An Integral Representation of Kekulé Numbers, and Double Integrals Related to Smarandache Sequences

John M. Campbell

Toronto, ON

jmaxwellcampbell@gmail.com

Abstract

We present an integral representation of Kekulé numbers for $P_2(n)$ benzenoids. Related integrals of the form $\int_{-\pi}^{\pi} \frac{\cos(nx)}{\sin^2 x + k} dx$ are evaluated. Conjectures relating double integrals of the form $\int_0^m \int_{-\pi}^{\pi} \frac{\cos(2nx)}{k + \sin^2 x} dx\,dk$ to Smarandache sequences are presented.

1 Introduction

It is well-known that some characteristics of Kekulé structures may be enumerated in terms of recursive sequences [4] [6] [7] [8] [15]. A variety of discrete formulas for $K(B)$ (the number of Kekulé structures in a benzenoid system B) are known [4].

The existence of Kekulé structures in benzenoid systems is commonly considered to be an algebraic problem. A well-known discrete identity follows: letting A denote the adjacency matrix of a benzenoid system B with n vertices, $\det A = (-1)^{\frac{n}{2}} K(B)^2$ (so a benzenoid system has Kekulé structures iff the matrix A is non-singular) [5] [8], a result discovered by Dewar and Longuet-Higgins (1952) and rigorously proven in 1980 by Cvetković (et al.) [4].

Inspired by Fourier analysis, we prove an integral equation for Kekulé numbers for pyrenes on a string with hexagons removed from both sides ($K(P_2(n))$), and prove an explicit closed form evaluation of $\int_{-\pi}^{\pi} \frac{\cos(nx)}{\sin^2 x + k} dx$.

We conjecture how the related expressions $\int_0^m \int_{-\pi}^{\pi} \frac{\cos(2nx)}{k + \sin^2 x} dx\,dk$ may be used to represent (quadratic) continued fractions, and conjecture that double integrals of this form correspond to sequences such as the square root of smallest square of the type $k^2(k+1)$ and the number of solutions to $x^2 \equiv 0 \mod n$, establishing unexpected number theoretic implications. Many of the sequences discussed below may be described as Smarandache sequences, such as core(n).

2 Main Problems and Results

Given the tetravalency of carbon, it becomes evident that the number of Kekulé structures of a benzenoid hydrocarbon is equal to the number of linear factors of the benzenoid system. Given the work of Ohkami and Hosoya, the following recurrence formula for the Kekulé

numbers for pyrenes on a string (i.e. a system of linearly annelated pyrenes, pyrenes being a characteristic subunit of all-benzenoid systems) of the form $K(P_2(n))$ holds [4] [15]:

$$K(P_n) = 10K(P_{n-1}) - K(P_{n-2}) \tag{1}$$

Consider the companion recursion sequence of (1) given by $d_n = 10d_{n-1} - d_{n-2}$; $d_0 = 1$, $d_1 = 5$ [17]. Surprisingly, these recursion sequences may be used to evaluate the following integral, letting $c_n = K(P_n)$:

Lemmma 1.

$$\int_{-\pi}^{\pi} \frac{\cos(nx)}{2 + \sin^2 x} dx = \frac{(-1)^n + 1}{2} \pi \left(-c_{\lfloor \frac{n}{2} \rfloor} + d_{\lfloor \frac{n}{2} \rfloor} \sqrt{\frac{2}{3}} \right)$$

Proof. First consider the non-zero values of the above equation; use induction. Let $P(n)$ be the statement "$\int_{-\pi}^{\pi} \frac{\cos(2nx)}{2+\sin^2 x} dx = (-c_n + d_n \sqrt{\frac{2}{3}})\pi$". Suppose $P(n)$ holds. So we want $P(n-2) \wedge P(n-1) \Rightarrow P(n)$. Verify that $P(n)$ holds for all $n < m$ for some $2 < m$.

We have $K(P_n) = 10K(P_{n-1}) - K(P_{n-2})$ (1) and $d_n = 10d_{n-1} - d_{n-2}$; $d_0 = 1$, $d_1 = 5$ [17]. So by the assumption of $P(n)$ we have:

$$\int_{-\pi}^{\pi} \frac{10\cos(2(n-1)x)}{2+\sin^2 x} dx = 10 \left(-c_{n-1} + d_{n-1} \sqrt{\frac{2}{3}} \right) \pi$$

$$\int_{-\pi}^{\pi} \frac{\cos(2(n-2)x)}{2+\sin^2 x} dx = \left(-c_{n-2} + d_{n-2} \sqrt{\frac{2}{3}} \right) \pi$$

So it remains to prove that:

$$\int_{-\pi}^{\pi} \frac{10\cos(2(n-1)x) - \cos(2(n-2)x) - \cos(2nx)}{2+\sin^2 x} dx = 0 \tag{2}$$

It is elementary to evalute the above integral as follows:

$$\int_{-\pi}^{\pi} \frac{10\cos(2(n-1)x) - \cos(2(n-2)x) - \cos(2nx)}{2+\sin^2 x} dx = \frac{4\sin(2n\pi)}{n-1}$$

So (2) holds, letting n be an integer (greater than 1).

