APÉRY’S IRRATIONALITY PROOF, MIRROR SYMMETRY AND
BEUKERS’S MODULAR FORMS

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ABSTRACT. In this paper, we will study the connections between Apéry’s proof of the irrationality of \( \zeta(3) \) and the mirror symmetry of Calabi-Yau threefolds. From the mysterious sequences in Apéry’s proof, we will construct a fourth order Picard-Fuchs equation that has a large complex structure limit. The mirror map associated to it is the modular form with respect to \( \Gamma_1(6) \) found by Beukers, while the instanton expansion of a rescaled Yukawa coupling give us another modular form found by Beukers. We will show how mirror symmetry provides further enlightening explanations to Beukers’s and many others’ enlightening explanations to Apéry’s mysterious proof.

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1. Introduction

In 1978, Apéry proved the irrationality of

\( \zeta(3) = \sum_{n=1}^{\infty} \frac{1}{n^3} = 1.2020569031595942854 \cdots \) \hspace{3em} (1.1)

in a rather miraculous way \cite{[1]}. He constructed two very mysterious sequences

\[ A_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \],

\[ B_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \left( \sum_{m=1}^{n} \frac{1}{m^3} + \sum_{m=1}^{k} \frac{(-1)^{m-1}}{2m^3 \binom{n}{m} \binom{n+m}{m}} \right) \], \hspace{3em} (1.2)

both of which are the solutions of the recursion equation

\( (n+1)^3 x_{n+1} - (34n^3 + 51n^2 + 27n + 5)x_n + n^3 x_{n-1} = 0 \) \hspace{3em} (1.3)

with initial conditions respectively

\( (A_0, A_1) = (1, 5) \) and \( (B_0, B_1) = (0, 6) \). \hspace{3em} (1.4)
Apéry proved that $A_n \in \mathbb{Z}$ for all $n \geq 0$, which is a very remarkable property. Since if we compute $A_n$ recursively from the recursion 1.3, we need to divide by $n^3$ at each step, therefore we should a priori expect that $A_n$ has denominator $(n!)^3$. Hence the integrality of $A_n$ is rather surprising. Equally surprising is the property that we have a very good denominator bound for $B_n$

$$d_n^3 B_n \in \mathbb{Z}, \forall n \geq 0,$$ \hspace{1cm} (1.5)

The readers are referred to [10] for a much better explanation about how remarkable these two properties are! Then Apéry proved that the sequence $B_n/A_n$ converges to $\zeta(3)$ fast enough to apply Dirichlet’s irrationality criterion. Even though the sequence $B_n$ is not integral after $n = 2$, nevertheless this can be cured by multiplying both $A_n$ and $B_n$ by $d_n^3$ [1, 10].

The development of many enlightening explanations to Apéry’s mysterious proof has been a wonderful chapter in the history of mathematics [10]. In particular, Beukers has many interesting works on this area. In this paper, we will further enlighten the works of Beukers and many others using the methods in the mirror symmetry of Calabi-Yau threefolds, which we briefly explain now. We will construct a power series $\Pi_0(\varphi)$ from $B_n$ of the form

$$\Pi_0(\varphi) = B_0 + \sum_{n=1}^{\infty} (B_n - B_{n-1}) \varphi^n = 6\varphi + \frac{327}{4} \varphi^2 + \frac{14843}{9} \varphi^3 + \cdots.$$ \hspace{1cm} (1.6)

It is the solution of a fourth order differential equation $\mathcal{D}\Pi_0(\varphi) = 0$, where the Picard-Fuchs operator $\mathcal{D}$ is given by

$$\mathcal{D} = (\varphi - 1)^4 \left( (\varphi^2 - 34\varphi + 1) \theta^4 + (\varphi - 1)^3 (81\varphi^2 + 46\varphi + 1) \theta^3 
- 24(\varphi - 1)^2 \varphi (3\varphi^2 + 12\varphi + 1) \theta^2 + 4(\varphi - 1)\varphi (7\varphi^3 + 107\varphi^2 + 77\varphi + 1) \theta 
- 4\varphi^2 (\varphi^3 + 49\varphi^2 + 115\varphi + 27) \right), \quad \theta = \varphi \frac{d}{d\varphi}.$$ \hspace{1cm} (1.7)

Next, we define a new variable $\varphi$ by $\varphi := 1/\phi$, it is very surprising that the following power series constructed from $A_n$

$$\varpi_0(\varphi) = A_0 + \sum_{n=1}^{\infty} (A_n - A_{n-1}) \varphi^n = 1 + 4\varphi + 68\varphi^2 + 1372\varphi^3 + \cdots.$$ \hspace{1cm} (1.8)

is also a solution of $\mathcal{D}$. What is more, in a small neighborhood of $\varphi = 0$, there exist another three solutions of the form

$$\varpi_1(\varphi) = \frac{1}{(2\pi i)} (\varpi_0(\varphi) \log \varphi + h_1(\varphi)),$$ 

$$\varpi_2(\varphi) = \frac{1}{(2\pi i)^2} (\varpi_0(\varphi) \log^2 \varphi + 2h_1(\varphi) \log \varphi + h_2(\varphi)),$$ 

$$\varpi_3(\varphi) = \frac{1}{(2\pi i)^3} (\varpi_0(\varphi) \log^3 \varphi + 3h_1(\varphi) \log^2 \varphi + 3h_2(\varphi) \log \varphi + h_3(\varphi)),$$ \hspace{1cm} (1.9)
where \( h_1(\varphi), h_2(\varphi) \) and \( h_3(\varphi) \) are power series of the form
\[
h_i(\varphi) = \sum_{j=1}^{\infty} c_{i,j} \varphi^j, \quad c_{i,j} \in \mathbb{Q}.
\] (1.10)

The four solutions \( \{\varpi_i(\varphi)\}_{i=0}^{3} \) form a basis of the solution space of \( \mathcal{D} \), and \( \varphi = 0 \) will be called the large complex structure limit of \( \mathcal{D} \).

