A systematic method for parametrising periodic minimal surfaces : the F-RD surface

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Abstract. — An algorithm for the exact construction of triply periodic minimal surfaces recently developed by the author is illustrated simply with the first parametrisation of the F-RD surface discovered by Alan Schoen. An exact expression for the F-RD Weierstrass function is derived, from which all quantitative features of this surface may be readily established.

Introduction.

While geometry has been a key participant in all stages of the development of the physical sciences, explanation of the increasing diversity of bicontinuous microstructures observed in condensed matter [1] provides a challenge to conventional geometric intuition. Recently, infinite periodic minimal surfaces (IPMS) have been adopted as the basis of a vocabulary for this evolving language of structure. It is an open question as to whether this specific class of periodic surfaces possess any real significance in the context of the physical systems, however their utility as a means of classification is undeniable. The cubic IPMS of genus three — the D, P and G surfaces — are most frequently invoked, in modelling the structures underlying a variety of molecular self-assemblies [2]. It has been postulated that these particular IPMS are favoured on the basis of surface homogeneity [3], that is, they represent the most uniform interfacial scenario attainable globally. Bicontinuous phases related to higher genus IPMS may also occur, with the region of their existence in the phase diagram increasing with decreasing sample purity. This expectation has been borne out by recent experiments [4].

With the advent of sophisticated measurement techniques, the principal limitation to the possible observation and recognition of topologically complex structures remains the incomplete knowledge regarding accompanying IPMS descriptions. This problem has been partially redressed by the discovery of a multitude of new IPMS by Schoen [5] and, lately, by Koch and Fischer [6]. These IPMS were isolated empirically, without the precise mathematical specification of the surface necessary for quantitative comparison with observed systems. Many of the Schoen examples have now been parametrised by Karcher [7].

A systematic procedure for the parametrisation of a general IPMS has recently been developed by the author [8]. There the method was verified with a greatly simplified rederivation of Neovius' description of the C(P) surface, then utilised in deriving the first parametrisations of the hexagonal HS2 and orthorhombic PT surfaces of Koch and Fischer, together with those of the new orthorhombic IPMS and new pentagonal surface (denoted VAL and pCLP, respectively) arising from earlier work with Hyde [9, 10]. While the general formulation of the procedure is mathematically involved, the fundamentals are simple and its application should be accessible to experimentalists seeking classification of observed structures. With a view to this aim we illustrate the method here with the first parametrisation of the F-RD surface of Schoen. The choice of this example is physically motivated — the F-RD surface is a cubic IPMS of relatively simple topology (in fact, the lowest genus cubic IPMS of Schoen remaining undescribed) and thus may be expected to occur in bicontinuous media.

The F-RD surface.

The topology and symmetry of the F-RD surface is specified in Schoen's report [5] ; we briefly summarise the information relevant to the parametrisation here. The fundamental translational unit of the IPMS, displayed in figure 1, has a genus of six and the space group symmetry Fm3m $\left(\text{or F}\,\frac{4}{m}\,\bar{3}\,\frac{2}{m}\right)$. Accordingly the IPMS contains mirror planes in the absence of any on-surface two-fold rotational axes (as is the case for the I-WP surface [11]) so the two labyrinths partitioned by the interface are geometrically distinct (and are characterised by the types F and RD). The translational unit is constructed from a basic surface element or Flächenstück (identified in Fig. 1) delimited by four mirror planes of the surface. Propagation of this basic element by repeated reflection in the bounding mirror planes, until the full set of symmetries are exhausted, generates the translational unit, thus comprising 48 such elements. The intersection of a mirror plane with the surface is referred to as a plane line of curvature. Two pairs of such curves defining the basic element intersect perpendicularly. The remaining two pairs intersect at angles of $\pi/3$ and $\pi/4$ at points of 3-fold and 4-fold perpendicular rotational symmetry of the surface, respectively. These are degenerate points of the surface, called flat points, at which the Gaussian curvature is zero. The degree of these flat points — the number of revolutions about the surface normal vector at this point traced out by the normal vector along any circuit on the surface enclosing the point — is 2 and 3, respectively.