For odd values of n for $\int_{-\pi}^{\pi} \frac{\cos(nx)}{2+\sin^2 x} dx$, interpret the integrand as a shifted skew-symmetric function. So it remains to prove that $\frac{\cos(n(x+\frac{\pi}{2}))}{2+\sin^2(x+\frac{\pi}{2})} = -\frac{\cos(n(-x+\frac{\pi}{2}))}{2+\sin^2(-x+\frac{\pi}{2})}$, which is elementary. $\qquad \square$

Theorem 1.

$$K(P_n) = -\frac{\int_{-\pi}^{\pi} \frac{\cos(2nx)}{2+\sin^2 x} dx}{\pi} + (-1)^n \cos(2n \sin^{-1} \sqrt{3}) \sqrt{\frac{2}{3}}$$

Proof. An alternative evaluation of d_n, from Jasinski (2008) [17] , follows:

$$d_n = (-1)^n \cos(2n \sin^{-1} \sqrt{3})$$

So given Lemma 1 , Theorem 1 holds.

$\square$

Lemmma 2. *Let y_n be defined by the following integer sequence: $y_n = (4k+2)y_{n-1} - y_{n-2}$, $y_0 = 0$, $y_1 = 4$ for some fixed k. Let z_n be defined by the following integer sequence: $z_n = (4k+2)z_{n-1} - z_{n-2}$, $z_0 = 1$, $z_1 = 2k+1$ for some fixed k. Then:*

$$\int_{-\pi}^{\pi} \frac{\cos(nx)}{k + \sin^2 x} dx = \frac{(-1)^n + 1}{2} \pi(-y_{\lfloor \frac{n}{2} \rfloor} + z_{\lfloor \frac{n}{2} \rfloor} \sqrt{\frac{2}{T_k}}) \tag{3}$$

Proof. First consider the non-zero values of the above equation; use induction. Let $P(n, k)$ be the statement, for fixed k, $\int_{-\pi}^{\pi} \frac{\cos(2nx)}{k + \sin^2 x} dx = \pi(-y_n + z_n \sqrt{\frac{2}{T_k}})$. We want: $P(n-2, k) \wedge P(n-1, k) \Rightarrow P(n, k)$. So by the assumption of $P(n, k)$ we have:

$$\int_{-\pi}^{\pi} \frac{(4k+2)\cos(2(n-1)x)}{k + \sin^2 x} dx = (4k+2)\pi(-y_{n-1} + z_{n-1} \sqrt{\frac{2}{T_k}})$$

So we must prove that $\int_{-\pi}^{\pi} \frac{(4k+2)\cos(2(n-1)x) - \cos(2(n-2)x) - \cos(2nx)}{k + \sin^2 x} dx = 0$, which is elementary:

$$\int_{-\pi}^{\pi} \frac{(4k+2)\cos(2(n-1)x) - \cos(2(n-2)x) - \cos(2nx)}{k + \sin^2 x} dx = \frac{4\sin(2n\pi)}{n-1}$$

By induction we must also prove that $\forall k \in \mathbb{R}(P(0, k) \wedge P(1, k))$.
It is elementary to establish that:

$$\int_{-\pi}^{\pi} \frac{1}{k + \sin^2 x} dx = \frac{2\sqrt{1 + \frac{1}{k}}\pi}{1 + k}$$

So $P(0, k)$ holds for all k. As for $P(1, k)$, it is elementary to establish that:

$$\int_{-\pi}^{\pi} \frac{\cos(2x)}{k + \sin^2 x} dx = \frac{(-4\sqrt{k}\sqrt{1+k}\pi + (1+2k)(\pi + 2i\ln(-\frac{i}{\sqrt{\frac{k}{1+k}}}) + i\ln(\frac{k}{1+k})))}{\sqrt{k}\sqrt{1+k}}$$

So we must prove:

$$\frac{(-4\sqrt{k}\sqrt{1+k}\pi + (1+2k)(\pi + 2i\ln(-\frac{i}{\sqrt{\frac{k}{1+k}}}) + i\ln(\frac{k}{1+k})))}{\sqrt{k}\sqrt{1+k}} = (-4 + (2k+1)\sqrt{\frac{4}{k(k+1)}})\pi$$

$$\Leftrightarrow -4\sqrt{k}\sqrt{1+k}\pi + (1+2k)(\pi + 2i\ln(-\frac{i}{\sqrt{\frac{k}{1+k}}}) + i\ln(\frac{k}{1+k})) = -4\sqrt{k}\sqrt{k+1}\pi + (4k+2)\pi$$

3

$$\Leftrightarrow (1+2k)(\pi + 2i\ln(-\frac{i}{\sqrt{\frac{k}{1+k}}}) + i\ln(\frac{k}{1+k})) = (4k+2)\pi \Leftrightarrow 2i\ln(-\frac{i}{\sqrt{\frac{k}{1+k}}}) + i\ln(\frac{k}{1+k}) = \pi$$

$$\Leftrightarrow \ln(-\frac{1+k}{k}) + \ln(\frac{k}{1+k}) = -\pi i \Leftrightarrow \ln(-\frac{1+k}{k}) + \ln(\frac{k}{1+k}) = -\pi i \Leftrightarrow \ln(-1) = -\pi i$$

So the proof by induction is complete.

Let $f(x, n, k)$ be an elementary periodic function of the form $f : \mathbb{Z}^+ \times \mathbb{R}^2 \to \mathbb{R}$ given by the expression $\frac{\cos((2n+1)x)}{k+\sin^2 x}$ for fixed integers n and fixed k.