However, we do not know whether \( \mathcal{D} \) is the Picard-Fuchs operator of a one-parameter mirror pair of Calabi-Yau threefolds. But nevertheless we can still proceed and define the mirror map by inverting the equation
\[
\tau = \varpi_1(\varphi)/\varpi_0(\varphi),
\] (1.11)

which gives us a \( q \)-expansion of \( \varphi \) that will be denoted by \( \varphi(q) \) \( (q = \exp 2\pi i \tau) \). In fact, \( \varphi(q) \) is the modular form (with respect to \( \Gamma_1(6) \)) found by Beukers [10]
\[
\varphi(q) = q \prod_{n=1}^{\infty} \frac{(1 - q^{2n})^{12}(1 - q^{6n})^{12}}{(1 - q^{2n})^{12}(1 - q^{3n})^{12}}.
\] (1.12)

Follow mirror symmetry, we can compute the Yukawa coupling \( \mathcal{Y} \) directly from the operator \( \mathcal{D} \)[5], which is given by
\[
\mathcal{Y} = \frac{(1 - \varphi)^2}{\varphi^3(\varphi^2 - 34\varphi + 1)^{5/4}}.
\] (1.13)

But it turns out that the following rescaled Yukawa coupling \( \mathcal{Y}^R \) is more interesting
\[
\mathcal{Y}^R = \frac{1}{(\varphi^2 - 34\varphi + 1)^{1/4}} \mathcal{Y} = \frac{(1 - \varphi)^2}{\varphi^3(\varphi^2 - 34\varphi + 1)^{3/2}}.
\] (1.14)

From mirror symmetry, the symplectic normalization of \( \mathcal{Y}^R \) is defined by [4, 5]
\[
\mathcal{Y}_{\tau\tau\tau}^R = \frac{1}{\varpi_0(\varphi)^2} \mathcal{Y}^R \cdot \left( \frac{1}{2\pi i} \frac{d\varphi}{d\tau} \right)^3.
\] (1.15)

Plug the mirror map \( \varphi(q) \) 1.12 into this expression, we get the instanton expansion of \( \mathcal{Y}_{\tau\tau\tau}^R \), which is another modular form with respect to \( \Gamma_1(6) \) found by Beukers [2, 10]
\[
\mathcal{Y}_{\tau\tau\tau}^R(q) = \prod_{n=1}^{\infty} \frac{(1 - q^{2n})^7(1 - q^{3n})^7}{(1 - q^{2n})^5(1 - q^{6n})^5}.
\] (1.16)

Therefore, using the methods in mirror symmetry, we have found a very interesting explanation to Beukers’s works [2].

On the other hand, using numerical methods, we have obtained the expansion of \( \Pi_0(\phi) \) with respect to the basis \( \{\varpi_i(\varphi)\}_{i=0}^{3} \)
\[
\Pi_0(\phi) = (-20\zeta(3)) - \frac{1}{4}(2\pi i)^3 \varpi_0(\varphi) + (12\zeta(3) + (2\pi i)^3) \varpi_1(\varphi)
\]
\[
+ (-12\zeta(3) - \frac{3}{2}(2\pi i)^3) \varpi_2(\varphi) + (2\pi i)^3 \varpi_3(\varphi).
\] (1.17)

Furthermore, the monodromy matrix of the vector \( (\varpi_0(\varphi), \varpi_1(\varphi), \varpi_2(\varphi), \varpi_3(\varphi))^T \) at the singularities of \( \mathcal{D} \) can also be numerically computed, and our results have shown their entries...
lie in the ring \(\mathbb{Q}[\zeta(3)/(2\pi i)^3]\). Both numerical results are well-known properties if we assume mirror symmetry [6].

The outline of this paper is as follows. In Section 2, we will briefly review some results of Beukers and others about Apéry’s proof, in particular the modular form found by Beukers in [2]. We will also study the mirror symmetry of the family of K3 surfaces constructed in the paper [3]. In Section 3, we will construct a fourth order Picard-Fuchs operator and solve it in a small neighborhood of the large complex structure limit. In Section 4, we will compute the Yukawa coupling and its instanton expansion. We will show that the instanton expansion of a rescaled Yukawa coupling gives us a modular form found by Beukers. In Section 5, we will give some interesting numerical results about the fourth order Picard-Fuchs operator, e.g. its monodromy matrices. In Section 6, we will list several interesting open questions.

