere centered at z_j. For a generic crossing, this index is ± 1 [1, 12].

Proposition 4. *The first Chern number of the scattering bundle is given by*

$$c_1(\Sigma, P) = \sum_{0<(z_j)_0<\pi} Index(z_j) + \sum_\alpha \ell_\alpha c_1(\Sigma, P_\alpha^T)\,, \tag{5.9}$$

where $c_1(\Sigma, P_\alpha^T)$ is the Chern number associated with the α^{th} spectral projection of the hermitian matrix $T(y_i)$ of Eq. (5.3a) *and $\ell_\alpha = (\theta_\alpha(\pi) - \theta_\alpha(0))/2\pi$.*

Remark. If the S-matrix has no eigenvalue crossings, the first term on the rhs of Eq. (5.9) is absent. Furthermore, in the absence of level crossings, two windings ℓ_α and ℓ_β can differ by at most one. Since $\sum_\alpha c_1(\Sigma, P_\alpha^T) = 0$, the second term on the rhs of Eq. (5.9) is bounded by $\sum_\alpha |c_1(\Sigma, P_\alpha^T)|$.

Proof of Proposition 4 (given Theorem 1). Since $\omega(P)$ is closed, $d\theta \wedge \omega(P) = d(\theta\omega(P))$, so

$$2\pi \int_{Y/\{Z\}} s_1(y) = \sum_\alpha \sum_Z \int_{S^2} \theta_\alpha(y)\omega_1(P_\alpha^S) + \sum_\alpha \left(\int_{\pi\times\Sigma} \theta_\alpha(\pi, y_1, y_2)\omega_1(P_\alpha^S) - \int_{0\times\Sigma} \theta_\alpha(0, y_1, y_2)\omega_1(P_\alpha^S) \right). \tag{5.10}$$

By Prop. 1, $\omega_1(P_\alpha^S) + \omega_1(P_\beta^S) = \omega_1(P_\alpha^S + P_\beta^S)$. Since $P_\alpha^S + P_\beta^S$ is smooth near the α, β level crossing the j^{th} crossing contributes

$$\int_{S^2} (\theta_\alpha(y)\omega_1(P_\alpha^S) + \theta_\beta(y)\omega(P_\beta^S)) = 2\pi n(z_j) \int_{S^2} \omega_1(P_\alpha^S)\,. \tag{5.11}$$

This gives the first sum on the rhs of Eq. (5.9). By our normalization $\theta_\alpha(0, y_1, y_2) = -\pi$. Since $\sum_\alpha \omega(P_\alpha^S) = 0$, the integral over $0 \times \Sigma$ vanishes. Now $\theta_\alpha(\pi, y_1, y_2) = \pi(2\ell_\alpha - 1)$. Since the spectral projections for $S(\pi - 0, y)$ and $T(y)$ coincide, the integral over $\pi \times \Sigma$ gives the second term on the rhs of Eq. (5.9). □

VI. Proof of Main Theorem

This section is a proof of Theorem 1 given the hypotheses in Sect. V. We shall first prove Eq. (5.5) for the first Chern number and then outline how the general case is treated.

By assumption our scattering "potential" h is supported on a disk of radius M for some integer M.

Now pick an integer $L \gg M$ and apply a Dirichlet condition at L. If L is chosen large enough, this causes only a small change in the wavefunctions of the bound states, and their curvatures are only slightly deformed. Since the Chern numbers of the bound states are topological invariants, this implies that they are unchanged. Thus the Dirichlet condition at L also does not change the Chern class of the complementary part of the spectrum, corresponding to the energy interval $[-2,2]$.

The cutoff at L breaks the system up into two noninteracting subsystems. The exterior states, supported on $\{n > L\}$, have absolutely continuous spectrum and are completely independent of $\{y_i\}$. These states contribute nothing to the curvature and are henceforth ignored. The interior states, supported on $\{n < L\}$, have a discrete, in fact finite, spectrum. This spectrum contains small perturbations of the discrete eigenvalues of the original problem, plus a number of new eigenvalues between -2 and 2. Since the space of states supported on $\{n < L\}$ is a subspace of the original Hilbert space, by the variational principle the number of eigenvalues below -2 for the system cut off at L cannot exceed the number for the original unregularized system, namely the number of bound states with energy below -2. Since each of these states remains, there can be no others. Similarly, new states with energy greater than 2 cannot appear.

