Matej Bel University

Acta Universitatis Matthiae Belii
series Mathematics
Volume 27

BELIANUM

2019

Acta Universitatis Matthiae Belii, Series Mathematics
ISSN 1338-712X

Editorial office:
Acta Universitatis Matthiae Belii, ser. Mathematics
Department of Mathematics, Faculty of Natural Sciences
Matej Bel University
Tajovského 40
974 01 Banská Bystrica
Slovakia
E-mail: actamath@savbb.sk

Scope of Journal: Acta Universitatis Matthiae Belii, series Mathematics, publishes original research articles and survey papers in all areas of mathematics and theoretical computer science. Occasionally valuable papers dealing with applications of mathematics in other fields can be published.

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Matej Bel University
Faculty of Natural Sciences

Acta Universitatis Matthiae Belii
series Mathematics

Volume 27

BELIANUM
Banská Bystrica, 2019

Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 3–13, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

The Numerical Solutions of linear and Non-Linear Volterra Integral Equations of the Second Kind using Variational Iteration Method

Fawziah M. Al-Saar
Department of Mathematics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004 (M.S.), India
Department of Mathematics, Amran University, Amran, Yemen
ombraah20016@gmail.com

Kirtiwant P. Ghadle
Department of Mathematics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004 (M.S.), India
drkp.ghadle@gmail.com

Abstract

This article provides approximate solutions to some linear and nonlinear Volterra-Integral equations of the second kind by using the Variational Iteration Method (VIM). Conversion Volterra's integral equation to an initial value problem or Volterra integro-differential equation is considered. The convergence of the method is also considered to provide rapidly convergent successive approximations to the exact solution if such a closed form solution exists. A comparison of the approximate solutions of this method with the Adomian decomposition method and an exact solution will be demonstrated through numerical examples to shows that the method is reliable, accurate and readily implemented.

Received 30 June 2019
Accepted in final form 16 December 2019
Communicated with Víctor Jiménez López.

Keywords Volterra integral equations, Lagrange multiplier, variational iteration method.
MSC(2010) 45D05, 65K15.

1 Introduction

Several authors in engineering and physical sciences have studied and used different numerical methods to solve Volterra Integral equations. In recent years, many of these numerical methods gave reliable and accurate solutions. [9] applied the two-step Laplace decomposition method for solving nonlinear Volterra integral equations. [8] used the homotopy analysis method for solving linear integral equations. [11] implemented a new modified of Adomian decomposition method by the Taylor expansion of the components apart from the zeroth of the Adomian series solution for Volterra integral equation of the second kind. [10] employed the Taylor collocation method to approximate solutions and convergence analysis for the Volterra-Fredholm integral equations, and [1] combined Laplace transform with analytical methods for solving Volterra integral equations with a convolution kernel. [6] studied the reliable modified of Laplace Adomian decomposition method to solve nonlinear interval Volterra-Fredholm integral equations. [7] constructed the numerical solution of nonlinear Volterra-Fredholm integral equations by variational iteration method.[12] used modified variational iteration method for the numerical solutions of some non-linear Fredholm integro-differential equations of the second kind. [5] studied recent advances in reliable methods for solving Volterra-Fredholm integral and integro-differential equations. [3] implemented the usage of the homotopy analysis method for solving fractional Volterra-Fredholm integro-differential equation of the second kind. [2] introduced the approximate solutions using the Adomian decomposition method and its modification for solving Fredholm integral equations. [4] employed modified the Adomian decomposition method to solve fuzzy Volterra-Fredholm integral equations. [14] used iterative methods to solve two-dimensional nonlinear Volterra-Fredholm integro-differential equations.

In this article, we consider linear Volterra integral equation of the second kind of the form

$$y(x) = f(x) + \lambda \int_a^{x)} k(x,t)y(t)dt, \tag{1.1}$$

and nonlinear Volterra integral equation of the second kind is represented by the form

$$y(x) = f(x) + \int_a^{x} k(x,t)F(y(t))dt, \tag{1.2}$$

where the kernel $K(x,t)$ and the function $f(x)$ are given real valued functions, λ is a parameter and $F(y(x))$ is a nonlinear function of $y(x)$ and the unknown function $y(x)$ appears inside and outside the integral sign.

The structure of this article is organized as follows: In the second section we present linear and nonlinear Volterra integral equations of the second kind were solved by variational iteration method which uses a few numbers of iterations. Section 3 presents our numerical examples and graphical results will demonstrate the efficiency of the method and will be shown that the method is accurate and readily implemented compared to some exact solutions. Finally, the conclusion will be in Section 4.

2 VIM for solving Volterra integral equations

To use the variational iteration method for solving Volterra integral equations, it is necessary to convert the integral equation to an equivalent initial value problem or to an equivalent integro-differential equation.

To convert Equation (1.1) to equivalent initial value problems [13] we achieved simply by differentiating both sides of Volterra equation with respect to x as many times as we need to get rid of the integral sign and come out with a differential equation. The conversion of Volterra equations requires the use of Leibnitz rule for differentiating the integral at the right hand side. The initial conditions can be obtained by substituting $x = 0$ into $y(x)$ and its derivatives.

2.1 Linear Volterra integral equations:

For the purpose of illustration of the methodology to the variational iteration method, we begin by considering a nonlinear differential equation of the formal form

$$L(y) + N(y) = g(x), \tag{2.1}$$

where L and N are linear and nonlinear operators respectively, $g(x)$ is a known analytical function and y is an unknown function to be determined. He [13] introduced method where a correction function for Equation (2.1) can be written as

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi)(Ly_n(\xi) + N\tilde{y}(\xi) - g(\xi))d\xi, \tag{2.2}$$

Where λ is a general Lagrange's multiplier, noting that in this method λ may be a constant or a function, and $\tilde{y_n}$ is a restricted value that means it behaves like a constant, hence $\delta\tilde{y_n} = 0$, where δ is the variational derivative.

For the complete use of the variational iteration method, we should follow two steps, first, we determine the Lagrange multiplier $\lambda(\xi)$ that will be identified optimally, second, we substitute the result into Equation (2.2) where the restrictions should be omitted.

Taking the variation of Equation (2.2) with respect to the independent variable y we find

$$\frac{\delta y_{n+1}}{\delta y_n} = 1 + \frac{\delta}{\delta y_n}\left(\int_0^x \lambda(\xi)(Ly_n(\xi) + N\tilde{y_n(\xi)} - g(\xi))d\xi\right), \tag{2.3}$$

integration by parts is usually used for the determination of the Lagrange multiplier $\lambda(\xi)$. In other words, we can use

$$\begin{aligned}
\int_0^x \lambda(\xi)y_n'(\xi)d\xi &= \lambda(\xi)y_n(\xi) - \int_0^x \lambda'(\xi)y_n(\xi)d\xi\\
\int_0^x \lambda(\xi)y_n''(\xi)d\xi &= \lambda(\xi)y_n'(\xi) - \lambda'(\xi)y_n(\xi) + \int_0^x \lambda''(\xi)y_n(\xi)d\xi\\
\int_0^x \lambda(\xi)y_n'''(\xi)d\xi &= \lambda(\xi)y_n''(\xi) - \lambda'(\xi)y_n'(\xi) + \lambda''(\xi)y_n(\xi) - \int_0^x \lambda'''(\xi)y_n(\xi)d\xi\\
\int_0^x \lambda(\xi)y_n^{iv}(\xi)d\xi &= \lambda(\xi)y_n'''(\xi) - \lambda'(\xi)y_n''(\xi) + \lambda''(\xi)y_n'(\xi) - \lambda'''(\xi)y_n(\xi) + \int_0^x \lambda^{iv}(\xi)y_n(\xi)d\xi
\end{aligned} \tag{2.4}$$

and so on.

Having determined the Lagrange multiplier $\lambda(\xi)$, the successive approximations y_{n+1}, $n \geq 0$, of the solution $y(x)$ will be readily obtained upon using selective function $y_0(x)$. However, for fast convergence, the function $y(x)$ should be selected by using the initial conditions as follows:

$$\begin{aligned}
&y_0(x) = y(0), \text{ for first order } y_n',\\
&y_0(x) = y(0) + xy_0', \text{ for second order } y_n'',\\
&y_0(x) = y(0) + xy_n' + \frac{1}{2!}x^2y_0'', \text{ for third order } y_n''',
\end{aligned}$$

and so on. Consequently, the solution

$$y(x) = \lim_{n\longrightarrow\infty} y_n(x). \tag{2.5}$$

The determination of the Lagrange multiplier plays a major role in the determination of the solution of the problem. In what follows, we write generally iteration formulae that show ODE, its corresponding Lagrange multiplier,and its correction functional respectively:

$$y^{(n)} + f(y(\xi), y'(\xi), \ldots, y^{(n)}(\xi)) = 0, \lambda = (-1)^n\frac{1}{(n-1)!}(\xi - x)^{n-1}$$

$$y_{n+1} = y_n + (-1)^n\int_0^x \frac{1}{(n-1)!}(\xi - x)^{n-1}[y_n''' + f(y_n, \ldots, y_n^{(n)})]d\xi, \tag{2.6}$$

for $n \geq 1$

2.2 Nonlinear Volterra integral equation:

For solving Equation (1.2) by variational iteration method [15], first we differentiate once from both sides of Equation (1.2), with respect to x:

$$y'(x) = f'(x) + k(x,x)F(y(x)) + \int_0^x \frac{\partial k(x,t)}{\partial x} F(y(t))dt, \tag{2.7}$$

now we apply variational iteration method to Equation (2.7). According to this method correction functional can be written in the following form:

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda \left(y_n'(s) - f'(s) - k(s,s)F(\tilde{y}_n(s)) - \int_0^s \frac{\partial k(s,t)}{\partial s} F(\tilde{y}_n(t)dt) \right) ds, \tag{2.8}$$

to make the above correction functional stationary with respect to y_n, we have:

$$\begin{aligned} \delta y_{n+1}(x) &= \delta y_n(x) + \delta \int_0^x \lambda \left(y_n'(s) - f'(s) - k(s,s)F(\tilde{y}_n(s)) - \int_0^s \frac{\partial k(s,t)}{\partial s} F(\tilde{y}_n(t)dt) \right) \\ &= \delta y_n(x) + \int_0^x \lambda,(s)\delta(y_n'(s))ds = \delta y_n(x) + \lambda(x)\delta y_n(x) + \int_0^x \lambda'(s)\delta y_n(s)ds = 0, \end{aligned} \tag{2.9}$$

from the above relation for any δy_n, we obtain the Euler-Lagrange equation:

$$\lambda'(s) = 0, \tag{2.10}$$

with the following natural boundary condition:

$$\lambda(x) + 1 = 0, \tag{2.11}$$

using equations (2.10) and (2.11), Lagrange multiplier can be identified optimally as follows:

$$\lambda(s) = 1, \tag{2.12}$$

substituting the identified Lagrange multiplier into Equation (2.8) we obtain the following iterative relation:

$$y_{n+1}(x) = y_n(x) + \int_0^x \left(y_n'(s) - f'(s) - k(s,s)F(y_n(s)) - \int_0^s \frac{\partial k(s,t)}{\partial s} F(y_n(t)dt) \right) ds, \tag{2.13}$$

we can obtain the exact solution or an approximate solution to the Equation (1.2) by starting from $y_0(x)$. Also in some Volterra integral equations by differentiating from integral equation, for example when the kernel is independent of x, we obtain a differential equation then we solve it by using variational iteration method.

3 Illustrative examples

In this section we solve three examples of the linear and nonlinear of Volterra integral equations which have solved in [13]. Numerical results show that our proposed method has a high accuracy.

