

Adiabatic Curvature and the S–Matrix

**Lorenzo Sadun
Joseph E. Avron**

Vienna, Preprint ESI 291 (1995)

December 11, 1995

Supported by Federal Ministry of Science and Research, Austria
Available via <http://www.esi.ac.at>

ADIABATIC CURVATURE AND THE S -MATRIX

by

Lorenzo Sadun¹ and Joseph E. Avron²

Abstract

We study the relation of the adiabatic curvature associated to scattering states and the scattering matrix. We show that there cannot be any formula relating the two locally. However, the first Chern number, which is proportional to the integral of the curvature, *can* be computed by integrating a 3-form constructed from the S -matrix. Similar formulas relate higher Chern classes to integrals of higher degree forms constructed from scattering data. We show that level crossings of the on-shell S -matrix can be assigned an index so that the first Chern number of the scattering states is the sum of the indices. We construct an example which is the natural scattering analog of Berry's spin 1/2 Hamiltonian.

December 1995

AMS 1995 Subject Classification: 81U20, 58Z05, also 14L30, 34L40, 81Q30

1994 PACS numbers: 03.65.Bz, also 03.80+r, 02.40Re

¹ Department of Mathematics, University of Texas, Austin, TX 78712, USA.
Email: sadun@math.utexas.edu. Research supported in part by an NSF Mathematical Sciences Postdoctoral Fellowship and Texas ARP Grant 003658-037

² Department of Physics, Israel Institute of Technology, Haifa, Israel.
Email: avron@physics.technion.ac.il. Research supported in part by GIF, DFG and the Fund for Promotion of Research at the Technion.

I. Motivation

In the quantum Hall effect, the conductance is related to a Chern number — the integral of the adiabatic curvature [1,2]. In many systems, conductance admits a description in terms of scattering data via Landauer type formulas [3]. This seems to suggest that there may be a direct and general link between adiabatic curvature and/or Chern numbers, on the one hand, and scattering data on the other. The study of this relation is the central theme of the work presented here. As we shall see, there is no such (pointwise) link between scattering data and adiabatic curvature, but there *is* such a link between scattering data and Chern numbers.

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”. This limits the applications of our results to the usual transport theory since transport of charge to infinity typically involves deformations at infinity.

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 [4]. Because of this, it may not be too surprising that scattering can sometime fail to know about the adiabatic curvature due to local deformations. From this point of view it is perhaps more remarkable that the S -matrix nevertheless determines the Chern numbers.

There is also a mathematical motivation for studying the geometry and topology of vector bundles from the perspective of scattering theory. 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 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. Our results can be phrased as stating that the scattering data determine the topology of such bundles, but not their local curvature.

We shall see that for a class of tight-binding models the first Chern class of the scattering bundle is determined by an explicit 3-form constructed from scattering data:

$$s_3(y) = \frac{1}{4\pi^2} \sum_{\alpha} d\theta_{\alpha}(y) \wedge \Omega(P_{\alpha}^S). \quad (1.1)$$

Here P_{α}^S is the α -th spectral projection of the on-shell scattering matrix $S(y)$, and $\theta_{\alpha}(y)$ is half the corresponding phase shift, i.e.,

$$S(y)P_{\alpha}^S(y) = \exp i\theta_{\alpha}(y)P_{\alpha}^S(y). \quad (1.2)$$

$y_0 = k$ parameterizes the energy and $\{y_j\}, j = 1, \dots, \ell$ are additional parameters that parameterize the deformation of the Hamiltonian. $\Omega(P)$ is the trace of the usual adiabatic curvature associated to the projection P ; see Eq. (2.1) below. If

$S(y)$ is a non-degenerate $n \times n$ matrix, then $\alpha = 1, \dots, n$ and P_α^S is a rank-1 orthogonal projection in \mathbb{C}^n .

Integrating $s_3(y)$ over the band of scattering energies parameterized by y_0 gives a closed 2-form on the space of parameters governing the deformation of the system. We shall see that the cohomology class of this 2-form is the first Chern class of the infinite-dimensional vector bundle in question.

In general, only unitary invariant properties of the on-shell S -matrix have physical significance [5]. The phase shifts are, of course, unitary invariant. $\Omega(P_\alpha^S)$ is not. Rather, under the transformation $S \rightarrow U^\dagger S U$, $P_\alpha^S \rightarrow U^\dagger P_\alpha^S U$ and

$$\Omega(P_\alpha^S) \rightarrow \Omega(P_\alpha^S) + d \operatorname{Tr}(P_\alpha^S U^\dagger dU). \quad (1.3)$$

It follows that the 3-form $s_3(y)$ is not invariant under y -dependent unitary transformations, but its cohomology class *is* invariant. First Chern numbers, which are periods of this three form, are invariant, as they should be.

