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Third-order link integrals

Mitchell A Berger†

Department of Mathematical Sciences, University of St Andrews, St Andrews, UK

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Abstract. The Gauss link integral measures simple linking between two curves. Helicity integrals, which are related to the Hopf invariant, similarly measure the net linking of a set of field lines (for example vortex lines or magnetic lines of force). However, these quadratic integrals do not always detect links involving three or more curves. We present an invariant cubic integral which can indeed detect linkage when the quadratic integrals vanish: for example the integral distinguishes the Borromean rings from three unlinked rings. This integral is based on an algebraic topology construct, the Massey triple product.

1. Introduction and definitions

Results from the pure mathematical literature can be made accessible to physicists and applied mathematicians by translating them into common physical language. This paper discusses an object from algebraic topology, the Massey triple product (Massey 1958, 1968, Fenn 1983), and reformulates it in terms of vector fields and the familiar operations of div, grad, and curl. The triple product (a mapping between cohomology classes) leads to a topological invariant which measures the third order linking of a set of closed curves. For example, it can distinguish the Borromean rings from three unlinked rings (see figure 1). We will derive an integral form for this invariant, and give an intuitive description of how it works.

The need for third- or higher-order integral invariants has been discussed by Edwards (1968) (see also Moffatt 1981). Edwards was searching for topological constraints on the statistical mechanics of polymer entanglements. He derived an expression which seemed to distinguish the Borromean rings from unlinked rings. Unfortunately, the derivation involved integrating an ill-defined function, and hence did not yield a sensible result (see end of section 3 below).

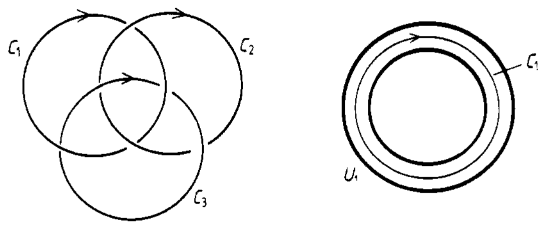

Figure 1. The Borromean rings. The curves C_i are enclosed inside small tubes U_i.

† Present address: Department of Mathematics, University College London, London, UK.

Consider three closed curves C_i, $i=1,2,3$ (see figure 1). We have put arrows on the curves to give them a direction. The curves are surrounded by toroidal volumes U_i. We will assume that these volumes are thin so that they do not intersect each other. The boundary surfaces will be called ∂U_i. Finally, let U' denote space external to the three tori ($U' = \mathscr{R}^3 - U_1 \cup U_2 \cup U_3$).

We suppose that the volumes contain magnetic (i.e. divergence-free) fields $\boldsymbol{B}_1$, $\boldsymbol{B}_2$, $\boldsymbol{B}_3$. The fields point in the same direction as the axial curves C_i, and do not cross the boundaries: $\boldsymbol{B}_i \cdot \hat{n}|_{\partial U_i} = 0$. Each field has a net flux in the axial direction Φ_i. Also, the magnetic fields have vector potentials $\boldsymbol{A}_i$, where $\nabla \times \boldsymbol{A}_i = \boldsymbol{B}_i$.

2. Second-order linking

First consider the situation where some of the curves link each other in pairs. Thus in figure 2 C_2 links both C_1 and C_3, but C_1 and C_3 are unlinked. This pair-wise linking can be detected by computing the Gauss integrals

$$\mathscr{L}_{ij} = \frac{1}{4\pi} \oint \oint \mathrm{d}\boldsymbol{r}_i \times \mathrm{d}\boldsymbol{r}_j \cdot \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3} \tag{1}$$

or the helicity integrals

$$\mathscr{H}_{ij} = \int_{U_i} \boldsymbol{A}_j \cdot \boldsymbol{B}_i \, \mathrm{d}^3 x_i . \tag{2}$$

One can readily show (Moreau 1961, Moffat 1969) that

$$\mathscr{H}_{ij} = \mathscr{H}_{ji} = \mathscr{L}_{ij} \Phi_i \Phi_j \qquad i \neq j. \tag{3}$$

For $i=j$ the Gauss integral is not invariant to deformations of the curve C_i. On the other hand $\mathscr{H}_{ii}$ is indeed invariant; it measures the twisting of magnetic field lines within U_i about the axis C_i, plus the coiling of the axis itself (Fuller 1978, Berger and Field 1984).

