Notes for the Master Thesis

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Sammanfattning

This is a collection of notes pertaining to concepts I needed to learn for my master's thesis.

Innehåll

1 Mathematical Prior

The Residue Theorem The residue theorem states that for a function $f(z)$ with a pole of order n at z_0, the integral of f about a positively oriented contour around z_0 satisfies

$$\oint \frac{\mathrm{d}z}{2\pi i} f(z) = \mathrm{Res}(f, z_0),$$

with

$$\mathrm{Res}(f, z_0) = \frac{1}{(n-1)!} \lim_{z \to z_0} \frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}} \left((z - z_0)^n f(z) \right).$$

Differential Forms The set of p-forms, or differential forms, is the set of $(0, p)$ tensors that are completely antisymmetric. They are constructed using the wedge product, defined as

$$\bigwedge_{k=1}^{p} d\chi^{\mu_k} = \sum_{\sigma \in S_p} \mathrm{sgn}(\sigma) \bigotimes_{k=1}^{p} d\chi^{\mu_{\sigma(k)}}.$$

Here S_p is the set of permutations of p elements. There exists

$$n_p^N = \binom{N}{k}$$

basis elements. We note that the wedge product is antisymmetric under the exchange of two basis elements. Hence, once an ordering of indices has been chosen, any permutation will simply create a linearly dependent map.

Consider now some antisymmetric tensor ω. Introducing the antisymmetrizer

$$\bigotimes_{k=1}^{p} d\chi^{[\mu_{\sigma(k)}]} = \frac{1}{p!} \sum_{\sigma \in S_p} \mathrm{sgn}(\sigma) \bigotimes_{k=1}^{p} d\chi^{\mu_{\sigma(k)}},$$

the symmetry yields

$$\omega = \omega_{\mu_1 \ldots \mu_p} \bigotimes_{k=1}^{p} d\chi^{\mu_{\sigma(k)}} = \omega_{\mu_1 \ldots \mu_p} \bigotimes_{k=1}^{p} d\chi^{[\mu_{\sigma(k)}]} = \frac{1}{p!} \omega_{\mu_1 \ldots \mu_p} \bigwedge_{k=1}^{p} d\chi^{\mu_k}.$$

In other words, we can antisymmetrize the components of ω to write it as a differential form.

The Exterior Derivative We define the exterior derivative of a differential form according to

$$d\omega = \frac{1}{p!} \partial_{\mu_1} \omega_{\mu_2 \ldots \mu_{p+1}} \bigwedge_{k=1}^{p+1} d\chi^{\mu_k},$$

which is a $p+1$-form.

Matrix-Valued Differential Forms A matrix-valued differential form is a differential form whose components are matrices. For these we need to define a slightly different wedge product according to

$$(A \wedge B)^a{}_b = A^a{}_c \wedge B^c{}_b.$$

In words, its components are found by computing the matrix product of the corresponding components of A and B, but using the wedge product instead of the normal multiplication. The output of this is then a new matrix-valued differential form. Their exterior derivatives are defined as for normal differential forms. We will use greek indices for the differential form structure and latin indices for the matrix structure.

Non-Abelian Gauge Theory - an Example We define the field strength 2-form

$$F = dA + A^2,$$

where we now suppress wedge products, as tensor products will not appear. By definition we have

$$A^2 = (A_\mu d\chi^\mu) \wedge (A_\nu d\chi^\nu) = \frac{1}{2}(A_\mu A_\nu - A_\nu A_\mu) d\chi^\mu d\chi^\nu = \frac{1}{2}[A_\mu, A_\nu] d\chi^\mu d\chi^\nu.$$

Now, F is a differential form, meaning we can write $F = \frac{1}{2} F_{\mu\nu} d\chi^\mu d\chi^\nu$. As for dA we have

$$dA = \partial_\mu A_\nu d\chi^\mu d\chi^\nu = \frac{1}{2}(\partial_\mu A_\nu - \partial_\nu A_\mu) d\chi^\mu d\chi^\nu,$$

where we in the last step explicitly antisymmetrized the result. Thus we have

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu].$$

Next, defining the gauge covariant derivative

$$\vec{\boldsymbol{\nabla}}_\mu = \partial_\mu + A_\mu.$$

We then have

$$\left[\vec{\boldsymbol{\nabla}}_\mu, \vec{\boldsymbol{\nabla}}_\nu\right] = [\partial_\mu, \partial_\nu] + [A_\mu, A_\nu] + [\partial_\mu, A_\nu] - [\partial_\nu, A_\mu].$$

For the first commutator, all components have the same matrix structure, so they commute. For the last two terms we will need to use the product rule to find

$$[\partial_\mu, A_\nu] = \partial_\mu A_\nu - A_\nu \partial_\mu = (\partial_\mu A_\nu) + A_\nu \partial_\mu - A_\nu \partial_\mu = (\partial_\mu A_\nu),$$

with the brackets highlighting the terms that are self-contained and do not act as operators. Thus we have

$$\left[\vec{\boldsymbol{\nabla}}_\mu, \vec{\boldsymbol{\nabla}}_\nu\right] = (\partial_\mu A_\nu) - (\partial_\nu A_\mu) + [A_\mu, A_\nu] = F_{\mu\nu}.$$

Next, for two vector fields we have

$$F(X, Y) = \frac{1}{2}\left[\vec{\boldsymbol{\nabla}}_\mu, \vec{\boldsymbol{\nabla}}_\nu\right] d\chi^\mu(X) d\chi^\nu(Y) = \frac{1}{2}\left[\vec{\boldsymbol{\nabla}}_\mu, \vec{\boldsymbol{\nabla}}_\nu\right](X^\mu Y^\nu - X^\nu Y^\mu).$$

We have

$$\vec{\boldsymbol{\nabla}}_\rho X^\mu Y^\nu = \partial_\rho X^\mu Y^\nu + A_\rho (X^\mu Y^\nu) = Y^\nu \partial_\rho (X^\mu) + X^\mu \partial_\rho (Y^\nu) + X^\mu Y^\nu \partial_\rho + A_\rho X^\mu Y^\nu,$$

and in particular

$$\begin{aligned}
\vec{\boldsymbol{\nabla}}_\nu X^\mu Y^\nu =& Y^\nu \partial_\nu (X^\mu) + X^\mu \partial_\nu (Y^\nu) + X^\mu Y^\nu \partial_\nu + A_\nu X^\mu Y^\nu = Y^\nu \partial_\nu (X^\mu) + X^\mu \partial_\nu (Y^\nu) + X^\mu \vec{\boldsymbol{\nabla}}_Y, \\
\vec{\boldsymbol{\nabla}}_\mu X^\mu Y^\nu =& Y^\nu \partial_\mu (X^\mu) + X^\mu \partial_\mu (Y^\nu) + Y^\nu \vec{\boldsymbol{\nabla}}_X.
\end{aligned}$$

Thus we have

$$\begin{aligned}
\vec{\boldsymbol{\nabla}}_\mu \vec{\boldsymbol{\nabla}}_\nu X^\mu Y^\nu =& \partial_\mu Y^\nu \partial_\nu (X^\mu) + \partial_\mu X^\mu \partial_\nu (Y^\nu) + \partial_\mu X^\mu \vec{\boldsymbol{\nabla}}_Y + A_\mu X^\mu \vec{\boldsymbol{\nabla}}_Y \\
=& \partial_\mu Y^\nu \partial_\nu (X^\mu) + \partial_\mu X^\mu \partial_\nu (Y^\nu) + (\partial_\mu X^\mu) \vec{\boldsymbol{\nabla}}_Y + \vec{\boldsymbol{\nabla}}_X \vec{\boldsymbol{\nabla}}_Y, \\
\vec{\boldsymbol{\nabla}}_\nu \vec{\boldsymbol{\nabla}}_\mu X^\mu Y^\nu =& \partial_\nu Y^\nu \partial_\mu (X^\mu) + \partial_\nu X^\mu \partial_\mu (Y^\nu) + (\partial_\nu Y^\nu) \vec{\boldsymbol{\nabla}}_X + \vec{\boldsymbol{\nabla}}_Y \vec{\boldsymbol{\nabla}}_X
\end{aligned}$$