A similar construction gives the higher Chern classes of the infinite dimensional bundle associated to P . Let $F(P)$ be the adiabatic curvature operator whose trace is $\Omega(P)$; see Eq. (2.1). The $2n$ -form $\frac{1}{n!(2\pi)^n} \operatorname{Tr}(F(P)^n)$ is closely related to the n -th Chern class of the bundle of scattering states defined by P . (P is infinite dimensional). This form is cohomologous to the integral over y_0 of the $2n+1$ form

$$s_{2n+1}(y) = \frac{1}{n!(2\pi)^{n+1}} \sum_\alpha d\theta_\alpha(y) \wedge \operatorname{Tr}(F(P_\alpha^S)^n), \quad (1.4)$$

which is computed from scattering data (and where P_α^S are finite dimensional).

In section II we review the theory of adiabatic curvature for finite dimensional projections and its extension to infinite dimensions. In section III we give a family of examples that show that the adiabatic curvature cannot, in general, be computed pointwise from the S -matrix. In these examples there is a nonzero curvature associated to two parameters, but the S -matrix is independent of one of the parameters. In section IV we state precise hypotheses under which the 3-form $s_3(y)$ computes first Chern numbers. We also show how these Chern numbers are related to numerical indices associated to level crossings of the S -matrix. In Section V we work a key example, the natural scattering analog of Berry's spin Hamiltonian. Section VI is the proof of the main theorem, as stated in Section IV. In Section VII we consider some exceptional cases and generalize our results to cover higher Chern classes. Finally, we include an appendix reviewing scattering in tight binding models.

II. Preliminaries–Geometry of Projections

Let X be a space of parameters with local coordinates $y = (y_1, \dots, y_\ell)$. Let $P(y)$ be a family of orthogonal finite dimensional projections that depends smoothly on $y \in X$. $\text{Range}(P)$ is a vector bundle over X with a natural connection. We are interested in the trace of the resulting curvature:

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

By abuse of language we call $\Omega(P)$, as well as the underlying operator $F(P) = -iPdP \wedge dPP$, the adiabatic curvature associated to P . If, for each y , $P(y)$ is a one dimensional projection and $\Psi(y)$ is a normalized vector in the range of $P(y)$ (depending smoothly on y) then Eq. (2.1) reduces to

$$\Omega(P) = \text{Im} \langle d\Psi | \wedge | d\Psi \rangle.\tag{2.2}$$

In the opposite extreme, when $P = 1$, Eq. (2.1) says that $\Omega(P) = 0$.

If P_1 and P_2 are mutually orthogonal, i.e., $P_1 P_2 = P_2 P_1 = 0$, with P_1 and P_2 smooth, orthogonal and finite dimensional, then

$$\Omega(P_1 + P_2) = \Omega(P_1) + \Omega(P_2).\tag{2.3}$$

As a special case, if the Hilbert space is finite-dimensional and $P_\perp = 1 - P$, then

$$\Omega(P) + \Omega(P_\perp) = 0.\tag{2.4}$$

But what if the range of P is infinite-dimensional? In the rest of this section we shall show that the Hilbert-Schmidt condition $\text{Tr}|\partial_j P|^2 < \infty$ guarantees that things carry over to infinite dimensional projections in a Hilbert space.

Proposition 1

Let P be a family of smooth orthogonal projections. If dP , $P_\perp dPP$ or $PdPP_\perp$ is Hilbert-Schmidt, then

1. dP , $P_\perp dPP$ and $PdPP_\perp$ are all Hilbert-Schmidt.
2. $\Omega(P)$ and $\Omega(P_\perp)$ are well defined and finite.
3. If dP_1 and dP_2 are Hilbert-Schmidt, with P_1 and P_2 mutually orthogonal projections, then Eq. (2.3) holds.
4. If dP is Hilbert-Schmidt, then Eq. (2.4) hold.

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

$$\partial_j P = P(\partial_j P)P_\perp + P_\perp(\partial_j P)P,\tag{2.5}$$

which implies statement 1. Consequently,

$$(\partial_j P)(\partial_k P) = P(\partial_j P)P_\perp(\partial_k P)P + P_\perp(\partial_j P)P(\partial_k P)P_\perp. \quad (2.6)$$

The product of two Hilbert-Schmidt operators is trace class [10], so $\Omega(P)$ and $\Omega(P_\perp)$ are finite. The anticommutativity of forms and commutativity of the trace (for products of Hilbert-Schmidt operators) gives Eq. (2.3), as follows:

$$\begin{aligned} \Omega(P_1 + P_2) &= \text{Tr}(P_1 + P_2)(dP_1 + dP_2) \wedge (dP_1 + dP_2)(P_1 + P_2) \\ &= \Omega(P_1) + \Omega(P_2) + \text{Tr}(P_1 dP_1 \wedge dP_2 P_1 + P_2 dP_2 \wedge dP_1 P_2) \\ &\quad + \text{Tr}(P_2 dP_1 \wedge dP_2 P_2 + P_1 dP_2 \wedge dP_1 P_1) \\ &\quad + \text{Tr}(P_1 dP_2 \wedge dP_2 P_1 + P_2 dP_1 \wedge dP_1 P_2). \end{aligned} \quad (2.7)$$