Example 1. Consider the following linear Volterra integral equation with the exact solution $y(x) = e^x$

$$y(x) = 1 + x + \frac{x^2}{2} + \frac{1}{2}\int_0^x (x-t)^2 y(t)dt, \tag{3.1}$$

differentiate both sides of Equation (3.1) with respect to x by using Leibnitz rule gives the integro-differential equation

$$y'(x) = 1 + x + \int_0^x (x-t)y(t)dt, \qquad y(0) = 1, \tag{3.2}$$

applyig the variational iteration method to Equation (3.2) we get the correction functional

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi \left(y_n'(\xi) - 1 - \xi - \int_0^\xi (\xi - s)\tilde{y}_n(s)ds \right) d\xi, \tag{3.3}$$

we find the Lagrange multiplier

$$\lambda = -1, \tag{3.4}$$

substituting this value of the Lagrange multiplier into the functional Equation (3.3) gives the iteration formula

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi \left(y_n'(\xi) - 1 - \xi - \int_0^\xi (\xi - s)y_n(s)ds \right) d\xi, \tag{3.5}$$

using the initial conditions to select $y_0(x) = y(0) = 1$ and use it into Equation 3.5 we get

$$\begin{aligned} y_0(x) &= 1, \\ y_1(x) &= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}, \\ y_2(x) &= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \frac{x^6}{6!}, \\ y_n(x) &= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \frac{x^6}{6!} + \cdots + \frac{x^n}{n!}, \end{aligned} \tag{3.6}$$

which converges to the exact solution $y(x) = e^x$

Figure 1 shows the comparison between the exact solution and the approximate solution

Table 1. Numerical results of Example 1, N = 4.

x	$y_{Exact}(x)$	$y_{Appr.}(x)$	$E_4(y)$
0.1	1.105170918	1.105170918	———
0.2	1.221402758	1.221402758	———
0.3	1.349858808	1.349858808	———
0.4	1.491824698	1.491824698	———
0.5	1.648721271	1.648721270	1×10^{-9}
0.6	1.822118800	1.822118799	1×10^{-9}
0.7	2.013752707	2.013752699	8×10^{-9}
0.8	2.225540928	2.225540897	31×10^{-9}
0.9	2.459603111	2.459603007	104×10^{-9}
1.0	2.718281828	2.718281526	302×10^{-9}

obtained by the VIM. It is seen from Fig.1 the solution obtained by the proposed method nearly identical to the exact solution. In this example, the simplicity and accuracy of the proposed method is illustrated by computing the absolute error $E_4(x)$.

The accuracy of the result can be improved by introducing more terms of the approximate solutions. In Table 1, VIM solutions is compared with the exact solution of the

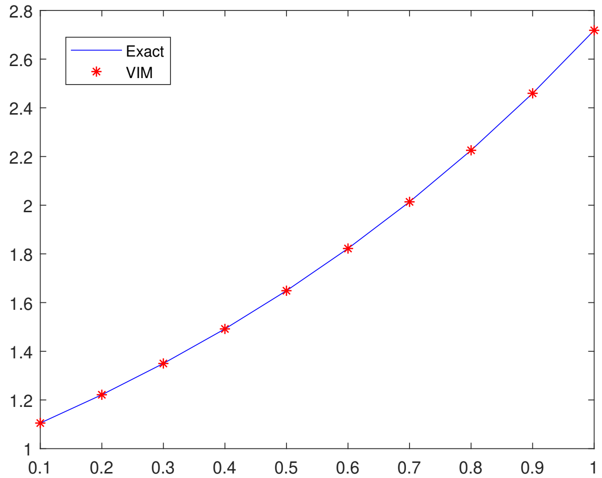

Figure 1. Comparison between exact and approximate solutions for Example 1

Volterra integral Equation (3.1). There is good agreement between exact and approximate solution obtained by proposed method. The table also shows the absolute error between the exact and approximate solutions.

Example 2. Consider the following nonlinear Volterra integral equation with the exact solution $y(x) = tan(x)$

$$y(x) = x + \int_0^x y^2(t)dt, \tag{3.7}$$

differentiate both sides of Equation (3.7) with respect to x by using Leibnitz rule gives the integro-differential equation

$$y'(x) = 1 + \int_0^x y^2(t), \qquad y(0) = x, \tag{3.8}$$

applyig the variational iteration method VIM to Equation (3.7) we get the correction functional

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi \left(y'_n(\xi) - 1 \int_0^\xi \tilde{y}_n^2(s)ds \right) d\xi, \tag{3.9}$$

we find the Lagrange multiplier

$$\lambda = -1, \tag{3.10}$$

substituting this value of the Lagrange multiplier into the functional (3.9) gives the iteration formula

$$y_{n+1}(x) = y_n(x) - \int_0^x \left(y'_n(\xi) - 1 - \int_0^\xi (y_n^2(s)ds \right) d\xi, \tag{3.11}$$

using the initial conditions to select $y_0(x) = y(0) = 1$ and use it into Equation (3.11) we get

$$y_0(x) \quad = \quad x,$$

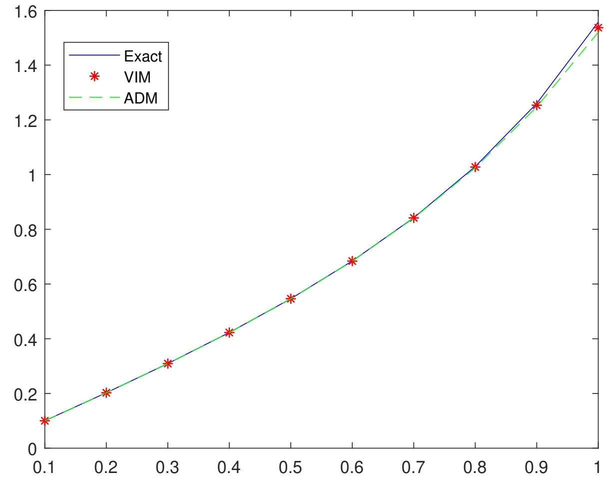

Figure 2. Comparison between exact and approximate solutions for Example 2

$$\begin{aligned} y_1(x) &= x + \frac{x^3}{3}, \\ y_2(x) &= x + \frac{x^3}{3} + \frac{2x^5}{15} + \frac{x^7}{63}, \\ y_3(x) &= x + \frac{x^3}{3} + \frac{2x^5}{15} + \frac{17x^7}{315} + \frac{342x^9}{25515} + \frac{1206x^{11}}{467775} + \frac{4x^{13}}{12285} + \frac{x^{15}}{59535}, \quad (3.12) \end{aligned}$$

which converges to the exact solution $y(x) = tan(x)$

Table 2. Numerical results of Example 2, N = 4.

x	$y_{Exact}(x)$	VIM	ADM	$E_4(y_{VIM})$	$E_4(y_{ADM})$
0.1	0.100334672	0.100334672	0.100334672	—	—
0.2	0.202710035	0.202710031	0.202710024	4×10^{-9}	11×10^{-9}
0.3	0.309336249	0.309336071	0.309335802	178×10^{-9}	447×10^{-9}
0.4	0.422793218	0.422790712	0.422787088	2.506×10^{-6}	6.13×10^{-6}
0.5	0.546302489	0.546282438	0.546254960	20.015×10^{-6}	47.538×10^{-6}
0.6	0.684136808	0.684023632	0.683878765	113.176×10^{-6}	258.043×10^{-6}
0.7	0.842288380	0.841782292	0.841187184	506.088×10^{-6}	1.101196×10^{-3}
0.8	1.029638557	1.027714288	1.025675297	1.924269×10^{-3}	3.96326×10^{-3}
0.9	1.260158218	1.253633063	1.247544849	6.525155×10^{-3}	12.613369×10^{-3}
1.0	1.557407725	1.536959360	1.520634921	20.448365×10^{-3}	36.772804×10^{-3}

Figure 2 shows the comparison between the exact solution and the approximate solutions obtained by the VIM and ADM. It is seen from Figure 2 the solution obtained by the proposed method nearly identical to the exact solution. In this example, the simplicity and accuracy of the proposed method is illustrated by computing the absolute error $E_4(x)$.

The accuracy of the result can be improved by introducing more terms of the approximate solutions. In Table 2, VIM solutions is compared with ADM and the exact solution of the Volterra integral Equation (3.1). There is good agreement between exact and approximate solution obtained by proposed method. The table also shows the absolute error between the exact and approximate solutions. VIM is better than ADM and it has more accuracy.

Example 3. Consider the following linear Volterra integral equation with the exact solution $y(x) = x + cos(x)$

$$y(x) = 1 + x + \frac{x^3}{3!} - \int_0^x (x-t)y(t)dt, \tag{3.13}$$

differentiate both sides of Equation (3.13) with respect to x by using Leibnitz rule gives the integro-differential equation

$$y'(x) = 1 + \frac{x^2}{2} - \int_0^x y(t)dt, \qquad y(0) = 1, \tag{3.14}$$

we obtain the initial value problem by differentiating Equation (3.14) again

$$y''(x) = x - y(x), \qquad y(0) = 1, y'(0) = 1, \tag{3.15}$$

(a) Applyig the variational iteration method to Equation (3.14) we get the correction functional

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi)\left(y_n'(\xi) - 1 - \frac{\xi^2}{2} - \int_0^\xi \tilde{y}_n(s)ds\right)d\xi, \tag{3.16}$$

we find the Lagrange multiplier of the first order

$$\lambda = -1, \tag{3.17}$$

substituting this value of the Lagrange multiplier into the functional Equation (3.15) gives the iteration formula

$$y_{n+1}(x) = y_n(x) - \int_0^x \left(y_n'(\xi) - 1 - \frac{\xi^2}{2} - \int_0^\xi (y_n(s)ds\right)d\xi, \tag{3.18}$$

using the initial conditions to select $y_0(x) = y(0) = 1$ and use it into Equation (3.18) we get

$$\begin{aligned}
y_0(x) &= 1,\\
y_1(x) &= 1 + x - \frac{x^2}{2!} + \frac{x^3}{3!},\\
y_2(x) &= 1 + x - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^5}{5!},\\
y_3(x) &= 1 + x - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^7}{7!},\\
y_n(x) &= x + \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots + \frac{(-1)^n x^{2n}}{(2n)!}\right),
\end{aligned} \tag{3.19}$$

which gives the exact solution $y(x) = x + cos(x)$

(b) Applying the variational iteration method to Equation (3.14) we get the correction functional

$$y_{n+1}(x) = y_n(x) + \int_0^x \lambda(\xi)\,(y_n''(\xi) + \tilde{y}_n(\xi))\,d\xi, \tag{3.20}$$

we find the Lagrange multiplier for second order

$$\lambda = \xi - x, \tag{3.21}$$

substituting this value of the Lagrange multiplier into the functional (3.20) gives the iteration formula

$$y_{n+1}(x) = y_n(x) + \int_0^x (\xi - x)\,(y_n''(\xi) + y_n(\xi) - \xi)\,d\xi, \tag{3.22}$$

using the initial conditions to select $y_0(x) = y(0) + xy_0' = 1 + x$ and use it into Equation (3.22) we get

$$\begin{aligned}
y_0(x) &= 1 + x, \\
y_1(x) &= 1 + x - \frac{x^2}{2!}, \\
y_2(x) &= 1 + x - \frac{x^2}{2!} + \frac{x^4}{4!}, \\
y_3(x) &= 1 + x - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!}, \\
y_n(x) &= x + \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots + \frac{(-1)^n x^{2n}}{(2n)!}\right),
\end{aligned} \tag{3.23}$$

which gives the exact solution $y(x) = x + cos(x)$.