The final result is found by first computing the difference of the above. One then notes down the result of swapping X and Y in that difference and subtracting that from what you have. First, the two connections net their commutator. The lone connections are found twice after the subtaction. Next, for the other terms the derivative can act on either factor or move to the right. The two former have terms with opposite sign cancelling them, and

$$\begin{aligned}
\left[\vec{\boldsymbol{\nabla}}_\mu, \vec{\boldsymbol{\nabla}}_\nu\right](X^\mu Y^\nu - X^\nu Y^\mu) =&2\left[\vec{\boldsymbol{\nabla}}_X, \vec{\boldsymbol{\nabla}}_Y\right] + 2\left((\partial_\mu X^\mu)\vec{\boldsymbol{\nabla}}_Y - (\partial_\nu Y^\nu)\vec{\boldsymbol{\nabla}}_X\right) \\
&+ 2(Y^\nu(\partial_\nu X^\mu) + X^\mu(\partial_\nu Y^\nu))\partial_\mu - 2(Y^\nu(\partial_\mu X^\mu) + X^\mu(\partial_\mu Y^\nu))\partial_\nu \\
=&2\left[\vec{\boldsymbol{\nabla}}_X, \vec{\boldsymbol{\nabla}}_Y\right] + 2\left((\partial_\mu X^\mu)\vec{\boldsymbol{\nabla}}_Y - (\partial_\nu Y^\nu)\vec{\boldsymbol{\nabla}}_X\right) \\
&+ 2[Y, X]^\mu\partial_\mu + 2(X^\mu(\partial_\nu Y^\nu)\partial_\mu - Y^\nu(\partial_\mu X^\mu)\partial_\nu) \\
=&2\left[\vec{\boldsymbol{\nabla}}_X, \vec{\boldsymbol{\nabla}}_Y\right] + 2\left((\partial_\mu X^\mu)Y^\nu A_\nu - (\partial_\nu Y^\nu)X^\mu A_\mu\right) + 2[Y, X]^\mu\partial_\mu \\
=&2\left(\left[\vec{\boldsymbol{\nabla}}_X, \vec{\boldsymbol{\nabla}}_Y\right] + [Y, X]^\mu A_\mu + [Y, X]^\mu\partial_\mu\right),
\end{aligned}$$

and thus

$$F(X, Y) = \left[\vec{\boldsymbol{\nabla}}_X, \vec{\boldsymbol{\nabla}}_Y\right] - \vec{\boldsymbol{\nabla}}_{[X,Y]}.$$

As for the exterior derivative of the field strength, we have

$$\begin{aligned}
dF =&\frac{1}{2}\partial_\mu F_{\nu\rho} d\chi^\mu d\chi^\nu d\chi^\rho \\
=&\frac{1}{2}\left(\partial_\mu(A_\nu A_\rho) - \partial_\mu(A_\rho A_\nu)\right) d\chi^\mu d\chi^\nu d\chi^\rho \\
=&\frac{1}{2}\left(\partial_\mu(A_\nu)A_\rho + A_\nu\partial_\mu(A_\rho) - \partial_\mu(A_\rho)A_\nu - A_\rho\partial_\mu(A_\nu)\right) d\chi^\mu d\chi^\nu d\chi^\rho,
\end{aligned}$$

as we have for any differential form F that $ddF = \partial_\mu\partial_\nu F_I d\chi^\mu d\chi^\nu d\chi^I = 0$, using the notation I to refer to some set of indices. Now, by comparison we have

$$FA - AF = \frac{1}{2}[F_{\mu\nu}, A_\rho] d\chi^\mu d\chi^\nu d\chi^\rho = \frac{1}{2}\left(F_{\mu\nu}A_\rho - A_\mu F_{\nu\rho}\right) d\chi^\mu d\chi^\nu d\chi^\rho,$$

using the properties of the indices under cyclic permutation. We find

$$\begin{aligned}
F_{\mu\nu}A_\rho - A_\mu F_{\nu\rho} =& \left(\partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]\right) A_\rho - A_\mu\left(\partial_\nu A_\rho - \partial_\rho A_\nu + [A_\nu, A_\rho]\right) \\
=&\partial_\mu(A_\nu)A_\rho - \partial_\nu(A_\mu)A_\rho - A_\mu\partial_\nu A_\rho + A_\mu\partial_\rho A_\nu,
\end{aligned}$$

and permuting indices cyclically we find

$$dF + AF - FA = 0,$$

which is a so-called Bianchi identity.

Next we study the form F^2. We have

$$dF^2 = d(F)F + FdF = (FA - AF)F + F(FA - AF).$$

Computing the trace of this involves computing the trace of objects of the form

$$F_{\mu_1\mu_2}A_{\mu_3}F_{\mu_4\mu_5}\bigwedge_{i=1}^{5} d\chi^{\mu_i}.$$

We note that if the first factor of F can be moved to the right in the trace, we will have shown that it is zero. Traces are invariant under cyclic permutation of matrices, so we can certainly move the components themselves. As for the differential forms, moving the first and second ones to the right requires either passing through 3 others, providing no net sign and yielding

$$\mathrm{tr}\left(dF^2\right) = d\,\mathrm{tr}\left(F^2\right) = 0.$$

Similarly we may consider the form F^n. Its trace is

$$d\,\mathrm{tr}(F^n) = n\,\mathrm{tr}\left(F^{n-1}dF\right) = n\,\mathrm{tr}\left(F^{n-1}(FA - AF)\right).$$

By the exact same argument we must have

$$d\,\mathrm{tr}(F^n) = 0.$$

Alternatively, let us prove that

$$dF^n = F^n A - AF^n.$$

Evidently it holds for $n = 1$. Next, assuming it to hold for some particular n, it follows that

$$\begin{aligned} dF^{n+1} =& d(F^n)F + F^n dF \\ =& (F^n A - AF^n)F + F^n(FA - AF) \\ =& F^{n+1}A - AF^{n+1}, \end{aligned}$$

completing the proof. Using the properties of the trace and the cyclic permutivity of the indices, we reobtain the same result.

The form F^2 is of some more interest. We have

$$F^2 = (dA)^2 + A^2 dA + d(A)A^2 + A^4.$$

Let us compute its trace. The last term is the easiest to handle as it is a contraction of a symmetric matrix product with an antisymmetric differential form, and is thus zero. Antisymmetrizing the components does not help due to the trace, which allows you to cyclically permute the matrices without changing the sign. Antisymmetrizing they start with the opposite sign of another term related to the first one by cyclic permutation, and it must be zero. As for the others we have

$$\begin{aligned} \mathrm{tr}\big((dA)^2 + A^2 dA + d(A)A^2\big) =& \mathrm{tr}\left(d(AdA) + \frac{2}{3}(A^2 dA + d(A)A^2 + Ad(A)A)\right) \\ =& \mathrm{tr}\left(d(AdA) + \frac{2}{3} dA^3\right) \\ =& d\,\mathrm{tr}\left((AdA) + \frac{2}{3}A^3\right). \end{aligned}$$

Let us finally investigate the topological invariance of integrals of F^2. Under a small deformation of A, we have

$$\begin{aligned} \delta\,\mathrm{tr}(F^n) =& n\,\mathrm{tr}\big(F^{n-1}\,\delta F\big) \\ =& n\left(\mathrm{tr}\big(F^{n-1} d\,\delta A\big) + \mathrm{tr}\big(F^{n-1}\,\delta A\, A\big) + \mathrm{tr}\big(F^{n-1} A\,\delta A\big)\right) \\ =& n\left(\mathrm{tr}\big(F^{n-1} d\,\delta A\big) - \mathrm{tr}\big(AF^{n-1}\,\delta A\big) + \mathrm{tr}\big(F^{n-1} A\,\delta A\big)\right) \\ =& n\,\mathrm{tr}\big(dF^{n-1}\,\delta A\big). \end{aligned}$$

Integration of Differential Forms Consider a set of p tangent vectors X_i. The corresponding coordinate displacements are $\mathrm{d}\chi_i^a = X_i^a\,\mathrm{d}t_i$, with no sum over i. We would now like to compute the p-dimensional volume defined by the X_i and $\mathrm{d}t_i$. We expect that if any of the X_i are linearly dependent the volume should be zero. We also expect that the volume be linear in the X_i. This implies

$$\mathrm{d}V_p = \omega(X_1, \ldots, X_p)\,\mathrm{d}t_1 \ldots \mathrm{d}t_p$$

for some differential form ω. We now define the integral over the p-volume S over the p-form ω as

$$\int_S \omega = \int \mathrm{d}t_1 \ldots \int \mathrm{d}t_p\,\omega(\dot{\gamma}_1, \ldots, \dot{\gamma}_p).$$

Here the γ_i are the set of curves that span S, the dot symbolizes the derivative with respect to the individual curve parameters and the right-hand integration is performed over the appropriate set of parameter values.

