Cubic surfaces and *q*-numerical ranges

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Abstract. Let A be an $n \times n$ complex matrix and $0 \le q \le 1$. The boundary of the q-numerical range of A is the orthogonal projection of a hypersurface defined by the dual surface of the homogeneous polynomial

 $F(t, x, y, z) = \det(t I_n + x(A + A^*)/2 + y(A - A^*)/(2i) + z A^*A).$

We construct different types of cubic surfaces S_F corresponding to the homogeneous polynomial F(t, x, y, z) induced by some 3×3 matrices. The degree of the boundary of the Davis-Wielandt shell of a 3×3 upper triangular matrix is determined by the cubic surface S_F .

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1. Introduction

Let A be an $n \times n$ complex matrix and $0 \le q \le 1$. The q-numerical range of A is defined and denoted as

$$W_q(A) = \{ \zeta^* A \xi : \xi, \zeta \in \mathbf{C}^n, \xi^* \xi = \zeta^* \zeta = 1, \zeta^* \xi = q \},\$$

where ξ^* denotes the transpose of the coordinate-wise complex conjugate of the vector $\xi \in \mathbf{C}^n$. It is well known (see [18]) that $W_q(A)$ is a convex subset of C. Its star-shaped generalization is studied in [15]. When q = 1, $W_q(A)$ reduces to the classical numerical range $W(A) = \{\xi^*A\xi : \xi \in \mathbf{C}^n, \xi^*\xi = 1\}$. For n = 3, there has been a number of interesting papers on their numerical ranges ([3, 5, 6, 16]). Furthermore, a comprehensive study of the numerical range of 3×3 matrices can be found in [7, 8] which classify the shapes of the numerical range via the homogeneous polynomial

$$F(t, x, y) = \det(t I_n + x(A + A^*)/2 + y(A - A^*)/(2i)),$$

where A^* stands for the Hermitian adjoint of A.

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The study of the q-numerical range is closely related to the so-called *Davis-Wielandt shell* of $A \in M_n$ which is defined as

$$DW(A) = \{ (\xi^* A\xi, \xi^* A^* A\xi) : \xi \in \mathbf{C}^n, \xi^* \xi = 1 \}.$$

(see [4, 10]). Consider the homogeneous polynomial

$$F(t, x, y, z) = \det(t I_n + x(A + A^*)/2 + y(A - A^*)/(2i) + z A^*A),$$
(1)

which defines the algebraic variety $S_F = \{ [(t, x, y, z] \in \mathbb{CP}^3 : F(t, x, y, z) = 0 \}$. Let G(t, x, y, z) = 0 be the dual surface of S_F . We consider a hypersurface in the 4-dimensional Euclidean space

$$S = \{(x, y, u, v) \in \mathbf{R}^4 : u^2 + v^2 = h(x + iy)^2\},\$$

where $h(z) = \sup\{w \in \mathbf{R} : (z, w) \in DW(A)\}$. Define an orthogonal projection π_q of \mathbf{R}^4 onto $\mathbf{C} \cong \mathbf{R}^2$ by

$$\pi_q((x, y, u, v)) = (qx + \sqrt{1 - q^2}u) + i(qy + \sqrt{1 - q^2}v).$$

Then the range $W_q(A)$ is given by $W_q(A) = \pi_q(S)$ (cf. [4]). Every boundary point (z, w) of DW(A) satisfies $G(1, \Re(z), \Im(z), w) = 0$ or the point lies on a multi-tangent of the surface $G(1, \Re(z), \Im(z), w) = 0$. If the surface F(t, x, y, z) = 0 has no singular point, then the range $W_q(A)$ is given by

$$\pi_q\{(x, y, u, v) \in \mathbf{R}^4 : G(1, x, y, x^2 + y^2 + u^2 + v^2) = 0\}.$$

The range $W_q(A)$ is essentially determined by the form G(t, x, y, z), and hence by the form $F_A(t, x, y, z) = F(t, x, y, z)$. If we replace A by UAU^* for some unitary matrix U, the associated form $F_{UAU^*}(t, x, y, z)$ coincides with $F_A(t, x, y, z)$. Thus the range $W_q(A)$ is invariant under a unitary similarity. The relation $W_q(A) = \pi_q(A)$ is rewritten as

$$W_q(A) = \{qz + \sqrt{1 - q^2}wh(z) : z \in W(A), w \in \mathbf{C}, |w| \le 1\}.$$