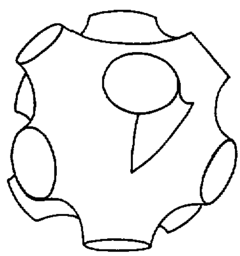

Fig. 1. — The fundamental unit of the F-RD surface comprising 48 of the surface elements shown.

Parametrisation of the F-RD surface.

Mapping a minimal surface into the plane, such that a surface point (x, y, z) is Gauss mapped to the point of intersection of its surface normal vector with the unit sphere centred there, and in turn stereographically projected to a complex number ω, the inverse function was shown by Weierstrass [12] to have the general form

$$(x, y, z) = \mathrm{Re} \int^{\omega} (1 - \omega'^2, i(1 + \omega'^2), 2\,\omega')\, R(\omega')\, \mathrm{d}\omega' \qquad (1)$$

for some complex function $R(\omega)$. The image of the basic element of the F-RD surface in the complex plane under this composite map is the shaded polygon in figure 2. For an IPMS the corresponding Weierstrass function $R(\omega)$ is multivalued, and more specifically, each generic surface normal vector image ω is shared by the same (finite) number of points (x, y, z) on the translational unit. Hence the Gauss map of this unit gives the multiple covering of the unit sphere (and the complex plane on projection) comprising this number of sheets. This number is a topological constant, and is equal to the genus less one for an orientable IPMS [9]. For the genus six F-RD surface the translational unit Gauss map image must then comprise five sheets. This is apparent from figure 2 — just as successive reflections of the basic surface element in its bounding planes yields the set of 48 such elements forming the translational unit, in the Gauss map image repeated reflection of the spherical geodesic polygon in its edges generates a set of 48 such polygons tessellating a five-sheeted spherical covering.

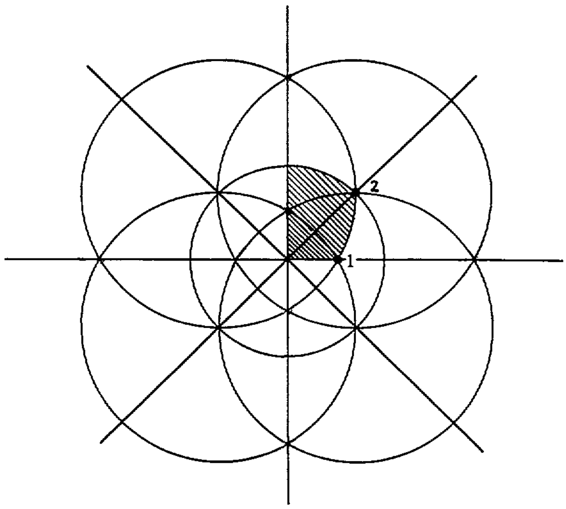

Fig. 2. — Projected Gauss map image of the F-RD surface element.

For the special surface normal vector images ω of flat points, the number of points on the unit possessing this normal is only equal to the generic value if each is counted with the multiplicity of its flat point degree. Accordingly, above the image ω on the multiple covering, the set of points, numbering this degree, corresponding to the flat point are identified as equivalent. We regard the associated set of sheets as pinned at this common point, which is referred to as a branch point of order the degree less one. The projected Gauss map image with structure imposed by this identification is the Riemann surface of the Weierstrass function $R(\omega)$. For the F-RD surface the branch point structure of the Riemann surface is generated by the propagation of the first and second order branch points (labelled in Fig. 2, and corresponding to the flat points of degree two and three, respectively, on the periphery of the basic surface element) at the $2\pi/3$ and $3\pi/4$ vertices of the polygon in the tessellation of the five sheets.