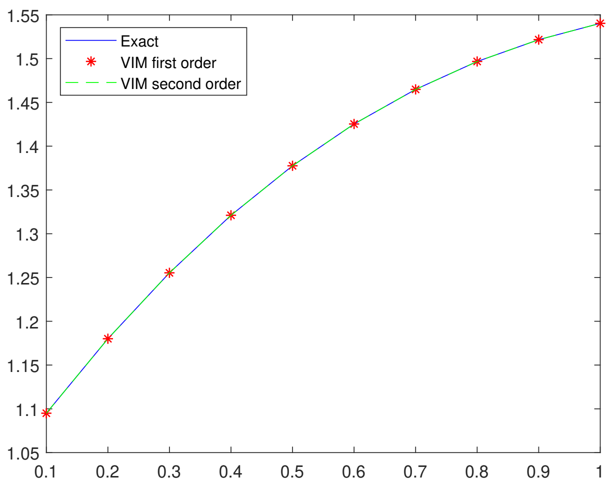

Figure 3. Comparison between exact and approximate solutions for Example 3

Figure 3 shows the comparison between the exact solution and the approximate solution obtained by the VIM of the first order and the second order respectively. It is seen from Figure 3 the solution obtained by the proposed method nearly identical to the exact solution. In this example, the simplicity and accuracy of the proposed method is illustrated by computing the absolute error $E_4(x)$ .The accuracy of the result can be improved by introducing more terms of the approximate solutions. In Table 3, VIM solutions are compared with the exact solution of the Volterra integral Equation (3.13). There is good agreement between the exact and approximate solution obtained by the proposed method. The table also shows the absolute error between the exact and approximate solutions and the approximate solution is obtained from the second order is accuracy more than that is obtained from first order with the same iterations.

Table 3. Numerical results of Example 3, N = 4.

x	$y_{Exact}(x)$	VIM 1^{st}order	VIM 2^{nd} order	$E_4(y)$ 1^{st}order	$E_4(y)$ 2^{nd} order
0.1	1.095004165	1.095004165	1.095004165	———	———
0.2	1.180066578	1.180066580	1.180066578	10×10^{-9}	———
0.3	1.255336489	1.255336531	1.255336488	42×10^{-9}	1×10^{-9}
0.4	1.321060994	1.321061303	1.321060978	309×10^{-9}	16×10^{-9}
0.5	1.377582562	1.377584015	1.377582465	1.453×10^{-6}	97×10^{-9}
0.6	1.425335615	1.425340754	1.425335520	5.139×10^{-6}	415×10^{-9}
0.7	1.464842187	1.464857105	1.464840765	14.918×10^{-6}	1.422×10^{-6}
0.8	1.496706709	1.496744188	1.496702578	37.479×10^{-6}	4.131×10^{-6}
0.9	1.521609968	1.521694288	1.521599388	84.32×10^{-6}	10.58×10^{-6}
1.0	1.540302306	1.540277778	1.540277778	173.884×10^{-6}	24.528×10^{-6}

4 Conclusion

In this article, the variational iteration method has been successfully employed to obtain the approximate and analytical solution of linear and nonlinear Volterra integral equation of the second kind. The results showed that the convergence, powerful and efficient of this technique was in a good agreement with the exact, analytical and approximate solutions for wide classes of problems. The solution is obtained by the our proposed method has high accuracy and also VIM better than Adomian decomposition method. The computations associated with the examples in this work were performed using Maple 17.

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Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 15–30, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

Non-neighbor sum-connectivity index and ABC index

S.B. Chandrakala
Department of Mathematics, Nitte Meenakshi Institute of Technology, Yelahanka, Bengaluru, India. Pin 560 064
chandrakalasb14@gmail.com

G.R. Roshini*
Department of Mathematics, Nitte Meenakshi Institute of Technology, Yelahanka, Bengaluru, India. Pin 560 064
gr.roshini@gmail.com

B. Sooryanarayana
Department of Mathematics, Dr.Ambedkar Institute of Technology, B.D.A. Outer Ring Road, Mallathahalli, Bengaluru, Karnataka State, India. Pin 560 056
dr_bsnrao@dr-ait.org

Michaela Mihoková
Department of Mathematics, Faculty of Natural Sciences, Matej Bel University, Tajovského 40, 974 01 Banská Bystrica, Slovakia
michaela.mihokova@umb.sk

Abstract

Topological indices have a significant importance in the study of physicochemical properties of chemical compounds. Among them, degree based topological indices have played a prominent role to study the chemical properties of nanostructure materials. In this paper, we compute non-neighbor sum-connectivity index (SCI), non-neighbor ABC index, multiplicative non-neighbor SCI and multiplicative non-neighbor ABC index for some standard classes of graphs and for corona products of some graphs. We have also obtained the same for some nano-structures.

Received September 22, 2019
Revised December 12, 2019
Accepted in final form December 22, 2019
Communicated with Miroslav Haviar.

Keywords topological index, non-neighbor vertices, SCI, ABC index, nano-structures.
MSC(2010) 97K30, 05C07.

1 Introduction

We consider a graph G to be a finite, undirected, simple graph having n vertices with m edges. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G, $d_G(u)$ denotes the degree of a vertex u, δ and Δ be the minimum degree and the maximum degree of a graph G respectively, $d(u,v)$ is the distance between the vertices u and v. A vertex $v \in V(G)$ is called a full degree vertex, if $d_G(v) = n-1$. Also, uv represents an edge between the two vertices u and v. For undefined terminologies we refer to [3].

*corresponding author

A topological index is a numeric value mathematically derived from the graph representing a molecule. The mathematical and computational chemistry involving the computation of topological indices is a trending research topic. Topological indices are of two main categories, one depends on vertex distance and the other depends on vertex degree.

Zagreb indices are the oldest among the topological indices, given by Gutman and Trinajstic [2] defined as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} [d_G(u) \times d_G(v)].$$

As the years passed many degree based topological indices were introduced, among which sum-connectivity index (SCI) and atom bond connectivity (ABC) index are two such topological indices. Sum-connectivity index, which was introduced in 2009 [14], is defined as

$$SCI(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^{-1/2}.$$

Atom-bond connectivity (ABC) index, which was introduced in 1998 [1], is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) \times d_G(v)}}.$$

The first multiplicative topological index was introduced in 1984 by Narumi and Katayama [6] and it is defined as

$$NK(G) = \prod_{u \in V(G)} d_G(u).$$

Some of the non-neighbor topological indices are studied in [8]. Also, some work on Randic and multiplicative topological indices can be referred in [9, 10, 11].

Motivated by these works, we define non-neighbor sum-connectivity index, non-neighbor ABC index and multiplicative non-neighbor sum-connectivity index, multiplicative non-neighbor ABC index. We define a set $\overline{N_G(u)}$ of non-neighbors of a vertex u as $\overline{N_G(u)} = \{v \in V(G) : d(u,v) \neq 1\}$ and a non-neighbor degree $\overline{d_G(u)}$ of u as $\overline{d_G(u)} = n - 1 - d_G(u)$, where n is the order of the graph G. Let $\overline{\delta}$ and $\overline{\Delta}$ denotes the minimum non-neighbor degree and the maximum non-neighbor degree of a graph G, respectively. Throughout this paper we use the notation NN for non-neighbor.

Definition 1. Non-neighbor SCI (NN-SCI):

$$\overline{SCI(G)} = \sum_{uv \in E(G)} [\overline{d_G(u)} + \overline{d_G(v)}]^{-1/2}$$

Definition 2. Multiplicative non-neighbor SCI:

$$\Pi\overline{SCI(G)} = \prod_{uv \in E(G)} [\overline{d_G(u)} + \overline{d_G(v)}]^{-1/2}$$

Definition 3. Non-neighbor ABC index (NN-ABC):

$$\overline{ABC(G)} = \sum_{uv \in E(G)} \sqrt{\frac{\overline{d_G(u)} + \overline{d_G(v)} - 2}{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

Definition 4. Multiplicative non-neighbor ABC index:

$$\Pi\overline{ABC(G)} = \prod_{uv \in E(G)} \sqrt{\frac{\overline{d_G(u)} + \overline{d_G(v)} - 2}{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

Boron nanotubes have been considered as excellent nanomaterial because of their remarkable properties such as high chemical stability, high resistance to oxidation at high temperatures and being a stable wide band-gap semiconductor, due to which they can be used for applications at high temperatures or in corrosive environments such as batteries, fuel cells, super capacitors, high speed machines as solid lubricants. The stability, mechanical and electronic properties have been discussed in [7, 13]. In 2009, Y. Liu et al. [12] predicted a new class of boron nanotubes, which are covered by hexagons and triangles. Such a nanotube was called Tri-Hexagonal boron nanotube and its 3D perception is shown in the Figure 1. Some of the degree based topological indices are studied for Tri-Hexagonal boron nanotube in [5].

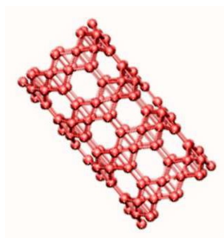

Figure 1. A 3D perception of Tri-Hexagonal boron nanotube.

In this article, NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index are introduced. In Section 2, these new indices are obtained for some classes of graphs. In Section 3, the indices are computed for some corona products of graphs. Finally, in Section 4, the new indices are computed for some nano-structures.

Proposition 5. *For a graph G of order $n \geq 3$ with the diameter $diam(G) \geq 2$,*

(i) $\overline{SCI(G)}$, $\Pi\overline{SCI(G)}$ *exist and* $\overline{SCI(G)}$, $\Pi\overline{SCI(G)} > 0$,

(ii) *if* $\overline{ABC(G)}$, $\Pi\overline{ABC(G)}$ *exist, then there does not exist a full degree vertex in G. Moreover,* $\overline{ABC(G)}$, $\Pi\overline{ABC(G)} \geq 0$.

Proposition 6. *Let G be a connected graph of order $n \geq 3$. Then for each $u \in V(G)$, $\overline{d_G(u)} \geq 0$.*

Proposition 7. *Let G be a connected graph of order n and size m. Then*

$$\sum_{u \in V(G)} \overline{d_G(u)} = n(n-1) - 2m.$$

2 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index for some classes of graphs

Here formulas for NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of a k-regular graph, a cycle, a path, a complete bipartite graph, a star graph and a wheel graph are computed.

Theorem 8. *For a k-regular graph G of order $n \geq 3$ with $2 \leq k \leq n-2$,*

$$\overline{SCI(G)} = \frac{nk}{2\sqrt{2(n-1-k)}} \qquad \text{and} \qquad \overline{ABC(G)} = \frac{nk}{n-1-k}\sqrt{\frac{n-2-k}{2}}.$$

Proof. A k-regular graph of order $n \geq 3$ has $nk/2$ number of edges. In these graphs the NN-degree of each vertex is $n-1-k$. Hence for a k-regular graph G,

$$\overline{SCI(G)} = \frac{nk}{2}\left[\frac{1}{\sqrt{2(n-1-k)}}\right] = \frac{nk}{2\sqrt{2(n-1-k)}}$$

and

$$\overline{ABC(G)} = \frac{nk}{2}\left[\sqrt{\frac{2(n-1-k)-2}{(n-1-k)^2}}\right] = \frac{nk}{n-1-k}\sqrt{\frac{n-2-k}{2}}.$$

□

Corollary 9. *For a k-regular graph G of order $n \geq 3$ with $2 \leq k \leq n-2$,*

$$\Pi\overline{SCI(G)} = [2(n-1-k)]^{-\frac{nk}{4}} \quad \text{and} \quad \Pi\overline{ABC(G)} = \left[\frac{\sqrt{2(n-2-k)}}{n-1-k}\right]^{\frac{nk}{2}}.$$

Corollary 10. *For a cycle C_n $(n \geq 4)$,*

$$\overline{SCI(C_n)} = n[2(n-3)]^{-\frac{1}{2}} \ ; \quad \overline{ABC(C_n)} = \frac{n}{n-3}\sqrt{2(n-4)}$$

and

$$\Pi\overline{SCI(C_n)} = [2(n-3)]^{-\frac{n}{2}} \ ; \quad \Pi\overline{ABC(C_n)} = \left[\frac{\sqrt{2(n-4)}}{n-3}\right]^{n}.$$

Remark 11. The diameter of a complete graph is 1 and hence NN-topological indices are not defined for it.