We therefore look for the states with energy between -2 and 2. For $L > n > M$, the wavefunctions take the form

$$\psi_{m,\alpha}(n) = \zeta_\alpha(k, y)(\exp(-ikn) + \exp(i(\theta_\alpha + kn))) , \tag{6.1}$$

where ψ takes values in $\mathbb{C}^N$, $\zeta_\alpha(k, \{y_i\})$ is an eigenvector of $S(k, \{y_i\})$ with eigenvalue $\exp(i\theta_\alpha(y))$, and the "energy bands," $k_{m\alpha}(\{y_i\})$, solve

$$\theta_\alpha(k, \{y_i\}) + 2kL = (2m-1)\pi, \quad m = 1, \ldots, L + \ell_\alpha - 1 . \tag{6.2}$$

Equation (6.2) is equivalent to the Dirichlet condition $\psi(L) = 0$. Although $k = 0$ is a solution to Eq. (6.2) with $m = 0$, $\psi_{0,\alpha}$ is identically zero, so this solution is not counted. Similarly $k = \pi$ solves Eq. (6.2) for $m = L + \ell$, but this also generates the zero wavefunction.

We temporarily suppress the α index and, as before, write $y_0 = k$. We also write ω for ω_1. Subscripts on ω will refer to spatial indices, so ω_{12} is the component of ω in the 1-2 plane, etc.

Taking derivatives we find that, for fixed m, $\partial k/\partial y_j = -(\partial\theta/\partial y_j)/2L$. We also define a density-of-states function

$$\rho(k) = (2L + d\theta/dk)/2\pi . \tag{6.3}$$

Of course, $1/\rho(k)$ is not precisely the spacing between levels. Rather,

$$\rho(k_m)(k_{m+1} - k_{m-1})/2 = 1 + O(L^{-3}) . \tag{6.4}$$

Each energy level $k_m(y)$ satisfying Eq. (6.2) is associated to two line bundles. One is the sub-bundle of the trivial Hilbert space bundle $\Sigma \times \ell_2$ spanned by ψ_m. The other is the sub-bundle of $\Sigma \times \mathbb{C}^N$ spanned by $\zeta(k, y)$. These two bundles are isomorphic, as the limiting behavior of ψ defines ζ, and as each ζ, together with a solution to Eq. (6.2), defines an eigenfunction ψ. Isomorphic bundles have the same Chern classes, so we may compute the Chern class of the ψ bundle by integrating the curvature of the ζ bundle. This is just the restriction to the surface $k_m(y)$ of the 2-form $\omega(P^S)$ on $I \times X$.

Two tangents to the surface $k_m(\{y_j\})$ are $(-\partial_1\theta/2L, 1, 0)$ and $(-\partial_2\theta/2L, 0, 1)$. Applying ω to these two vectors, we find that ω, restricted to the surface $k_m(\{y_j\})$, equals $f(k_m(y), y_1, y_2)\, dy^1 \wedge dy^2$, where

$$f(y) = \omega_{12} + \frac{\omega_{20}\partial_1\theta + \omega_{01}\partial_2\theta}{2L} . \tag{6.5}$$

So we can write, using Eq. (A.5),

$$c_1(\Sigma, P) = \frac{1}{2\pi} \sum_{\alpha=1}^{n} \sum_{m=1}^{L+\ell_\alpha-1} \int_\Sigma f_\alpha(k_{\alpha,m}(y), y_1, y_2)\, dy_1 \wedge dy_2 . \tag{6.6}$$

Next we replace the sum over m with an integral over k_0, using the fact that

$$f(k_m, y_1, y_2) = \int_{(k_{m-1}+k_m)/2}^{(k_m+k_{m+1})/2} f(k, y_1, y_2)\rho(k)\, dk + O(L^{-2}) . \tag{6.7}$$