As the Riemann surface is finite-sheeted, the Weierstrass function of an IPMS is algebraic, and is hence specified by a polynomial equation of degree equal to the number of sheets [13]. The Weierstrass function of the F-RD surface is then the solution of the quintic equation

$$a_5(\omega)R^5 + a_4(\omega)R^4 + a_3(\omega)R^3 + a_2(\omega)R^2 + a_1(\omega)R + a_0(\omega) = 0 \tag{2}$$

for a particular set of six polynomials $a_5(\omega), .., a_0(\omega)$. The parametrisation of this surface is then completed on combining equations (1) and (2) once these polynomials have been specified.

As the Gauss map image of the surface element of an IPMS tessellates a spherical covering, this polygon must be triangulated by one of the fifteen basic Schwarz tiles [14]. The IPMS of cubic symmetry are derived from the Schwarz case 4 tiling of the unit sphere by the 48 reflection images of the geodesic triangle with vertex angles ($\pi/4$, $\pi/3$, $\pi/2$) (equivalent to projection of the hexakis octahedron onto a concentric sphere). This underlying triangular tiling is shown in stereographic projection in figure 2. For this orientation the 6, 8 and 12 vertices of angle $\pi/4$, $\pi/3$ and $\pi/2$ in the tiling are positioned at $\{0, \infty, e^{i\pi/4} e^{im\pi/2}\}$, $\left\{\left(\frac{\sqrt{3} \pm 1}{\sqrt{2}}\right) e^{im\pi/2}\right\}$ and $\{\{(\sqrt{2} \pm 1) e^{i\pi/4}, 1\} e^{im\pi/2}\}$, respectively (where m is an integer).

The set of roots of each coefficient polynomial $a_M(\omega)$ are necessarily symmetric with respect to the underlying Schwarz tiling. Thus they must comprise the 6, 8 and/or 12 tiling vertices and/or the 24 (respectively 48) images of a general edge (respectively face) point. The polynomials with roots at the $\pi/4$, $\pi/3$ and $\pi/2$ vertices are

$$p_1 = \prod_{i=1}^{5} (\omega - \omega_i) = \omega(\omega^4 + 1) \tag{3a}$$

$$p_2 = \prod_{j=1}^{8} (\omega - \omega_j) = \omega^8 - 14\,\omega^4 + 1 \tag{3b}$$

$$p_3 = \prod_{k=1}^{12} (\omega - \omega_k) = \omega^{12} + 33\,\omega^8 - 33\,\omega^4 - 1 \tag{3c}$$

(where the $\pi/4$ vertex at infinity in the closed complex plane is suppressed in p_1). Further, for edges of the tessellated Riemann surface to represent plane lines of curvature on the IPMS, the degree of $a_M(\omega)$ must be 4M (again counting with the suppressed zero at infinity) [8]. These facts are then sufficient to specify the form of each coefficient polynomial — in particular equation (2) now becomes

$$\alpha_5 p_1^2 p_2 R^5 + \alpha_4 p_2^2 R^4 + \alpha_3 \begin{Bmatrix} p_1^2 \\ p_3 \end{Bmatrix} R^3 + \alpha_2 p_2 R^2 + \alpha_0 = 0 \tag{4}$$

where $\alpha_5, . . , \alpha_0$ are real numbers, and the braces indicate the two possibilities for the cubic term.

Additional information results from demanding consistency between equation (4) and the known branch point structure of the Riemann surface. Here we utilise the general observation that, local to a surface flat point of degree $b_0 + 1$, on the $b_0 + 1$ sheets of the Riemann surface pinned at the corresponding branch point (of order b_0) above the flat point normal vector image ω_0, the Weierstrass function branches have the asymptotic form [8]

$$R^{b_0+1}(\omega) \sim \gamma_0(\omega - \omega_0)^{-b_0} \cdot \omega \to \omega_0 \,. \tag{5}$$