But $P_1 dP_2 = P_1 dP_2 P_2$, so

$$\begin{aligned} &\text{Tr}(P_2 dP_1 \wedge dP_2 P_2 + P_1 dP_2 \wedge dP_1 P_1) \\ &= \text{Tr}(P_2 dP_1 P_1 \wedge P_1 dP_2 P_2 + P_1 dP_2 P_2 \wedge P_2 dP_1 P_1) = 0. \end{aligned} \quad (2.8)$$

The two remaining terms vanish similarly, using also the identity $P_1 dP_2 = -dP_1 P_2$. This establishes Eq. (2.3), of which Eq. (2.4) is a special case. \blacksquare

This proposition says that the curvature of infinite dimensional projections behaves just like that of finite dimensional projections if dP is Hilbert-Schmidt. In fact, if either P or its complement P_\perp is finite dimensional, then the curvature of the infinite dimensional piece can always be studied by looking at its finite dimensional complement.

Infinite dimensional projections can have some unusual curvatures, as the example below shows:

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:

$$(U(a, b)\psi)(x) = \exp(i b \Lambda(x - a)) \psi(x - a). \quad (2.9)$$

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

$$\begin{aligned} \Omega(P) &= da \wedge db \text{Tr} \left(Q\Lambda'Q + [Q\Lambda Q, Q\nabla Q] \right) \\ &= da \wedge db \text{Tr} Q\Lambda'Q. \end{aligned} \quad (2.10)$$

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

$$\Omega(P) = da \wedge db \text{Tr} P, \quad (2.11)$$

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? Perhaps 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.

An important fact about curvatures is that their integrals over closed regions of parameter space are quantized. For finite dimensional bundles this is a standard result of Chern-Weil theory. See e.g. [6, 7] for the theory of Chern classes for finite dimensional bundles and [8, 9] for its extension to infinite dimensional bundles.

For infinite dimensional bundles, the existence of Chern classes depends on the structure group. The group $U(H)$ of unitary operators on the infinite dimensional Hilbert space H is too big. 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. For each integer p let $U_p(H)$ be the subspace of $U_c(H)$ such that $U - I$ is in L^p . In particular, $p = 1$ means trace class and $p = 2$ means Hilbert-Schmidt. As long as the structure group can be reduced to $U_c(H)$, Chern classes are well defined topologically. Freed [9] showed that, when the structure group is U_p , the Chern-Weil formulas for c_i in terms of curvature hold for all $i \geq p$.

The situation where dP is Hilbert-Schmidt is 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 [8] showed how to construct the determinant bundle of P , from which one can show that the first Chern class is represented by $\Omega/2\pi$. In short, we have the following

Proposition 2

Let P be a family of orthogonal projections such that dP is Hilbert-Schmidt, and let Σ be a (smooth) closed 2-surface in parameter space. Then

$$c_1(\Sigma, P) = \frac{1}{2\pi} \int_{\Sigma} \Omega(P) \quad (2.12)$$

is an integer.

III. Curvature Is Not Computable from Scattering Data

Here we construct examples that show that curvature is not necessarily detected by the S -matrix. In these examples the curvature associated to two parameters may be nonzero, but the S -matrix is independent of one of the parameters.

Let V be any reasonable perturbation of the Laplacian in one dimension so 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

$$H(a, b) = U(a, b) \left(-\frac{d^2}{dx^2} + V \right) U^\dagger(a, b) = \left(-i \frac{d}{dx} - b \Lambda'(x - a) \right)^2 + V(x - a), \quad (3.1)$$

where U is as in Eq. (2.9). 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 $|x| \rightarrow \infty$,

$$\psi_y(x) = e^{ib\Lambda(\pm\infty)} \psi_{k,0,0}(x - a). \quad (3.2)$$

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

$$S(k, a, b) = \begin{pmatrix} r_R(k) e^{2ika} & t_L(k) e^{ib\Delta\Lambda} \\ t_R(k) e^{\pm ib\Delta\Lambda} & r_L(k) e^{\pm 2ika} \end{pmatrix}, \quad (3.3)$$

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 $\text{Tr} Q(-\Delta + \Lambda^2)Q < \infty$. Let $P = 1 - Q$. P is the projection on the (positive energy) scattering states. From proposition 1 and example 1 we have that

$$\Omega(P) = -\Omega(Q) = -da \wedge db \text{Tr } Q\Lambda'Q. \quad (3.4)$$

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

$$\Lambda'(x) = \begin{cases} 1 & |x| < L; \\ -1 & |x - 2L| < L; \\ 0 & \text{otherwise,} \end{cases} \quad (3.5)$$

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

IV. Chern Numbers Are Computable From Scattering Data

In this section we describe the main result of this paper, namely how the first Chern class of the scattering states can be computed from scattering data. This may be done either by integrating the 3-form $s_3(y)$ of Eq. (1.1) or by summing certain indices associated to scattering data. This section and the next contain explanations of these procedures, as well as some examples. The proofs of the formulas are deferred to section VI.