Note that $f(y)$ is defined by Eq. (6.5) for all y_0, not just for $y_0 = k_m(y)$. Some care is required for $f(k_1)$ and $f(k_{L+\ell-1})$. Equation (6.7) still applies, as long as we take $k_0 = 0$ and $k_{L+\ell} = \pi$. We also have that

$$\begin{aligned} \int_0^{k_1/2} f(y)\rho(y)\, dk &= f(0, y_1, y_2)/2 + O(L^{-1}) , \\ \int_{(\pi+k_{L+\ell-1})/2}^{\pi} f(y)\rho(y)\, dk &= f(\pi, y_1, y_2)/2 + O(L^{-1}) . \end{aligned} \tag{6.8}$$

Plugging (6.7) and (6.8) into (6.6) we find

$$c_1(\Sigma, P) = \frac{1}{2\pi} \sum_{\alpha=1}^{n} \int_{I\times\Sigma} f_\alpha(y)\rho_\alpha(y) - \frac{1}{4\pi} \int_\Sigma \sum_\alpha (f_\alpha(0, y_1, y_2) + f_\alpha(\pi, y_1, y_2)) + O(L^{-1}) . \tag{6.9}$$

By Eq. (2.4) $\sum_\alpha \omega(P_\alpha^S)$ is identically zero, so $\sum_\alpha f_\alpha(0, y_1, y_2) + \sum_\alpha f_\alpha(\pi, y_1, y_2) = O(L^{-1})$. We are thus left with the triple integral of $\sum_\alpha f_\alpha(y)\rho_\alpha(y)$. But

$$f(y)\rho(y) = \frac{L}{\pi}\omega_{12} + \frac{1}{2\pi}(\omega_{20}\partial_1\theta + \omega_{01}\partial_2\theta + \omega_{12}\partial_0\theta) + O(L^{-1}) . \tag{6.10}$$

Summing over α eliminates the $O(L)$ term, as $\sum_\alpha \omega(P_\alpha^S) = 0$. The $O(1)$ terms of Eq. (6.10), summed over α, are precisely $2\pi s_1(y)$. This shows that

$$c_1(\Sigma, P) = \int_{I\times\Sigma} s_1(y) + O(L^{-1}) . \tag{6.11}$$

Since $c_1(\Sigma,P)$ and $\int_{I\times\Sigma} s(y)$ are independent of L, the $O(L^{-1})$ correction must in fact be zero. This establishes Theorem 1 for the case $k=1$.

The proof for other values of k is almost identical, and so is only sketched here. The form $s_k(y)$ is defined everywhere except at level crossings. Near level crossings $s_k = O(d^{-2k})$, which is integrable in dimension $2k+1$.

As before, we apply a cutoff at a large distance L and examine the finite number of interior states. By Proposition 3, c_k for the bundle of interior states is the sum of the c_k's of the individual eigenbundles. Eigenstates of the Hamiltonian are in 1-1 correspondence with eigenstates of the S-matrix on the energy bands (6.2). Since the integral of ω_k is topological, we can use the curvature of the eigenbundles of S, restricted to the energy bands, to compute the topological class of the eigenbundles of H. The form $\omega_k(P_\alpha^S)$, restricted to the surface $k_m(y)$, takes the form $f(y)\,dy^1 \wedge \cdots \wedge dy^{2k}$, where

$$f(y) = \omega_{1\ldots 2k} + \frac{1}{2L}\sum_{i=1}^{2k}(-1)^i \partial_i \theta \omega_{0,\ldots,i-1,\hat{i},i+1,\ldots,2k}\,, \tag{6.12}$$

where $\hat{i}$ denotes that the subscript i is not included. We replace the sum over m with an integral over k. As before, this involves multiplying $f(y)$ by the density of states:

$$f(y)\rho(y) = \frac{L}{\pi}\omega_{1,\ldots,2k} + \frac{1}{2\pi}(d\theta \wedge \omega_k)_{0,1,\ldots,2k}\,. \tag{6.13}$$

Summing over α and integrating eliminates the $O(L)$ term, since the trivial $\mathbb{C}^N$ bundle has zero invariants. What remains is the integral of $s_k(y)$. □