Furthermore, if the boundary of the range DW(A) has a flat portion on the plane $a_1x_1 + a_2x_2 + a_3x_3 + a_0 = 0$, then the real point (a_0, a_1, a_2, a_3) is a singular point of the surface S_F . Thus the number of the flat portions of the boundary of the range DW(A) is less than or equal to the number of the singular points of the surface S_F (cf. [5]). The analysis of the degree of the boundary equation of $W_q(A)$ is closely related to the study of the singularities of the surface S_F .

Cubic surfaces is a classical subject in algebraic geometry. Schläfli [17] gave a foundation of its classification theory (see also [2, 9]). It is of great interest in computer aided geometric design (cf. [1, 14]). In this paper, we study the Davis-Wielandt shells of certain 3×3 upper triangular matrices from a viewpoint of the types of singularities occuring on the cubic surfaces S_F corresponding to the matrices.

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2. Singular points of cubic surfaces

Let F(t, x, y, z) be an irreducible complex cubic form in the polynomial ring $\mathbf{C}[t, x, y, z]$. Suppose that $(t, x, y, z) = (1, x_0, y_0, z_0)$ is a singular point of the algebraic surface S_F , that is, $F(1, x_0, y_0, z_0) = F_t(1, x_0, y_0, z_0) = F_x(1, x_0, y_0, z_0) = F_y(1, x_0, y_0, z_0) = F_z(1, x_0, y_0, z_0) = 0$.

In this case, we assume that

$$F(1, x_0 + x, y_0 + y, z_0 + z) = \alpha_{11}x^2 + \alpha_{22}y^2 + \alpha_{33}z^2 + 2\alpha_{12}xy + 2\alpha_{13}xz + 2\alpha_{23}yz + F_3(x, y, z),$$
(2)

where $F_3(x, y, z)$ is homogeneous of degree 3. If the cubic surface S_F has non isolated singularities, then the singularity set is a line (cf. [2] page 252, [13]). A fundamental classification of a singularity is provided by the types of the quadratic form $\alpha_{11}x^2 + \alpha_{22}y^2 + \alpha_{33}z^2 + 2\alpha_{12}xy + 2\alpha_{13}xz + 2\alpha_{23}yz$. Consider the symmetric matrix

$$\alpha = \begin{bmatrix} \alpha_{11} \ \alpha_{12} \ \alpha_{13} \\ \alpha_{12} \ \alpha_{22} \ \alpha_{23} \\ \alpha_{13} \ \alpha_{23} \ \alpha_{33} \end{bmatrix}$$

corresponding to the coefficients of the quadratic terms in (2). Firstly we consider an exceptional case $\alpha_{11} = \alpha_{22} = \alpha_{33} = 0$, $\alpha_{12} = \alpha_{13} = \alpha_{23} = 0$, or equivalently $F(t, x, y) = F_3(x, y, z)$. If the irreducible cubic curve $F_3(x, y, z) = 0$ has no singular point, the surface S_F has no singular point. If $F_3(x, y, z) = 0$ has a node or a cusp, then the surface S_F has a line of singularities.

Secondly we consider a generic case $\alpha \neq 0$. In this case, if the surface S_F has a singular point $(1, x_0, y_0, z_0)$, then the surface $F(t, x_0t + x, y_0t + y, z_0t + z) = 0$ is expressed as $t(a_{11}x^2 + a_{22}y^2 + a_{33}z^2 + 2a_{12}xy + 2a_{13}xz + 2a_{23}yz) + F_3(x, y, z) = 0$. For instance, we assume that $a_{33} \neq 0$. The surface S_F has a rational parametrization

$$t = -\frac{F_3(x, y, 1)}{a_{33} + 2a_{13}x + 2a_{23}y + a_{11}x^2 + 2a_{12}xy + a_{22}y^2}$$