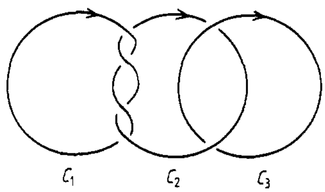

Figure 2. Three curves with $\mathscr{L}_{12} = 2$, $\mathscr{L}_{13} = 0$, and $\mathscr{L}_{23} = -1$.

Next consider the Borromean rings in figure 1. For these rings all the Gauss integrals vanish. The numbers $\mathscr{L}_{ij}$ (or $\mathscr{H}_{ij}$) do not distinguish the Borromean rings from three unlinked rings. In the following sections, however, we will present third-order analogues of $\mathscr{L}_{ij}$ and $\mathscr{H}_{ij}$ which do make this distinction.

3. The Massey fields

We consider configurations where all the second-order linking numbers vanish, i.e.

$$\mathscr{L}_{ij} = \mathscr{H}_{ij} = 0 \qquad i \neq j. \tag{4}$$

First we construct some new vector fields out of combinations of the vector potentials A_i. For the moment, we restrict ourselves to the region U' outside of the three tubes U_i. Let

$$\begin{aligned} G_1(x) &= A_2(x) \times A_3(x) \\ G_2(x) &= A_3(x) \times A_1(x) \qquad \text{for } x \in U'. \\ G_3(x) &= A_1(x) \times A_2(x) \end{aligned} \tag{5}$$

These fields are divergence free in U': for example

$$\nabla \cdot G_1 = B_2 \cdot A_3 - B_3 \cdot A_2 = 0$$

because the fields B_i do not enter U'. The extension of these fields to all space will be discussed below. The linking number $\mathcal{M}$, in essence, will measure the linking of the field lines of G_i with the field lines of B_i.

Two more sets of vector fields are needed. Let F_i be a vector potential for G_i,

$$\nabla \times F_i = G_i. \tag{6}$$

Finally, define the Massey fields

$$\begin{aligned} M_1 &= A_3 \times F_3 - A_2 \times F_2 \\ M_2 &= A_1 \times F_1 - A_3 \times F_3 \\ M_3 &= A_2 \times F_2 - A_1 \times F_1. \end{aligned} \tag{7}$$

The Massey triple product is (in the context of three-dimensional vector fields) the set of all possible Massey fields modulo gauge transformations of A_i and F_i.) Two immediate properties of the Massey fields are

$$M_1 + M_2 + M_3 = 0 \tag{8}$$

and

$$\nabla \cdot M_i(x) = 0 \qquad \text{for } x \in U'. \tag{9}$$

(For example, $\nabla \cdot M_1 = A_2 \cdot G_2 - A_3 \cdot G_3 = 0$.)

In order to evaluate F_i, we need to know what G_i looks like inside the tubes U_1, U_2 and U_3. The vector potential F_i will exist only if $\nabla \cdot G_i = 0$ everywhere. Thus we need to find a divergence-free extension of G_i inside the tubes. This extension exists only when the Gauss linkages (and helicities) between pairs of tubes vanish. No matter how we extend G_1 into tube 2, for example, the flux of G_1 out of the boundary of tube 2 is

$$\begin{aligned} \int_{\partial U_2} G_1 \cdot \hat{n}\, \mathrm{d}^2x &= \int_{\partial U_2} A_2 \times A_3 \cdot \hat{n}\, \mathrm{d}^2x \\ &= \int_{U_2} \nabla \cdot A_2 \times A_3\, \mathrm{d}^3x \\ &= \int_{U_2} A_3 \cdot B_2\, \mathrm{d}^3x. \end{aligned}$$

By equation (2), then,

$$\int_{U_2} \nabla \cdot G_1\, \mathrm{d}^3x = \int_{\partial U_2} G_1 \cdot \hat{n}\, \mathrm{d}^2x = \mathcal{H}_{23}. \tag{10}$$