On the tessellation of the five sheets, over each $\pi/4$ vertex ω_i of the underlying tiling in figure 2 three sheets are pinned at a second order branch point with the remaining two sheets unbranched. The five branches are then given asymptotically *via* equation (5) by

$$R^3(\omega) \sim \gamma_i(\omega - \omega_i)^{-2} \text{ (once)}, \; R(\omega) \sim \gamma_i' \text{(twice)} : \omega \to \omega_i \,. \tag{6}$$

Substituting the first form into equation (4), the requirement that the quintinc and quadratic terms are of leading (and equal) asymptotic order in $(\omega - \omega_i)$ implies that the quartic term cannot be present (that is, $\alpha_4 = 0$) and that the first of the two options for the cubic term applies. Hence the form of the polynomial equation must now be

$$\alpha_5 p_1^2 p_2 R^5 + \alpha_3 p_1^2 R^3 + \alpha_2 p_2 R^2 + \alpha_0 = 0 \tag{7}$$

for which, on substitution of the second form of equation (6), the quadratic and constant terms are of equal leading order (namely zero), as required. Similarly, equation (7) is now consistent with the fact that, over each $\pi/3$ vertex ω_j of the Schwarz tiling the pair of sheets pinned at a first order branch point, and the three unbranched sheets, display the asymptotics

$$R^2(\omega) \sim \gamma_j(\omega - \omega_j)^{-1} \text{ (once)}, \ R(\omega) \sim \gamma_j' \text{(three times} \quad \omega \to \omega_j \,. \tag{8}$$

The final stage of the parametrisation is the determination of the real coefficients α_5, α_3, α_2 and α_0. Clearly one such unknown may be divided out of equation (7) while another may be chosen without loss of generality by a suitable scaling of $R(\omega)$ (amounting to a choice of units for the coordinate axes), leaving two parameters to be specified. This is achieved by analysing the Riemann surface structure on the five unbranched sheets above the $\pi/2$ vertices ω_k of the underlying tiling. From figure 2, each such point is covered once by four polygons meeting with common $\pi/2$ vertex there, and four times as an interior point of the polygon. In the latter case the four coverings are related by reflection in the two perpendicular underlying tiling edges intersecting at the point, and accordingly the four corresponding Weierstrass function values at this point occur as a repeated pair. For example, evaluating equation (7) at $\omega = 1$ (where, from equations (3a) and (3b), $p_1(1) = 2$ and $p_2(1) = -12$) there must exist real constants α and a and a complex conjugate pair $(c, \bar{c})$ such that

$$-48\,\alpha_5 R^5 + 4\,\alpha_3 R^3 - 12\,\alpha_2 R^2 + \alpha_0 = \alpha(R-a)(R-c)^2(R-\bar{c})^2 \,. \tag{9}$$

Equating coefficients yields the pair of homogeneous relations

$$16\,\alpha_2\alpha_3 = 25\,\alpha_0\alpha_5 \,, \quad -135\,\alpha_2^2\alpha_5 = \alpha_3^3 \tag{10}$$

thus removing the final two degrees of freedom. Choosing, say $\alpha_5 = 1$, $\alpha_3 = -15$, $\alpha_2 = 5$ and $\alpha_0 = -48$, the Weierstrass function of the F-RD surface is then given by

$$p_1^2 p_2 R^5 - 15\,p_1^2 R^3 + 5\,p_2 R^2 - 48 = 0 \tag{11}$$

where p_1 and p_2 are the Weierstrass polynomials of the I-WP and D surfaces, given in equations (3a) and (3b).