If the matrix α is non-singular, the point $(1, x_0, y_0, z_0)$ is called an ordinary double point (also called A_1 point). If α is singular with rank r, for r = 2, the singular point $(1, x_0, y_0, z_0)$ is called a biplanar double point (or a binode). If r = 1, the singular point $(1, x_0, y_0, z_0)$ is called a uniplanar double point (or a unode). If r = 0, or $\alpha = 0$, the singular point $(1, x_0, y_0, z_0)$ is a called a triple point. Biplanar double points are classified into four types. Suppose that $(1, x_0, y_0, z_0)$ is a biplanar double point of S_F . By changing the variables, we may assume that $\alpha_{13} = \alpha_{23} = \alpha_{31}$ $= \alpha_{32} = \alpha_{33} = 0, \alpha_{11}\alpha_{22} - \alpha_{12}^2 \neq 0$. Under these assumptions, if $F_3(0, 0, 1) \neq 0$, the point $(1, x_0, y_0, z_0)$ is a biplanar double point A_2 . We are interested in the real cubic form F(t, x, y, z) given by (1), which is hyperbolic with respect to (1, 0, 0, 0), that is, the cubic equation $F(t, x_0, y_0, z_0) = 0$ in t has 3 real roots counting multiplicities for every $(x_0, y_0, z_0) \in \mathbf{R}^3$. If we replace A^*A in equation (1) by an arbitrary 3×3 hermitian matrix K, we can construct a real irreducible hyperbolic form F for which the surface F(t, x, y, z) = 0 has non-isolated singularities. An example is given by

$$A = \begin{bmatrix} 1+i & 0 & 0\\ 0 & 1+i & 0\\ 0 & 0 & 3i \end{bmatrix}, \quad K = \begin{bmatrix} 0 & 2 & 0\\ 2 & 0 & 1\\ 0 & 1 & 0 \end{bmatrix}.$$

In the sequel, we shall treat the case the cubic surface F(t, x, y, z) has isolated singularities. For more singularity classification of cubic surfaces, we refer the reader to Bruce and Wall [2] and references therein. There are 21 types of cubic surfaces in referring to isolated singularities listed on the webpage of Labs [11]. Nice models of cubic surfaces can be found on the webpage [12]. In Section 3, we show that the following 6 typical types of cubic surfaces actually occur as surfaces S_F corresponding to some matrices:

- [I]: no singularity;
- [II]: one ordinary double point A_1 ;
- [IV]: two ordinary double points $2A_1$;
- [VIII]: three ordinary double points $3A_1$;
- [IX]: two biplanar double points $2A_2$;
- [XVII]: two biplanar double points $2A_2$ and one ordinary double point A_1 .

Let A be a 3×3 matrix, and F(t, x, y, z) the corresponding homogeneous polynomial. In [2], the *class* of an irreducible cubic surface S_F with isolated singularities is defined. It is the number of tangent hyperplanes of S_F passing through a generic point. The class number is given by

$$12 - \sum_{j} \nu(P_j),\tag{3}$$

where P_j is a singular point of S_F and $\nu(P)$ is a positive number depending on the type of singularity at the point P. In particular, $\nu(P) = 2$ if P is an A_1 point, and $\nu(P) = 3$ if P is an A_2 point.

Notice that every boundary point P of the Davis-Wielandt shell of a matrix lies in the dual surface of the cubic surface if P does not lie on a flat portion. An algorithm for computing the boundary of the Davis-Wielandt shell of a 3×3 matrix can be found in [4, 5]. The class number (3) of the cubic surface S_F is exactly the degree of the boundary generating surface G(1, x, y, z) = 0 of the Davis-Wielandt shell of A.

3. Upper triangular matrices

We deal with the Davis-Wielandt shell of a 3×3 upper triangular matrix using the cubic surface S_F .

Theorem 1. Let A be the matrix given by

$$A = \begin{bmatrix} 2 \ 3 + \epsilon & 0\\ 0 & 0 & 2\\ 0 & 0 & -2 \end{bmatrix},$$

for $\epsilon = \pm 1$.

- (i) If $\epsilon = +1$, then the surface S_F has no singular points. The cubic surface is of type [I], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 12.
- (ii) If $\epsilon = -1$, the surface S_F has an ordinary double point at $(t, x, y, z) = (1, 0, 0, -\frac{1}{8})$. The cubic surface is of type [II], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 10.