Clearly $f(n, k)$ is symmetric (about the y-axis). Interpret $f(x, n, k)$ as a shifted skew-symmetric function. So we want that $f(x + \frac{\pi}{2}, n, k) = -f(-x + \frac{\pi}{2}, n, k)$. So we want:

$$\frac{\cos((2n+1)(x + \frac{\pi}{2}))}{k + \sin^2 x} = -\frac{\cos((2n+1)(-x + \frac{\pi}{2}))}{k + \sin^2 x}$$

$$\Leftrightarrow \cos((2n+1)x)\cos((2n+1)\frac{\pi}{2}) - \sin((2n+1)x)\sin((2n+1)\frac{\pi}{2}) =$$
$$-(\cos((2n+1)\frac{\pi}{2})\cos((2n+1)x) + \sin((2n+1)\frac{\pi}{2})\sin((2n+1)x))$$

Recall that n is an integer, so $\cos((2n+1)\frac{\pi}{2}) = 0$. So the proof is complete.

$\square$

Reinterpret z_n as a multivariable function given by $z_{n,k} = (4k+2)z_{n-1,k} - z_{n-2,k}$; $z_{0,k} = 1$, $z_{1,k} = 2k+1$. Using OEIS one notices that: $z_{n,1} = \cosh(2n\sinh^{-1} 1)$, $z_{n,2} = \cosh(2n\sinh^{-1}(\sqrt{2}))$, $z_{n,3} = \cosh(2n\sinh^{-1}(\sqrt{3}))$, $z_{n,4} = \cosh(2n\sinh^{-1}(2))$, ... The pattern is clear.

Reinterpret $y_{n,k}$ as a multivariable function given by $y_{n,k} = (4k+2)y_{n-1,k} - y_{n-2,k}$, $y_{0,k} = 0$, $y_{1,k} = 4$. Using OEIS one notices that:

$$y_{n,1} = \frac{1}{\sqrt{2}}((3 + 2\sqrt{2})^n - (3 - 2\sqrt{2})^n)$$

$$y_{n,2} = \frac{1}{\sqrt{6}}((5 + 2\sqrt{6})^n - (5 - 2\sqrt{6})^n)$$

Given the above results one deduces that:

$$y_{n,3} = \frac{1}{\sqrt{12}}((7 + 2\sqrt{12})^n - (7 - 2\sqrt{12})^n)$$

Also one may deduce that:

$$y_{n,4} = \frac{1}{\sqrt{20}}((9 + 2\sqrt{20})^n - (9 - 2\sqrt{20})^n)$$

So we conjecture:

4

Lemmma 3.

$$y_{n,k} = \frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^n - (2k+1-2\sqrt{k(k+1)})^n)$$

$$z_{n,k} = \cosh(2n\sinh^{-1}(\sqrt{k}))$$

Proof. We have $y_{n,k} = (4k+2)y_{n-1,k} - y_{n-2,k}$, $y_{0,k} = 0$, $y_{1,k} = 4$, and $z_{n,k} = (4k+2)z_{n-1,k} - z_{n-2,k}$; $z_{0,k} = 1$, $z_{1,k} = 2k+1$.

Let $P(n,k)$ represent the statement " $y_{n,k} = \frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^n - (2k+1-2\sqrt{k(k+1)})^n)$", for some fixed k. Verify that $P(0,k)$ and $P(1,k)$ hold:

$$y_{0,k} = \frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^0 - (2k+1-2\sqrt{k(k+1)})^0)$$

$$y_{1,k} = \frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^1 - (2k+1-2\sqrt{k(k+1)})^1)$$

So by the assumption of $P(n,k)$ we want $P(n-2,k) \wedge P(n-1,k) \Rightarrow P(n,k)$, and have:

$$(4k+2)y_{n-1,k} = (4k+2)\frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^{n-1} - (2k+1-2\sqrt{k(k+1)})^{n-1})$$

$$y_{n-2,k} = \frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^{n-2} - (2k+1-2\sqrt{k(k+1)})^{n-2})$$

So it remains to prove that:

$$\frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^n - (2k+1-2\sqrt{k(k+1)})^n) =$$

$$(4k+2)\frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^{n-1} - (2k+1-2\sqrt{k(k+1)})^{n-1})$$

$$-\frac{1}{\sqrt{k(k+1)}}((2k+1+2\sqrt{k(k+1)})^{n-2} - (2k+1-2\sqrt{k(k+1)})^{n-2})$$

$$\Leftrightarrow (2k+1+2\sqrt{k(k+1)})^n - (2k+1-2\sqrt{k(k+1)})^n =$$

$$(4k+2)((2k+1+2\sqrt{k(k+1)})^{n-1} - (2k+1-2\sqrt{k(k+1)})^{n-1})$$

$$-((2k+1+2\sqrt{k(k+1)})^{n-2} - (2k+1-2\sqrt{k(k+1)})^{n-2})$$

Simplify the right-hand side expression and the above equation holds.