Theorem 12. *For a path P_n $(n \geq 4)$,*

$$\overline{SCI(P_n)} = \frac{2}{\sqrt{2n-5}} + \sqrt{\frac{n-3}{2}} \quad \text{and} \quad \overline{ABC(P_n)} = 2\sqrt{\frac{2n-7}{(n-2)(n-3)}} + \sqrt{2(n-4)}.$$

Proof. Let $u \in V(P_n)$. Then

$$\overline{d_{P_n}(u)} = \begin{cases} n-2 & \text{if } d_{P_n}(u) = 1 \\ n-3 & \text{if } d_{P_n}(u) = 2 \end{cases} \qquad \text{and} \qquad |E(P_n)| = n-1.$$

By Definition 1 and 3,

$$\overline{SCI(P_n)} = \frac{2}{\sqrt{(n-2)+(n-3)}} + \frac{n-3}{\sqrt{2(n-3)}} = \frac{2}{\sqrt{2n-5}} + \sqrt{\frac{n-3}{2}}$$

and

$$\begin{aligned}\overline{ABC(P_n)} &= 2\sqrt{\frac{(n-2)+(n-3)-2}{(n-2)(n-3)}} + (n-3)\sqrt{\frac{2(n-3)-2}{(n-3)^2}} \\ &= 2\sqrt{\frac{2n-7}{(n-2)(n-3)}} + \sqrt{2(n-4)}.\end{aligned}$$

□

Corollary 13. *For a path P_n $(n \geq 4)$,*

$$\begin{aligned}\Pi\overline{SCI(P_n)} &= \frac{1}{2n-5}[2(n-3)]^{-\frac{n-3}{2}}, \\ \Pi\overline{ABC(P_n)} &= \left[\frac{2n-7}{(n-2)(n-3)}\right]\left[\frac{1}{n-3}\sqrt{2(n-4)}\right]^{n-3}.\end{aligned}$$

Proof.

$$\begin{aligned}\Pi\overline{SCI(P_n)} &= \left[\frac{1}{\sqrt{(n-2)+(n-3)}}\right]^2 \times \left[\frac{1}{\sqrt{2(n-3)}}\right]^{n-3} = \frac{1}{2n-5}[2(n-3)]^{-\frac{n-3}{2}}, \\ \Pi\overline{ABC(P_n)} &= \left[\sqrt{\frac{(n-2)+(n-3)-2}{(n-2)(n-3)}}\right]^2 \times \left[\sqrt{\frac{2(n-3)-2}{(n-3)^2}}\right]^{n-3} \\ &= \frac{2n-7}{(n-2)(n-3)}\left[\frac{1}{n-3}\sqrt{2(n-4)}\right]^{n-3}.\end{aligned}$$

□

Remark 14. $\overline{SCI(P_3)} = 2$, $\Pi\overline{SCI(P_3)} = 1$; indices $\overline{ABC(P_3)}$ and $\Pi\overline{ABC(P_3)}$ do not exist.

Theorem 15. *For a complete bipartite graph $K_{p,q}$,*

(i) $\overline{SCI(K_{p,q})} = \dfrac{pq}{\sqrt{p+q-2}}$, *where $p \geq 1$, $q \geq 2$ (or reverse order),*

(ii) $\overline{ABC(K_{p,q})} = pq\sqrt{\dfrac{p+q-4}{(p-1)(q-1)}}$, *where $p, q \geq 2$.*

Proof. Let V_1 and V_2 be the bi-partitions of $K_{p,q}$ with $|V_1| = p$ and $|V_2| = q$. Then for each $u \in V(K_{p,q})$, we have

$$\overline{d_{K_{p,q}}(u)} = \begin{cases} p-1 & \text{if } u \in V_1 \\ q-1 & \text{if } u \in V_2 \end{cases} \qquad \text{and} \qquad |E(K_{p,q})| = pq.$$

So, by Definition 1 and 3,

$$\overline{SCI(K_{p,q})} = pq\left[\frac{1}{\sqrt{(p-1)+(q-1)}}\right] = \frac{pq}{\sqrt{p+q-2}}$$

and

$$\overline{ABC(K_{p,q})} = pq\sqrt{\frac{(p-1)+(q-1)-2}{(p-1)(q-1)}} = pq\sqrt{\frac{p+q-4}{(p-1)(q-1)}}.$$

□

Corollary 16. *For a complete bipartite graph $K_{p,q}$,*

(i) $\Pi\overline{SCI(K_{p,q})} = [p+q-2]^{-\frac{pq}{2}}$, *where $p \geq 1$, $q \geq 2$ (or reverse order),*

(ii) $\Pi\overline{ABC(K_{p,q})} = \left[\frac{p+q-4}{(p-1)(q-1)}\right]^{\frac{pq}{2}}$, *where $p, q \geq 2$.*

Proof.

$$\Pi\overline{SCI(K_{p,q})} = \left[\frac{1}{\sqrt{(p-1)+(q-1)}}\right]^{pq} = [p+q-2]^{-\frac{pq}{2}}$$

and

$$\Pi\overline{ABC(K_{p,q})} = \left[\sqrt{\frac{p+q-4}{(p-1)(q-1)}}\right]^{pq} = \left[\frac{p+q-4}{(p-1)(q-1)}\right]^{\frac{pq}{2}}.$$

□

Corollary 17. *For a star graph $K_{1,n}$ $(n \geq 2)$,*

$$\overline{SCI(K_{1,n})} = \frac{n}{\sqrt{n-1}} \; ; \quad \overline{ABC(K_{1,n})} \text{ does not exist}$$

and

$$\Pi\overline{SCI(K_{1,n})} = (n-1)^{-\frac{n}{2}} \; ; \quad \Pi\overline{ABC(K_{1,n})} \text{ does not exist.}$$

Theorem 18. *For a wheel graph $W_{1,n}$ $(n \geq 4)$,*

$$\overline{SCI(W_{1,n})} = n\left[\frac{\sqrt{2}+1}{\sqrt{2(n-3)}}\right] \quad \textit{and} \quad \overline{ABC(W_{1,n})} \quad \textit{does not exist.}$$

Proof. For each vertex $u \in V(W_{1,n})$, we have

$$\overline{d_{W_{1,n}}(u)} = \begin{cases} 0 & \text{if } u \text{ is a central vertex} \\ n-3 & \text{otherwise} \end{cases} \qquad \text{and} \qquad |E(W_{1,n})| = 2n.$$

So, by Definition 1 and 3,

$$\overline{SCI(W_{1,n})} = \frac{n}{\sqrt{n-3}} + \frac{n}{\sqrt{2(n-3)}} = n\left[\frac{\sqrt{2}+1}{\sqrt{2(n-3)}}\right].$$

As $W_{1,n}$ has a full degree vertex, $\overline{ABC(W_{1,n})}$ does not exist. □

Corollary 19. *For a wheel graph $W_{1,n}$ $(n \geq 4)$,*

$$\Pi\overline{SCI(W_{1,n})} = [\sqrt{2}(n-3)]^{-n} \quad \textit{and} \quad \Pi\overline{ABC(W_{1,n})} \quad \textit{does not exist.}$$

Proof.

$$\Pi\overline{SCI(W_{1,n})} = \left(\frac{1}{\sqrt{n-3}}\right)^n \left[\frac{1}{\sqrt{2(n-3)}}\right]^n = [\sqrt{2}(n-3)]^{-n}$$

□

3 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of corona products of graphs

In this section, we give formulas for NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of a comb graph, a sunlet graph, a helm graph, a fan graph and a friendship graph.

The corona product $G \odot H$ [4] of two graphs G and H, is the graph obtained by taking one copy of G and $|V(G)|$ copies of H, and by joining each vertex of the i-th copy of H to the i-th vertex of G; where $1 \leq i \leq |V(G)|$.

Theorem 20. *For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,*

$$\begin{aligned}\overline{SCI(G)} &= 2\left[(4n-5)^{-\frac{1}{2}} + (4n-7)^{-\frac{1}{2}}\right] \\ &\quad + (n-2)\left[(4n-6)^{-\frac{1}{2}} + 2^{-1}(n-3)(n-2)^{-\frac{3}{2}}\right], \\ \overline{ABC(G)} &= \sqrt{\frac{2}{2n-3}}\left(\sqrt{\frac{4n-7}{n-1}} + \sqrt{\frac{4n-9}{n-2}}\right) + (n-2)\left[\frac{1}{\sqrt{n-1}} + \frac{n-3}{(n-2)^2}\sqrt{\frac{2n-5}{2}}\right].\end{aligned}$$

Proof. Let $u \in V(G)$. Then

$$\overline{d_G(u)} = \begin{cases} 2n-2 & \text{if } d_G(u) = 1 \\ 2n-3 & \text{if } d_G(u) = 2 \\ 2(n-2) & \text{if } d_G(u) = 3 \end{cases} \qquad \text{and} \qquad |E(G)| = 2n-1.$$

So, by Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= 2[(2n-2)+(2n-3)]^{-\frac{1}{2}} + 2[(2n-3)+(2n-4)]^{-\frac{1}{2}} \\ &\quad + (n-2)[(2n-2)+(2n-4)]^{-\frac{1}{2}} + (n-3)\left[2^2(n-2)\right]^{-\frac{1}{2}} \\ &= 2\left[(4n-5)^{-\frac{1}{2}} + (4n-7)^{-\frac{1}{2}}\right] + (n-2)\left[(4n-6)^{-\frac{1}{2}} + 2^{-1}(n-3)(n-2)^{-\frac{3}{2}}\right]\end{aligned}$$

and

$$\begin{aligned}\overline{ABC(G)} &= 2\sqrt{\frac{(2n-2)+(2n-3)-2}{(2n-2)(2n-3)}} + 2\sqrt{\frac{(2n-4)+(2n-3)-2}{(2n-4)(2n-3)}} \\ &\quad + (n-2)\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}} + (n-3)\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} \\ &= \sqrt{\frac{2}{2n-3}}\left(\sqrt{\frac{4n-7}{n-1}} + \sqrt{\frac{4n-9}{n-2}}\right) + (n-2)\left[\frac{1}{\sqrt{n-1}} + \frac{n-3}{(n-2)^2}\sqrt{\frac{2n-5}{2}}\right].\end{aligned}$$

□

Corollary 21. *For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,*

$$\Pi\overline{SCI(G)} = \left[2^{\frac{3n-8}{2}}(4n-5)(4n-7)(2n-3)^{\frac{n-2}{2}}(n-2)^{\frac{n-3}{2}}\right]^{-1},$$
$$\Pi\overline{ABC(G)} = 2^{-\frac{n+1}{2}}(n-1)^{-\frac{n}{2}}(4n-7)(4n-9)(2n-5)^{\frac{n-3}{2}}(2n-3)^{-2}(n-2)^{-(n-2)}.$$

Proof. For $G = P_n \odot K_1$,

$$\begin{aligned}\Pi\overline{SCI(G)} &= [(2n-2)+(2n-3)]^{-1}[(2n-3)+(2n-4)]^{-1}[(2n-2)\\ &\quad+(2n-4)]^{-\frac{n-2}{2}}\left[2^2(n-2)\right]^{-\frac{n-3}{2}}\\ &= \left[2^{\frac{3n-8}{2}}(4n-5)(4n-7)(2n-3)^{\frac{n-2}{2}}(n-2)^{\frac{n-3}{2}}\right]^{-1}\end{aligned}$$

and

$$\begin{aligned}\Pi\overline{ABC(G)} &= \left[\sqrt{\frac{(2n-2)+(2n-3)-2}{(2n-2)(2n-3)}}\right]^2\left[\sqrt{\frac{(2n-4)+(2n-3)-2}{(2n-4)(2n-3)}}\right]^2\\ &\quad\left[\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}}\right]^{n-2}\left[\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\right]^{n-3}\\ &= 2^{-\frac{n+1}{2}}(n-1)^{-\frac{n}{2}}(4n-7)(4n-9)(2n-5)^{\frac{n-3}{2}}(2n-3)^{-2}(n-2)^{-(n-2)}.\end{aligned}$$

□

Theorem 22. *For a sunlet graph $G = C_n \odot K_1$ $(n \geq 3)$*

$$\overline{SCI(G)} = \frac{n}{2}\left[2^{\frac{1}{2}}(2n-3)^{-\frac{1}{2}} + (n-2)^{-\frac{1}{2}}\right],$$
$$\overline{ABC(G)} = n\left[(n-1)^{-\frac{1}{2}} + 2^{-\frac{1}{2}}(n-2)^{-1}(2n-5)^{\frac{1}{2}}\right].$$