One more result will be needed before defining $\boldsymbol{G}_i$ inside the tubes. Note that outside of U_3 (for example), the magnetic field $\boldsymbol{B}_3$ vanishes and so $\nabla\times\boldsymbol{A}_3=0$. Thus in certain subregions of space $\boldsymbol{A}_3$ will be expressible as a gradient. In particular, the flux of $\boldsymbol{B}_3$ through any closed curve drawn inside U_2 vanishes. We can then write $\boldsymbol{A}_3=\nabla\phi_{(2)3}$ inside U_2. The subscript (2) has been added to remind us that this scalar field is, strictly speaking, *only* defined within U_2; it is dangerous to extend it elsewhere. We may define similar scalar functions such as $\boldsymbol{A}_2=\phi_{(3)2}$ in U_3, etc. Getting back to the extensions of $\boldsymbol{G}_i$, let

$$\boldsymbol{G}_1(\boldsymbol{x})=\begin{cases}\boldsymbol{A}_2\times\boldsymbol{A}_3 & \boldsymbol{x}\in U_1 \text{ and } U' \\ \boldsymbol{A}_2\times\boldsymbol{A}_3-\phi_{(2)3}\boldsymbol{B}_2 & \boldsymbol{x}\in U_2 \\ \boldsymbol{A}_2\times\boldsymbol{A}_3+\phi_{(3)2}\boldsymbol{B}_3 & \boldsymbol{x}\in U_3.\end{cases} \tag{11}$$

The field $\boldsymbol{G}_1$ is now divergence-free everywhere. The extensions of $\boldsymbol{G}_2$ and $\boldsymbol{G}_3$ can be found by permuting the indices.

(In Edwards (1968) an attempt was made to find a third-order link integral. Using our notation, the method involved letting $\boldsymbol{A}_1=\nabla\phi_1$ for a potential ϕ_1 defined in a certain region outside of U_3. However, ϕ_1 was then identified with the potential $\phi_{(3)1}$ defined inside U_3 (equations A11, A12). Unfortunately U_1 links the combined region where ϕ_1 and $\phi_{(3)1}$ were used. This means that there are closed paths where the line integral of $\boldsymbol{A}_1$ is non-zero, invalidating the assignment $\boldsymbol{A}_1=\nabla\phi_1$.)

4. Third-order linking numbers

We can now define the third-order linking number $\mathcal{M}$. Consider the surface integrals of the Massey fields at the boundaries of the tubes:

$$m_{ij}=\int_{\partial U_i}\boldsymbol{M}_j\cdot\hat{n}\,\mathrm{d}^2x \tag{12}$$

and define

$$\mathcal{M}\equiv(\Phi_1\Phi_2\Phi_3)^{-1}m_{12}. \tag{13}$$

The quantities m_{ij} and $\mathcal{M}$ have the following properties:

(i)

$$m_{ij}=0 \qquad \text{if } i=j. \tag{14}$$

(ii)

$$m_{12}=m_{23}=m_{31}=-m_{21}=-m_{32}=-m_{13}. \tag{15}$$

(iii)

$$m_{12}=\int_{U_1}\boldsymbol{B}_1\cdot(\boldsymbol{F}_1-\phi_{(1)2}\boldsymbol{A}_3)\,\mathrm{d}^3x. \tag{16}$$

(iv) The number $\mathcal{M}$ is invariant to the gauge transformations $A_i\rightarrow A_i+\nabla\mu_i$ and $\boldsymbol{F}_i\rightarrow\boldsymbol{F}_i+\nabla\psi_i$.

(v) Furthermore $\mathcal{M}$ is invariant to arbitrary motions of the volumes U_i.

Proof of (i). We will prove that $m_{11}=0$. In U_1, express A_2 and A_3 as gradients. The Massey field $\boldsymbol{M}_1$ becomes

$$\boldsymbol{M}_1=\nabla\phi_{(1)3}\times\boldsymbol{F}_3-\nabla\phi_{(1)2}\times\boldsymbol{F}_2. \tag{17}$$

Integrate by parts on ∂U_1 to obtain

$$\begin{aligned}
m_{11}&=\int_{\partial U_1}(\phi_{(1)2}\boldsymbol{G}_2-\phi_{(1)3}\boldsymbol{G}_3)\cdot\hat{n}\,\mathrm{d}^2x\\
&=\int_{\partial U_1}(\phi_{(1)2}\nabla\phi_{(1)3}\times\boldsymbol{A}_1-\phi_{(1)3}\boldsymbol{A}_1\times\nabla\phi_{(1)2})\cdot\hat{n}\,\mathrm{d}^2x\\
&=\int_{\partial U_1}\nabla(\phi_{(1)2}\phi_{(1)3})\times\boldsymbol{A}_1\cdot\hat{n}\,\mathrm{d}^2x\\
&=-\int_{\partial U_1}\phi_{(1)2}\phi_{(1)3}\boldsymbol{B}_1\cdot\hat{n}\,\mathrm{d}^2x.
\end{aligned}$$