As for $z_{n,k}$, we have: $z_{n,k} = (4k+2)z_{n-1,k} - z_{n-2,k}$; $z_{0,k} = 1$, $z_{1,k} = 2k+1$, and we want $z_{0,k} = 1$ and $z_{1,k} = 2k+1$:

$$z_{0,k} = \cosh(2 \times 0 \sinh^{-1}(\sqrt{k}))$$

$$z_{1,k} = \cosh(2\sinh^{-1}(\sqrt{k}))$$

Expand and simplify, and the above holds.

$$(4k+2)z_{n-1,k} = (4k+2)\cosh(2(n-1)\sinh^{-1}(\sqrt{k}))$$

$$z_{n-2,k} = \cosh(2(n-2)\sinh^{-1}(\sqrt{k}))$$

So it remains to prove that:

$$\cosh(2n\sinh^{-1}(\sqrt{k})) = (4k+2)\cosh(2(n-1)\sinh^{-1}(\sqrt{k})) - \cosh(2(n-2)\sinh^{-1}(\sqrt{k})) =$$
$$(4k+2)\cosh(2n\sinh^{-1}(\sqrt{k}) - 2\sinh^{-1}(\sqrt{k})) - \cosh(2n\sinh^{-1}(\sqrt{k}) - 4\sinh^{-1}(\sqrt{k}))$$

Expand and simplify, and the proof holds.

$\square$

Theorem 2.

$$\int_{-\pi}^{\pi} \frac{\cos(nx)}{k+\sin^2 x}dx =$$
$$\frac{(-1)^n+1}{2}\pi\left(-\frac{(2k+1+2\sqrt{k(k+1)})^{\lfloor \frac{n}{2}\rfloor} - (2k+1-2\sqrt{k(k+1)})^{\lfloor \frac{n}{2}\rfloor}}{\sqrt{k(k+1)}}\right.$$
$$\left. + \cosh(2\lfloor\frac{n}{2}\rfloor\sinh^{-1}(\sqrt{k}))\frac{2}{\sqrt{k(k+1)}}\right)$$

Proof. The above theorem follows from Lemma 2 and Lemma 3.

$\square$

Note that k is not restricted to integers. Integrating the above with respect to k yields strange results, often related to Smarandache sequences.

Consider the following function for even integers n:

$$f(n) = \frac{1}{48}(-5+i^n)(2+i^n)n\int_0^1\int_{-\pi}^{\pi}\frac{\cos(nx)}{t+\sin^2 x}dxdt$$

Consider:

$$f(10) = -41(-41+29\sqrt{2})\pi$$

$$f(12) = -140(-140 + 99\sqrt{2})\pi$$

$$f(14) = -239(-239 + 169\sqrt{2})\pi$$

$$f(16) = -816(-816 + 577\sqrt{2})\pi$$

$$f(18) = -1393(-1393 + 985\sqrt{2})\pi$$

Remarkably the sequence ..., 41, 140, 239, 816, 1393, ... corresponds to the numerators of the lower principal and intermediate convergents to $\sqrt{2}$ [9], and the sequence ..., 29, 99, 169, 577, 985 , ... corresponds to the denominators of the lower principal and intermediate convergents to $\sqrt{2}$ [1].

Conjecture 1. *Let A_n represent the numerator of the nth convergent to $\sqrt{2}$ and let P_n represent the nth Pell number, i.e. the denominator of the nth convergent to $\sqrt{2}$.*
If $\frac{n}{2}$ is even then:

$$\frac{1}{48}(-5 + i^n)(2 + i^n)n \int_0^1 \int_{-\pi}^\pi \frac{\cos(nx)}{t + \sin^2 x} dx dt = 2P_{n/2}(-2P_{n/2} + A_{n/2}\sqrt{2})\pi$$

If $\frac{n}{2}$ is odd then:

$$\frac{1}{48}(-5 + i^n)(2 + i^n)n \int_0^1 \int_{-\pi}^\pi \frac{\cos(nx)}{t + \sin^2 x} dx dt = A_{n/2}(-A_{n/2} + P_{n/2}\sqrt{2})\pi$$

(Note that the double integral $\int_{-1}^1 \int_{-\pi}^\pi \frac{\cos(nx)}{t+\sin^2 x} dx dt$ displays similar behaviour.)
Moreover,

Conjecture 2. *For all integers m, and for all even integers n, the expression*

$$\int_0^m \int_{-\pi}^\pi \frac{\cos(nx)}{t + \sin^2 x} dx dt$$

is equal to a number of the form $a(b + c\sqrt{d_m})\pi$, where d_m is equal to the mth smallest k such that $k^2(k + 1)$ is a square, and a, b, and c are rational.

The aforementioned sequence (2, 6, 3, 5, 30, 42,...) is given in [12]. To illustrate the above phenomenon, let $n = 4$, and evaluate the above double integral for $m = 1, 2, 3, ...$, and note the appearance of the aforementioned integer sequence (2, 6, 3, 5, 30, 42, ...):

$$4(-4 + 3\sqrt{2})\pi$$
$$4(-12 + 5\sqrt{6})\pi$$
$$8(-12 + 7\sqrt{3})\pi$$
$$8(-20 + 9\sqrt{5})\pi$$
$$4(-60 + 11\sqrt{30})\pi$$
$$4(-84 + 13\sqrt{42})\pi$$
$$8(-56 + 15\sqrt{14})\pi$$

Another example of the above double-integral-quadratic-convergent phenomenon:

Conjecture 3. *Let C_n represent the numerator of the nth convergent to $\sqrt{3}$ and let D_n represent the denominator of the nth convergent to $\sqrt{3}$. If $n \equiv 2 \mod 4$, then:*

$$\frac{1}{4}n \int_0^{\frac{1}{2}} \int_{-\pi}^{\pi} \frac{\cos(nx)}{t + \sin^2 x} dx dt = C_{\frac{n}{2}}(-C_{\frac{n}{2}} + D_{\frac{n}{2}}\sqrt{3})\pi$$

(A similar phenomenon holds for $n \equiv 0 \mod 4$.)