2. Beukers’s modular forms and K3 surfaces

In this section, we will briefly review some results of Beukers and others about the mysterious sequences in Apéry’s proof. First, let us recall that the modular group \(\Gamma_1(6)\) is the subgroup of \(\text{SL}(2, \mathbb{Z})\) that consists of matrices

\[
\begin{pmatrix}
a & b \\
c & d
\end{pmatrix} \in \text{SL}(2, \mathbb{Z}), \quad a \equiv d \equiv 1 (\text{mod } 6), \quad c \equiv 0 (\text{mod } 6).
\]

(2.1)

In the paper [2], Beukers found two modular forms with respect to \(\Gamma_1(6)\)

\[
T(q) = q \prod_{n=1}^{\infty} \frac{(1 - q^n)^{12}(1 - q^{6n})^{12}}{(1 - q^{2n})^{12}(1 - q^{3n})^{12}} = q - 12q^2 + 66q^3 - 220q^4 + \cdots.
\]

(2.2)

\[
F(q) = \prod_{n=1}^{\infty} \frac{(1 - q^{2n})^{7}(1 - q^{3n})^{7}}{(1 - q^n)^5(1 - q^{6n})^5} = 1 + 5q + 13q^2 + 23q^3 + \cdots.
\]

(2.3)

Here the variable \(q\) is defined by

\[
q := \exp 2\pi i \tau, \quad \tau \in \mathbb{H},
\]

(2.4)

where \(\mathbb{H}\) is the upper half complex plane. The modular form \(F(q)\) has an expansion with respect to \(T(q)\) of the form

\[
F(q) = \sum_{n=0}^{\infty} A_n T(q)^n,
\]

which explains the integrality of \(A_n\) since both modular forms have integral coefficients.

In 1984, Beukers and Peters discovered a very interesting connection between the sequences 1.2 and K3 surface [3]. Let us define a power series \(\mathcal{A}(\varphi)\) by

\[
\mathcal{A}_0(\varphi) := \sum_{n=0}^{\infty} A_n \varphi^n = 1 + 5\varphi + 73\varphi^2 + 1445\varphi^3 + \cdots.
\]

(2.5)

The recursion equation 1.3 is equivalent to the statement that \(\mathcal{A}(\varphi)\) is a solution of the differential equation \(\mathcal{L} \mathcal{A}(\varphi) = 0\), where the operator \(\mathcal{L}\) is defined by

\[
\mathcal{L} := \vartheta^3 - \varphi(34\vartheta^3 + 51\vartheta^2 + 27\vartheta + 5) + \varphi^2(\vartheta + 1)^3, \quad \vartheta = \varphi \frac{d}{d\varphi}.
\]

(2.6)
Moreover, $\mathcal{L}$ is the Picard-Fuchs operator of a pencil of K3 surfaces, which will be denoted by $[3, 10]$

$$\pi : \mathcal{X} \to \mathbb{P}^1,$$  

while the underlying real manifold of a smooth fiber will be denoted by $X$.

2.1. The Yukawa coupling. There exists a holomorphic twoform $\Omega_\varphi$ on $\mathcal{X}_\varphi$ that varies holomorphically with respect to $\varphi$. The Picard-Fuchs operator $\mathcal{L}$ can also be written as

$$\mathcal{L} = \varphi^3 (\varphi^2 - 34 \varphi + 1) \frac{d^3}{d\varphi^3} + 3 \varphi^2 (2 \varphi^2 - 51 \varphi + 1) \frac{d^2}{d\varphi^2} + \varphi (7 \varphi^2 - 112 \varphi + 1) \frac{d}{d\varphi} + (\varphi - 5) \varphi.$$  

(2.8)

Another independent solution of $\mathcal{L}$ is of the form

$$\mathcal{A}_1(\varphi) = \mathcal{A}_0(\varphi) \log \varphi + \sum_{n=1}^{\infty} C_n \varphi^n,$$  

(2.9)

where the coefficient $C_n$ is determined by the recursion equation

$$(n + 1)^3 C_{n+1} - (34n^3 + 51n^2 + 27n + 5) C_n + n^3 C_{n-1} + 3(n + 1)^2 A_{n+1} - 3 (34n^2 + 34n + 9) A_n + 3n^2 A_{n-1} = 0,$$  

(2.10)

with initial condition

$$C_1 = 12, \ C_2 = 210.$$  

(2.11)

Moreover, there is a third solution $\mathcal{A}_2(\varphi)$ of $\mathcal{L}$ given by

$$\mathcal{A}_2(\varphi) = \mathcal{A}_1^2(\varphi)/\mathcal{A}_0(\varphi),$$  

(2.12)

and $\{\mathcal{A}_i(\varphi)\}_{i=0}^2$ form a basis for the solution space of $\mathcal{L}$. From the paper $[7]$, there exist cohomology cycles $\{\alpha_i\}_{i=0}^2 \subset H^2(X, \mathbb{C})$ with pairing relations

$$\int_X \alpha_0 \wedge \alpha_2 = \int_X \alpha_2 \wedge \alpha_0 = 1, \ \int_X \alpha_1 \wedge \alpha_1 = 2, \ \int_X \alpha_i \wedge \alpha_j = 0 \text{ otherwise}$$  

(2.13)

such that the twoform $\Omega_\varphi$ has an expansion $[7]$

$$\Omega_\varphi = \mathcal{A}_0(\varphi) \alpha_0 + \mathcal{A}_1(\varphi) \alpha_1 - \mathcal{A}_2(\varphi) \alpha_2.$$  

(2.14)

Together with formula 2.13, we immediately deduce that

$$\int_X \Omega_\varphi \wedge \Omega_\varphi = \int_X \Omega_\varphi \wedge \frac{d\Omega_\varphi}{d\varphi} = 0.$$  

(2.15)