Proof. Firstly we treat case (i), that is $\epsilon = +1$. The derivative of the form F(t, x, y, z) with respect y is given by

$$F_y(t, x, y, z) = -2y (5t - 6x + 36z).$$
(4)

Hence, if S_F has a singular point, it lies on a hyperplane y = 0 or a hyperplane z = (-5t + 6x)/36. We compute the resultant $R_1(x, z)$ of F_t and F_x with respect to t, and the resultant $R_2(x, z)$ of F_t and F_z with respect to t under the assumption that y = 0. We obtain that

$$R_1(x,z) = -72(3x^2 - 16z^2)(9x^2 + 24xz + 80z^2),$$
(5)

$$R_2(x,z) = 192(3x+20z)^2(3x^2+8xz-144z^2), \tag{6}$$

which are products of linear factors. The equation $R_1(x, z) = R_2(x, z) = 0$ implies x = z = 0. Since $F(1, 0, 0, 0) = 1 \neq 0$, the surface S_F has no singular points on the hyperplane y = 0. Next we compute the resultant $R_3(x, z)$ of F_t and F_x with respect to t, and the resultant $R_4(x, z)$ of F_t and F_z with respect to t under the assumption that z = (-5t + 6x)/36. Then we have

$$R_3(x,z) = \frac{256}{729} (1521x^4 + 906x^2y^2 + 121y^4), \tag{7}$$

$$R_4(x,z) = \frac{4096}{729} (729x^4 + 886x^2y^2 + 81y^4).$$
(8)

These are also products of linear factors. The equation $R_3(x, y) = R_4(x, y) = 0$ implies x = y = 0. Because $F(1, 0, 0, 0) = 1 \neq 0$, the surface S_F has no singular points.

Secondly we treat case (*ii*), that is $\epsilon = -1$. The form F(t, x, y, z) associated with A satisfies the equation

$$F(1, x, y, -\frac{1}{8} + z) = -\frac{9}{2}x^2 - \frac{1}{2}y^2 + 64z^2 - 12(x^2 + y^2)z,$$
(9)

and hence $(1, 0, 0, -\frac{1}{8})$ is an ordinary double point of the cubic surface. On the hyperplane t = 0 at infinity, we have

$$F_x(0, x, y, z) = -24xz, F_y(0, x, y, z) = -24yz, F(0, x, y, z) = -12(x^2 + y^2)z.$$

These relations imply that the cubic surface S_F has no singular point on t = 0. On the affine 3-space t = 1, the equation

$$F(1, x, y, z) = 1 + 16z - 6x^2 - 2y^2 + 64z^2 - 12x^2z - 12y^2z$$
(10)

implies that the resultant of F_x and F_y with respect z, x, y are respectively given by

-192xy, -4y(1+6z), -12x(1+2z).

Since F(1, 0, y, -1/6) = 1/9, F(1, x, 0, -1/2) = 9, the singular point (1, x, y, z) of S_F necessarily satisfies x = y = 0. Then $F(1, 0, 0, z) = 1 + 16z + 64z^2 = (1 + 8z)^2$, and thus $z = -\frac{1}{8}$.

The class numbers (3) of (i) and (ii) are respectively 12 = 12 - 0 and 10 = 12 - 2, which are the degrees of the boundary generating surface of the respective DW(A).

Theorem 2. Let A be the upper triangular matrix given by

$$A = \begin{bmatrix} 1 & a & 0 \\ 0 & 1 & b \\ 0 & 0 & 0 \end{bmatrix},$$

a > 0, b > 0. Then

- (i) The corresponding cubic surface S_F has no singular points on the plane at infinity t = 0.
- (ii) If $a = \sqrt{1+b^2}$, the surface S_F has an ordinary double point at (t, x, y, z)= $(1, 2/b^2, 0, -1/b^2)$ and a pair of imaginary ordinary double points (t, x, y, z)= $(1, (1-b^2)/b^2, \pm i(b^2+1)/b^2, -1/b^2)$. The cubic surface is of type [VIII], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 6.
- (iii) If $a \neq \sqrt{1+b^2}$, the surface S_F has a pair of imaginary ordinary double points $(t, x, y, z) = (1, (1-b^2)/b^2, \pm i(b^2+1)/b^2, -1/b^2)$. The cubic surface is of type [IV], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 8.