VII. Threshold States

In this section we prove an extension of Theorem 1, allowing threshold states to exist at $k=0$ and $k=\pi$. That is, we replace Eq. (5.3a) and Eq. (5.3b) by more general limiting conditions. We no longer require all the eigenvalues of the S-matrix to approach -1 as $k\to 0$ or $k\to\pi$. Rather, some $+1$ eigenvalues may occur, corresponding to threshold states. Specifically, we assume that

$$S(y_0,\{y_j\})+1 = \begin{cases} 2B(\{y_j\}) + iy_0 A(\{y_j\}) + O(y_0^2) & \text{near } y_0 = 0\,; \\ 2R(\{y_j\}) + i(y_0-\pi)T(\{y_j\}) + O((y_0-\pi)^2) & \text{near } y_0 = \pi\,, \end{cases} \tag{7.1}$$

with $A(\{y_j\})$, $T(\{y_j\})$ smooth, Hermitian, matrix-valued functions that have no level crossings in X, and with $B(y_i)$, $R(y_i)$ orthogonal projections on $\mathbb{C}^N$ that depend smoothly on $\{y_i\}$. This implies that *Range*(B) and *Range*(R) are finite-dimensional bundles over X with well-defined Chern numbers.

Theorem 2. *Assume the above hypotheses. If Σ is an oriented surface in X, then the first Chern number of the bundle defined by P over Σ is*

$$c_1(\Sigma,P) = \frac{c_1(\Sigma,B)+c_1(\Sigma,R)}{2} + \int_{I\times\Sigma} s_1(y)\,. \tag{7.2}$$

The proof of Eq. (7.2) is almost identical to that of Eq. (5.5). The only difference is that, for the states in $Range(B)$, $\theta(0) = 0$ instead of $-\pi$, and as a result $k_1 = \pi/L + O(L^{-2})$, not $2\pi/L + O(L^{-2})$. Replacing the sum over m with an integral over k gives an integral with lower limit $k = 0$, not $k = k_1/2$. This, and similar considerations at $k = \pi$, cause Eq. (6.9) to be replaced by

$$c_1(\Sigma, P) = \frac{1}{2\pi} \sum_{\alpha=1}^{N} \int_{I\times\Sigma} f_\alpha(y)\rho_\alpha(y)d^3y$$
$$-\frac{1}{4\pi} \int_{\Sigma} \sum_{\beta \notin Range(B)} f_\beta(0, y_1, y_2) - \frac{1}{4\pi} \int_{\Sigma} \sum_{\gamma \notin Range(R)} f_\gamma(\pi, y_1, y_2) + O(L^{-1}) . \tag{7.3}$$

Since $\sum_\alpha f_\alpha(0, y_1, y_2) = O(L^{-1})$, a negative sum over $\beta \notin Range(B)$ can be replaced with a positive sum over $\beta \in Range(B)$, with a similar substitution for γ. As a result,

$$c_1(\Sigma, P) = \frac{1}{2\pi} \sum_{\alpha=1}^{N} \int_{I\times\Sigma} f_\alpha(y)\rho_\alpha(y)\, d^3y$$
$$+\frac{1}{4\pi} \int_{\Sigma} \sum_{\beta\in Range(B)} f_\beta(0, y_1, y_2) + \frac{1}{4\pi} \int_{\Sigma} \sum_{\gamma\in Range(R)} f_\gamma(\pi, y_1, y_2) \tag{7.4}$$
$$= \int_{I\times\Sigma} s_1(y) + c_1(\Sigma, B)/2 + c_1(\Sigma, R)/2 . \quad \square$$

The example of Sect. III, with $|B| = 1/2$, illustrates this theorem. There is no bound state, but there is a threshold at $k = \pi$ whose Chern number is $+1$. As k goes from 0 to π, θ_0 goes from $-\pi$ to π, as before, but θ_1 goes from $-\pi$ to 0. From Eq. (5.10) we see that the integral of s_1 is $-1/2$. Adding this to half the Chern number of the threshold state gives 0. This is indeed the Chern number of the scattering states, since, in the absence of bound states, the projection $P = 1$.

Appendix I. Scattering and Tight Binding Models

Here we recall some basic facts from scattering theory and tight-binding models on graphs, for Hamiltonians of the form (5.1).