Following mirror symmetry $[4, 5, 6]$, let us define the Yukawa coupling of this family by

$$\mathcal{Y} := \int_X \Omega_\varphi \wedge \frac{d^2 \Omega_\varphi}{d\varphi^2},$$  

(2.16)

While from formula 2.13, we have

$$\int_X \frac{d\Omega_\varphi}{d\varphi} \wedge \frac{d\Omega_\varphi}{d\varphi} = -\mathcal{Y}, \ \int_X \frac{d\Omega_\varphi}{d\varphi} \wedge \frac{d^2 \Omega_\varphi}{d\varphi^2} = -\frac{1}{2} \frac{d\mathcal{Y}}{d\varphi}, \ \int_X \Omega_\varphi \wedge \frac{d^3 \Omega_\varphi}{d\varphi^3} = \frac{3 d\mathcal{Y}}{2 d\varphi}.$$  

(2.17)

Hence from the form of $\mathcal{L}$ in formula 2.8, we deduce

$$\frac{3}{2} \varphi^3 (\varphi^2 - 34 \varphi + 1) \frac{d\mathcal{Y}}{d\varphi} + 3 \varphi^2 (2 \varphi^2 - 51 \varphi + 1) \mathcal{Y} = 0,$$  

(2.18)
solving which we obtain
\[ \Upsilon = \frac{C_1}{\varphi^2(\varphi^2 - 34\varphi + 1)}. \]  
(2.19)

On the other hand, from formula 2.17, we also have
\[ \Upsilon = -2 \left( A'_1(\varphi) - \mathcal{A}'_0(\varphi)\mathcal{A}'_2(\varphi) \right) \]  
(2.20)

Plug in the power series expansions of \( \mathcal{A}_i(\varphi) \), we get
\[ C_1 = -2. \]  
(2.21)

2.2. The mirror map. Following mirror symmetry [5, 6], the mirror map is defined by
\[ \tau = \frac{1}{2\pi i} \frac{A_1(\varphi)}{\mathcal{A}_0(\varphi)}. \]  
(2.22)

Let us define \( q \) by
\[ q = \exp 2\pi i \tau. \]  
(2.23)

Equation 2.22 can be inverted order by order, which gives us the \( q \)-expansion of the mirror map \( \varphi(q) \) [4, 5]
\[ \varphi(q) = q - 12q^2 + 66q^3 - 220q^4 + 95q^5 - 804q^6 + 1068q^7 - 1596q^8 + 3279q^9 + O(q^{10}), \]  
(2.24)

which is in fact equal to \( T(q) \) [10]. From formula 2.20, the Yukawa coupling \( \Upsilon \) can also be written as
\[ \Upsilon = -2\varphi_0^2(\varphi) \left( 2\pi i \frac{d\tau}{d\varphi} \right)^2, \]  
(2.25)

together with 2.19, we obtain
\[ \varphi_0^2(\varphi) \left( 2\pi i \frac{d\tau}{d\varphi} \right)^2 = \frac{1}{\varphi^2(\varphi^2 - 34\varphi + 1)}. \]  
(2.26)

The normalized Yukawa coupling with respect to the coordinate \( \tau \) is by definition
\[ \frac{1}{\varphi_0^2(\varphi)} \Upsilon \left( \frac{1}{2\pi i} \frac{d\varphi}{d\tau} \right)^2 = -2, \]  
(2.27)

which corresponds to the well-known fact in mirror symmetry that the Gromov-Witten invariants of K3 surfaces are trivial [7].

3. Picard-Fuchs equation and the large complex structure limit

From this section, we will apply the methods in the mirror symmetry of Calabi-Yau threefolds to further enlighten Apéry’s proof and the works of Beukers and many others. First, let us construct a power series \( \Pi_0(\phi) \) from the sequence 1.2 by
\[ \Pi_0(\phi) := B_0 + \sum_{n=1}^{\infty} (B_n - B_{n-1})\phi^n = 6\phi + \frac{327}{4}\phi^2 + \frac{14843}{9}\phi^3 + \cdots, \]  
(3.1)

which satisfies a fourth order Picard-Fuchs equation.
Lemma 3.1. \( \Pi_0(\phi) \) is a solution of the Picard-Fuchs operator \( \mathcal{D} \) that is defined by

\[
\mathcal{D} := (\phi - 1)^4 \left( \phi^2 - 34\phi + 1 \right) \theta^4 + (\phi - 1)^3 \left( 81\phi^2 + 46\phi + 1 \right) \theta^3 \\
- 24(\phi - 1)^2 \phi \left( 3\phi^2 + 12\phi + 1 \right) \theta^2 + 4(\phi - 1) \phi \left( 7\phi^3 + 107\phi^2 + 77\phi + 1 \right) \theta \\
- 4\phi^2 \left( \phi^3 + 49\phi^2 + 115\phi + 27 \right), \quad \theta = \phi \frac{d}{d\phi}.
\]

Proof. Suppose \( \mathcal{D} \) has a power series solution of the form

\[
\sum_{n=1}^{\infty} b_n \phi^n, \text{ with } b_1 = 6.
\]