The exact parametrisation of the F-RD surface is thus attained by substituting the Weierstrass function solutions of equation (11) into the representation (1). Although the quintic polynomial equation cannot be solved analytically, all required surface information (such as local coordinates and the global properties of surface-to-volume ratio, surface area and integral squared Gaussian curvature) can be extracted numerically in a simple and economical manner. The extent of the path integration in equation (1) may be restricted to the polygonal region of the complex plane shaded in figure 2, as the complete IPMS is then generated by mirror reflection in the bounding planar curves of the basic surface element. The corresponding polygonal region of the Riemann surface (that is, the corresponding branch of the Weierstrass function) is ascertained by determining the five root of equation (11) for a particular point ω on the real axis edge $0 < \omega < \frac{\sqrt{3}-1}{\sqrt{2}}$ of the polygon. These five roots comprise a real number and two complex conjugate pairs. The real roots represents the relevant function branch since this real axis segment is the image of a plane line of curvature on this sheet. The function value of this branch at a neighbouring point in the region is then determined *via* Newton's method using this real root as the initial estimate. Continuing this procedure, the entire basic surface element is thus constructed pointwise. The density of the array of such points necessary to yield accurate values for global properties of the IPMS is found by calculating the integral Gaussian curvature of the surface element. With the Gaussian curvature of the surface at the point with normal vector image ω given by [9]

$$K = -4(1 + |\omega|^2)^{-4} |R(\omega)|^{-2},$$

numerical integration of this quantity over the surface element must recover the exact value of $5\pi/12$ to within the desired tolerance.

Conclusion.

The above parametrisation demonstrates the utility of the general algorithm [8]. Application of the algorithm to a particular IPMS only assumes a knowledge of the generic Gauss map image of the basic surface element, specified by the degree of each flat point and the nature of the position of its image with respect to the corresponding Schwarz spherical tiling (i.e. whether it lies at a vertex, or on an edge, or in the interior, of a triangular tile). Such information may be inferred from soap film experiments, and has been extensively tabulated for the minimal balance surfaces of Koch and Fischer [15]. Having established the basic structure of the Gauss map image, the determination of the Weierstrass function polynomial equation up to a number of real constants (that is, up to the stage embodied in equation (7) for the F-RD surface) is then straightforward for any IPMS.

The symmetries relating the special sets of points on the IMPS fundamental unit, possessing common normal vectors imaged at vertices of the Schwarz tiling, in turn imply relations between the corresponding Weierstrass function values, yielding additional constraints on the polynomial equation. This reduces the number of nontrivial constants remaining in the parametrisation to the number of degrees of freedom of the Gauss map consistent with these symmetries. By definition these constraints are purely algebraic. For the F-D surface the consistency condition (Eq. (9)) for the polynomial equation is readily solved (as given in Eq. (10)). For IPMS of higher genus and/or lower symmetry this procedure becomes algebraically lengthy and produces multiple solutions, from which the desired one must be chosen in accordance with the known Weierstrass function behaviour. However this is not a severe deficiency in most situations of physical interest since the inferred genera and symmetry of periodic structures observed in bicontinuous media lie within the range of practical applicability of the procedure.

The algorithm suffices if the number of undetermined constants is equal to the number of free variables associated with the crystallographic group of the IPMS. The symmetry criteria thus impose a one-to-one correspondence between the Gauss map and the IPMS, and yield a purely algebraic surface parametrisation. This is the case for the F-RD surface (in which the cubic symmetry admits no degrees of freedom) and for the majority of the IPMS discovered by Schoen and by Koch and Fischer.

There are however surfaces for which the algorithm alone is insufficient, and must be supplemented with additional considerations [7]. In these cases the number of variables unconstrained by the algorithm exceeds that of the IPMS space group. This circumstance is not unnatural since the approach is based upon the Gauss map and the symmetries derived from it — the resulting algebraic constraints represent locally necessary conditions which may not completely fix the desired global surface symmetry. This then entails the introduction of global closure conditions, stipulating that the IPMS is that member of the continuum of locally admissable surfaces which locks into the crystallographic sites. These constraints, involving determination of surface coordinates and hence integration of the Weierstrass function, are strictly transcendental. Such a situation arises in analysing the Bonnet associate family of an IPMS (obtained on replacing the Weierstrass function $R(\omega)$ by $e^{i\theta} R(\omega)$, $0 < \theta < \frac{\pi}{2}$). As the Gauss map is totally insensitive to the Bonnet transformation, the existence of an associate IPMS to, say, the F-RD surface derived above can only be ascertained by solution of a complicated transcendental equation.

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