Hypotheses: We consider tight-binding models with a finite number of scattering channels and a compactly supported scattering potential that depends on a parameter space X with coordinates $\{y_i\}$. (See the appendix for a discussion of tight-binding models). The on-shell S -matrix $S(y)$ is a finite dimensional $n \times n$ matrix, which we assume depends smoothly on all variables y . We assume $S(y)$ has level crossings on a set Z of codimension 3 or higher, and that the 3-form $s_3(y) = O(d^{\perp 2})$ near the crossings, where d is the distance from y to Z . Finally, we assume that the S -matrix approaches -1 at the edges of the spectrum. More precisely, we assume that

$$S(y_0, \{y_i\}) + 1 = \begin{cases} i y_0 A(\{y_i\}) + O(y_0^2) & \text{near } y_0 = 0; \\ i (y_0 - \pi) T(\{y_i\}) + O((y_0 - \pi)^2) & \text{near } y_0 = \pi, \end{cases} \quad (4.1)$$

with $A(\{y_i\})$, $T(\{y_i\})$ smooth, Hermitian, matrix-valued functions that have no level crossings in X .

Conventions: $y_0 = k$ parameterizes the energy. The band of scattering states is the interval $k \in [0, \pi]$. The phase shifts are normalized so that $\theta_\alpha(y_0 = 0) = -\pi$; the values of θ_α for all y_0 follow by continuity. ℓ_α is the winding of θ_α , i.e.,

$$2\pi\ell_\alpha = \theta_\alpha(\pi) + \pi. \quad (4.2)$$

Our hypotheses imply that ℓ_α is an integer and is independent of the parameters $\{y_i\}$.

Remark 1: We have chosen to state the hypotheses in terms of the scattering data only. These assumptions have spectral consequences, and some parts of the hypotheses could be phrased in terms of spectral conditions. In particular, the hypotheses imply that embedded and threshold states do not enter or leave the interval $k = [0, \pi]$ as $\{y_i\}$ are varied. For more on this see the appendix.

Remark 2: The smoothness of $S(y)$ implies smoothness of the 3-form $s_3(y)$ of Eq. (1.1) away from eigenvalue crossings. The assumption about the form of singularities near crossings holds if the crossings are generic. In the generic situation $S(y)$ has, away from the edges of the band, eigenvalue crossings of multiplicity two on a set of codimension 3. Near a crossing at a point z_j , $S(y)$, projected on the relevant two-dimensional space, can be approximated by

$$e^{i\theta(y)} \left(1 + i \sum_{\ell, m} \sigma_\ell g_{\ell m}(z_j) (y - z_j)_m + O((y - z_j)^2) \right), \quad (4.3)$$

with g a real, rank 3 matrix, and with σ denoting the triplet of Pauli matrices. The overall phase $\theta(y) = (\theta_\alpha(y) + \theta_\beta(y))/2$ is smooth, even at $y = z_j$. Near such a crossing $s_3(y) = O(d^{\perp 2})$.

Remark 3: The assumption that the S -matrix near the edges of the spectrum assumes the form Eq (4.1) seems very special. In fact it is not, since the S -matrix is known to have universal limiting values under a range of circumstances [11]. The exceptions are when threshold states (zero energy resonances) occur. For more on this condition in the context of tight binding hamiltonians, see the appendix.

The following example of a system that obeys the hypotheses may be instructive:

Example 2: Consider a half-line tight-binding model with (real) potential $V(n) = v\delta_{n,0}$ and hopping $t_{n,n+1} = 1$, $n \geq 0$. The on-shell scattering matrix is a complex number of modulus one (the reflection amplitude) given by

$$S(k, v) = -\frac{v - z}{v - 1/z}, \quad z = e^{ik}. \quad (4.4)$$

The energy is $E = z + 1/z$. There is one bound state if $|v| > 1$ which becomes a threshold state when $v = \pm 1$. At the edge of the continuous spectrum ($z = \pm 1$), $S(k, v) = -1$ for all $v \neq \pm 1$.

Theorem 1: *Assume the above hypotheses. The integral of the 3-form $s_3(y)$ over the spectral interval $I = (0, \pi)$ is a closed 2-form on X . The cohomology class of this 2-form is the first Chern class of the bundle of scattering states in the spectral interval I . In particular, if Σ is an oriented surface in X , then the first Chern number of the bundle defined by P over Σ is*

$$c_1(\Sigma, P) = \int_{I \times \Sigma} s_3(y). \quad (4.5)$$

Remark 4: The tight-binding assumption is made to make the entire continuous spectrum be a single band, and the proof is tailored to this case. It should be straightforward to prove similar results for compact perturbations of periodic potentials (either on the continuum or on a lattice) subject to similar conditions on the S -matrix. In addition, the formula Eq. (4.5) is the simplest in a class of formulas for the Chern number. More complicated formulas hold if Eq. (4.1) is replaced by other limiting values for the S -matrix that occur when threshold states exist at $y_0 = 0$ or $y_0 = \pi$. These formulas are discussed in section VII.