Stokes' Theorem Stokes' theorem relates the integral of a differential form $d\omega$ over some subset V of a manifold to an integral over ∂V of another differential form. It states that

$$\int_V d\omega = \oint_{\partial V} \omega.$$

2 Topology

Topological Spaces Let X be a set and $T = \{U_i | i \in I\}$ be a collection of subsets of X (I is some set of indices). The pair (X, T) (sometimes we only explicitly write X) is defined as a topological space if

- $\emptyset,\ X \in T$.
- If J is any subcollection of I, the family $\{U_j | j \in J\}$ satisfies
$$\bigcup_{j \in J} U_j \in T.$$
- If J is any finite subcollection of I, the family $\{U_j | j \in J\}$ satisfies
$$\bigcap_{j \in J} U_j \in T.$$

If the two satisfy the definition, we say that T gives a topology to X. The U_i are called its open sets.

Two cases of little interest are $T = \{\emptyset,\ X\}$ and T being the collection of all subsets of X. The two are called the trivial and discrete topologies respectively.

Metrics A metric is a map $d : X \times X \to \mathbb{R}$ that satisfies

- $d(x, y) = d(y, x)$.
- $d(x, x) \geq 0$, with equality applying if and only if $x = y$.
- $d(x, y) + d(y, z) \geq d(x,)z$.

Metric Spaces Suppose X is endowed with a metric. The collection of open disks

$$U_\varepsilon = \{x \in X | d(x, x_0) < \varepsilon\}$$

then gives a topology to X called the metric topology. The pair forms a metric space.

Continuous Maps A map between two topological spaces X and Y is continuous if its inverse maps an open set in Y to an open set in X.

Neighborhoods N is a neighborhood of x if it is a subset of X and x belongs to at least one open set contained within N.

Hausdorff Spaces A topological space is a Hausdorff space if, for any two points x, y, there exists neighborhoods U_x, U_y of the two points that do not intersect. This is an important type of topological space, as examples in physics are practically always within this category.

Homeomorphisms A homeomorphism (not to be confused with a homomorphism, however hard it may be) is a continuous map between two topological spaces with a continuous inverse. Two topological spaces are homeomorphic if there exists a homeomorphism between them.

Homotopy Types Two topological spaces belong to the same homotopy type if there exists a continuous map from one to the other. This is a more relaxed version of homeomorphicity, as we no longer require the map to be invertible.

Donuts and Coffee Mugs Homeomorphicity defines an equivalence relation between topological spaces. This means that we can define topological spaces into categories based on homeomorphicity.

We are now in a position to introduce the poor man's notion of topology, which considers two bodies as equivalent if one can be deformed into the other without touching two parts of the surface or tearing a part of the body. These continuous deformations correspond to homeomorphisms, but we will try to keep the discussions more to the abstract.

Topological Invariants An important question pertaining to this division of topological spaces is what separates the different categories. One possible answer is so-called topological invariants, quantities which are invariant under homeomorphism. The issue with this answer is that the full set of topological invariants has not been identified, hence they can only be used to verify that two topological spaces belong to different categories.

Subgroups and Equivalence Let H be a subgroup of an (Abelian) group G. We say that x and y are equivalent if

$$x - y \in H.$$

The addition operation is the group operation, a smart choice of notation as G is Abelian. We denote the corresponding equivalence class as $[x]$ and the set of all such classes is the quotient space $\frac{G}{H}$. From this we have a natural operation

$$[x] + [y] = [x + y]$$

on the quotient space.

3 Quantum Pumps

Berry Phase, Connection and Curvature Consider a system with a Hamiltonian and eigenstates parametrized by some set of parameters χ - that is, we have for each value of χ a set of eigenstates

$$\mathcal{H}(\chi)\left|n(\chi)\right\rangle = E_n(\chi)\left|n(\chi)\right\rangle .$$

The adiabatic theorem tells us that if R is varied such that the Hamiltonian changes sufficiently slowly, a state which is initialized to an eigenstate at $t = 0$ will evolve to a corresponding eigenstate at a later time. In the general case we have

$$\left|\psi_n(t)\right\rangle = e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int\limits_0^t \mathrm{d}\tau E_n(\tau)} \left|n(\chi(t))\right\rangle .$$

The former factor is the complex exponential of the so-called Berry phase. Inserting this into the Schrödinger equation we find

$$\gamma_n = i\int\limits_0^t \mathrm{d}\tau \, \left\langle n(\chi(\tau))\right| \frac{\partial}{\partial\tau} \left|n(\chi(\tau))\right\rangle .$$

Noting that

$$\frac{\partial}{\partial\tau}\left|n(\chi(\tau))\right\rangle = \frac{\mathrm{d}R}{\mathrm{d}\tau} \cdot \vec{\boldsymbol{\nabla}}_R \left|\chi(R)\right\rangle ,$$

we can define the Berry connection

$$A_n = i\left\langle n(\chi)\right| \vec{\boldsymbol{\nabla}}_\chi \left|n(\chi)\right\rangle$$

and find

$$\gamma_n = i\int\limits_C \mathrm{d}\chi \cdot A_n.$$

C is the orbit in parameter space traversed during the time evolution.

In a slightly more sophisticated manner, the Berry connection may be taken to be a 1-form

$$A_n = i \langle n(R)| \partial_\mu |n(R)\rangle d\chi^\mu.$$

Due to Stokes' theorem, the line integral of the Berry connection about some closed path is related to the surface integral of its exterior derivative, termed the Berry curvature. Its components are

$$\Omega^{(2)}_{n,\mu\nu} = \partial_\mu A_{n,\nu} - \partial_\nu A_{n,\mu},$$

and we have

$$\int_{\partial S} A_n = \frac{1}{2} \int_S \mathrm{d}\chi^\mu \wedge \mathrm{d}\chi^\nu \, \Omega^{(2)}_{n,\mu\nu}.$$

A More Sophisticated Definition From this point on we switch to the more compact notation

$$\partial_\mu |n\rangle = |\partial_\mu n\rangle$$

and suppress the parameter dependence. The Berry curvature is given by

$$\Omega^{(2)} = dA_n = \frac{1}{2}(\partial_\mu A_{n,\nu} - \partial_\nu A_{n,\mu}) d\chi^\mu \wedge d\chi^\nu,$$

and we find

$$\Omega^{(2)}_{\mu\nu} = i \left(\langle \partial_\mu n | \partial_\nu n \rangle + \langle n | \partial_\mu \partial_\nu n \rangle - \langle \partial_\nu n | \partial_\mu n \rangle - \langle n | \partial_\nu \partial_\mu n \rangle \right) = i \left(\langle \partial_\mu n | \partial_\nu n \rangle - \langle \partial_\nu n | \partial_\mu n \rangle \right).$$

This can be expressed without derivatives of the state. To do that we differentiate the eigenvalue expression to yield

$$\partial_\mu \mathcal{H} |n\rangle + \mathcal{H} |\partial_\mu n\rangle = \partial_\mu E_n |n\rangle + E_n |\partial_\mu n\rangle.$$

Using the orthogonality of the eigenstates, we have for some $n \neq m$ that

$$\langle m | \partial_\mu \mathcal{H} | n \rangle = (E_n - E_m) \langle m | \partial_\mu n \rangle.$$

We can now solve for the inner product on the left-hand side and its complex conjugate, as well as sum over m, to find

$$\Omega^{(2)}_{\mu\nu} = i \sum_{m \neq n} \frac{\langle n | \partial_\mu \mathcal{H} | m \rangle \langle m | \partial_\nu \mathcal{H} | n \rangle - \text{c.c}}{(E_n - E_m)^2}.$$

Finally we introduce a third definition

$$\Omega^{(2)} = \frac{i}{2} \oint \frac{\mathrm{d}z}{2\pi i} \operatorname{tr}\big(G d\mathcal{H} G^2 d\mathcal{H}\big).$$

G is given by $(z - \mathcal{H})^{-1}$ and the integral is a counter-clockwise contour integral around the energy of the state in consideration. There is also the appearance of the exterior derivative of the Hamiltonian.