Plug it into the Picard-Fuchs operator, we obtain a recursion equation about \( b_n \)

\[
(n + 2)(n + 3)^3 b_{n+3} - (n + 2) \left( 38n^3 + 271n^2 + 652n + 528 \right) b_{n+2} + (143n^4 + 626n^3 + 780n^2 \\
- 50n - 455) b_{n+1} - 2 \left( 106n^4 - 53n^3 - 240n^2 + 60n + 230 \right) b_n + (143n^4 - 769n^3 + 1305n^2 \\
- 475n - 400) b_{n-1} + (-38n^4 + 385n^3 - 1470n^2 + 2504n - 1604) b_{n-2} + (n - 3)^4 b_{n-3} = 0,
\]

with initial condition

\[
b_1 = 6, b_2 = \frac{327}{4}, b_3 = \frac{14843}{9}, b_4 = \frac{10924447}{288}, b_5 = \frac{8503393807}{9000}, b_6 = \frac{223313780023}{9000}.
\]

Apply the recursion equation 1.3 repeatedly, we find that the sequence

\[
b_n = B_n - B_{n-1}, \quad n \geq 1
\]

satisfies the recursion equation 3.4 and the initial condition 3.5, which proves this lemma.

From the form of the Picard-Fuchs operator \( \mathcal{D} \), it has regular singularities at

\[
\phi = 0, 1, (1 + \sqrt{2})^4, (1 + \sqrt{2})^{-4}, \infty.
\]

Now let us define a new variable \( \varphi \) by

\[
\varphi := 1/\phi.
\]

With respect to \( \varphi \), \( \mathcal{D} \) (up to a multiplication by \( \varphi^6 \)) can be written as

\[
\mathcal{D} = (\varphi - 1)^4 \left( \varphi^2 - 34\varphi + 1 \right) \vartheta^4 + (\varphi - 1)^3 \varphi \left( \varphi^2 + 46\varphi + 81 \right) \vartheta^3 \\
- 24(\varphi - 1)^2 \varphi \left( \varphi^2 + 12\varphi + 3 \right) \vartheta^2 + 4(\varphi - 1) \varphi \left( \varphi^3 + 77\varphi^2 + 107\varphi + 7 \right) \vartheta \\
- 4\varphi \left( 27\varphi^3 + 115\varphi^2 + 49\varphi + 1 \right), \quad \vartheta = \varphi \frac{d}{d\varphi}.
\]

Let us define a new power series \( \varpi_0(\varphi) \) from the sequence 1.2 by

\[
\varpi_0(\varphi) = (1 - \varphi)\varphi(\varphi) = A_0 + \sum_{n=1}^{\infty} (A_n - A_{n-1})\varphi^n = 1 + 4\varphi + 68\varphi^2 + 1372\varphi^3 + \cdots,
\]

and we have the following important lemma.

Lemma 3.2. The power series \( \varpi_0(\varphi) \) is a solution of the Picard-Fuchs operator \( \mathcal{D} \) 3.9.
Proof. Suppose $D$ has a power series solution of the form
\[ \sum_{n=0}^{\infty} a_n \varphi^n, \text{ with } a_0 = 1. \] (3.11)
Plug it into $D$, we obtain a recursion equation about $a_n$
\[
(n + 3)a_{n+3} + (-38n^4 - 385n^3 - 1470n^2 - 2504n - 1604)a_{n+2} + (143n^4 + 769n^3 + 1305n^2 \\
+ 475n - 400)a_{n+1} - 2 (106n^4 + 53n^3 - 240n^2 - 60n + 230) a_n + (143n^4 - 626n^3 + 780n^2 \\
+ 50n - 455)a_{n-1} - (n - 2) (38n^3 - 271n^2 + 652n - 528) a_{n-2} + (n - 3)(n - 2)a_{n-3} = 0 
\] (3.12)
with initial condition
\[ a_0 = 1, a_1 = 4, a_2 = 68, a_3 = 1372, a_4 = 31556, a_5 = 786004. \] (3.13)
Apply the recursion equation \ref{eq:recursion} repeatedly, we find that the sequence
\[ a_0 = A_0, a_n = A_n - A_{n-1}, n \geq 1 \] (3.14)
satisfies the recursion equation \ref{eq:recursion} and the initial condition \ref{eq:initial}, which proves this lemma. \hfill \Box

In a small neighborhood of the point $\varphi = 0$, the Picard-Fuchs operator $D$ can be solved by the Frobenius method \cite{8}. More explicitly, we look at the equation
\[ D \left( \varphi^\epsilon \sum_{k=0}^{\infty} a_k(\epsilon) \varphi^k \right) = 0, \] (3.15)
where $\epsilon$ is a formal index and $a_k(\epsilon)$ is a number. To the lowest order, this differential equation gives us the indicial equation
\[ \epsilon^4 = 0, \] (3.16)
hence there exist another three solutions of the form \cite{8}
\[
\varpi_1(\varphi) = \frac{1}{(2\pi i)} (\varpi_0(\varphi) \log \varphi + h_1(\varphi)), \\
\varpi_2(\varphi) = \frac{1}{(2\pi i)^2} \left( \varpi_0(\varphi) \log^2 \varphi + 2h_1(\varphi) \log \varphi + h_2(\varphi) \right), \\
\varpi_3(\varphi) = \frac{1}{(2\pi i)^3} \left( \varpi_0(\varphi) \log^3 \varphi + 3h_1(\varphi) \log^2 \varphi + 3h_2(\varphi) \log \varphi + h_3(\varphi) \right).
\] (3.17)
Here $h_1(\varphi)$, $h_2(\varphi)$ and $h_3(\varphi)$ are power series
\[ h_i(\varphi) = \sum_{n=1}^{\infty} c_{i,n} \varphi^n \] (3.18)
that are determined uniquely by the recursion equations and initial conditions given by the Picard-Fuchs equation.