Remark 5: If the system is made of disconnected pieces, it is possible to arrange for embedded eigenvalues, associated with a compact part of the system, to lie in the energy interval associated to the scattering states. These embedded eigenstates can carry Chern numbers, but are irrelevant to the problem we study here. The caveat “bundle of scattering states” in the theorem indicates that we are not including these eigenstates.

Remark 6: Since $|y|^{\perp 2}$ is integrable in three dimensions, the integral in Eq. (4.5) is absolutely convergent.

Let $Y = I \times X$. The eigenvalues and eigenvectors of the on-shell S -matrix have a consistent labeling in $Y/\{\text{crossings}\}$. By the assumptions about $A(y)$ in Eq. (4.1), there is a consistent labeling of the spectrum on the section $y_0 \times X$ with y_0 near zero. Since codimension 3 crossings do not destroy simple connectivity, this labeling propagates to $Y/\{\text{crossings}\}$.

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. 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

$$Index(z_j) = n(z_j) c_1(P_\alpha^S, S^2(z_j)), \quad (4.6)$$

where $S^2(z_j)$ is a small sphere centered at z_j . For a generic crossing, as described in Remark 2,

$$c_1(P_\alpha^S, S^2(z_j)) = \text{sgn } \det g(z_j). \quad (4.7)$$

A consequence of theorem 1 is:

Proposition 3: The Chern numbers are given by

$$c_1(\Sigma, P) = \sum_{0 < (z_j)_0 < \pi} Index(z_j) + \sum_{\alpha} \ell_{\alpha} c_1(P_{\alpha}^T, \Sigma), \quad (4.8)$$

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. (4.1) and ℓ_{α} is the winding given in Eq. (4.2).

Proof of Proposition 3 (given Theorem 1): Since $\Omega(P)$ is closed, $d\theta \wedge \Omega(P) = d(\theta\Omega(P))$, so

$$\begin{aligned} 4\pi^2 \int_{Y/\{\text{crossings}\}} s_3(y) &= \sum_{\alpha} \sum_{\text{crossings}} \int_{S^2} \theta_{\alpha}(y) \Omega(P_{\alpha}^S) \\ &+ \sum_{\alpha} \left(\int_{\pi \times \Sigma} \theta_{\alpha}(\pi, y_1, y_2) \Omega(P_{\alpha}^S) - \int_{0 \times \Sigma} \theta_{\alpha}(0, y_1, y_2) \Omega(P_{\alpha}^S) \right). \end{aligned} \quad (4.9)$$

Near the α, β level crossing $\Omega(P_{\alpha}^S) + \Omega(P_{\beta}^S) = O(1)$, so the j -th crossing contributes

$$\int_{S^2} (\theta_{\alpha}(y) \Omega(P_{\alpha}^S) + \theta_{\beta}(y) \Omega(P_{\beta}^S)) = 2\pi n(z_j) \int_{S^2} \Omega(P_{\alpha}^S). \quad (4.10)$$

This gives the first sum on the rhs of Eq. (4.8). 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. (4.8). ■

V. Example—Scattering of Spin 1/2 Particles

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} . This is an example that satisfies the conditions for theorem 1 and propositions 1 and 3, and is one where the Chern number for the scattering states is non-zero for $|\vec{B}| > 1/2$. 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 $h(\vec{B}) = \vec{B} \cdot \vec{\sigma} + |B|$, and consider the following tight binding Hamiltonian $H(\vec{B})$ on the non-negative integers:

$$(H(\vec{B})\psi)(n) = \psi(n+1) + \psi(n-1) + \delta_{n0} h(\vec{B})\psi(n), \quad (5.1)$$

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

The absolutely continuous spectrum is the interval $[-2, 2]$. It is free of embedded eigenvalues and is all of the spectrum if $|B| < 1/2$. For $|B| > 1/2$ the spectrum also has one bound state with energy $2|B| + \frac{1}{2|B|}$. The bound state for $|\vec{B}| > 1/2$ has an exponentially localized wave function

$$\psi_0(y) = (2|B|)^{\perp n} \vec{B} \cdot \vec{\sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (5.2)$$

Let P be the projection onto the scattering states. $P_\perp = 1 - P$ is the projection onto the bound states. Since P_\perp is smooth and finite rank, we can use Eq. (2.4) and Eq. (2.2) to compute the adiabatic curvature of P :

$$\Omega(P) = -\Omega(P_\perp) = \begin{cases} 0 & \text{if } |\vec{B}| < 1/2; \\ -\omega(\vec{B}) & \text{if } |\vec{B}| > 1/2, \end{cases} \quad (5.3)$$

where

$$\omega(\vec{B}) = \frac{1}{2|B|^3} (B_1 dB_2 \wedge dB_3 + B_2 dB_3 \wedge dB_1 + B_3 dB_1 \wedge dB_2) \quad (5.4)$$

is half the spherical angle 2-form. Integrating this we find that for a 2-sphere S^2 enclosing the origin in the 3-dimensional space of magnetic fields,

$$c_1(S^2, P) = \begin{cases} 0, & \text{if } |B| < 1/2; \\ -1 & \text{if } |B| > 1/2. \end{cases} \quad (5.5)$$