Does this correspond to our previous notion of the Berry curvature? To investigate, let us rewrite the above operators as

$$\mathcal{H} = \sum_n E_n |n\rangle\langle n|, \quad G = \sum_n \frac{1}{z - E_n} |n\rangle\langle n|.$$

Next we note that

$$G dG^{-1} = -dG G^{-1} = -G d\mathcal{H},$$

hence

$$G dG^{-1} G dG^{-1} G = G d\mathcal{H} G d\mathcal{H} G,$$

and by cyclic permutation we have

$$\begin{aligned}
\operatorname{tr}\big(GdG^{-1}GdG^{-1}G\big) &= \operatorname{tr}(Gd\mathcal{H}Gd\mathcal{H}G)\\
&= \operatorname{tr}\big(G\partial_\mu\mathcal{H}G\partial_\nu\mathcal{H}G\big)d\chi^\mu d\chi^\nu\\
&= \operatorname{tr}\big(G\partial_\nu\mathcal{H}G^2\partial_\mu\mathcal{H}\big)d\chi^\mu d\chi^\nu\\
&= -\operatorname{tr}\big(Gd\mathcal{H}G^2 d\mathcal{H}\big).
\end{aligned}$$

As a warmup to the final computation, consider a case where the spectrum is parameter-independent. In the eigenbasis of the Hamiltonian we generally have

$$\begin{aligned}
dG^{-1} &= \sum_n \left(-\partial_\mu E_n \,|n\rangle\langle n| + (z-E_n)\left(|\partial_\mu n\rangle\langle n| + |n\rangle\langle\partial_\mu n|\right)\right) d\chi^\mu,\\
dG &= \sum_n \left(\frac{\partial_\mu E_n}{(z-E_n)^2}\,|n\rangle\langle n| + \frac{1}{z-E_n}\left(|\partial_\mu n\rangle\langle n| + |n\rangle\langle\partial_\mu n|\right)\right) d\chi^\mu,
\end{aligned}$$

and thus in this case

$$GdG^{-1}GdG^{-1}G = \sum \frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\,|1\rangle\langle 1|\left(|\partial_\mu 2\rangle\langle 2| + |2\rangle\langle\partial_\mu 2|\right)|3\rangle\langle 3|\left(|\partial_\nu 4\rangle\langle 4| + |4\rangle\langle\partial_\nu 4|\right)|5\rangle\langle 5|\,e^{\mu\nu},$$

where the natural numbers are summed over and we abbreviate the differential form basis vector. Multiplying this out we have

$$\begin{aligned}
GdG^{-1}GdG^{-1}G &= \sum \frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\,|1\rangle\left(\langle 1|\partial_\mu 2\rangle\,\delta_{23} + \delta_{12}\,\langle\partial_\mu 2|3\rangle\right)\left(\langle 3|\partial_\nu 4\rangle\,\delta_{45} + \delta_{34}\,\langle\partial_\nu 4|5\rangle\right)\langle 5|\,e^{\mu\nu}\\
&= \sum |1\rangle\left(\frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\,\langle 1|\partial_\mu 2\rangle\,\delta_{23}\,\langle 3|\partial_\nu 4\rangle\,\delta_{45}\right.\\
&\quad + \frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\,\langle 1|\partial_\mu 2\rangle\,\delta_{23}\delta_{34}\,\langle\partial_\nu 4|5\rangle\\
&\quad + \frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\,\langle\partial_\mu 2|3\rangle\,\langle 3|\partial_\nu 4\rangle\,\delta_{45}\\
&\quad \left.+ \frac{(z-E_2)(z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\,\langle\partial_\mu 2|3\rangle\,\delta_{34}\,\langle\partial_\nu 4|5\rangle\right)\langle 5|\,e^{\mu\nu}\\
&= \sum |1\rangle\left(\frac{1}{z-E_1}\,\langle 1|\partial_\mu 2\rangle\,\langle 2|\partial_\nu 4\rangle\,\langle 4| + \frac{z-E_2}{(z-E_1)(z-E_5)}\,\langle 1|\partial_\mu 2\rangle\,\langle\partial_\nu 2|5\rangle\,\langle 5|\right.\\
&\quad \left.+ \frac{1}{z-E_3}\,\langle\partial_\mu 1|3\rangle\,\langle 3|\partial_\nu 4\rangle\,\langle 4| + \frac{1}{z-E_5}\,\langle\partial_\mu 1|3\rangle\,\langle\partial_\nu 3|5\rangle\,\langle 5|\right) e^{\mu\nu},
\end{aligned}$$

and

$$\begin{aligned}
\operatorname{tr}\big(GdG^{-1}GdG^{-1}G\big) &= \sum\left(\frac{1}{z-E_1}\,\langle 1|\partial_\mu 2\rangle\,\langle 2|\partial_\nu 4\rangle\,\langle 4|1\rangle + \frac{z-E_2}{(z-E_1)(z-E_5)}\,\langle 1|\partial_\mu 2\rangle\,\langle\partial_\nu 2|5\rangle\,\langle 5|1\rangle\right.\\
&\quad \left.+ \frac{1}{z-E_3}\,\langle\partial_\mu 1|3\rangle\,\langle 3|\partial_\nu 4\rangle\,\langle 4|1\rangle + \frac{1}{z-E_5}\,\langle\partial_\mu 1|3\rangle\,\langle\partial_\nu 3|5\rangle\,\langle 5|1\rangle\right) e^{\mu\nu}\\
1 &= \sum\left(\frac{1}{z-E_1}\,\langle 1|\partial_\mu 2\rangle\,\langle 2|\partial_\nu 4\rangle\,\delta_{41} + \frac{z-E_2}{(z-E_1)(z-E_5)}\,\langle 1|\partial_\mu 2\rangle\,\langle\partial_\nu 2|5\rangle\,\delta_{51}\right.\\
&\quad \left.+ \frac{1}{z-E_3}\,\langle\partial_\mu 1|3\rangle\,\langle 3|\partial_\nu 4\rangle\,\delta_{41} + \frac{1}{z-E_5}\,\langle\partial_\mu 1|3\rangle\,\langle\partial_\nu 3|5\rangle\,\delta_{51}\right) e^{\mu\nu}\\
&= \sum\left(\frac{1}{z-E_1}\,\langle 1|\partial_\mu 2\rangle\,\langle 2|\partial_\nu 1\rangle + \frac{z-E_2}{(z-E_1)^2}\,\langle 1|\partial_\mu 2\rangle\,\langle\partial_\nu 2|1\rangle\right.\\
&\quad \left.+ \frac{1}{z-E_3}\,\langle\partial_\mu 1|3\rangle\,\langle 3|\partial_\nu 1\rangle + \frac{1}{z-E_1}\,\langle\partial_\mu 1|3\rangle\,\langle\partial_\nu 3|1\rangle\right) e^{\mu\nu}.
\end{aligned}$$

Let us now perform the contour integral about a particular energy E_n. All of them are equal to 1 if and only if n is equal to the index that appears in the denominator, hence

$$\begin{aligned}\Omega^{(2)} =& -\frac{i}{2}\sum \left(\langle n|\partial_\mu 1\rangle \langle 1|\partial_\nu n\rangle + \langle n|\partial_\mu 1\rangle \langle \partial_\nu 1|n\rangle + \langle \partial_\mu 1|n\rangle \langle n|\partial_\nu 1\rangle + \langle \partial_\mu n|1\rangle \langle \partial_\nu 1|n\rangle\right) e^{\mu\nu} \\ =& -\frac{i}{2}\sum \left(-\langle \partial_\mu n|1\rangle \langle 1|\partial_\nu n\rangle + \langle \partial_\mu n|1\rangle \langle 1|\partial_\nu n\rangle + \langle 1|\partial_\mu n\rangle \langle \partial_\nu n|1\rangle - \langle \partial_\mu n|1\rangle \langle 1|\partial_\nu n\rangle\right) e^{\mu\nu} \\ =& \frac{i}{2}\left(\langle \partial_\mu n|\partial_\nu n\rangle - \langle \partial_\nu n|\partial_\mu n\rangle\right) e^{\mu\nu},\end{aligned}$$

and thus

$$\Omega^{(2)}_{\mu\nu} = i\left(\langle \partial_\mu n|\partial_\nu n\rangle - \langle \partial_\nu n|\partial_\mu n\rangle\right).$$