One may easily conclude that the above phenomenon does not hold for all rational m; consider:

Conjecture 4. *For all even positive n,*

$$n \int_0^{\frac{1}{3}} \int_{-\pi}^{\pi} \frac{\cos(nx)}{t + \sin^2 x} dx dt = \frac{4 \times 3^{\frac{n}{2}} - 4}{3^{\frac{n}{2}}}\pi$$

Further conjectures related to number theory follow:

Conjecture 5. *Consider the sequence of numbers given by:*

$$\int_0^m \int_{-\pi}^{\pi} \frac{\cos(2x)}{t + \sin^2 x} dx dt$$

Factoring the maximum integer from these expressions, the resulting coefficient of the square root is given by the sequence of the number of solutions to $x^2 \equiv 0 \mod n$.

This sequence (1, 1, 2, 1, 1, 1, 2, 3, 1, 1, 2, 1, 1, 1, 4, 1, ...) is given by [18]. Note the appearance of this sequence (and of [12]), evaluating the above double integral for $m = 1, 2, 3, ...$:

$4(-1+\sqrt{2})\pi$, $4(-2+\sqrt{6})\pi$, $4(-3+2\sqrt{3})\pi$, $8(-2+\sqrt{5})\pi$, $4(-5+\sqrt{30})\pi$, $4(-6+\sqrt{42})\pi$, $4(-7+2\sqrt{14})\pi$, $8(-4+3\sqrt{2})\pi$, $12(-3+\sqrt{10})\pi$, $4(-10+\sqrt{110})\pi$, $4(-11+2\sqrt{33})\pi$, $8(-6+\sqrt{39})\pi$, $4(-13+\sqrt{182})\pi$, $4(-14+\sqrt{210})\pi$, $4(-15+4\sqrt{15})\pi$, $16(-4+\sqrt{17})\pi$, ...

Factoring the maximum integer from these expressions, note the sequence of (the absolute value of the) initial negative coefficients (1, 2, 3, 2, 5, 6, 7, 4, 3, 10, 11, 6, 13, 14, 15, 4, ...), which corresponds to the Smarandache sequence [10]. We conjecture that:

Conjecture 6. *Consider the sequence of numbers given by:*

$$\int_0^m \int_{-\pi}^{\pi} \frac{\cos(2x)}{t + \sin^2 x} dx dt$$

Factoring the maximum integer from these expressions, the (absolute value of the) resulting negative coefficient is given by the sequence given by the smallest number whose square is divisible by n: (1, 2, 3, 2, 5, 6, 7, 4, 3, 10, 11, 6, 13, 14, 15, 4, 17, 6, ...).

Conjecture 7. *Consider the sequence of numbers given by, for $m = 1, 2, 3, ...$:*

$$\int_0^{\frac{m+1}{m}} \int_{-\pi}^{\pi} \frac{\cos(2x)}{t + \sin^2 x} dx dt$$

Factoring the maximum integer from these numbers, the (absolutel value of the) resulting negative coefficient is given by the smallest number whose square is divisible by n.

Again the Smarandache sequence [10] arises.
Consider the sequence of numbers given by, for $m = 1, 2, 3, ...$:

$$\int_0^{\frac{m+1}{m}} \int_{-\pi}^{\pi} \frac{1}{t + \sin^2 x} dx dt$$

Unexpected patterns arise in the evaluation of the above double integral. Let:

$$\int_0^{\frac{m+1}{m}} \int_{-\pi}^{\pi} \frac{1}{t + \sin^2 x} dx dt = -\pi(\ln(a_m^2) - 2\ln(b_m + c_m \sqrt{d_m}))$$

Using Sloane's online sequence recognition tool, we conjecture that:

Conjecture 8. b_m *corresponds to* **A165367**, *the trisection* $a(n) =$ **A026741** $(3 * n + 2)$, *where* **A026741** *is n if n odd, $n/2$ if n even.* a_m^2 *corresponds to* **A168077**, *which is* $a(2n) =$**A129194**$(2n)/2$; $a(2n+1) =$ **A129194**$(2n+1)$, *where* **A129194** *is* $n^2(\frac{3}{4} - (-1)^{\frac{n}{4}})$.

We presently leave as open problems the evaluation of c_m and d_m (defined above).
Let:

$$\int_0^{\frac{m+1}{m}} \int_{-\pi}^{\pi} \frac{\cos(4x)}{t + \sin^2 x} dx dt = \pi a_m(-b_m + c_m \sqrt{d_m})$$

Using Sloane's online sequence recognition tool, we conjecture that:

Conjecture 9. c_m *corresponds to* **A165367**, *the trisection* $a(n) =$ **A026741** $(3 * n + 2)$, *where* **A026741** *is n if n odd, $n/2$ if n even.*

Let:

$$\int_0^{m \times \sqrt{2}} \int_{-\pi}^{\pi} \frac{1}{t + \sin^2 x} dx dt = 2\pi \ln(1 + 2m\sqrt{2} + a_m \sqrt{b_m(2m + \sqrt{2})})$$