Now we recompute this Chern number from theorem 1. The scattering matrix is (see Appendix)

$$S(k, \vec{B}) = -\frac{h(\vec{B}) - z}{h(\vec{B}) - 1/z}, \quad (5.6)$$

where $z = \exp ik$, $0 \leq k \leq \pi$. Since the spectrum of $h(\vec{B})$ is $\{0, 2|B|\}$, S is smooth for k real and \vec{B} away from the sphere $|\vec{B}| = 1/2$. S satisfies the basic hypotheses in particular Eq. (4.1) holds with $A(\vec{B}) = 2/(h(\vec{B}) - 1)$ and $T(\vec{B}) = 2/(h(\vec{B}) + 1)$. The eigenvalues and adiabatic curvature for the corresponding spectral projections of S are:

$$\exp i\theta_0(k, \vec{B}) = -z^2, \quad \exp i\theta_1(k, \vec{B}) = -(2|\vec{B}| - z)/(2|\vec{B}| - 1/z), \quad (5.7)$$

$$\Omega(P_0^S) = -\Omega(P_1^S) = -\omega(\vec{B}). \quad (5.8)$$

The windings of θ are thus

$$\ell_0 = 1, \quad \ell_1 = \begin{cases} 1 & \text{for } |\vec{B}| < 1/2; \\ 0 & \text{for } |\vec{B}| > 1/2. \end{cases} \quad (5.9)$$

It follows that the 3-form of Eq. (1.1) is

$$s_3(y) = \frac{1}{4\pi^2} (d\theta_1 - d\theta_0) \wedge \omega(\vec{B}). \quad (5.10)$$

Integrating s_3 over $I \times S^2$, or using proposition 3, we confirm that the Chern number of the scattering states is given by Eq. (5.6).

VI. Derivation of Eq. (4.5)

This section is a proof of formula Eq. (4.5) in theorem 1 given the hypotheses in section IV. By assumption our scattering potential is compactly supported, hence 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 therefore does not change the Chern classes of these states. Thus it 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 $\{x > L\}$, 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 $\{x < L\}$, 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 $\{x < L\}$ is a subspace of the original Hilbert space, by the variational principle the number of negative eigenvalues for the system cut off at L cannot exceed the number for the original unregularized system, namely the number of negative energy bound states. 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 $L > |x| > M$, the wavefunctions take the form

$$\psi_{m,\alpha}(x) = \zeta_\alpha(k, y) \left(\exp(-ik|x|) + \exp(i(\theta_\alpha + k|x|)) \right), \quad (6.1)$$

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

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

Eq. (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 $y_0 = k$. 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

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

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

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

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

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

So we can write

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

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

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

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 $f(k_{L+\ell+1})$. Eq. (6.7) still applies, as long as we take $k_0 = 0$ and $k_{L+\ell} = \pi$. We also have that

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

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

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

By Eq. (2.3) and Eq. (2.4), $\sum_{\alpha} \Omega(P_{\alpha}^S)$ is identically zero, so $\sum_{\alpha} f_{\alpha}(0, y_1, y_2) + \sum_{\alpha} f_{\alpha}(\pi, y_1, y_2) = O(L^{\perp 1})$. We are thus left with the triple integral of $\sum_{\alpha} f_{\alpha}(y) \rho_{\alpha}(y)$. But

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

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 $2\pi s_3(y)$. This shows that

$$c_1(\Sigma, P) = \int_{I \times \Sigma} s(y) + O(L^{\perp 1}). \quad (6.11)$$

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

VII. Threshold States and Higher Chern Classes

In this section we prove two extensions of theorem 1. The first extension is to allow threshold states to exist at $k = 0$ and $k = \pi$. The second extension is to compute the higher Chern classes of the bundle $Range(P)$ in term of scattering data.

For the first extension the hypotheses are as in theorem 1, except that the eigenvalues of the S matrix do not all have to approach -1 as $k \rightarrow 0$ or $k \rightarrow \pi$. Rather, some $+1$ eigenvalues may occur, corresponding to threshold states. Specifically, we assume that

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

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*

$$c_1(\Sigma, P) = \frac{c_1(\Sigma, B) + c_1(\Sigma, R)}{2} + \int_{I \times \Sigma} s_3(y). \quad (7.2)$$

The proof of Eq. (7.2) is almost identical to that of Eq. (4.5). The only difference is that, for the states in $Range(B)$, $\theta(0) = 0$ instead of $-\pi$, and as a result $k_1 = \pi/L + O(L^{\perp 2})$, not $2\pi/L + O(L^{\perp 2})$. 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