However $\boldsymbol{B}_1\cdot\hat{n}=0$ since $\boldsymbol{B}_1$ stays inside U_1. Thus $m_{11}=0$.

Proof of (ii). By equation (8), $m_{11}+m_{12}+m_{13}=0$. Thus

$$m_{12}=-m_{13}. \tag{18}$$

Let us now show also that

$$m_{23}=-m_{13}. \tag{19}$$

Consider a large sphere S enclosing all three tubes U_i. By equation (9) the divergence of $\boldsymbol{M}_3$ vanishes in the region between S and the boundaries ∂U_i. The divergence theorem then tells us that

$$m_{13}+m_{23}+m_{33}=\int_S\boldsymbol{M}_3\cdot\hat{n}\,\mathrm{d}^2x. \tag{20}$$

We can now apply the same reasoning as in the proof of (i), by writing $\boldsymbol{A}_i=\nabla\phi_{(S)i}$, $i=1,2,3$, to show that $\int_S\boldsymbol{M}_3\cdot\hat{n}\,\mathrm{d}^2x=0$. As $m_{33}=0$ this proves equation (19). The other equalities in (ii) can be proved using $m_{21}+m_{22}+m_{23}=0$, etc.

Proof of (iii). Inside U_1,

$$\begin{aligned}
\nabla\cdot\boldsymbol{M}_2&=\boldsymbol{B}_1\cdot\boldsymbol{F}_1-\boldsymbol{A}_1\cdot\boldsymbol{G}_1+\boldsymbol{A}_3\cdot\boldsymbol{G}_3\\
&=\boldsymbol{B}_1\cdot\boldsymbol{F}_1-\boldsymbol{A}_1\cdot(\boldsymbol{A}_2\times\boldsymbol{A}_3)+\boldsymbol{A}_3\cdot(\boldsymbol{A}_1\times\boldsymbol{A}_2-\phi_{(1)2}\boldsymbol{B}_1)\\
&=\boldsymbol{B}_1\cdot(\boldsymbol{F}_1-\phi_{(1)2}\boldsymbol{A}_3).
\end{aligned}$$

Proof of (iv). First consider the gauge transformation $\boldsymbol{F}_1\to\boldsymbol{F}_1+\nabla\psi_1$. Gauge transformations involving $\boldsymbol{F}_2$ and $\boldsymbol{F}_3$ can be dealt with by permutation of the indices. The change in m_{12} is

$$\begin{aligned}
\delta m_{12}&=\int_{\partial U_1}(\boldsymbol{A}_1\times\nabla\psi_1)\cdot\hat{n}\,\mathrm{d}^2x\\
&=\int_{\partial U_1}(\psi_1\boldsymbol{B}_1)\cdot\hat{n}\,\mathrm{d}^2x
\end{aligned}$$

after an integration by parts. But $\boldsymbol{B}_1\cdot\hat{n}$ vanishes at ∂U_1 so $\delta m_{12}=0$.

Next let $\boldsymbol{A}_1\to\boldsymbol{A}_1+\nabla\mu_1$. Equation (16) for m_{12} only involves $\boldsymbol{A}_1$ through its curl, $\boldsymbol{B}_1$. Since $\delta\boldsymbol{B}_1=0$ for this gauge transformation, $\delta m_{12}=0$ as well. Finally, the fluxes Φ_1, Φ_2, and Φ_3 are invariant to gauge transformations (as well as motions of the tubes).

Proof of (v). It suffices to consider the motion of only one tube, say U_3. Arbitrary motions or deformations of the three tubes can be built up from such single motions. The movement of U_3 can be generated by a velocity field $\boldsymbol{V}$; the change in $\boldsymbol{B}$ is

$$\partial \boldsymbol{B}_3/\partial t = \nabla \times (\boldsymbol{V} \times \boldsymbol{B}_3). \tag{21}$$

By (iv), we can choose the gauge of $\boldsymbol{A}_3$ so that

$$\partial \boldsymbol{A}_3/\partial t = (\boldsymbol{V} \times B_3). \tag{22}$$

This vanishes away from U_3. Thus by equation (16) $\partial m_{12}/\partial t = 0$.