Let us now go to the general case. It will contain an operator product

$$\begin{aligned}&|1\rangle\langle 1| \left(-\partial_\mu E_2 |2\rangle\langle 2| + (z-E_2)\left(|\partial_\mu 2\rangle\langle 2| + |2\rangle\langle \partial_\mu 2|\right)\right) |3\rangle\langle 3| \left(-\partial_\nu E_4 |4\rangle\langle 4| + (z-E_4)\left(|\partial_\nu 4\rangle\langle 4| + |4\rangle\langle \partial_\nu 4|\right)\right) |5\rangle\langle 5| \\ =& |1\rangle \left(-\partial_\mu E_2 \delta_{12}\delta_{23} + (z-E_2)\left(\langle 1|\partial_\mu 2\rangle \delta_{23} + \delta_{12}\langle \partial_\mu 2|3\rangle\right)\right)\left(-\partial_\nu E_4 \delta_{34}\delta_{45} + (z-E_4)\left(\langle 3|\partial_\nu 4\rangle \delta_{45} + \delta_{34}\langle \partial_\nu 4|5\rangle\right)\right)\langle 5|,\end{aligned}$$

and the trace will turn this to

$$\left(-\partial_\mu E_2 \delta_{12}\delta_{23} + (z-E_2)\left(\langle 1|\partial_\mu 2\rangle \delta_{23} + \delta_{12}\langle \partial_\mu 2|3\rangle\right)\right)\left(-\partial_\nu E_4 \delta_{34}\delta_{45} + (z-E_4)\left(\langle 3|\partial_\nu 4\rangle \delta_{45} + \delta_{34}\langle \partial_\nu 4|5\rangle\right)\right)\delta_{15}.$$

Each bracket has three terms, so let us denote their products (after adding the extra factors) as a_{ij}, with i and j denoting which terms from each of the brackets are multiplied. We know that when tracing $a_{22}+a_{23}+a_{32}+a_{33}$, we get the result. We will thus have completed the proof if we can show that the others yield no net contribution. First we have

$$\begin{aligned}\sum a_{11} =& \sum \frac{1}{(z-E_1)(z-E_3)(z-E_5)}\left(-\partial_\mu E_2 \delta_{12}\delta_{23}\right)\left(-\partial_\nu E_4 \delta_{34}\delta_{45}\right)\delta_{15} e^{\mu\nu} \\ =& \sum \frac{\partial_\mu (E_2)\partial_\nu (E_4)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\delta_{23}\delta_{34}\delta_{45}\delta_{15} e^{\mu\nu} \\ =& \sum \frac{\partial_\mu (E_1)\partial_\nu (E_1)}{(z-E_1)^3} e^{\mu\nu}.\end{aligned}$$

This is identically zero as it contains a contraction of symmetric components with the antisymmetric differential form basis. As for the others we have

$$\begin{aligned}\sum a_{12} &= -\sum \frac{\partial_\mu E_2 (z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\delta_{23}\langle 3|\partial_\nu 4\rangle \delta_{45}\delta_{15} e^{\mu\nu} = -\sum \frac{\partial_\mu E_1}{(z-E_1)^2}\langle 1|\partial_\nu 1\rangle e^{\mu\nu}, \\ \sum a_{13} &= -\sum \frac{\partial_\mu E_2 (z-E_4)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\delta_{23}\delta_{34}\langle \partial_\nu 4|5\rangle \delta_{15} e^{\mu\nu} = -\sum \frac{\partial_\mu E_1}{(z-E_1)^2}\langle \partial_\nu 1|1\rangle e^{\mu\nu}, \\ \sum a_{21} &= -\sum \frac{\partial_\nu E_4 (z-E_2)}{(z-E_1)(z-E_3)(z-E_5)}\langle 1|\partial_\mu 2\rangle \delta_{23}\delta_{34}\delta_{45}\delta_{15} e^{\mu\nu} = -\sum \frac{\partial_\nu E_1}{(z-E_1)^2}\langle 1|\partial_\mu 1\rangle e^{\mu\nu}, \\ \sum a_{31} &= -\sum \frac{\partial_\nu E_4 (z-E_2)}{(z-E_1)(z-E_3)(z-E_5)}\delta_{12}\langle \partial_\mu 2|3\rangle \delta_{34}\delta_{45}\delta_{15} e^{\mu\nu} = -\sum \frac{\partial_\nu E_1}{(z-E_1)^2}\langle \partial_\mu 1|1\rangle e^{\mu\nu},\end{aligned}$$

and these all cancel each other exactly, completing the proof.

Properties of Parametrized States We will now derive some useful properties of derivatives of states of parametrized systems. Because orthogonality is preserved we have

$$\partial_\mu \langle m|n\rangle = \langle \partial_\mu m|n\rangle + \langle m|\partial_\mu n\rangle = 0.$$

Because the identity is also preserved we have

$$\sum |\partial_\mu n\rangle\langle n| + |n\rangle\langle \partial_\mu n| = 0.$$

The Single Spin Consider a single spin-$\frac{1}{2}$ in an external field of length 1. The Hamiltonian is

$$\mathcal{H} = h_x\sigma_x + h_y\sigma_y + h_z\sigma_z,$$

with the external field being restricted in length. With respect to the σ_z eigenstates at $\theta = \phi = 0$, which are of course angle-independent, we have

$$|{\downarrow}\rangle_{\theta,\phi} = \begin{bmatrix} -\sin\left(\frac{\theta}{2}\right)e^{-i\phi} \\ \cos\left(\frac{\theta}{2}\right) \end{bmatrix}, \ |{\uparrow}\rangle_{\theta,\phi} = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right)e^{-i\phi} \\ \sin\left(\frac{\theta}{2}\right) \end{bmatrix}, \tag{1}$$

and thus

$$A_{-,\theta} = 0,\ A_{-,\phi} = \sin^2\left(\frac{\theta}{2}\right),\ A_{+,\theta} = 0,\ A_{+,\phi} = \cos^2\left(\frac{\theta}{2}\right).$$

The Berry curvature is then

$$\Omega^{(2)}_{\pm,\theta\phi} = \mp\frac{1}{2}\sin(\theta).$$

This implies that the Berry phase induced after an adiabatic cycle is equal to half the subtended solid angle.

Higher Berry Curvature and the KS Invariant For an infinite $1d$ system, $\Omega^{(2)}$ might diverge. A convergent quantity might instead be found by splitting the Hamiltonian into a sum of local terms working at a finite range, i.e.

$$\mathcal{H} = \sum_{p\in\mathbb{Z}} \mathcal{H}_p.$$

The quantity

$$F^{(2)}_{pq} = \frac{i}{2}\oint \frac{\mathrm{d}z}{2\pi i}\,\mathrm{tr}\big(Gd\mathcal{H}_pG^2d\mathcal{H}_q\big)$$

then decays exponentially with respect to $|p-q|$ if the Hamiltonian is gapped, and is thus well-defined. Next we can construct the two-form

$$F^{(2)}_q = \sum_{p\in\mathbb{Z}} F^{(2)}_{pq} = \frac{i}{2}\oint \frac{\mathrm{d}z}{2\pi i}\,\mathrm{tr}\big(Gd\mathcal{H}G^2d\mathcal{H}_q\big).$$

Its exterior derivative is given by

$$dF^{(2)}_q = \sum_{p\in\mathbb{Z}} F^{(3)}_{pq}.$$

We have

$$\begin{aligned}
&\partial_\rho(G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q)e^{\rho\mu\nu} \\
&= \big(\partial_\rho G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\rho\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_p\partial_\rho G^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_pG^2\partial_\rho\partial_\nu\mathcal{H}_q\big)\,e^{\rho\mu\nu} \\
&= \big(\partial_\rho G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_p(\partial_\rho GG + G\partial_\rho G)\partial_\nu\mathcal{H}_q\big)\,e^{\rho\mu\nu} \\
&= \big(\partial_\rho\mathcal{H}G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_p(G\partial_\rho\mathcal{H}G^2 + G^2\partial_\rho\mathcal{H}G)\partial_\nu\mathcal{H}_q\big)\,e^{\rho\mu\nu} \\
&= \big(\partial_\rho\mathcal{H}G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_p(G\partial_\rho\mathcal{H}G^2 + G^2\partial_\rho\mathcal{H}G)\partial_\nu\mathcal{H}_q\big)\,e^{\rho\mu\nu} \\
&= \big(\partial_\rho\mathcal{H}G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_pG\partial_\rho\mathcal{H}G^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_pG^2\partial_\rho\mathcal{H}G\partial_\nu\mathcal{H}_q\big)\,e^{\rho\mu\nu},
\end{aligned}$$

and thus

$$\begin{aligned}
&\mathrm{tr}\big(\partial_\rho(G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q)\big)e^{\rho\mu\nu} \\
&= \mathrm{tr}\big(\partial_\rho\mathcal{H}G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_pG\partial_\rho\mathcal{H}G^2\partial_\nu\mathcal{H}_q + G\partial_\mu\mathcal{H}_pG^2\partial_\rho\mathcal{H}G\partial_\nu\mathcal{H}_q\big)e^{\rho\mu\nu} \\
&= \mathrm{tr}\big(\partial_\rho\mathcal{H}G\partial_\mu\mathcal{H}_pG^2\partial_\nu\mathcal{H}_q - G\partial_\rho\mathcal{H}G^2\partial_\mu\mathcal{H}_qG\partial_\nu\mathcal{H}_p + G\partial_\mu\mathcal{H}_pG^2\partial_\rho\mathcal{H}G\partial_\nu\mathcal{H}_q\big)e^{\rho\mu\nu}.
\end{aligned}$$