Proof. Let $u \in V(G)$. Then

$$\overline{d_G(u)} = \begin{cases} 2(n-1) & \text{if } d_G(u) = 1 \\ 2(n-2) & \text{if } d_G(u) = 3 \end{cases} \qquad \text{and} \qquad |E(G)| = 2n.$$

By Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= n[(2n-2)+(2n-4)]^{-\frac{1}{2}} + n[2(2n-4)]^{-\frac{1}{2}}\\ &= \frac{n}{2}\left[2^{\frac{1}{2}}(2n-3)^{-\frac{1}{2}} + (n-2)^{-\frac{1}{2}}\right]\end{aligned}$$

and

$$\begin{aligned}\overline{ABC(G)} &= n\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}} + n\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\\ &= n\left[(n-1)^{-\frac{1}{2}} + 2^{-\frac{1}{2}}(n-2)^{-1}(2n-5)^{\frac{1}{2}}\right].\end{aligned}$$

□

Corollary 23. *For a sunlet graph $G = C_n \odot K_1$ $(n \geq 3)$,*

$$\Pi\overline{SCI(G)} = \left[2^3(n-2)(2n-3)\right]^{-\frac{n}{2}} \quad \text{and} \quad \Pi\overline{ABC(G)} = \left[\frac{1}{n-2}\sqrt{\frac{2n-5}{2(n-1)}}\right]^n.$$

Proof.

$$\Pi\overline{SCI(G)} = [(2n-2)+(2n-4)]^{-\frac{n}{2}}[2(2n-4)]^{-\frac{n}{2}} = \left[2^3(n-2)(2n-3)\right]^{-\frac{n}{2}}$$

and

$$\Pi\overline{ABC(G)} = \left[\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}}\right]^n \left[\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\right]^n = \left[\frac{1}{n-2}\sqrt{\frac{2n-5}{2(n-1)}}\right]^n.$$

□

Theorem 24. *For a helm graph $G = W_{1,n} \odot K_1 \setminus v_o v_o^{'}$ $(n \geq 3)$, where v_o is the central vertex of $W_{1,n}$ and $v_o^{'}$ is the one and only vertex of K_1,*

$$\overline{SCI(G)} = n[(4n-5)^{-\frac{1}{2}} + 2^{-1}(n-2)^{-\frac{1}{2}} + (3n-4)^{-\frac{1}{2}}],$$

$$\overline{ABC(G)} = \frac{n}{\sqrt{2}}\left[\sqrt{\frac{4n-7}{(2n-1)(n-2)}} + \frac{\sqrt{2n-5}}{n-2} + \sqrt{\frac{3}{n}}\right].$$

Proof. For any $u \in V(G)$, we have

$$\overline{d_G(u)} = \begin{cases} 2n-1 & \text{if } d_G(u)=1 \\ 2(n-2) & \text{if } d_G(u)=4 \\ n & \text{if } d_G(u)=n \end{cases} \quad \text{and} \quad |E(G)| = 3n.$$

By Definition 1 and 3,

$$\overline{SCI(G)} = n\left\{[(2n-1)+(2n-4)]^{-\frac{1}{2}} + [2(2n-4)]^{-\frac{1}{2}} + [n+(2n-4)]^{-\frac{1}{2}}\right\} = n\left[(4n-5)^{-\frac{1}{2}} + 2^{-1}(n-2)^{-\frac{1}{2}} + (3n-4)^{-\frac{1}{2}}\right]$$

and

$$\overline{ABC(G)} = n\left[\sqrt{\frac{(2n-1)+(2n-4)-2}{(2n-1)(2n-4)}} + \sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} + \sqrt{\frac{n+(2n-4)-2}{n(2n-4)}}\right] = \frac{n}{\sqrt{2}}\left[\sqrt{\frac{4n-7}{(2n-1)(n-2)}} + \frac{\sqrt{2n-5}}{n-2} + \sqrt{\frac{3}{n}}\right].$$

□

Corollary 25. *For a helm graph $G = W_{1,n} \odot K_1 \setminus v_o v_o^{'}$ $(n \geq 3)$, where v_o is the central vertex of $W_{1,n}$ and $v_o^{'}$ is the one and only vertex of K_1,*

$$\Pi\overline{SCI(G)} = 2^{-n}\left[(4n-5)(n-2)(3n-4)\right]^{-\frac{n}{2}},$$

$$\Pi\overline{ABC(G)} = \left[\frac{3(4n-7)(2n-5)}{n(2n-1)(2n-4)^3}\right]^{\frac{n}{2}}.$$

Proof.

$$\Pi\overline{SCI(G)} = \left\{[(2n-1)+(2n-4)]^{-\frac{1}{2}} \times [2(2n-4)]^{-\frac{1}{2}} \times [n+(2n-4)]^{-\frac{1}{2}}\right\}^{n}$$
$$= 2^{-n}\left[(4n-5)(n-2)(3n-4)\right]^{-\frac{n}{2}}$$

and

$$\Pi\overline{ABC(G)} = \left[\sqrt{\frac{(2n-1)+(2n-4)-2}{(2n-1)(2n-4)}} \times \sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} \times \sqrt{\frac{n+(2n-4)-2}{n(2n-4)}}\right]^{n}$$
$$= \left[\frac{3(4n-7)(2n-5)}{n(2n-1)(2n-4)^3}\right]^{\frac{n}{2}}.$$

□

Theorem 26. *For a fan graph $f_n = K_1 \odot P_n$ $(n \geq 4)$,*

$$\overline{SCI(f_n)} = 2\left[(n-2)^{-\frac{1}{2}} + (2n-5)^{-\frac{1}{2}} + 2^{-\frac{3}{2}}(n-3)^{\frac{1}{2}}\right] + (n-2)(n-3)^{-\frac{1}{2}},$$

$\overline{ABC(f_n)}$ *does not exist.*

Proof. For any $u \in V(f_n)$, we have

$$\overline{d_{f_n}(u)} = \begin{cases} n-2 & \text{if } d_{f_n}(u) = 2 \\ n-3 & \text{if } d_{f_n}(u) = 3 \\ 0 & \text{if } d_{f_n}(u) = n \end{cases} \qquad \text{and} \qquad |E(f_n)| = 2n-1.$$

By Definition 1 and 3,

$$\overline{SCI(f_n)} = 2(n-2)^{-\frac{1}{2}} + (n-2)(n-3)^{-\frac{1}{2}} + 2\left[(n-2)+(n-3)\right]^{-\frac{1}{2}}$$
$$+ (n-3)[2(n-3)]^{-\frac{1}{2}}$$
$$= 2\left[(n-2)^{-\frac{1}{2}} + (2n-5)^{-\frac{1}{2}} + 2^{-\frac{3}{2}}(n-3)^{\frac{1}{2}}\right] + (n-2)(n-3)^{-\frac{1}{2}}.$$

As f_n has a full degree vertex, $\overline{ABC(f_n)}$ does not exist. □

Corollary 27. *For a fan graph $f_n = K_1 \odot P_n$ $(n \geq 4)$,*

$$\Pi\overline{SCI(f_n)} = \left[2^{\frac{n-3}{2}}(n-2)(2n-5)(n-3)^{\frac{2n-5}{2}}\right]^{-1} \quad \textit{and} \quad \Pi\overline{ABC(f_n)} \textit{ does not exist.}$$

Proof.

$$\Pi\overline{SCI(f_n)} = (n-2)^{-1}(n-3)^{-\frac{n-2}{2}}[(n-2)+(n-3)]^{-1}[2(n-3)]^{-\frac{n-3}{2}}$$
$$= \left[2^{\frac{n-3}{2}}(n-2)(2n-5)(n-3)^{\frac{2n-5}{2}}\right]^{-1}$$

□

Theorem 28. *For a friendship graph $F_n = K_1 \odot nK_2$ $(n \geq 2)$,*

$$\overline{SCI(F_n)} = 2^{\frac{1}{2}}n(n-1)^{-\frac{1}{2}}\left(1+2^{-\frac{3}{2}}\right) \qquad \textit{and} \qquad \overline{ABC(F_n)} \textit{ does not exist.}$$

Proof. For any $u \in V(F_n)$, we have

$$\overline{d_{F_n}(u)} = \begin{cases} 2n-2 & \text{if } d_{F_n}(u) = 2 \\ 0 & \text{if } d_{F_n}(u) = 2n \end{cases} \qquad \text{and} \qquad |E(F_n)| = 3n.$$

By Definition 1 and 3,

$$\overline{SCI(F_n)} = 2n[2(n-1)]^{-\frac{1}{2}} + n[4(n-1)]^{-\frac{1}{2}} = 2^{\frac{1}{2}} n(n-1)^{-\frac{1}{2}} \left(1 + 2^{-\frac{3}{2}}\right).$$

As F_n has a full degree vertex, $\overline{ABC(F_n)}$ does not exist. □

Corollary 29. *For a friendship graph* $F_n = K_1 \odot nK_2$ $(n \geq 2)$,

$$\Pi\overline{SCI(F_n)} = \left[2^2(n-1)^{\frac{3}{2}}\right]^{-n} \qquad \textit{and} \qquad \Pi\overline{ABC(F_n)} \textit{ does not exist.}$$

Proof. $\Pi\overline{SCI(F_n)} = [2(n-1)]^{-n}[2(2n-2)]^{-\frac{n}{2}} = \left[2^2(n-1)^{\frac{3}{2}}\right]^{-n}$ □

4 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of some nano-structures

In this section, we consider Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, Tri-Hexagonal boron nanotorus $THBC_3C_6[p,q]$ and Tri-Hexagonal boron-α nanotube $THBAC_3C_6[p,q]$. We will compute NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of these nano-structures. To compute certain topological indices of these, we will partition the edge set based on NN degrees of end vertices of each edge of the graph.

4.1 Tri-Hexagonal boron nanotube

In this section, we calculate some topological indices of $C_3C_6(H)[p,q]$, where p denotes the number of hexagons in a column and q denotes the number of hexagons in a row of the 2D graph of $G = C_3C_6(H)[p,q]$ nanotube. It is easy to see that $|V(G)| = 8pq$ and $|E(G)| = q(18p-1)$. The molecular graph of $G = C_3C_6(H)[p,q]$ nanotube is shown in the Figure 2.

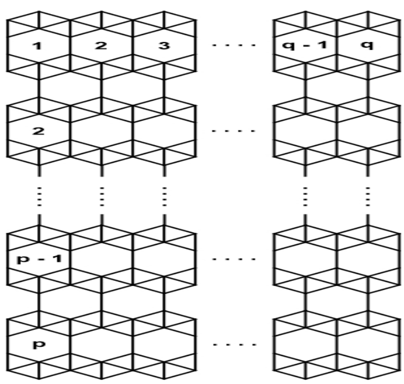

Figure 2. A 2D molecular graph of Tri-Hexagonal boron nanotube - $C_3C_6(H)[p,q]$.