Lemma 3.3.
\[ \varpi_1(\varphi) = \frac{1}{2\pi i} (1 - \varphi) \varpi_1(\varphi), \quad \varpi_2(\varphi) = \frac{1}{(2\pi i)^2} (1 - \varphi) \varpi_2(\varphi). \] (3.19)
Proof. If we plug \( \varpi_1(\varphi) \) into the Picard-Fuchs equation \( D\varpi_1(\varphi) = 0 \), we obtain the following recursion equation about \( c_{1,n} \)

\[
(n + 3)^4 c_{1,n+3} + (-38n^4 - 385n^3 - 1470n^2 - 2504n - 1604) c_{1,n+2} + (143n^4 + 769n^3 + 1305n^2 + 475n - 400)c_{1,n+1} - 2 (106n^4 + 53n^3 - 240n^2 - 60n + 230) c_{1,n} + (143n^4 - 626n^3 + 780n^2 + 50n - 455)c_{1,n-1} + (2 - n) (38n^3 - 271n^2 + 652n - 528) c_{1,n-2} + (n - 3)^3 (n - 2)c_{1,n-3} + 4(n + 3)^3 a_{n+3} + (-152n^3 - 1155n^2 - 2940n - 2504) a_{n+2} + (572n^3 + 2307n^2 + 2610n + 475) a_{n+1} - 2 (424n^3 + 159n^2 - 480n - 60) a_n + 2 (286n^3 - 939n^2 + 780n + 25) a_{n-1} + (-152n^3 + 1041n^2 - 2388n + 1832) a_{n-2} + (n - 3)^2(4n - 9)a_{n-3} = 0, \]

where \( a_n = A_n - A_{n-1}, \forall n \geq 1 \),

with initial condition

\[
c_{1,1} = 12, c_{1,2} = 198, c_{1,3} = 4228, c_{1,4} = 100387, c_{1,5} = \frac{12752512}{5}, c_{1,6} = \frac{339439818}{5}. \tag{3.21}
\]

The recursion equation 3.20 together with the initial condition 3.21 determine the sequence \( \{c_{1,n}\}_{n=1}^{\infty} \) uniquely. From formulas 2.10 and 2.1, we find that the solution to the recursion equation 3.20 and 3.21 are given by

\[
c_{1,1} = C_1, \ c_{1,n} = C_n - C_{n-1}, \ n \geq 2. \tag{3.22}
\]

Hence together with the equation

\[
\varpi_0(\varphi) = (1 - \varphi)\varpi_0(\varphi), \tag{3.23}
\]

this proves the first equation of the lemma, while the second one can be proved similarly. \( \square \)

Similarly the sequence \( \{c_{3,n}\}_{n=1}^{\infty} \) is uniquely determined by the recursion equation and initial condition given by the Picard-Fuchs equation \( D\varpi_3(\varphi) = 0 \). The solution \( \varpi_3(\varphi) \) is indeed the “new” thing! First, we have

\[
\varpi_0(\varphi)\varpi_3(\varphi) \neq \varpi_1(\varphi)\varpi_2(\varphi), \tag{3.24}
\]

thus the Picard-Fuchs operator \( D \) cannot be the symmetric cubic of a second order differential operator. Later when we numerically evaluate the monodromy of \( \varpi_i(\varphi) \) around singularities, we will show that it is the monodromy of \( \varpi_3(\varphi) \) that yields \( \zeta(3)/(2\pi i)^3 \).

The four solutions \( \{\varpi_i(\varphi)\}_{i=0}^{3} \) form a basis of the solution space of \( D \). Let us define a vector \( \varpi(\varphi) \) by

\[
\varpi(\varphi) = (\varpi_0(\varphi), \varpi_1(\varphi), \varpi_2(\varphi), \varpi_3(\varphi))^\top. \tag{3.25}
\]

The monodromy matrix of \( \varpi(\varphi) \) at \( \varphi = 0 \) is given by

\[
M_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 1 & 3 & 3 & 1 \end{pmatrix}. \tag{3.26}
\]
which is maximally unipotent. We will call \( \varphi = 0 \) the large complex structure limit of \( \mathcal{D} \), a terminology from the mirror symmetry of Calabi-Yau threefolds \([4, 5, 6]\). From now on, we will intuitively say \( \varphi \) is the parameter for the complex moduli space \( \mathcal{M}_C \) of \( \mathcal{D} \) \([4, 5, 6]\)

\[
\mathcal{M}_C := \mathbb{C} - \{0, 1, (1 + \sqrt{2})^4, (1 + \sqrt{2})^{-4}, \infty\}. \tag{3.27}
\]

4. **The Yukawa couplings and Instanton expansions**

First, let us look at the mirror map of the Picard-Fuchs operator \( \mathcal{D} \). Follow the mirror symmetry of Calabi-Yau threefolds, the mirror map of \( \mathcal{D} \) is defined by the equation

\[
\tau = \frac{\varpi_1(\varphi)}{\varpi_0(\varphi)} = \frac{1}{2\pi i} \left( \log \varphi + \frac{h_1(\varphi)}{\varpi_0(\varphi)} \right) = \frac{1}{2\pi i} \mathcal{A}_1(\varphi). \tag{4.1}
\]