5. Calculating the third-order linking number

First we show that $\mathcal{M} = 0$ for three unlinked rings, and then show that $\mathcal{M} = \pm 1$ for the Borromean rings. If a collection of rings is unlinked, that means each ring can be enclosed in its simply connected volume. Thus, for example, we can draw a simply connected surface S' where U_1 is completely inside S', but U_2 and U_3 are completely outside. The calculation of $\mathcal{M}$ proceeds as in the proofs of (i) and (ii). By analogy with equation (20) we write

$$m_{12} = \int_{S'} \boldsymbol{M}_2 \cdot \hat{n}\, \mathrm{d}^2 x. \tag{23}$$

The right-hand side can be shown to vanish by expressing the vector potentials $\boldsymbol{A}_i$ as gradients on S'. Thus $\mathcal{M} = 0$ for unlinked rings.

Let us consider the Borromean rings in a particularly simple geometry (see figure 3). Ring 1 (i.e. curve C_1) forms an ellipse in the $y-z$ plane and bounds an area S_1 within that plane. Similarly, C_2 and C_3 lie in the $z-x$ and $x-y$ planes, respectively. The unit normals to S_1, S_2, and S_3 are $\hat{x}$, $\hat{y}$, and $\hat{z}$. Curve C_1 pierces S_2 at two points, but does not touch S_3. Similarly C_2 pierces S_3 and C_3 pierces S_1.

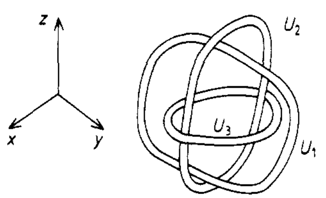

Figure 3. Geometry used for calculating $\mathcal{M}$.

Calculation will be simplified by choosing some rather special gauges for $\boldsymbol{A}_i$. Outside of the thin tubes U_i, let $\boldsymbol{A}_i$ be non-zero only for points on S_i. For these points

$$\begin{aligned} \boldsymbol{A}_1 &= \Phi_1 \delta(x) \hat{x} \\ \boldsymbol{A}_2 &= \Phi_2 \delta(y) \hat{y} \\ \boldsymbol{A}_3 &= \Phi_3 \delta(z) \hat{z}. \end{aligned} \tag{24}$$

(For a closed curve linking tube i, $\int \boldsymbol{A}_i \cdot \mathrm{d}\boldsymbol{l} = \Phi_i$ as required.)

Now let us calculate m_{12}, using equation (16). Since $\boldsymbol{A}_3 = 0$ inside U_1,

$$m_{12} = \int_{U_1} \boldsymbol{B}_1 \cdot \boldsymbol{F}_1\, \mathrm{d}^3 x. \tag{25}$$

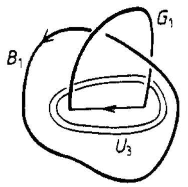

Figure 4. The vector field $\boldsymbol{G}_1$ links $\boldsymbol{B}_1$ in a right-handed sense.

The vector field $\boldsymbol{G}_1$ (see equation (11) and figure 4) is non-zero only on the line segment where S_2 intersects S_3, and inside U_2. Inside U_2 the scalar $\phi_{(2)3} = \Phi_3$ for points above $z=0$, and $\phi_{(2)3} = 0$ for points below $z=0$. Thus $\boldsymbol{G}_1 = -\Phi_3 \boldsymbol{B}_2$ in the upper half of U_2, and has net flux $\Phi_2\Phi_3$.

From the figure, the field lines of $\boldsymbol{G}_1$ link those of $\boldsymbol{B}_1$ in a right-handed sense, so the integral of $\boldsymbol{F}_1$ along a field line of $\boldsymbol{B}_1$ gives the value $+\Phi_2\Phi_3$. Thus $m_{12} = \Phi_1\Phi_2\Phi_3$ and by equation (13)

$$\mathcal{M} = 1. \tag{26}$$

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