Proof. Let g(t, x, y, z) = 4F(t, x, y, z). Firstly, we show that the surface g(t, x, y, z) = 0 has no singular points on the plane t = 0. We have

$$g(0, x, y, z) = -b^{2}(x^{2} + y^{2})(x + (a^{2} + 1)z).$$

Consider $g_z(0, x, y, z) = 0$, we may assume that (x, y, z) = (0, 0, 1) or $(x, y, z) = (1, \pm i, z)$. If (x, y, z) = (0, 0, 1) then $g_t(0, 0, 0, 1) = 4(a^2b^2 + b^2 + 1) \neq 0$, and

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thus $(x, y) = (1, \pm i)$. The condition $g_y(0, x, y, z) = 0$ implies that $z = -1/(a^2 + 1)$ and hence $g_x(0, x, y, z) = -b^2(3 - 1 - 2/(a^2 + 1)) = -2b^2(a^2 + 1 - 1)/(a^2 + 1)$ $= -2a^2b^2/(a^2 + 1) \neq 0$. This shows that the surface g(t, x, y, z) = 0 has no singular points on the plane t = 0.

Next, we deal with singular points of the surface g(t, x, y, z) = 0 on the affine space $t = 1, (x, y, z) \in \mathbb{C}^3$. Assume that (1, x, y, z) is a singular point of g(t, x, y. z) = 0. Then

$$g_y(1, x, y, z) = -2y(b^2x + (a^2b^2 + b^2)z + a^2 + b^2) = 0.$$
 (11)

Suppose

$$b^{2}x + (a^{2}b^{2} + b^{2})z + a^{2} + b^{2} = 0$$
(12)

in (11). Solve (12) for x = x(z). Then the equation g(1, x(z), y, z) = 0 becomes $4a^4(b^2z + 1)^2/b^4 = 0$. Thus $z = -1/b^2$, and $x = (1 - b^2)/b^2$. Further, we solve

$$g_z(1,(1-b^2)/b^2,y,-1/b^2) = -\frac{a^2+1}{b^2}(b^4y^2+(1+b^2)^2) = 0$$

in y. Then $y = \pm i((b^2 + 1)/b^2)$. Conversely the point $(t, x, y, z) = (1, (1 - b^2)/b^2, \pm i(b^2 + 1)/b^2, -1/b^2)$ satisfies the condition for singularity. We conclude that the singular points (1, x, y, z) with $y \neq 0$ are $(x, y, z) = ((1 - b^2)/b^2, \pm i(b^2 + 1)/b^2, -1/b^2)$.

Lastly, we deal with singular points of the surface g(t, x, y, z) = 0 on the plane y = 0. In this plane, $g_y(1, x, 0, z) = 0$ holds. Assume that (1, x, 0, y) is a singular point of g(t, x, y, z) = 0. We solve the equation

$$g_z(1, x, 0, z) = 8(a^2b^2 + b^2 + 1)z - (a^2b^2 + b^2)x^2 + (4b^2 + 8)x + 4a^2 + 8 = 0$$

in z = z(x). Then the resultant of g(1, x, 0, z(x)) and $g_x(1, x, 0, z(x))$ with respect to x is given by

$$-\frac{a^{12}b^8(a^2+1)^2(b^2+1)^4(a^2-1-b^2)^2}{16(a^2b^2+b^2+1)^5}$$

which does vanish if and only if $a = \sqrt{b^2 + 1}$. Thus in case (*iii*), $a \neq \sqrt{b^2 + 1}$, the cubic surface is of type [IV].

We assume $a = \sqrt{b^2 + 1}$ in (*ii*). Applying an Euclidean algorithm for g(1, x, 0, z(x))and $g_x(1, x, 0, z(x))$ with respect to x, we obtain that their common divisor $b^2x - 2$ = 0. Then the singular point (1, x, 0, z(x)) on the plane y = 0 satisfies $x = 2/b^2$ and z(x) is given by $z = -1/b^2$. Thus the surface S_F has three ordinary double points, the cubic surface is of type [VIII].