We will intuitively call \( \tau \) the parameter for the complexified Kähler moduli space \([4, 5, 6]\). The exponential of equation 4.1 becomes

\[
q = \varphi \exp \left( \frac{h_1(\varphi)}{\varpi_0(\varphi)} \right), \tag{4.2}
\]

whose inversion gives us the mirror map \( \varphi(q) \), and from Section 2.2, we have

\[
\varphi(q) = T(q). \tag{4.3}
\]

Hence we can assume that the complexified Kähler moduli space of \( \mathcal{D} \) is given by the modular curve with respect to \( \Gamma_1(6) \)

\[
\mathcal{M}_K := X_1(6). \tag{4.4}
\]

In the paper \([2]\), Beukers also studied the properties of the map defined by the modular form \( T(q) \). He showed that

\[
T(= \varphi): \tau_0 = i\infty \mapsto 0, \quad \tau_1 = \frac{i}{\sqrt{6}} \mapsto (1 + \sqrt{2})^{-4}, \quad \tau_2 = \frac{2}{5} + \frac{i}{5\sqrt{6}} \mapsto (1 + \sqrt{2})^4, \quad \tau_3 = \frac{1}{2} \mapsto \infty. \tag{4.5}
\]

From the results in this section, it has the interpretation that the mirror map \( \varphi(q) \) maps the special points \( \{\tau_0, \tau_1, \tau_2, \tau_3\} \) on the complexified Kähler moduli space \( \mathcal{M}_K \) to the boundary (singular) points of the complex moduli space \( \mathcal{M}_C \).

A very interesting question is whether there exists a one-paramater mirror pair of Calabi-Yau threefolds \((M, M^\vee)\) such that the complexified Kähler moduli space of \( M \) is \( \mathcal{M}_K \), while the complex moduli space of its mirror \( M^\vee \) is \( \mathcal{M}_C \). Moreover, we want the Picard-Fuchs operator of a holomorphic threeform \( \Omega_\varphi \), which is defined for a deformation of \( M^\vee \), to be exactly the operator \( \mathcal{D} \)

\[
\mathcal{D} \Omega_\varphi = 0. \tag{4.6}
\]

If such a mirror pair exists, then the Yukawa coupling \( \mathcal{Y} \) is defined by \([4, 5]\)

\[
\mathcal{Y} := \int_{M^\vee} \Omega_\varphi \wedge \frac{d^3}{d\varphi^3} \Omega_\varphi. \tag{4.7}
\]

Even though we do not know whether such a mirror pair exists or not, nevertheless we can still proceed and compute the Yukawa coupling \( \mathcal{Y} \) directly from the Picard-Fuchs operator.
$D \ [4, 5]$. Up to a nonzero constant, it is given by

$$\mathcal{Y} = \frac{1}{\varphi^3} \exp \left(-\frac{1}{2} \int \frac{1}{\varphi} \cdot (\varphi - 1)^3 \varphi (\varphi^2 + 46 \varphi + 81) \frac{d\varphi}{(\varphi - 1)^4 (\varphi^2 - 34 \varphi + 1)} \right) = \frac{(1 - \varphi)^2}{\varphi^3 (\varphi^2 - 34 \varphi + 1)^{5/4}}. \ (4.8)$$

Follow mirror symmetry, the symplectic normalization of the Yukawa coupling $\mathcal{Y}$ is defined by \cite{4, 5}

$$\mathcal{Y}_{\tau\tau\tau} = \frac{1}{\omega_0(\varphi)^2} \cdot \mathcal{Y} \cdot \left(\frac{1}{2\pi i \, d\tau}\right)^3. \ (4.9)$$

Plug the $q$-expansion of the mirror map $\varphi(q) \ 2.24$ into the formula \ref{4.9}, we obtain the instanton expansion of $\mathcal{Y}_{\tau\tau\tau}$

$$\mathcal{Y}_{\tau\tau\tau} = 1 - \frac{7q}{2} - \frac{285q^2}{8} - \frac{3635q^3}{16} - \frac{213405q^4}{128} - \frac{3678681q^5}{256} - \frac{139506681q^6}{1024} - \frac{2803163819q^7}{2048} - \frac{46859436061q^8}{32768} - \frac{10074477480605q^9}{65536} - \frac{442717425568755q^{10}}{262144} + \mathcal{O}(q^{11}). \ (4.10)$$

After a rescaling $q \to 4q$, the coefficients of this expansion become integral

$$\mathcal{Y}_{\tau\tau\tau}^{rs} = 1 - 14q - 570q^2 - 14540q^3 - 426810q^4 - 14714724q^5 - 558026724q^6 - 22425310552q^7 - 937189672122q^8 - 40297909922420q^9 - 1770869702275020q^{10} + \mathcal{O}(q^{11}). \ (4.11)$$

The instanton number $n_k, k \geq 1$ can be defined by the equation

$$\mathcal{Y}_{\tau\tau\tau}^{rs} = 1 + \sum_{k=1}^{\infty} n_k k^3 \frac{q^k}{1 - q^k}. \ (4.12)$$

The first several instanton numbers are given by

$$n_1 = -14, \ n_2 = -\frac{139}{2}, \ n_3 = -538, \ n_4 = -6660, \ n_5 = -\frac{2942942}{25}, \ \cdots \ ; \ (4.13)$$

which are not always integral. Hence the Yukawa coupling $\mathcal{Y}$ seems to be not very interesting.