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

Since $\sum_{\alpha} f_\alpha(0, y_1, y_2) = O(L^{\perp 1})$, 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,

$$\begin{aligned} c_1(\Sigma, P) = & \frac{1}{2\pi} \sum_{\alpha=1}^n \int_{I \times \Sigma} f_\alpha(y) \rho_\alpha(y) d^3 y \\ & + \frac{1}{4\pi} \int_{\Sigma} \sum_{\beta \in Range(B)} f_\beta(0, y_1, y_2) + \frac{1}{4\pi} \int_{\Sigma} \sum_{\gamma \in Range(R)} f_\gamma(\pi, y_1, y_2) \quad (7.4) \\ = & \int_{I \times \Sigma} s_3(y) + c_1(\Sigma, B)/2 + c_1(\Sigma, R)/2. \quad \blacksquare \end{aligned}$$

The example of section V, 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_3 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 $P = 1$.

We next turn our attention to higher Chern classes. For any family of projections P , let $F(P)$ be the operator-valued 2-form $-iPdP \wedge dPP$. The cohomology class of the $2n$ -form

$$\omega_n = \frac{1}{n!(2\pi)^n} Tr(F(P)^n) \quad (7.5)$$

is a topological invariant, a linear combination of the n -th Chern class and products of lower Chern classes. For example, if the first Chern class is zero, then ω_2 gives minus the 2nd Chern class.

Theorem 3: *Assume a tight-binding model with a finite number of scattering channels and a compactly supported scattering potential that depends on a $2k$ -dimensional compact oriented parameter space X with local coordinates $\{y_i\}$. Assume the S -matrix $S(y)$ depends smoothly on all variables and has level crossings at a finite number of points in $I \times X$, with $F(P_\alpha^S) = O(d^{\perp 2})$ near the level crossings, where d is the distance to the crossing. Assume that S has the limiting behavior given in Eq. (4.1). Then*

$$s_{2k+1}(y) = \frac{1}{k!(2\pi)^{k+1}} \sum_{\alpha} d\theta_{\alpha}(y) \wedge \text{Tr}(F(P_{\alpha})^k) \quad (7.6)$$

is defined almost everywhere, and

$$\int_X \omega_k = \int_{I \times X} s_{2k+1}. \quad (7.7)$$

The proof is almost identical to that of theorem 1, and so is only sketched here. The form $s_{2k+1}(y)$ is defined everywhere except at level crossings. Near level crossings $s_{2k+1} = O(d^{\perp 2k})$, 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. 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

$$f(y) = \omega_{1\dots 2k} + \frac{1}{2L} \sum_{i=1}^{2k} (-1)^i \partial_i \theta \omega_{0,\dots,i\perp 1,\hat{i},i+1,\dots,2k}, \quad (7.8)$$

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:

$$f(y)\rho(y) = \frac{L}{\pi} \omega_{1,\dots,2k} + \frac{1}{2\pi} (d\theta \wedge \omega_k)_{0,1,\dots,2k}. \quad (7.9)$$

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 $s_{2k+1}(y)$. ■

To construct an example for theorem 3, we recall the non-Abelian analog of Berry's spin-1/2 example. (For details, see [13]). Let $X = \mathbb{R}^5$ be the space of

real, symmetric, traceless 3×3 matrices Q . Consider a spin-3/2 particle with the Hamiltonian

$$h(Q) = |Q| + \sum_{i,j=1}^3 Q_{ij} J_i J_j, \quad (7.10)$$

where $|Q|^2 = \frac{3}{2} \text{Tr}(Q^2)$ and $\{J_i\}$ are the usual angular momentum operators. The spectrum of h is $\{0, 2|Q|\}$, and each eigenvalue is doubly degenerate. If we restrict ourselves to a 4-sphere S^4 enclosing the origin in X , then the upper eigenbundle has 2nd Chern number $c_2 = +1$, while the lower eigenbundle has $c_2 = -1$.

We can now duplicate the construction of Section V. Consider a spin-3/2 particle on a semi-infinite chain with potential $V(n) = h(Q)\delta_{n0}$. Our parameter space is a 4-sphere of the form $|Q| = \text{constant}$. As before, there is continuous spectrum over the energy range $[-2, 2]$. If $|Q| > 1/2$ there is a bound state with energy $2|Q| + \frac{1}{2|Q|}$. This bound state is doubly degenerate and has (2nd) Chern number $+1$. The scattering states therefore have (2nd) Chern number 0 if $|Q| < 1/2$ and -1 if $|Q| > 1/2$. The 5-form $s_5(y)$ is proportional to $d\theta_0 - d\theta_1$ times the area form on S^4 , and integrating s_5 over $I \times S^4$ correctly computes the Chern number in all cases.

VIII. Appendix: Scattering and Tight Binding Models

Here we recall some basic facts from scattering theory and tight-binding models on graphs.