Theorem 30. *For Tri-Hexagonal boron nanotube $G = C_3C_6(H)[p,q]$, where $p, q \geq 1$,*

$$\overline{SCI(G)} = q\left[\frac{6}{\sqrt{16pq-10}} + \frac{(2p-1)}{\sqrt{2(8pq-5)}} + \frac{6(2p-1)}{\sqrt{16pq-11}} + \frac{2p}{\sqrt{4pq-3}}\right],$$

$$\overline{ABC(G)} = \frac{q}{\sqrt{8pq-6}}\left[6\sqrt{\frac{4pq-3}{2pq-1}} + \frac{\sqrt{2}(2p-1)(8pq-6)}{8pq-5}\right.$$
$$\left. + 6(2p-1)\sqrt{\frac{16pq-13}{8pq-5}} + 4p\sqrt{\frac{8pq-7}{4pq-3}}\right].$$

Proof. There are four partitions of the edge set corresponding to their NN degrees of end vertices of G, which are

$$E_1 = E_{(8pq-4,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = 8pq-4 \ and \ \overline{d_G(v)} = 8pq-6\};$$
$$|E_1| = 6q$$
$$E_2 = E_{(8pq-5,8pq-5)} = \{uv \in E(G) | \overline{d_G(u)} = \overline{d_G(v)} = 8pq-5\};$$
$$|E_2| = q(2p-1)$$
$$E_3 = E_{(8pq-5,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = 8pq-5 \ and \ \overline{d_G(v)} = 8pq-6\};$$
$$|E_3| = 6q(2p-1)$$
$$E_4 = E_{(8pq-6,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = \overline{d_G(v)} = 8pq-6\};$$
$$|E_4| = 4pq$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\overline{SCI(G)} = \frac{6q}{\sqrt{(8pq-4)+(8pq-6)}} + \frac{q(2p-1)}{\sqrt{2(8pq-5)}}$$
$$+ \frac{6q(2p-1)}{\sqrt{(8pq-5)+(8pq-6)}} + \frac{4pq}{\sqrt{2(8pq-6)}}$$
$$= q\left[\frac{6}{\sqrt{16pq-10}} + \frac{2p-1}{\sqrt{2(8pq-5)}} + \frac{6(2p-1)}{\sqrt{16pq-11}} + \frac{2p}{\sqrt{4pq-3}}\right],$$

$$\overline{ABC(G)} = 6q\sqrt{\frac{(8pq-4)+(8pq-6)-2}{(8pq-4)(8pq-6)}} + q(2p-1)\sqrt{\frac{2(8pq-5)-2}{(8pq-5)^2}}$$
$$+ 6q(2p-1)\sqrt{\frac{(8pq-5)+(8pq-6)-2}{(8pq-5)(8pq-6)}} + 4pq\sqrt{\frac{2(8pq-6)-2}{(8pq-6)^2}}$$
$$= \frac{q}{\sqrt{8pq-6}}\left[6\sqrt{\frac{4pq-3}{2pq-1}} + \frac{\sqrt{2}(2p-1)(8pq-6)}{8pq-5}\right.$$
$$\left. + 6(2p-1)\sqrt{\frac{16pq-13}{8pq-5}} + 4p\sqrt{\frac{8pq-7}{4pq-3}}\right],$$

which is the required result. □

Corollary 31. *For Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, where $p,q \geq 1$,*

$$\Pi\overline{SCI(G)} = 2^{-\frac{q}{2}(6p-1)}(8pq-5)^{-\frac{q}{2}(2p-1)}(8pq-6)^{-2pq} \times (16pq-10)^{-3q}(16pq-11)^{-3q(2p-1)},$$

$$\Pi\overline{ABC(G)} = 2^{\frac{q}{2}(6p+11)}(4pq-3)^{3q}(8pq-4)^{-3q}(8pq-5)^{-4q(2p-1)}(8pq-6)^{-q(9p+\frac{1}{2})} \times (8pq-7)^{2pq}(16pq-13)^{3q(2p-1)}.$$

4.2 Tri-Hexagonal boron nanotorus

In this section, we calculate some topological indices of $THBC_3C_6[p,q]$, where p denotes the number of hexagons in a column and q denotes the number of hexagons in a row of the 2D graph of $G = THBC_3C_6[p,q]$ nanotorus. It is easy to see that $|V(G)| = 8pq$ and $|E(G)| = 18pq$. The molecular graph of $G = THBC_3C_6[p,q]$ nanotorus is shown in the Figure 3.

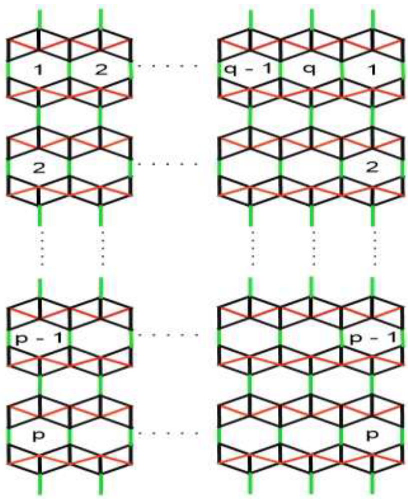

Figure 3. A 2D molecular graph of Tri-Hexagonal boron nanotorus - $THBC_3C_6[p,q]$.

Theorem 32. *For Tri-Hexagonal boron nanotorus $G = THBC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\overline{SCI(G)} = 2pq\left[\frac{1}{\sqrt{2(8pq-5)}} + \frac{6}{\sqrt{16pq-11}} + \frac{1}{\sqrt{4pq-3}}\right],$$

$$\overline{ABC(G)} = 4pq\left[\frac{\sqrt{4pq-3}}{8pq-5} + 3\sqrt{\frac{16pq-13}{(8pq-5)(8pq-6)}} + \frac{\sqrt{2(8pq-7)}}{8pq-6}\right].$$

Proof. There are three partitions of the edge set corresponding to their NN degrees of end vertices of G, which are

$$\begin{aligned} E_1 &= E_{(8pq-5,8pq-5)} = \{uv \in E(G)|\ \overline{d_G(u)} = \overline{d_G(v)} = 8pq-5\};\\ |E_1| &= 2pq\\ E_2 &= E_{(8pq-5,8pq-6)} = \{uv \in E(G)|\ \overline{d_G(u)} = 8pq-5 \ and\ \overline{d_G(v)} = 8pq-6\};\\ |E_2| &= 12pq\\ E_3 &= E_{(8pq-6,8pq-6)} = \{uv \in E(G)|\ \overline{d_G(u)} = \overline{d_G(v)} = 8pq-6\};\\ |E_3| &= 4pq \end{aligned}$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\begin{aligned} \overline{SCI(G)} &= \frac{2pq}{\sqrt{2(8pq-5)}} + \frac{12pq}{\sqrt{(8pq-5)+(8pq-6)}} + \frac{4pq}{\sqrt{2(8pq-6)}}\\ &= 2pq\left[\frac{1}{\sqrt{2(8pq-5)}} + \frac{6}{\sqrt{16pq-11}} + \frac{1}{\sqrt{4pq-3}}\right],\\ \overline{ABC(G)} &= 2pq\sqrt{\frac{2(8pq-5)-2}{(8pq-5)^2}} + 12pq\sqrt{\frac{(8pq-5)+(8pq-6)-2}{(8pq-5)(8pq-6)}}\\ &+ 4pq\sqrt{\frac{2(8pq-6)-2}{(8pq-6)^2}}\\ &= 4pq\left[\frac{\sqrt{4pq-3}}{8pq-5} + 3\sqrt{\frac{16pq-13}{(8pq-5)(8pq-6)}} + \frac{\sqrt{2(8pq-7)}}{8pq-6}\right], \end{aligned}$$

which is the required result. □

Corollary 33. *For Tri-Hexagonal boron nanotorus $THBC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\begin{aligned} \Pi\overline{SCI(G)} &= \left[2^5(8pq-5)(16pq-11)^6(4pq-3)^2\right]^{-pq},\\ \Pi\overline{ABC(G)} &= \left[2^{-6}(4pq-3)^{-9}(8pq-5)^{-8}(8pq-7)^2(16pq-13)^6\right]^{pq}. \end{aligned}$$

4.3 Tri-Hexagonal boron-α nanotorus

In this section, we calculate some topological indices of $THBAC_3C_6[p,q]$, where p denotes the number of rows and q denotes the number of columns of the 2D graph of $G = THBAC_3C_6[p,q]$ nanotorus. It is easy to see that $|V(G)| = 4pq/3$ and $|E(G)| = 7pq/2$. The molecular graph of $G = THBAC_3C_6[p,q]$ nanotorus is shown in the Figure 4.

Theorem 34. *For Tri-Hexagonal boron-α nanotorus $G = THBAC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\begin{aligned} \overline{SCI(G)} &= \frac{pq}{2}\left[\frac{3}{2\sqrt{\frac{2}{3}pq-3}} + \frac{4}{\sqrt{\frac{8}{3}pq-13}}\right],\\ \overline{ABC(G)} &= \frac{pq}{2\sqrt{\frac{4}{3}pq-6}}\left[3\sqrt{\frac{\frac{4}{3}pq-7}{\frac{2}{3}pq-3}} + 4\sqrt{\frac{\frac{8}{3}pq-15}{\frac{4}{3}pq-7}}\right]. \end{aligned}$$

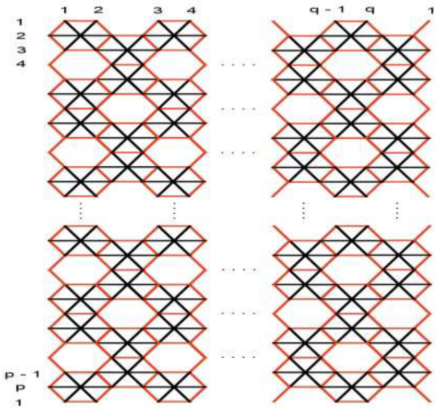

Figure 4. A 2D molecular graph of Tri-Hexagonal boron-α nanotorus - $THBAC_3C_6[p,q]$.

Proof. There are two partitions of the edge set corresponding to their NN degrees of end vertices of G, which are

$$\begin{aligned}
E_1 &= E_{(\frac{4}{3}pq-6,\frac{4}{3}pq-6)} = \left\{uv \in E(G)|\ \overline{d_G(u)} = \overline{d_G(v)} = \frac{4}{3}pq-6\right\};\\
|E_1| &= \frac{3}{2}pq\\
E_2 &= E_{(\frac{4}{3}pq-6,\frac{4}{3}pq-7)} = \left\{uv \in E(G)|\ \overline{d_G(u)} = \frac{4}{3}pq-6 \ and\ \overline{d_G(v)} = \frac{4}{3}pq-7\right\};\\
|E_2| &= 2pq
\end{aligned}$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\begin{aligned}
\overline{SCI(G)} &= \frac{3pq}{2\sqrt{2\left(\frac{4}{3}pq-6\right)}} + \frac{2pq}{\sqrt{\left(\frac{4}{3}pq-6\right)+\left(\frac{4}{3}pq-7\right)}}\\
&= \frac{pq}{2}\left[\frac{3}{2\sqrt{\frac{2}{3}pq-3}} + \frac{4}{\sqrt{\frac{8}{3}pq-13}}\right],\\
\overline{ABC(G)} &= \frac{3}{2}pq\sqrt{\frac{2\left(\frac{4}{3}pq-6\right)-2}{\left(\frac{4}{3}pq-6\right)^2}} + 2pq\sqrt{\frac{\left(\frac{4}{3}pq-6\right)+\left(\frac{4}{3}pq-7\right)-2}{\left(\frac{4}{3}pq-6\right)\left(\frac{4}{3}pq-7\right)}}\\
&= \frac{pq}{2\sqrt{\frac{4}{3}pq-6}}\left[3\sqrt{\frac{\frac{4}{3}pq-7}{\frac{2}{3}pq-3}} + 4\sqrt{\frac{\frac{8}{3}pq-15}{\frac{4}{3}pq-7}}\right],
\end{aligned}$$

which is the required result. □

Corollary 35. *For Tri-Hexagonal boron-α nanotorus $THBAC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\Pi\overline{SCI(G)} = \left[2^{\frac{3}{2}}\left(\frac{2}{3}pq-3\right)^{\frac{3}{4}}\left(\frac{8}{3}pq-13\right)\right]^{-pq},$$

$$\Pi\overline{ABC(G)} = \left[2^{-\frac{7}{4}}\left(\frac{4}{3}pq-7\right)^{-\frac{1}{4}}\left(\frac{2}{3}pq-3\right)^{-\frac{5}{2}}\left(\frac{8}{3}pq-15\right)\right]^{pq}.$$

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Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 31–50, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

On selected developments in the theory of natural dualities

Miroslav Haviar*
Faculty of Natural Sciences, M Bel University,
Tajovského 40, 974 01 Banská Bystrica, Slovakia
miroslav.haviar@umb.sk

Abstract

This is a survey on selected developments in the theory of natural dualities where the author had the opportunity to make with his foreign colleagues several breakthroughs and move the theory forward. It is aimed as author's reflection on his works on the natural dualities in Oxford and Melbourne over the period of twenty years 1993-2012 (before his attention with the colleagues in universal algebra and lattice theory has been fully focused on the theory of canonical extensions and the theory of bilattices). It is also meant as a remainder that the main problems of the theory of natural dualities, *Dualisability Problem* and *Decidability Problem for Dualisability*, remain still open.