Using Sloane's online sequence recognition tool, we conjecture that:

Conjecture 10. b_m *corresponds to the Smarandache sequence* **A007913**, *which is the squarefree part of* $n : a(n) = $ *smallest positive number m such that n/m is a square.*

Note that the Smarandache sequence corresponding to b_m is also referred to as core(m) [11]. We thus have related Fourier-type integrals to squarefree numbers (through [11]), given that the above double integrals may be represented as follows, by Fubini's theorem:

9

$$\int_0^m \left(\int_{-\pi}^{\pi} \frac{\cos(nx)}{t + \sin^2 x} dx\right) dt$$

$$= \int_{-\pi}^{\pi} \cos(nx)(-\ln(\sin^2 x) + \ln(m + \sin^2 x))dx$$

Conjecture 10 may easily be extended to all non-perfect-square integers, with the Smarandache sequence **A007913** [11] again arising.

We presently leave the above conjectures as open problems. A closed form evaluation of $\int_q^m \int_{-\pi}^{\pi} \frac{\cos(nx)}{t+\sin^2 x} dx dt$ would be ideal, especially considering the multifarious connections to number theory.

3 Other Results from Fourier Analysis

Consider elementary 2π-periodic functions of the form $f : \mathbb{Q}^2 \times \mathbb{R} \to \mathbb{C}$ given by $f(x) = \ln(\sin(ax)+\cos(bx))$, where a and b are rational. Letting $a = 1$ and $b = 1$ the evaluation of the sine and cosine Fourier coefficients of $f(x)$ results in expressions involving $_2F_1(1, -\frac{n}{2}, 1-\frac{n}{2}, i)$, which is not defined for positive even integers n. We evaluate the aforementioned coefficients as follows:

Proposition 1.

$$\forall n \in \mathbb{Z}^+ \left(\int_{-\pi}^{\pi} \cos(nx)\ln(\sin x + \cos x)dx = \right.$$

$$\left. (-1)^{\lfloor \frac{n+3}{4}\rfloor} \frac{(-1)^{n+1}+1}{\sqrt{2}} \frac{1}{2\lfloor \frac{n}{2}\rfloor + 1} i\pi + \lfloor \frac{(n+3) \bmod 4}{3}\rfloor (-1)^{\lfloor \frac{n}{4}\rfloor} \frac{2\pi}{n}\right)$$

Proposition 2.

$$\forall n \in \mathbb{Z}^+ \left(\int_{-\pi}^{\pi} \sin(nx)\ln(\sin x + \cos x)dx = \frac{(-1)^{\lfloor \frac{n+5}{4}\rfloor}((-1)^{n+3}+1)\pi i}{\sqrt{2}n} - \frac{\lfloor \frac{(n+5) \bmod 4}{3}\rfloor (-1)^{\lfloor \frac{n+2}{4}\rfloor}\pi}{2\lfloor \frac{n}{4}\rfloor + 1}\right)$$

Note that the former series may be expressed using the Kronecker symbol and related modular forms [19], and that $\lfloor \frac{(n+3) \bmod 4}{3}\rfloor (-1)^{\lfloor \frac{n}{4}\rfloor}$ corresponds to the inverse of the 8th cyclotomic polynomial [13].

Given Proposition 1 and Proposition 2, determine the Fourier series for $\ln(\sin x + \cos x)$:

$$\ln(\sin x + \cos x) = \frac{i(\pi + i\ln 2)}{2}$$

$$+ \sum_{n=1}^{\infty} \cos(nx)\left((-1)^{\lfloor \frac{n+3}{4}\rfloor} \frac{(-1)^{n+1}+1}{\sqrt{2}} \frac{1}{2\lfloor \frac{n}{2}\rfloor + 1} i + \lfloor \frac{(n+3) \bmod 4}{3}\rfloor (-1)^{\lfloor \frac{n}{4}\rfloor} \frac{2}{n}\right)$$

$$+ \sin(nx)\left(\frac{(-1)^{\lfloor \frac{n+5}{4}\rfloor}((-1)^{n+3}+1)i}{\sqrt{2}n} - \frac{\lfloor \frac{(n+5) \bmod 4}{3}\rfloor (-1)^{\lfloor \frac{n+2}{4}\rfloor}}{2\lfloor \frac{n}{4}\rfloor + 1}\right))$$

Letting $x = \pi$, use the above technique to prove:

$$-\frac{\pi}{\sqrt{2}} = \sum_{n=1}^{\infty} \frac{(-1)^{\lfloor \frac{n+3}{4} \rfloor}((-1)^{n+1} + 1)}{2\lfloor \frac{n}{2} \rfloor + 1}$$

$$-\frac{\ln 2}{4} = \sum_{n=1}^{\infty} \frac{\lfloor \frac{(n+3) \bmod 4}{3} \rfloor (-1)^{\lfloor \frac{n}{4} \rfloor}}{n}$$

To conclude, in addition to presenting the above two series, we have rigorously proven the new evaluation of $\int_{-\pi}^{\pi} \frac{\cos(nx)}{k + \sin^2 x} dx$, and have presented unusual connections between Fourier-type double integrals and Smarandache number theory.