Discrete Schrödinger Operators for Graphs:

For an arbitrary graph there is a conventional notion of a discrete Schrödinger operator associated with the graph. For each vertex v we have a real potential $V(v)$, and for each pair of adjacent vertices we have a hopping amplitude $t_{vv'}$ satisfying $t_{vv'} = \bar{t}_{v'v}$. We consider the Hermitian operator H defined by

$$(H\psi)(v) = \sum t_{vv'}\psi(v') + V(v)\psi(v). \quad (A.1)$$

Consider a graph with n strands going to infinity, which we label by $\alpha \in 1, \dots, n$. Let x be an integer label of the vertices along a given strand (so that the point at infinity corresponds to $x = \infty$). The function $\exp \pm ikx$, with $0 \leq k \leq \pi$, is a plane wave. We henceforth assume that $t_{vv'} = 1$ and $V(v) = 0$ for all but a finite number of vertices. These assumptions guarantee absolutely continuous spectrum, with multiplicity n , for the momentum interval $[0, \pi]$, corresponding to the energy interval $[-2, 2]$.

Bound States: Bound states with exponentially decaying solutions behave at infinity like $(\pm 1)^n e^{\pm \kappa n}$ 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 . (The condition that ψ vanishes at a vertex is codimension 2 in the complex case and codimension 1 in the real case. This has to occur on all strands simultaneously.) For a connected system, our hypotheses in section IV 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 at least four strands go to infinity. In the complex case there need be at least two strands. The example in section V 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 $\psi(x) \rightarrow \zeta_{out} e^{ikx} + \zeta_{in} e^{\perp ikx}$ as $x \rightarrow \infty$. The on-shell S -matrix is the defined by

$$\zeta_{out} = S(k) \zeta_{in}. \quad (A.2)$$

Since there is no distinguished basis in \mathbb{C}^n , one focuses on unitary invariant properties of $S(k)$.

There is a class of graphs for which there is a simple formula for the on-shell S -matrix. Consider first a compact graph, and let h be the tight binding Hamiltonian for the graph (either with or without spin). Now attach an infinite strand (with free evolution on the strand) to each vertex of the graph. The scattering states are determined by the solutions of

$$(h - E)(\psi_{in} + \psi_{out}) = -(\psi_{in}/z + z\psi_{out}). \quad (A.4)$$

It follows that

$$S = -\frac{h - z}{h - 1/z}, \quad (A.5)$$

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. (4.1) holds with $A = 2/(h - 1)$, $T = 2/(h + 1)$.

The condition $\text{Ker}(h \mp 1) = 0$ 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 section 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 $h(y) = u(y)h_0 u^\dagger(y)$, with h_0 a fixed Hermitian matrix (whose spectrum does not contain ± 1), and with $u(y)$ a family of unitary matrices.

Acknowledgment. The authors gratefully acknowledge the hospitality of the Erwin Schrödinger Institute and to the ITP, Technion, where part of this work was done. We also thank Dan Freed for helpful discussions on the topology of infinite dimensional bundles.

References

- [1] D. J. Thouless, M. Kohmoto, P. Nightingale and M. den Nijs, *Quantum Hall conductance in a two dimensional periodic potential*, Phys. Rev. Lett. **49**, 40, (1982).
- [2] B. Simon, *Holonomy, the quantum adiabatic theorem and Berry's phase*, Phys. Rev. Lett. **51**, 2167 (1983); M.V. Berry, Proc. Roy. Soc. A **392**, 45–57, (1984)
- [3] R. Landauer, *IBM J. of Research and Development* **32** (1988)
- [4] V.A. Marchenko, *Sturm Liouville operators and their applications*, Birkhauser, (1986).
- [5] M. SH. Birman and D.R. Yafaev, *Spectral properties of the scattering matrix*, St. Petersburg Math. J. **4**, 1055–1079, (1993); *The spectral shift function, the work of M.G. Krein and its further developments*, *ibid* 833–870.
- [6] J. Milnor and J. Stasheff, *Characteristic Classes*, Princeton University Press and University of Tokyo Press, Princeton, 1974.
- [7] B.A. Dubrovin, A.T. Fomenko and S.P. Novikov, *Modern Geometry— Methods and Applications*, Vol. II, Springer, (1984)
- [8] A. Pressley and G. Segal, *Loop Groups*, Oxford University Press, (1988).
- [9] D. Freed, *An Index Theorem for Families of Fredholm Operators Parameterized by a Group*, Topology **27** (1988) 279–300.
- [10] B. Simon, *Trace Ideals and their Applications*, Cambridge University Press, (1979)
- [11] A. Jensen and T. Kato. *Spectral Properties of Schrödinger Operators and Time-Decay of the Wave Functions*, Duke. Math. J. **46** 583–611 (1979)
- [12] W. Thirring, *Quantum Mechanics of Atoms and Molecules*, Springer, (1979)
- [13] J.E. Avron, L. Sadun, J. Segert and B. Simon, *Chern Numbers, Quaternions, and Berry's Phases in Fermi Systems*, Commun. Math. Phys **124**, 595–627 (1989)