Theory of natural dualities is a general theory for quasi-varieties of algebras that generalizes 'classical' dualities such as *Stone duality* for Boolean algebras, *Pontryagin duality* for abelian groups, *Priestley duality* for distributive lattices, and *Hofmann-Mislove-Stralka duality* for semilattices. We present a brief background of the theory and then illustrate its applications on our study of Entailment Problem, Problem of Endodualisability versus Endoprimality and then a famous Full versus Strong Problem with related developments.

Received December 29, 2019
Accepted in final form January 12, 2019
Communicated with Ján Karabáš.

Keywords natural duality, entailment, endodualisability, endoprimality, full and strong dualities.
MSC(2010) Primary 08C20; Secondary 06D50.

1 Introduction

In 1936 M.H. Stone published a seminal work on duality theory, exhibiting a dual equivalence between the category of all Boolean algebras and the category of all Boolean spaces [44]. Almost at the same time L. Pontryagin showed that the category of abelian groups is dually equivalent to the category of compact topological abelian groups [37], [38]. The most important step toward the development of general duality theory was Priestley's duality for distributive lattices: the category of all distributive lattices was shown to be dually equivalent to the category of all compact totally-order disconnected ordered topological spaces (since then called Priestley spaces) [41], [42]. Shortly after that, K.H. Hofmann, M. Mislove and A. Stralka developed a duality for semilattices [34]. The general duality theory, called *Natural duality theory*, grew out from these four dualities, in a monumental work by B.A. Davey and H. Werner [26]. Its rapid development over the next two decades is covered in the survey papers by B. A. Davey [4] and by H. A. Priestley [43], and in the monographs by D. M. Clark and B. A. Davey [2] and by J. G. Pitkethly and B. A. Davey [36]. The author's focus here is on selected developments

*The author gratefully acknowledges support from Slovak grant VEGA 1/0337/16.

in the theory over the period of twenty years 1993-2012 where he had the opportunity and privilege to make, mainly with H. A. Priestley and B. A. Davey in Oxford and Melbourne, certain breakthroughs and move the theory forward.

The theory has proven to be a valuable tool in algebra, algebraic logic, certain parts of computer science, and even in theoretical physics as demonstrated by the author's survey in this journal on free orthomodular lattices [31]. This year's second (and expectedly final) survey is also meant as a remainder that the main problems of the theory, the *Dualisability Problem* and the Decidability Problem for Dualisability, remain still open.

Generally speaking, the theory of natural dualities concerns the topological representation of algebras. The main idea of the theory is that, given a quasi-variety $\boldsymbol{\mathcal{A}} = \mathbb{ISP}(\mathbf{M})$ of algebras generated by an algebra $\mathbf{M}$, one can often find a topological relational structure $\underset{\sim}{M}$ on the underlying set M of $\mathbf{M}$ such that a dual equivalence exists between $\boldsymbol{\mathcal{A}}$ and a suitable category $\boldsymbol{\mathcal{X}}$ of topological relational structures of the same type as $\underset{\sim}{M}$. Requiring the relational structure of $\underset{\sim}{M}$ to be *algebraic over* $\mathbf{M}$, all the requisite category theory "runs smoothly" (we refer to [2]). A uniform way of representing each algebra $\mathbf{A}$ in the quasi-variety $\boldsymbol{\mathcal{A}}$ as an algebra of continuous structure-preserving maps from a suitable structure $\mathbf{X} \in \boldsymbol{\mathcal{X}}$ into $\underset{\sim}{M}$ can be obtained. In particular, the representation is relatively simple and useful for free algebras in $\boldsymbol{\mathcal{A}}$ as was demonstrated also in [31].

The motivation for the natural duality theory goes back to the question "Why in 1614 did the Scottish philosopher and mathematician John Napier, Laird of Merchiston in Scotland, invent the logarithm?" ([6]). To quote from his 1619 book [35]:

"Seeing there is nothing (*right well-beloved Students of the Mathematics*) *that is so troublesome to mathematical practice, nor that doth more molest and hinder calculators, than the multiplications, divisions, square and cubical extractions of great numbers, which besides the tedious expense of time are for the most part subject to many slippery errors, I began therefore to consider in my mind by what certain and ready art I might remove those hindrances. ... I found at length some excellent brief rules ... which together with the hard and tedious multiplications, divisions, and extractions of roots, doth also cast away from the work itself even the very numbers themselves that are to be multiplied, divided and resolved into roots, and putteth other numbers in their place which perform as much as they can do, only by addition and subtraction, division by two or division by three."*

A *natural duality* is a form of logarithm which is applied to algebraic structures rather than to numbers: it takes difficult problems concerning algebras and converts them into simpler yet equivalent problems concerning completely different mathematical structures just as a logarithm converts a difficult multiplication of positive real numbers into a simpler yet equivalent addition of entirely different (and not necessarily positive) real numbers. Given a finite algebra $\mathbf{A}$, a natural duality based on $\mathbf{A}$ is the exact analogue of a logarithm, $\log_a$, to the base a for some positive real number $a \neq 1$ and $\mathbf{A}$ is said to *admit a natural duality* if a natural duality based on $\mathbf{A}$ exists. Just as $\log_a$ does not exist if a is not positive or $a = 1$, a natural duality based on $\mathbf{A}$ need not exist. ([6])

In Section 2 we present a brief background of the theory of natural dualities with its main two open problems, the *Dualisability Problem* and the Decidability Problem for Dualisability. In Sections 3 and 4 we illustrate the application of the theory on the study of entailment and endodualisability developed by the author in a close collaboration with H.A. Priestley and B.A. Davey. In Section 5 we give an overview of later developments of the theory in the author's collaboration with B. Davey's research group, where our focus is mainly on a famous Full versus Strong Problem.

2 The basic scheme of the theory of natural dualities and its main open problems

We now recall the basic scheme of the theory more precisely. Let $\mathbf{M} = (M; F)$ be a finite algebra. Let $\underset{\sim}{M} = (M; G, H, R, \mathcal{T})$ be a discrete topological structure, i.e. a non-empty set M endowed with (finite) families G, H and R of operations, partial operations and relations, respectively, and with a discrete topology $\mathcal{T}$. We recall that the graph of an n-ary (partial) operation $g\colon M^n \to M$ is the $(n+1)$-ary relation

$$\operatorname{graph}(g) = \{\, (x_1, \ldots, x_n, g(x)) \mid (x_1, \ldots, x_n) \in M^n \,\} \subseteq M^{n+1}.$$

We say that the structure $\underset{\sim}{M}$ is *algebraic over* $\mathbf{M}$ if the relations in R and the graphs of the operations and partial operations in $G \cup H$ are subalgebras of appropriate powers of $\mathbf{M}$. Hence a unary (partial) operation is algebraic over $\mathbf{M}$ if and only if it is a (partial) endomorphism of $\mathbf{M}$.

Let $\boldsymbol{\mathcal{A}} = \mathbb{ISP}(\mathbf{M})$ be the quasi-variety generated by a finite algebra $\mathbf{M}$ and assume that $\underset{\sim}{M} = (M; G, H, R, \mathcal{T})$ is algebraic over $\mathbf{M}$. Let $\boldsymbol{\mathfrak{X}} = \mathbb{IS}_c\mathbb{P}^+(\underset{\sim}{M})$ be the 'topological quasi-variety' generated by $\underset{\sim}{M}$, i.e. the class of all structures which are embeddable as closed substructures into powers of $\underset{\sim}{M}$. For any algebra $\mathbf{A} \in \boldsymbol{\mathcal{A}}$, let $D(\mathbf{A})$ denote the set of all $\boldsymbol{\mathcal{A}}$-homomorphisms $\mathbf{A} \to \mathbf{M}$. Since $\underset{\sim}{M}$ is algebraic over $\mathbf{M}$, $D(\mathbf{A})$ can naturally be understood as a substructure of $\underset{\sim}{M}^A$, and so as a member of $\boldsymbol{\mathfrak{X}}$.

Let $X \subseteq M^I$ for some non-empty set I and let $r \subseteq M^n$ be an n-ary relation on M. We say that a map $\varphi\colon X \to M$ preserves the relation r if $[\varphi(\tilde{\mathrm{x}}_1), \ldots, \varphi(\tilde{\mathrm{x}}_n)] \in r$ for all $\tilde{\mathrm{x}}_1 = (x_{1i})_{i \in I}, \ldots, \tilde{\mathrm{x}}_n = (x_{ni})_{i \in I}$ such that $[x_{1i}, \ldots, x_{ni}] \in r$ for every $i \in I$. We say that φ preserves an n-ary (partial) operation if φ preserves its graph as an $(n+1)$-ary relation.

Let $\mathbf{X}$ be a structure in $\boldsymbol{\mathfrak{X}}$. By an $\boldsymbol{\mathfrak{X}}$-morphism $\varphi\colon \mathbf{X} \to \underset{\sim}{M}$ we mean a continuous structure-preserving map, i.e. a continuous map preserving all (partial) operations in $G \cup H$ and all relations in R. Let $E(\mathbf{X})$ be the set of all $\boldsymbol{\mathfrak{X}}$-morphisms $\mathbf{X} \to \underset{\sim}{M}$. Again, since $\underset{\sim}{M}$ is algebraic over $\mathbf{M}$, $E(\mathbf{X})$ can be understood as a subalgebra of $\mathbf{M}^X$, i.e. a member of $\boldsymbol{\mathcal{A}}$.

The (hom-)functors $D\colon \boldsymbol{\mathcal{A}} \to \boldsymbol{\mathfrak{X}}$ and $E\colon \boldsymbol{\mathfrak{X}} \to \boldsymbol{\mathcal{A}}$ are contravariant and dually adjoint. Moreover, for any $\mathbf{A} \in \boldsymbol{\mathcal{A}}$ and for any $\mathbf{X} \in \boldsymbol{\mathfrak{X}}$, we have maps $e_A : \mathbf{A} \to ED(\mathbf{A})$ and $\varepsilon_X : \mathbf{X} \to DE(\mathbf{X})$ given by evaluation, *viz.*

$$\begin{aligned} e_A(a)(h) &= h(a) \quad \text{for every } a \in A \text{ and } h \in D(\mathbf{A}), \\ \varepsilon_X(y)(\varphi) &= \varphi(y) \quad \text{for every } y \in X \text{ and } \varphi \in E(\mathbf{X}), \end{aligned}$$

which are embeddings. We say that $\underset{\sim}{M}$ *yields a pre-duality on* $\boldsymbol{\mathcal{A}}$. In general, such a scheme provides us with a canonical way of constructing, via hom-functors, a dual adjunction between a category of algebras $\boldsymbol{\mathcal{A}} = \mathbb{ISP}(\mathbf{M})$, generated by a finite algebra $\mathbf{M}$, and a category $\boldsymbol{\mathfrak{X}} = \mathbb{IS}_c\mathbb{P}^+(\underset{\sim}{M})$ of structured topological spaces, generated by the alter ego $\underset{\sim}{M}$ of the algebra $\mathbf{M}$.