Bound States. Bound states with exponentially decaying solutions behave at infinity like $(\pm 1)^n e^{-\kappa n}$ with $\kappa > 0$ and have energies $\pm 2\cosh\kappa$. These are always outside the continuous spectrum $[-2, 2]$. Eigenvalues embedded in the continuous spectrum $[-2, 2]$, if they exist, are associated with compactly supported eigenfunctions. Complex hermitian Hamiltonians with embedded eigenvalues are of codimension $2N$ while real symmetric Hamiltonians with embedded eigenvalues are of codimension N. This is because, for an eigenfunction ψ to be compactly supported, ψ must vanish at N vertices, the ends of each strand. The condition that ψ vanishes at a vertex is codimension 2 in the complex case and codimension 1 in the real case. For a connected system, our hypotheses in Sect. V preclude embedded eigenvalues, as these would conflict with the unitarity of S on $\mathbb{C}^N$. In the real case this is the generic setting if $N \geqq 4$. In the complex case one needs $N \geqq 2$. The example in Sect. III is of this type since one strand with spin is equivalent to two strands without spin.

Scattering States. Let ψ be a solution of the difference equation $(H - 2\cos k)\psi = 0$ with $k \in [0, \pi]$. To each such ψ we can associate two vectors in $\mathbb{C}^N$ so that $\psi(x) \to \zeta_{out} e^{ikx} + \zeta_{in} e^{-ikx}$ as $x \to \infty$. The on-shell S-matrix is defined by

$$\zeta_{out} = S(k)\zeta_{in} . \tag{A.1}$$

There is a class of tight binding models for which there is a simple formula for the on-shell S-matrix. Consider the Hamiltonian Eq. (5.1), where only h_{00} is different from zero, and let $h = h_{00}$ be an $N \times N$ Hermitian matrix. The scattering states are determined by the solutions of

$$(h - E)(\psi_{in} + \psi_{out}) = -(\psi_{in}/z + z\psi_{out}) . \tag{A.2}$$

It follows that

$$S = -\frac{h - z}{h - 1/z} , \tag{A.3}$$

where $z = \exp ik$ and the energy is $E = z + 1/z$. At the edges of the continuous spectrum, where $z = \pm 1$, the phase shifts are $\exp i\theta_\alpha = -1$, except in the special case where h has eigenvalues ± 1. If $h \mp 1$ is invertible, the S-matrix at the edges of the spectrum is -1 and Eq. (5.3a) holds with $A = 2/(h - 1)$, $T = 2/(h + 1)$.

The condition $Ker(h \mp 1) = 0$ is a codimension 1 condition, (since h is a hermitian matrix). It follows that a generic matrix family $h(y)$ may violate the conditions in the hypotheses in Sect. IV. This is not surprising, as the hypotheses do not allow bound states to appear or disappear. If two Hamiltonians have different numbers of bound states, then any path between them must contain a point where the hypotheses are violated. On the other hand, it is easy to construct examples where the nature of the spectrum does not change, and where the hypotheses are satisfied. For example, take $h(y) = u(y)h_0u^\dagger(y)$, with h_0 a fixed Hermitian matrix (whose spectrum does not contain ± 1), and with $u(y)$ a family of unitary matrices.

Appendix II. Chern–Weil Theory

Here we review the essentials of Chern–Weil theory, first for finite dimensional bundles and then for infinite dimensional bundles. See [5, 10] for details on the theory of Chern classes for finite dimensional bundles and [6, 11] for its extension to infinite dimensional bundles.

Given a manifold M, a fiber bundle E over M with structure group G, and a connection on that bundle, we may define a *classifying map* f from M to an infinite dimensional manifold BG, the *classifying space* of G. Two G-bundles over M, with isomorphic fibers, are isomorphic if and only if their classifying maps are homotopic. Moreover, there is a G-bundle EG over BG, called the *universal bundle*, such that the principal bundle associated to E is the pullback of EG by f. Indeed, the connection on E is just the pullback of a universal connection on EG, and the curvature of E is just the pullback of the curvature of EG.

Next we specialize to unitary bundles. The classifying space $BU(n)$ is the quotient of a contractible space (namely $EU(n)$) by $U(n)$. The cohomology ring of $BU(n)$ is freely generated by a 2-dimensional class C_1, a 4-dimensional class $C_2, \ldots$, and a $2n$-dimensional class C_n. That is, as a ring, $H^*(BU(n), \mathbb{Z}) \simeq \mathbb{Z}[C_1, \ldots, C_n]$. The cohomology classes C_k are called the Chern classes of $BU(n)$. By definition,

the Chern classes of the bundle E over M (denoted $C_k(E)$) are the pullbacks of these integral classes by the classifying map f. Since homotopic maps induce the same pullbacks in cohomology, $C_k(E)$ depends only on the topology of E and not on the connection.