On the other hand, it turns out that the following rescaled Yukawa coupling

$$\mathcal{Y}^R := \frac{1}{(\varphi^2 - 34 \varphi + 1)^{1/4}} \mathcal{Y} = \frac{(1 - \varphi)^2}{\varphi^3 (\varphi^2 - 34 \varphi + 1)^{3/2}} \ (4.14)$$

is more interesting. Its symplectic normalization is defined by

$$\mathcal{Y}_{\tau\tau\tau}^R = \frac{1}{\omega_0(\varphi)^2} \cdot \mathcal{Y}^R \cdot \left(\frac{1}{2\pi i \, d\tau}\right)^3 = \frac{1}{\varphi (\varphi^2 - 34 \varphi + 1)^{1/2}} \left(\frac{1}{2\pi i \, d\tau}\right). \ (4.15)$$

From formula \ref{2.26}, we obtain

$$\mathcal{A}(\varphi) = \mathcal{Y}_{\tau\tau\tau}^R. \ (4.16)$$

Thus under the mirror map, $\mathcal{Y}_{\tau\tau\tau}^R$ is sent to the modular form $F(q)$. The upshot is that the mirror symmetry of Calabi-Yau threefolds provides a geometric explanation to Beukers’s modular forms and the formula \ref{2.4}.
5. Some numerical results

In this section, we will provide some numerical results, which at least hint the similarities between the properties of $D$ and that of mirror symmetry [6]. Since $\Pi_0(\phi)$ is a solution of the Picard-Fuchs operator $D$, therefore with respect to the basis $\{\varpi_i(\varphi)\}_{i=0}^3$, it admits an expansion of the form

$$\Pi_0(\phi) = \sum_{i=0}^3 \tau_i \varpi_i(\varphi), \ \tau_i \in \mathbb{C}. \quad (5.1)$$

However, the number $\tau_i$ is technically very difficult to compute analytically, and the method developed in the paper [9] does not work since $D$ has more singularities. Using numerical method [8], we obtain

$$\tau_0 = -20\zeta(3) - \frac{1}{4}(2\pi i)^3, \ \tau_1 = 12\zeta(3) + (2\pi i)^3, \ \tau_2 = -12\zeta(3) - \frac{3}{2}(2\pi i)^3, \ \tau_3 = (2\pi i)^3. \quad (5.2)$$

The appearances of $\zeta(3)$ and $(2\pi i)^3$ in $\tau_i$ are exactly what we have expected from the theory of mirror symmetry. For more details, the readers are referred to the paper [6].

We have also numerically computed the monodromy matrices of $\varpi(\varphi)$ at the singularities of $D$ using the numerical method in [8]. The monodromy matrix of $\varpi(\varphi)$ at $(1 + \sqrt{2})^{-4}$ numerically agrees with

$$\left( \begin{array}{cccc} 0 & 0 & -6 & 0 \\ 0 & 1 & 0 & 0 \\ -1/6 & 0 & 0 & 0 \\ -17 \zeta(3)/(2\pi i)^3 & 0 & -102 \zeta(3)/(2\pi i)^3 & 1 \end{array} \right). \quad (5.3)$$

The monodromy matrix of $\varpi(\varphi)$ at $\varphi = 1$ numerically agrees with the identity matrix, while the monodromy matrix of $\varpi(\varphi)$ at $\varphi = (1 + \sqrt{2})^4$ numerically agrees with

$$\left( \begin{array}{cccc} -24 & -120 & -150 & 0 \\ 10 & 49 & 60 & 0 \\ -25/6 & -20 & -24 & 0 \\ 5/2 - 425 \zeta(3)/(2\pi i)^3 & 12 - 2040\zeta(3)/(2\pi i)^3 & 15 - 2550 \zeta(3)/(2\pi i)^3 & 1 \end{array} \right). \quad (5.4)$$

Therefore our numerical results have implied that the entries of the monodormy matrices of $\varpi(\varphi)$ at singularities lie in the ring $\mathbb{Q}[\zeta(3)/(2\pi i)^3]$, which is a well-known property in mirror symmetry [6].

Another thing that is very interesting to notice is that, the number $\zeta(3)/(2\pi i)^3$ only occur in the monodromy of $\varpi_3(\varphi)$. First, from Section 3, we deduce that the periods $\varpi_j(\varphi)$ with $j = 0, 1, 2$ comes from that of a family of K3 surfaces, i.e.

$$\varpi_j(\varphi) = \frac{1}{(2\pi i)^j} \varphi_j(\varphi), \ j = 0, 1, 2. \quad (5.5)$$

Therefore, the monodromy of $\varpi_j(\varphi)$ is determined by that of $\varphi_j(\varphi)$, which of course cannot have $\zeta(3)/(2\pi i)^3$ occur in the entries of its monodromy. In this sense, it is only the solution $\varpi_3(\varphi)$ that is the new to $D$. 
6. Further prospects

We will end this paper with several open questions.

(1) Does there exist a one-parameter family of Calabi-Yau threefolds whose Picard-Fuchs operator is $D$?

(2) If such a one-parameter family of Calabi-Yau threefolds exists, does it have any connections with the family of K3 surfaces found by Beukers and Peters in [3]? Or more specifically, what is the connection between the Picard-Fuchs operators $D$ and $L$?

(3) Could the method in this paper be generalized to study other irrational proofs of interesting numbers like the zeta values?

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