Somehow we are to find

$$F^{(3)}_{pq} = \frac{i}{6}\oint \frac{\mathrm{d}z}{2\pi i}\,\mathrm{tr}\big(G^2 d\mathcal{H} G d\mathcal{H}_p G d\mathcal{H}_q - G d\mathcal{H} G^2 d\mathcal{H}_p G d\mathcal{H}_q\big) - (p \leftrightarrow q).$$

To compute this we expand in eigenstates of the Hamiltonian according to

$$\begin{aligned} G^2 d\mathcal{H} G d\mathcal{H}_p G d\mathcal{H}_q &= \sum \frac{|1\rangle\langle 1|\,|2\rangle\langle 2|\,d\mathcal{H}\,|3\rangle\langle 3|\,d\mathcal{H}_p\,|4\rangle\langle 4|\,d\mathcal{H}_q}{(z-E_1)(z-E_2)(z-E_3)(z-E_4)} \\ &= \sum \frac{|1\rangle\langle 1|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(z-E_1)^2(z-E_2)(z-E_3)}. \end{aligned}$$

Let us now compute the contour integral around the ground state. The contributions from where only one number is zero is

$$\begin{aligned} &\sum - |0\rangle\langle 0|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q \left(\frac{1}{(E_0-E_2)^2(E_0-E_3)} + \frac{1}{(E_0-E_2)(E_0-E_3)^2}\right) \\ &\quad + \frac{|1\rangle\langle 1|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(E_0-E_1)^2(E_0-E_3)} + \frac{|1\rangle\langle 1|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_1)^2(E_0-E_2)}. \end{aligned}$$

Introducing

$$G_0 = \sum_{n\neq 0} \frac{1}{E_0 - E_n}\,|n\rangle\langle n|\,,$$

this can be written as

$$- |0\rangle\langle 0|\,\big(d\mathcal{H} G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_q + d\mathcal{H} G_0 d\mathcal{H}_p G_0^2 d\mathcal{H}_q\big) + G_0^2 d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p G_0 d\mathcal{H}_q + G_0^2 d\mathcal{H} G_0 d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q.$$

Similarly, when two of the numbers are zero we get the contribution

$$\begin{aligned} &\sum \frac{1}{2}\left(2\frac{|0\rangle\langle 0|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(E_0-E_3)^3} + 2\frac{|0\rangle\langle 0|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_2)^3}\right) - 2\frac{|1\rangle\langle 1|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_1)^3} \\ &= |0\rangle\langle 0|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p G_0^3 d\mathcal{H}_q + |0\rangle\langle 0|\,d\mathcal{H} G_0^3 d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q - 2G_0^3 d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q. \end{aligned}$$

Finally, if none or all of them are zero there is no contribution. Next, we have

$$G d\mathcal{H} G^2 d\mathcal{H}_p G d\mathcal{H}_q = \sum \frac{|1\rangle\langle 1|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(z-E_1)(z-E_2)^2(z-E_3)}.$$

The contributions after computing the contour integral are

$$\begin{aligned} &\sum - |1\rangle\langle 1|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q \left(\frac{1}{(E_0-E_1)^2(E_0-E_3)} + \frac{1}{(E_0-E_1)(E_0-E_3)^2}\right) \\ &\quad + \frac{|0\rangle\langle 0|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(E_0-E_2)^2(E_0-E_3)} + \frac{|1\rangle\langle 1|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_1)(E_0-E_2)^2} \\ &= - G_0^2 d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p G_0 d\mathcal{H}_q - G_0 d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p G_0^2 d\mathcal{H}_q + |0\rangle\langle 0|\,d\mathcal{H} G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_q + G_0 d\mathcal{H} G_0^2 d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q \end{aligned}$$

when one number is zero and

$$\begin{aligned} &\sum \frac{1}{2}\left(2\frac{|0\rangle\langle 0|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|3\rangle\langle 3|\,d\mathcal{H}_q}{(E_0-E_3)^3} + 2\frac{|1\rangle\langle 1|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_1)^3}\right) - 2\frac{|0\rangle\langle 0|\,d\mathcal{H}\,|2\rangle\langle 2|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q}{(E_0-E_2)^2} \\ &= |0\rangle\langle 0|\,d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p G_0^3 d\mathcal{H}_q + G_0^3 d\mathcal{H}\,|0\rangle\langle 0|\,d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q - 2\,|0\rangle\langle 0|\,d\mathcal{H} G_0^3 d\mathcal{H}_p\,|0\rangle\langle 0|\,d\mathcal{H}_q \end{aligned}$$

when two are. The final result is thus

$$\begin{aligned} F^{(3)}_{pq} &= \frac{i}{6}\Big(- \big\langle d\mathcal{H} G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_q\big\rangle - \big\langle d\mathcal{H} G_0 d\mathcal{H}_p G_0^2 d\mathcal{H}_q\big\rangle + \big\langle d\mathcal{H}_p G_0 d\mathcal{H}_q G_0^2 d\mathcal{H}\big\rangle \\ &\quad + \big\langle d\mathcal{H}_q G_0^2 d\mathcal{H} G_0 d\mathcal{H}_p\big\rangle + \langle d\mathcal{H}\rangle\big\langle d\mathcal{H}_p G_0^3 d\mathcal{H}_q\big\rangle + \big\langle d\mathcal{H} G_0^3 d\mathcal{H}_p\big\rangle\langle d\mathcal{H}_q\rangle \\ &\quad - 2\big\langle d\mathcal{H}_q G_0^3 d\mathcal{H}\big\rangle\langle d\mathcal{H}_p\rangle + \big\langle d\mathcal{H}_p G_0 d\mathcal{H}_q G_0^2 d\mathcal{H}\big\rangle + \big\langle d\mathcal{H}_p G_0^2 d\mathcal{H}_q G_0 d\mathcal{H}\big\rangle \\ &\quad - \big\langle d\mathcal{H} G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_q\big\rangle - \big\langle d\mathcal{H}_q G_0 d\mathcal{H} G_0^2 d\mathcal{H}_p\big\rangle - \langle d\mathcal{H}\rangle\big\langle d\mathcal{H}_p G_0^3 d\mathcal{H}_q\big\rangle \\ &\quad - \langle d\mathcal{H}_p\rangle\big\langle d\mathcal{H}_q G_0^3 d\mathcal{H}\big\rangle + 2\big\langle d\mathcal{H} G_0^3 d\mathcal{H}_p\big\rangle\langle d\mathcal{H}_q\rangle\Big) - (p \leftrightarrow q) \\ &= \frac{i}{6}\Big(-2\big\langle d\mathcal{H} G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_q\big\rangle - \big\langle d\mathcal{H} G_0 d\mathcal{H}_p G_0^2 d\mathcal{H}_q\big\rangle + 2\big\langle d\mathcal{H}_p G_0 d\mathcal{H}_q G_0^2 d\mathcal{H}\big\rangle \\ &\quad + \big\langle d\mathcal{H}_p G_0^2 d\mathcal{H}_q G_0 d\mathcal{H}\big\rangle + \big\langle d\mathcal{H}_q G_0^2 d\mathcal{H} G_0 d\mathcal{H}_p\big\rangle - \big\langle d\mathcal{H}_q G_0 d\mathcal{H} G_0^2 d\mathcal{H}_p\big\rangle \\ &\quad + 3\big\langle d\mathcal{H} G_0^3 d\mathcal{H}_p\big\rangle\langle d\mathcal{H}_q\rangle - 3\big\langle d\mathcal{H}_q G_0^3 d\mathcal{H}\big\rangle\langle d\mathcal{H}_p\rangle\Big) - (p \leftrightarrow q), \end{aligned}$$

where all the expectation values are computed in the ground state.