The class numbers (3) of (i) and (ii) are respectively 12 = 12 - 0 and 10 = 12 - 2, which are the degrees of the boundary generating surfaces of the respective DW(A).

We consider the cubic form corresponding to a nilpotent matrix

$$A = \begin{bmatrix} 0 & a & c \\ 0 & 0 & b \\ 0 & 0 & 0 \end{bmatrix}$$

We assume $a \neq 0$, and we may assume a = 1. We also assume that b > 0 and $c \in \mathbf{R}$. We deal with the matrix

$$A = \begin{bmatrix} 0 & 1 & c \\ 0 & 0 & b \\ 0 & 0 & 0 \end{bmatrix}, \ b > 0, \ c \in \mathbf{R},$$
(13)

Theorem 3. Let A be the matrix as in (13).

- (i) If b = 1, the surface S_F has two biplanar double points (0, 1, i, c/b) and (0, 1, -i, c/b), and one ordinary double point (1, 2c, 0, c² 1). The cubic surface is of type [XVII], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 4.
- (ii) If $b \neq 1$, the surface S_F has two biplanar double points (0, 1, i, c/b) and (0, 1, -i, c/b). The cubic surface is of type [IX], and the boundary generating surface of the Davis-Wielandt shell DW(A) lies in a polynomial surface of degree 6.

Proof. By direct computations, a pair of points (t, x, y, z) = (0, 1, i, c/b), (0, 1, -i, c/b) are biplanar double points of type A_2 , and the surface S_F has no other singular points on the plane t = 0 at infinity. We examine singular points on the affine 3-space : $t = 1, (x, y, z) \in \mathbb{C}^3$. For b = 1, the surface S_F has an ordinary double point at $(t, x, y, z) = (1, 2c, 0, c^2 - 1)$. The cubic surface is of type [XVII].

For $0 < b, b \neq 1$, we will show that there is no singular point of the surface S_F on the affine 3-space t = 1, $(x, y, z) \in \mathbb{C}^3$, and thus the cubic surface is of type [IX]. We define the polynomial g(x, y, z) and compute that

$$g(x, y, z) = 4F(1, x, y, z)$$

= $bcx^3 + bcxy^2 - b^2(x^2 + y^2)z - (b^2 + c^2 + 1)(x^2 + y^2)$
 $+4b^2z^2 + -4bcxz + 4(b^2 + c^2 + 1)z + 4.$

Then $g_y(x, y, z) = -2y(-bcx + b^2z + b^2 + c^2 + 1) = 0$. Suppose (x_0, y_0, z_0) is a singular point of g = 0 with $y_0 \neq 0$. We set $h = -bcx + b^2z + b^2 + c^2 + 1$. We find the resultant of g and h with respect to z is $4b^4 \neq 0$. Thus there is no such a singular point. So we assume that $(x_0, 0, z_0)$ is a singular point of g = 0. Then $g_z(x_0, 0, z_0) = 8b^2z - b^2x^2 - 4bcx + 4b^2 + 4c^2 + 4$. Solve $g_z(x, 0, z) = 0$ with respect to z, and substitute the solution z = k(x) into $g_x(x, 0, z) = 0$, we obtain $(bx - 2c)(b^2x^2 - 4bcx + 4b^2 + 4c^2 + 4) = 0$. We set $m(x) = b^2x^2 - 4bcx + 4b^2 + 4c^2 + 4$. Then the resultant m(x) and g(x, 0, k(x)) with respect to x is $16b^8 \neq 0$. This implies that bx - 2c = 0, we have x = 2c/b, and then $z = (2c^2 - b^2 - 1)/(2b^2)$. Hence $F = -(b-1)^2(b+1)^2/b^2 \neq 0$, and thus the surface F = 0 has no singular point in the affine 3-space.

The class numbers (3) of (i) and (ii) are respectively $4 = 12 - 2 \times 3 - 2$ and $6 = 12 - 2 \times 3$, which are the degrees of the boundary generating surfaces of the respective DW(A).

Remark 1. We have found in Theorems 1-3 six types of cubic surfaces related with the Davis-Wielandt shell DW(A) of 3×3 matrices. It is open whether there exist cubic surfaces other than types (I), (II), (IV), (VIII), (IX), (XVII) related with some 3×3 matrices.

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