4   Appendix

Mathematica function for Theorem 2:

```
  Theorem2 =
Simplify[FunctionExpand[(-(((2#1 + 1 + 2 Sqrt[#1 (#1 + 1)])^
Floor[#2/2] - (2 #1 + 1 - 2 Sqrt[#1 (#1 + 1)])^
Floor[#2/2])/Sqrt[#1 (#1 + 1)]) + (Cosh[
2 Floor[#2/2] ArcSinh[Sqrt[#1]]]*(2/Sqrt[#1 (#1 + 1)]))))*
Pi*((((-1)^#2) + 1)/(2))]] &
```

Integration results for Conjecture 8:

$$-\pi(\ln(4) - 2\ln(7 + 3\sqrt{5})),$$
$$-\pi(\ln(25) - 2\ln(17 + 2\sqrt{66})),$$
$$-\pi(\ln(9) - 2\ln(10 + \sqrt{91})),$$
$$-\pi(\ln(49) - 2\ln(23 + 4\sqrt{30})),$$
$$-\pi(\ln(16) - 2\ln(13 + 3\sqrt{17})),$$
$$-\pi(\ln(81) - 2\ln(29 + 2\sqrt{190})),$$
$$-\pi(\ln(25) - 2\ln(16 + \sqrt{231})),$$
$$-\pi(\ln(121) - 2\ln(35 + 4\sqrt{69})),$$
$$-\pi(\ln(36) - 2\ln(19 + 5\sqrt{13})),$$
$$-\pi(\ln(169) - 2\ln(41 + 6\sqrt{42})),$$
$$-\pi(\ln(49) - 2\ln(22 + \sqrt{435})),$$
$$-\pi(\ln(225) - 2\ln(47 + 8\sqrt{31})),$$
$$-\pi(\ln(64) - 2\ln(25 + \sqrt{561})),$$
$$-\pi(\ln(289) - 2\ln(53 + 6\sqrt{70})),$$
$$-\pi(\ln(81) - 2\ln(28 + \sqrt{703})),$$
$$-\pi(\ln(361) - 2\ln(59 + 4\sqrt{195})),$$
$$-\pi(\ln(100) - 2\ln(31 + \sqrt{861})), \ldots$$

As indicated above, the sequence 4, 25, 9, 49, 16, 81, 25, 121, 36, 169, 49, 225, 64, 289, 81, 361, 100, ... corresponds to **A168077** [2], and the sequence 7, 17, 10, 23, 13, 29, 16, 35, 19, 41, 22, 47, 25, 53, 28, 59, 31, ... corresponds to **A165367** [3].

Integration results for Conjecture 9:

$$4(-12 + 5\sqrt{6})\pi,$$
$$2(-15 + 4\sqrt{15})\pi,$$
$$\tfrac{8}{9}(-28 + 11\sqrt{7})\pi,$$
$$\tfrac{3}{2}(-15 + 7\sqrt{5})\pi,$$
$$\tfrac{4}{25}(-132 + 17\sqrt{66})\pi,$$
$$\tfrac{2}{9}(-91 + 10\sqrt{91})\pi,$$
$$\tfrac{8}{49}(-120 + 23\sqrt{30})\pi,$$
$$\tfrac{3}{8}(-51 + 13\sqrt{17})\pi,$$
$$\tfrac{4}{81}(-380 + 29\sqrt{190})\pi,$$
$$\tfrac{2}{25}(-231 + 16\sqrt{231})\pi,$$
$$\tfrac{8}{121}(-276 + 35\sqrt{69})\pi,$$
$$\tfrac{5}{18}(-65 + 19\sqrt{13})\pi,$$
$$\tfrac{12}{169}(-252 + 41\sqrt{42})\pi,$$
$$\tfrac{2}{49}(-435 + 22\sqrt{435})\pi,$$
$$\tfrac{16}{225}(-248 + 47\sqrt{31})\pi,$$
$$\tfrac{1}{32}(-561 + 25\sqrt{561})\pi,$$
$$\tfrac{12}{289}(-420 + 53\sqrt{70})\pi,$$
$$\tfrac{2}{81}(-703 + 28\sqrt{703})\pi,$$
$$\tfrac{8}{361}(-780 + 59\sqrt{195})\pi,$$
$$\tfrac{1}{50}(-861 + 31\sqrt{861})\pi, ...$$

As indicated above the sequence 5, 4, 11, 7, 17, 10, 23, 13, 29, 16, 35, 19, 41, 22, 47, 25, 53, 28, 59, 31 corresponds to **A165367** [3].

Integration results for Conjecture 10:

$$2\pi \ln(1 + 2\sqrt{2} + 2\sqrt{2 + \sqrt{2}}),$$
$$2\pi \ln(1 + 4\sqrt{2} + 2\sqrt{2(4 + \sqrt{2})}),$$
$$2\pi \ln(1 + 6\sqrt{2} + 2\sqrt{3(6 + \sqrt{2})}),$$
$$2\pi \ln(1 + 8\sqrt{2} + 4\sqrt{8 + \sqrt{2}}),$$
$$2\pi \ln(1 + 10\sqrt{2} + 2\sqrt{5(10 + \sqrt{2})}),$$
$$2\pi \ln(1 + 12\sqrt{2} + 2\sqrt{6(12 + \sqrt{2})}),$$