On $BU(n)$, one can relate the cohomology classes C_k to the curvature of the natural connection on $EU(n)$. Such formulas are called Chern–Weil formulas. The simplest such formula states that the form ω_1 is in the cohomology class C_1, hence that the period $c_1(\Sigma, P)$ equals the cohomology class $C_1(P)$ applied to the homology class of Σ, and hence that $c_1(\Sigma, P)$ is an integer. Other formulas relate ω_k to C_k. In the special case that C_k is the lowest nonvanishing Chern class, they state that the cohomology class of ω_k *is* C_k. In all cases these formulas show that the periods of ω_k are topological invariants. Once such formulas are established on $BU(n)$, they apply to M as well, since both the Chern classes and the curvature forms on M are pullbacks of the corresponding objects on $BU(n)$.

For infinite dimensional bundles, the existence of Chern classes depends on the structure group. The full group $U(H)$ of unitary operators on the infinite dimensional Hilbert space H is contractible, so $BU(H)$ is contractible, so every $U(H)$-bundle is trivial. To obtain nontrivial characteristic classes, one must reduce the structure group to a small enough subgroup of $U(H)$, where Chern classes are defined and can be expressed by curvature formulas.

Let $U_c(H)$ be the space of unitary operators U with $U - I$ compact. An element of U_c is the norm limit of a sequence of operators U with $U - I$ having finite rank. It should be no surprise, then, that the cohomology of BU_c is the same as the direct limit of the $BU(n)$, namely $H^*(BU_c, \mathbb{Z}) = \mathbb{Z}[C_1, C_2, \ldots]$. Thus, whenever the structure group of a unitary bundle can be reduced to $U_c(H)$, Chern classes are well defined topologically. For each integer p, let $U_p(H)$ be the subspace of $U_c(H)$ such that $U - I$ is in the p^{th} Schatten ideal $\mathcal{I}^p$. In particular, U_1 means $U - I$ is trace class and U_2 means $U - I$ is Hilbert–Schmidt. Freed [6] showed that, when the structure group is U_p, the Chern–Weil formulas for c_k hold for all $k \geqq p$.

The situation where dP is Hilbert–Schmidt is, at first glance, intermediate between U_1 and U_2. For any path γ, the operator U^γ that gives parallel transport along the path may be obtained by integrating the equation $dU = [dP, P]U$ along the path, with initial condition $U = 1$. Since the right-hand side is Hilbert–Schmidt, every path γ has $U^\gamma - I$ Hilbert–Schmidt, so our structure group reduces to U_2. However, we have more. The curvature is trace class and holonomies along closed null-homotopic loops are actually in U_1. Pressley and Segal [11] showed how to construct the determinant bundle of P, from which one can show that the first Chern class is indeed represented by ω_1.

Finally we consider additivity properties. Let P and Q be orthogonal projections with $PQ = 0$ and with dP and dQ both Hilbert–Schmidt. The bundle defined by the range of $P + Q$ is the direct sum of the bundle defined by P and the bundle defined by Q. On this direct sum bundle we consider two different connections. The first is the adiabatic connection of $P + Q$. The second is the direct sum of the adiabatic connection of P and the adiabatic connection of Q. The curvature of the second connection is just the direct sum of the curvature of the adiabatic connection of P and the adiabatic connection on Q.

Let $\omega_k(P + Q)$ be constructed by Eq. (2.2) from the curvature of the first connection, and let $\omega_k'(P + Q)$ be constructed in the same way from the curvature of

the second connection. Since the periods ω_k are topological invariants,

$$\int_\Sigma \omega_k(P+Q) = \int_\Sigma \omega'_k(P+Q)\,. \tag{A.4}$$

However, $\omega'_k(P+Q)$ is just the sum of $\omega_k(P)$ and $\omega_k(Q)$, so

$$\int_\Sigma \omega_k(P+Q) = \int_\Sigma \omega_k(P) + \int_\Sigma \omega_k(Q)\,. \tag{A.5}$$

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