This quantity is somewhat difficult to manage, but one can reduce it somewhat. First, states excited outside of the support of $\mathcal{H}_p$ and $\mathcal{H}_q$ do not contribute, as they are orthogonal to the ground state and can pass through $\mathcal{H}_p$ and $\mathcal{H}_q$, as well as their exterior derivatives. By a similar token, $F^{(3)}_{pq}$ is non-zero only if $\mathcal{H}_p$ and $\mathcal{H}_q$ have overlapping support. This also implies that the only terms in the Hamiltonian that contribute are the ones with support overlapping with both $\mathcal{H}_p$ and $\mathcal{H}_q$.

Using these quantities we can construct a 3-form Berry curvature

$$\Omega^{(3)}(f) = \frac{1}{2}\sum_{p,q\in\mathbb{Z}} F^{(3)}_{pq}(f(q) - f(p)).$$

f is some sigmoid function, its particular shape turning out to be unimportant. A simple choice is $f(p) = \Theta(p-a)$ for some $a \in \mathbb{Z} + \frac{1}{2}$. For this particular choice we have

$$\begin{aligned}
\Omega^{(3)}(f) =& \frac{1}{2}\sum_{p,q\in\mathbb{Z}} F^{(3)}_{pq}(\Theta(q-a) - \Theta(p-a)) \\
=& \frac{1}{2}\sum_{p\in\mathbb{Z},\ q>a} F^{(3)}_{pq}(1-\Theta(p-a)) - \frac{1}{2}\sum_{p\in\mathbb{Z},\ q<a} F^{(3)}_{pq}\Theta(p-a) \\
=& \frac{1}{2}\sum_{p<a,\ q>a} F^{(3)}_{pq} - \frac{1}{2}\sum_{p>a,\ q<a} F^{(3)}_{pq} \\
=& \sum_{p<a,\ q>a} F^{(3)}_{pq},
\end{aligned}$$

using the antisymmetry of $F^{(3)}_{pq}$.

Finally we can define the KS invariant

$$Q_{\mathrm{KS}} = \int \Omega^{(3)}(f),$$

which is performed over the full parameter space of the Hamiltonian. This is a topological invariant.

The Dimerized Spin Chain Consider an infinite spin chain with Hamiltonian

$$\mathcal{H}_{1d} = \sum_{p\in\mathbb{Z}} \mathcal{H}^1_p(w) + \sum_{p\in 2\mathbb{Z}+1} \mathcal{H}^{2,+}_{p,p+1}(w) + \sum_{p\in 2\mathbb{Z}} \mathcal{H}^{2,-}_{p,p+1}(w).$$

The parameter takes values on S^3. There are three kinds of terms here. The first is

$$\mathcal{H}^1_p(w) = (-1)^p(w_1\sigma^1_p + w_2\sigma^2_p + w_3\sigma^3_p),$$

which is some fluctuating on-site term. The two others are

$$\mathcal{H}^{2,\pm}_{p,p+1}(w) = g^{\pm}(w)\sum_{\mu=1,2,3} \sigma^\mu_p \sigma^\mu_{p+1},$$

with two functions

$$g^+(w) = \begin{cases} w_4, & 0 \le w_4 \le 1, \\ 0, & \text{otherwise}, \end{cases} \qquad g^-(w) = \begin{cases} -w_4, & -1 \le w_4 \le 0, \\ 0, & \text{otherwise}. \end{cases}$$

This type of interaction defines five distinct regimes:

- $w_4 = 1$, where there is only odd-even bonding.
- $0 < w_4 < 1$, where there is odd-even bonding and on-site interactions.
- $w_4 = 0$, where there is only on-site interaction.
- $-1 < w_4 < 0$, where there is even-odd bonding and on-site interactions.

- $w_4 = 1$, where there is only even-odd bonding.

To compute the 3-form Berry curvature and KS invariant, we rewrite the Hamiltonian as a sum of local terms. These are

$$\mathcal{H}_p(w) = \mathcal{H}_p^1(w) + x\mathcal{H}_{p,p+1}^{2,\pm}(w) + (1-x)\mathcal{H}_{p-1,p}^{2,\mp}(w).$$

The top sign is for odd p. The new parameter x is an extra control parameter, taken to be fixed. Its introduction is an explicit representation of the ambiguity of the choice of local terms.

For the sigmoid function f we choose a Heaviside function, this time leaving us with two variants - f with $a \in 2\mathbb{Z} - \frac{1}{2}$ and f' with $a \in 2\mathbb{Z} + \frac{1}{2}$. To see how they differ, consider the regime $w_4 > 0$. In this case f splits the dimer in two and f' switches on between two dimers.

Because the local terms in the Hamiltonian only interact at range 1 in either direction, the eigenstates of the system for any parameter choice are product states over each dimer. This means

$$\Omega^{(3)}(f) = \Omega^{(3)}(f') = F^{(3)}_{a-\frac{1}{2},a+\frac{1}{2}},$$

with the particular choice of a distinguishing the two cases. $\Omega^{(3)}(f)$ is only non-trivial if the sites $a \pm \frac{1}{2}$ belong to the same dimer, hence $\Omega^{(3)}(f) = 0$ unless $w_4 > 0$ and $\Omega^{(3)}(f') = 0$ unless $w_4 < 0$.

We will need to diagonalize the dimer, so we first transform the basis from an angle-independent one into one parallel with the Zeeman field using a unitary operator U. This transforms states according to $|\psi\rangle \to |\psi\rangle_{\theta,\phi} = U|\psi\rangle$ and any operator according to $A \to a = UAU^\dagger$, the explicit angle dependence having been removed from the left-hand side of both equalities. The small-letter notation will be useful for clarification when a matrix representation is invoked. Having applied this transformation we choose simultaneous eigenstates of $S'_{z,p} + S'_{z,p+1}$ and $(S'_p + S'_{p+1})^2$, which are also eigenstates of $(S'_p)^2$ and $(S'_{p+1})^2$. The vector appearing in the Zeeman term has length $\sqrt{1-w_4^2}$, meaning

$$h_p = -2\sqrt{1-w_4^2}S'_{z,p} + 4xw_4 S'_p \cdot S'_{p+1}, \; h_{p+1} = 2\sqrt{1-w_4^2}S_{z,p+1} + 4(1-x)w_4 S'_p \cdot S'_{p+1}$$

for $p = a - \frac{1}{2}$. Furthermore, as

$$S'_p \cdot S'_{p+1} = \frac{1}{2}((S'_p + S'_{p+1})^2 - (S'_p)^2 - (S'_{p+1})^2),$$

we have

$$h_p = -\sqrt{1-w_4^2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} + 2xw_4 \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{bmatrix},$$
$$h_{p+1} = \sqrt{1-w_4^2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} + (1-x)w_4 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}$$

in the eigenbasis of total spin, and the total dimer Hamiltonian is

$$h = w_4 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix} - 2\sqrt{1-w_4^2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

The eigenstates $|1,1\rangle$ and $|1,-1\rangle$ are still eigenstates of the total Hamiltonian, with energy w_4. In addition there are two eigenstates found by diagonalizing

$$\begin{bmatrix} w_4 & -2\sqrt{1-w_4^2} \\ -2\sqrt{1-w_4^2} & -3w_4 \end{bmatrix}.$$

The energies are $\pm 2 - w_4$, with eigenstates

$$\frac{1}{\sqrt{2}}\begin{bmatrix} -\sqrt{1+w_4} & \sqrt{1-w_4} \\ \sqrt{1-w_4} & \sqrt{1+w_4} \end{bmatrix}.$$

We proceed by introducing hyperspherical coordinates

$$w_1 = \sin(\alpha)\cos(\theta),\ \ w_2 = \sin(\alpha)\sin(\theta)\cos(\phi),\ \ w_3 = \sin(\alpha)\sin(\theta)\sin(\phi),\ \ w_4 = \cos(\alpha),$$

for which we have

$$h_p = -\sin(\alpha)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} + x\cos(\alpha)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix},$$

$$h_{p+1} = \sin(\alpha)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} + (1-x)\cos(\alpha)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix},$$

$$h_p + h_{p+1} = h = \cos(\alpha)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix} - 2\sin(\alpha)\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