$$2\pi \ln(1 + 14\sqrt{2} + 2\sqrt{7(14 + \sqrt{2})}),$$
$$2\pi \ln(1 + 16\sqrt{2} + 4\sqrt{2(16 + \sqrt{2})}),$$
$$2\pi \ln[1 + 18\sqrt{2} + 6\sqrt{18 + \sqrt{2}}),$$
$$2\pi \ln[1 + 20\sqrt{2} + 2\sqrt{10(20 + \sqrt{2})}),$$
$$2\pi \ln[1 + 22\sqrt{2} + 2\sqrt{11(22 + \sqrt{2})}),$$
$$2\pi \ln[1 + 24\sqrt{2} + 4\sqrt{3(24 + \sqrt{2})}),$$
$$2\pi \ln[1 + 26\sqrt{2} + 2\sqrt{13(26 + \sqrt{2})}),$$
$$2\pi \ln[1 + 28\sqrt{2} + 2\sqrt{14(28 + \sqrt{2})}),$$
$$2\pi \ln[1 + 30\sqrt{2} + 2\sqrt{15(30 + \sqrt{2})}),$$
$$2\pi \ln[1 + 32\sqrt{2} + 8\sqrt{32 + \sqrt{2}}),$$
$$2\pi \ln[1 + 34\sqrt{2} + 2\sqrt{17(34 + \sqrt{2})}),$$
$$2\pi \ln[1 + 36\sqrt{2} + 6\sqrt{2(36 + \sqrt{2})}),$$
$$2\pi \ln[1 + 38\sqrt{2} + 2\sqrt{19(38 + \sqrt{2})}),$$
$$2\pi \ln[1 + 40\sqrt{2} + 4\sqrt{5(40 + \sqrt{2})}), ...$$

As indicated above, the sequence 1, 2, 3, 1, 5, 6, 7, 2, 1, 10, 11, 3, 13, 14, 15, 1, 17, 2, 19, 5, ... corresponds to the Smarandache sequence **A007913** [11].

References

[1] B. Cloitre. $a(1) = 1$; $a(2n + 1) = 2a(2n) - a(2n - 1)$, $a(2n) = 4a(2n - 1) - a(2n - 2)$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A079496

[2] P. Curtz . $a(2n) = $ A129194$(2n)/2$; $a(2n+1) = $ A129194$(2n+1)$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A168077

[3] P. Curtz. Trisection a(n) = A026741(3*n+2). The Online Encyclopedia of Integer Sequences. http://oeis.org/A165367

[4] S. Cyvin and I. Gutman. Kekulé Structures in Benzenoid Hydrocarbons. Lecture Notes in Chemistry, Edited by G. Berthier, M. Dewar, H. Fischer. Springer-Verlag, 1988. p.14., 25-26, p.280-285.

[5] Z. Fuji, G. Xiaofeng, C. Ropngsi. The Existence of Kekulé Structures in a Benzenoid System. Advances in the Theory of Benzenoid Hydrocarbons. Topics in Current Chemistry. Edited by I. Gutman and S. Cyvin. Springer-Verlag, 1990. p. 183.

[6] I. Gutman and S. Cyvin. Introduction to the Theory of Benzenoid Hydrocarbons. Springer-Verlag. 1989. p.54-56.

[7] H. Hosoya. Sequences of Polyomino and Polyhex Graphs whose Perfect Matching Numbers are Fibonacci or Lucas Numbers: The Golden Family Graphs of a New Category. 2004. http://www.scipress.org

[8] P. John and H. Sachs. Calculating the Numbers of Perfect Matchings and of Spanning Trees, Pauling's Orders, the Characteristic Polynomial, and the Eigenvectors of a Benzenoid System. Advances in the Theory of Benzenoid Hydrocarbons. Topics in Current Chemistry. Edited by I. Gutman and S. Cyvin. Springer-Verlag, 1990. p. 148, 164, 169.

[9] C. Kimberling. Numerators of the lower principal and intermediate convergents to $2^{1/2}$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A143608

[10] R. Muller. Smallest number whose square is divisible by n. The Online Encyclopedia of Integer Sequences. http://oeis.org/A019554

[11] R. Muller. Squarefree part of $n : a(n) =$ smallest positive number m such that n/m is a square. The Online Encyclopedia of Integer Sequences. http://oeis.org/A007913

[12] A. Murthy and M. Srikanth. Smallest k such that $n(n+1) * k$ is a square. The Online Encyclopedia of Integer Sequences. http://oeis.org/A083481

[13] S. Plouffe. Inverse of 8th cyclotomic polynomial. The Online Encyclopedia of Integer Sequences. http://oeis.org/A014017

[14] N. Sloane . $a(0) = 1$, $a(1) = 3$; for $n > 1$, $a(n) = 6a(n-1) - a(n-2)$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A001541

[15] N. Sloane. $a(0) = 0$, $a(1) = 4$, $a(n) = 10 * a(n-1) - a(n-2)$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A122652

[16] N. Sloane. $a(n) = 6a(n-1) - a(n-2)$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A005319

[17] N. Sloane. $a(n) = 10a(n-1) - a(n-2)$; $a(0) = 1$, $a(1) = 5$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A001079

[18] N. Sloane. (1) Number of solutions to $x^2 \equiv 0(\mod n)$. (2) Also square root of largest square dividing n. (3) Also $Max_{d|n} GCD[d, n/d]$. The Online Encyclopedia of Integer Sequences. http://oeis.org/A000188

[19] E. Weisstein. $a(n) = (2/n)$, where (k/n) is the Kronecker symbol. The Online Encyclopedia of Integer Sequences. http://oeis.org/A091337