The eigenstates of individual spin are given in equation 1, and we then have

$$|1,1\rangle_{\theta,\phi} = \begin{bmatrix} \cos^2\left(\frac{\theta}{2}\right)e^{-2i\phi} \\ \frac{1}{\sqrt{2}}\sin(\theta)e^{-i\phi} \\ \sin^2\left(\frac{\theta}{2}\right) \\ 0 \end{bmatrix},\ |1,0\rangle_{\theta,\phi} = \begin{bmatrix} -\frac{1}{\sqrt{2}}\sin(\theta)e^{-2i\phi} \\ \cos(\theta)e^{-i\phi} \\ \frac{1}{\sqrt{2}}\sin(\theta) \\ 0 \end{bmatrix},\ |1,-1\rangle_{\theta,\phi} = \begin{bmatrix} \sin^2\left(\frac{\theta}{2}\right)e^{-2i\phi} \\ -\frac{1}{\sqrt{2}}\sin(\theta)e^{-i\phi} \\ \cos^2\left(\frac{\theta}{2}\right) \\ 0 \end{bmatrix},\ |0,0\rangle_{\theta,\phi} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ e^{-i\phi} \end{bmatrix}$$

with respect to the total spin basis for $\theta = \phi = 0$. We can then explicitly write

$$U = \begin{bmatrix} \cos^2\left(\frac{\theta}{2}\right)e^{-2i\phi} & -\frac{1}{\sqrt{2}}\sin(\theta)e^{-2i\phi} & \sin^2\left(\frac{\theta}{2}\right)e^{-2i\phi} & 0 \\ \frac{1}{\sqrt{2}}\sin(\theta)e^{-i\phi} & \cos(\theta)e^{-i\phi} & -\frac{1}{\sqrt{2}}\sin(\theta)e^{-i\phi} & 0 \\ \sin^2\left(\frac{\theta}{2}\right) & \frac{1}{\sqrt{2}}\sin(\theta) & \cos^2\left(\frac{\theta}{2}\right) & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{bmatrix}.$$

Let us also derive an expression for G_0. The eigenstates of the Hamiltonian in the angle-dependent basis are

$$v_{-2-\cos(\alpha)} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ \sqrt{1-\cos(\alpha)} \\ 0 \\ \sqrt{1+\cos(\alpha)} \end{bmatrix},\ v_{\cos(\alpha),1} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},\ v_{\cos(\alpha),2} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix},\ v_{2-\cos(\alpha)} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ -\sqrt{1+\cos(\alpha)} \\ 0 \\ \sqrt{1-\cos(\alpha)} \end{bmatrix}.$$

Forming these into a matrix V and computing VDV^{-1} for

$$D = \begin{bmatrix} -\frac{1}{2(1+\cos(\alpha))} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2(1+\cos(\alpha))} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \end{bmatrix}$$

nets us

$$g_0 = \begin{bmatrix} -\frac{1}{2(1+\cos(\alpha))} & 0 & 0 & 0 \\ 0 & -\frac{1}{8}(1+\cos(\alpha)) & 0 & \frac{1}{8}\sin(\alpha) \\ 0 & 0 & -\frac{1}{2(1+\cos(\alpha))} & 0 \\ 0 & \frac{1}{8}\sin(\alpha) & 0 & -\frac{1}{8}(1-\cos(\alpha)) \end{bmatrix}.$$

The three angles are now neatly separated, as ϕ and θ only enter in U and α only enters in the combination of eigenstates after U has been applied. Using the explicit formula we then have

$$\begin{aligned} F^{(3)}_{p,p+1} = &\frac{i}{6}\Big(-2\left\langle d\mathcal{H}G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_{p+1}\right\rangle - \left\langle d\mathcal{H}G_0 d\mathcal{H}_p G_0^2 d\mathcal{H}_{p+1}\right\rangle + 2\left\langle d\mathcal{H}_p G_0 d\mathcal{H}_{p+1} G_0^2 d\mathcal{H}\right\rangle \\ &+ \left\langle d\mathcal{H}_p G_0^2 d\mathcal{H}_{p+1} G_0 d\mathcal{H}\right\rangle + \left\langle d\mathcal{H}_{p+1} G_0^2 d\mathcal{H} G_0 d\mathcal{H}_p\right\rangle - \left\langle d\mathcal{H}_{p+1} G_0 d\mathcal{H} G_0^2 d\mathcal{H}_p\right\rangle \\ &+ 3\left\langle d\mathcal{H}G_0^3 d\mathcal{H}_p\right\rangle\left\langle d\mathcal{H}_{p+1}\right\rangle - 3\left\langle d\mathcal{H}_{p+1}G_0^3 d\mathcal{H}\right\rangle\left\langle d\mathcal{H}_p\right\rangle\Big) - (p \leftrightarrow p+1). \end{aligned}$$

In order to get non-trivial results, we must compute these expectation values in an angle-dependent basis. To that end, we note that all the operators involved only depend on α in the angle-dependent basis. We then write $A = U^\dagger a U$ and consider its expectation value in some angle-dependent state $|\psi\rangle = U^\dagger |\psi\rangle_{\theta,\phi}$. We then have

$$\langle\psi|A|\psi\rangle = \langle\psi|UU^\dagger a U U^\dagger|\psi\rangle_{\theta,\phi} = \langle\psi|a|\psi\rangle_{\theta,\phi}\,.$$

This means, for instance, that

$$\begin{aligned}\left\langle d\mathcal{H}G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_{p+1}\right\rangle &= \left\langle U(d\mathcal{H}G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_{p+1})_{\theta,\phi}U^\dagger\right\rangle_{\theta,\phi}\\ &= \left\langle Ud(U^\dagger hU)U^\dagger g_0^2 Ud(U^\dagger h_p U)U^\dagger g_0 Ud(U^\dagger h_{p+1}U)U^\dagger\right\rangle_{\theta,\phi}\end{aligned}$$

By antisymmetry we may compute any component of this form, so we choose $F^{(3)}_{p,p+1,\alpha\theta\phi}$, for which the two latter terms vanish.

This is going to take some time, so let's start. We have

$$\begin{aligned}&\left\langle d\mathcal{H}G_0^2 d\mathcal{H}_p G_0 d\mathcal{H}_{p+1}\right\rangle\\ &= -\frac{i}{64}\cos(\theta)\left(\cos(\alpha)-1\right)\left(2\sin(\alpha)\cos^2(\alpha) - 2\cos^3(\alpha) - 5\sin(\alpha)\cos(\alpha) + 3\cos(\alpha)^2 + \sin(\alpha) + 4\cos(\alpha) + 3\right)\end{aligned}$$

Using the explicit formula above we somehow find

$$\Omega^{(3)}_{\alpha\theta\phi} = \frac{1}{2}(2+\cos(\alpha))\tan^2\left(\frac{\alpha}{2}\right)\sin(\theta)$$

for $0 < \alpha < \frac{\pi}{2}$. We then have

$$\begin{aligned}Q_{\text{KS}} &= \int_{S^3}\Omega^{(3)}_{\alpha\theta\phi} = \frac{1}{2}\int_0^{\frac{\pi}{2}}\int_0^{\pi}\int_0^{2\pi} \mathrm{d}\alpha\,\mathrm{d}\theta\,\mathrm{d}\phi\,(2+\cos(\alpha))\tan^2\left(\frac{\alpha}{2}\right)\sin(\theta)\\ &= 2\pi\int_0^{\frac{\pi}{2}}\mathrm{d}\alpha\,(2+\cos(\alpha))\tan^2\left(\frac{\alpha}{2}\right) = 2\pi.\end{aligned}$$

What if we were to use a different sigmoid? Swapping to f', which is zero for $w_4 > 0$. Elsewhere we find

$$\Omega^{(3)}_{\alpha\theta\phi} = \frac{1}{2}(2-\cos(\alpha))\cot^2\left(\frac{\alpha}{2}\right)\sin(\theta),$$

and thus

$$\begin{aligned}Q_{\text{KS}} &= 2\pi\int_{\frac{\pi}{2}}^{\pi}\mathrm{d}\alpha\,(2-\cos(\alpha))\cot^2\left(\frac{\alpha}{2}\right)\\ &= -2\pi\int_{\frac{\pi}{2}}^{0}\mathrm{d}\beta\,(2-\cos(\pi-\beta))\cot^2\left(\frac{\pi-\beta}{2}\right)\\ &= 2\pi\int_0^{\frac{\pi}{2}}\mathrm{d}\beta\,(2+\cos(\beta))\tan^2\left(\frac{\beta}{2}\right)\\ &= 2\pi,\end{aligned}$$

and indeed the choice of sigmoid was irrelevant.