Let $\underset{\sim}{M} = (M; G, H, R, \mathcal{T})$ be an algebraic structure over $\mathbf{M}$, so that $\underset{\sim}{M}$ yields a pre-duality on $\boldsymbol{\mathcal{A}} = \mathbb{ISP}(\mathbf{M})$. We say that $\underset{\sim}{M}$ *yields a natural duality on* $\boldsymbol{\mathcal{A}}$ if for every $\mathbf{A} \in \boldsymbol{\mathcal{A}}$ the embedding e_A is an isomorphism, i.e. the evaluation maps $e_A(a)$ $(a \in A)$ are the only $\boldsymbol{\mathfrak{X}}$-morphisms from $D(\mathbf{A})$ to $\underset{\sim}{M}$; we notice that they represent then the elements a of $\mathbf{A}$. Sometimes we say that $G \cup H \cup R$ *yields a (natural) duality on* $\boldsymbol{\mathcal{A}}$ or that $\underset{\sim}{M}$ *is dualisable.* We further say that $\underset{\sim}{M}$ (or $G \cup H \cup R$) yields a *full duality* on $\boldsymbol{\mathcal{A}}$ if $\underset{\sim}{M}$ yields a duality on $\boldsymbol{\mathcal{A}}$ and for every $\mathbf{X} \in \boldsymbol{\mathfrak{X}}$ the embedding ε_X is also an isomorphism. In such a case the categories $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathfrak{X}}$ are dually equivalent via categorical anti-isomorphisms D and E which are inverse to each other. Finally, we say that $\underset{\sim}{M}$ (or $G \cup H \cup R$) yields a *strong* *duality* on $\mathcal{A}$ if it yields a full duality on $\mathcal{A}$ and $\underset{\sim}{M}$ is injective in the category $\mathfrak{X}$ (with respect to embeddings). A famous *Full versus Strong Problem*, which dated back to the beginnings of the theory of natural dualities and was open for about twenty-five years asked:

Problem 2.1. (Full versus Strong Problem) *Is every full duality strong?*

We have not claimed above that it is always possible, for a given algebra $\mathbf{M}$, to choose a structure $\underset{\sim}{M}$ on M yielding a duality on $\mathbb{ISP}(\mathbf{M})$. Indeed, for some finite algebras $\mathbf{M}$ there is no choice of alter ego $\underset{\sim}{M}$ for which the resulting dual adjunction yields a duality between $\mathcal{A}$ and $\mathfrak{X}$; for example, the two-element implication algebra $\mathbf{I} = (\{0,1\}; \to)$, see [2, Chapter 10]. In fact, the main problem of the theory of natural dualities, the *Dualisability Problem*, remains still open:

Problem 2.2. (Dualisability Problem) *Which finite algebras are dualisable?*

At present, the Dualisability Problem seems to be unsolvable (cf. [36, page viii]). There are algebras $\mathbf{M}$ which fail to be dualizable (we refer to [26] or [4]). However, for a very wide range of algebras dualities do exist. For example, the NU-Duality Theorem ([26], Theorem 1.18 or [4], Theorem 2.8) guarantees that a duality on $\mathbb{ISP}(\mathbf{M})$ is available whenever $\mathbf{M}$ has a lattice reduct. Many further theorems which say how to choose an appropriate structure $\underset{\sim}{M}$ on M to obtain a duality, or a strong (thus full) duality, on $\mathbb{ISP}(\mathbf{M})$ can be found in [2] and in [36]. The Dualisability Problem might be formally undecidable, and in fact, the "holy grail" (cf. [36, page viii]) of some natural-duality theoreticians is the Decidability Problem for Dualisability:

Problem 2.3. (Decidability Problem for Dualisability) *Is there an algorithm for deciding whether or not any given finite algebra is dualisable?*

3 Entailment in natural dualities and our solution of the Entailment problem

Again assume a structure $\underset{\sim}{M} = (M; G, H, R, \mathcal{T})$ is algebraic over a finite algebra $\mathbf{M}$ and let r be an n-ary algebraic relation on M (i.e. a subalgebra of $\mathbf{M}^n$). We say that the structure $\underset{\sim}{M}$, or more often just $G \cup H \cup R$, *entails* r if for every $\mathbf{X} \in \mathfrak{X}$, each $\mathfrak{X}$-morphism $\varphi\colon \mathbf{X} \to \underset{\sim}{M}$ preserves r; we write $G \cup H \cup R \vdash r$. For relations r and s we write $r \vdash s$ in place of $\{r\} \vdash s$. We say that $G \cup H \cup R$ entails an n-ary (partial) operation h if it entails its graph as an $(n+1)$-ary relation, and that it entails a set R' of relations and (partial) operations if it entails each $r \in R'$.

3.1 Test Algebra Lemma and the Entailment problem

Central to the identification of the relations entailed from certain set $G \cup H \cup R$ is so-called Test Algebra Lemma. (It is formulated in entailment terms in [25], Lemma 2.3 and in [2], Lemma 8.1.3.) We present this statement and we notice that $\mathbf{s}$ always denotes the algebraic relation s considered as an algebra in $\mathcal{A}$.

Theorem 3.1. (Test Algebra Lemma) Let $\mathbf{M}$ be a finite algebra, let G, H, R be, respectively, sets (possibly empty) of operations, partial operations and relations which are algebraic over $\mathbf{M}$, and let s be an algebraic relation. Then the following are equivalent:

(1) $G \cup H \cup R$ entails s;

(2) $G \cup H \cup R$ entails s on $D(\mathbf{s})$.

Moreover, $G \cup H \cup R$ entails s whenever $G \cup H \cup R$ yields a duality on $\mathbf{s}$.

We often use the term *test algebra* for an algebra $\mathbf{A} \in \mathbb{ISP}(\mathbf{M})$ witnessing the failure of the structure $\underset{\sim}{M}$ to yield a duality on $\mathbb{ISP}(\mathbf{M})$.

It is important that provided a set $G \cup H \cup R$ yields a duality on $\boldsymbol{\mathcal{A}}$ then the duality is not destroyed by deleting from $G \cup H \cup R$ any element which is entailed by the remaining members. This is the key to obtaining so-called *economical dualities* which are easy to work with. A full discussion of the central role played by entailment in duality theory is presented in the paper [17]. In this paper we solved the Entailment Problem of duality theory that was formulated as follows:

Problem 3.2. (Entailment Problem) *Find an intrinsic description of the relations entailed by $G \cup H \cup R$.*

This problem was formulated as the first open problem of the natural dualities in the famous survey paper [4]. When this problem was firstly introduced, it was expected that the solution would be a semantic one in terms of a preservation theorem providing a list of finitary constructs which preserve entailment. By this is meant that if $(G \cup H \cup R) \vdash s$ then s would be obtainable from the set $G \cup H \cup R$ via a finite sequence of finitary constructs. In our solution to the problem in [17] we indeed firstly discovered a semantic solution, which was similar to the characterisation of the well-known *clone closure* Inv(Pol(R)) of a set of relations R (all 'invariants' of 'polymorphisms' preserving R) originally obtained in the famous pair of papers [1] by V. Bodnarčuk, L.A. Kalužnin, V.N. Kotov and B.A. Romov. Later on, we noticed that our semantic solution also arises as a direct application of a syntactic solution: a description of relations entailed by $G \cup H \cup R$ in terms of the first-order formulæ of the language with equality, $\boldsymbol{\mathcal{L}}_{\underset{\sim}{M}}$, associated with $\underset{\sim}{M}$. An important step towards the solution was the recognition that on a given set Ω of finitary algebraic relations on $\mathbf{M}$ the map $R \longmapsto \overline{R} := \{\, s \in \Omega \mid R \vdash s \,\}$ is a closure operator (*entailment closure*). And also the recognition that this closure operator is algebraic, in the sense that the closure of any set R is the union of the closures of its finite subsets (so that the lattice of closed sets is algebraic). This provided indirect evidence for a positive solution to the Entailment Problem.

3.2 Our syntactic solution of the Entailment problem

In [25] the important fact that entailment closure is algebraic was deduced as a corollary of the Test Algebra Lemma. In the paper [17] we extended the Test Algebra Lemma, upgrading it to the Test Algebra Theorem. This theorem provides our syntactic solution to the Entailment Problem:

Theorem 3.3. (The Test Algebra Theorem or Entailment in the duality sense) Let $\mathbf{M}$ be a finite algebra and let a structure $\underset{\sim}{M} = (M; G, H, R, \mathfrak{T})$ be algebraic over $\mathbf{M}$. Then the following are equivalent:

(1) $G \cup H \cup R$ entails s;

(2) $G \cup H \cup R$ entails s on $D(\mathbf{s})$;

(3) some finite subset of $G \cup H \cup R$ entails s on $D(\mathbf{s})$;

(4) $s = \{\, (u(\rho_1), \dots, u(\rho_n)) \mid u : D(\mathbf{s}) \to M$ preserves $G \cup H \cup R \,\}$;

(5) there exists a primitive positive formula $\Phi(x_1, \dots, x_n)$ in the language $\boldsymbol{\mathcal{L}}_{\underset{\sim}{M}}$ such that

  (i) $D(\mathbf{s}) \vdash \Phi(\rho_1, \dots, \rho_n)$ and
  (ii) $s = \{\, (c_1, \dots, c_n) \in M^n \mid M \vdash \Phi(c_1, \dots, c_n) \,\}$.

The most important part of our syntactic solution is that $(G \cup H \cup R) \vdash s$ if and only if there is a primitive positive formula Φ in the language $\mathcal{L}_{\underset{\sim}{M}}$ such that s may be obtained from $G \cup H \cup R$ via a *primitive positive construct*. We may take Φ to be the primitive positive type of $\rho_1, \dots, \rho_n$ in $D(\mathbf{s})$.

In duality theory, a set R of finitary algebraic relations on a finite algebra $\mathbf{M}$ entails a finitary algebraic relation s on the powers of $\underset{\sim}{M}$ (which are the duals of free algebras in the associated quasivariety $\boldsymbol{\mathcal{A}}$; see, for example, [26]) if and only if s can be obtained from R in the clone-theoretic case.

Therefore applying our results in the clone setting we derive a famous consequence due to V. Bodnarčuk, L.A. Kalužnin, V.N. Kotov and B.A. Romov [1]:

Theorem 3.4. (Entailment in the clone sense) Let R be a family of finitary relations on a finite set M and let $s \subseteq M^n$. Then the following are equivalent:

(1) $s \in \mathrm{Inv}(\mathrm{Pol}(R))$;

(2) R entails s on M^s;

(3) $s = \{(u(\rho_1), \dots, u(\rho_n)) \mid u : M^s \to M \text{ preserves } R\}$;

(4) there is some finite structure Z of type $(M; R)$ and elements $z_1, \dots, z_n \in Z$ such that $s = \{\, (u(z_1), \dots, u(z_n)) \mid u : Z \to M \text{ preserves } R \,\}$;

(5) $s = \{\, (c_1, \dots, c_n) \in M^n \mid M \vdash \Phi(c_1, \dots, c_n) \,\}$ for some primitive positive formula $\Phi(x_1, \dots, x_n)$ (in the language of the relational structure $(M; R)$).

3.3 Our semantic solution of the Entailment problem

Through the Test Algebra Theorem we are able to convert our syntactic solution to the Entailment Problem to a semantic solution, so obtaining a set of constructs sufficient to describe entailment. We only summarise the results below and sketch the main steps of our semantic solution while for all details of it and definitions of the constructs we refer to our paper [17] or to [2, 2.4.5 and 9.2.1].

In case $G \cup H = \emptyset$, the list of entailment constructs may be taken to be: *trivial relations*, *repetition removal*, *intersection*, *product*, and *retractive projection* (in which the natural projection map is required to be a retraction). As a consequence in the clone setting we have the result of [1] that $\mathrm{Inv}(\mathrm{Pol}(R))$ can be obtained from R by a finite number of applications of trivial relations, intersection, repetition removal, product and projection.

As is well known, arbitrary projection is not necessarily an allowable construct on structures of the form $D(\mathbf{A}) = \boldsymbol{\mathcal{A}}(\mathbf{A}, \mathbf{M})$. If it were, we could form the relational product of two relations, which is not guaranteed to lift to structures $D(\mathbf{A})$ which are not full powers. This explains why a set R of algebraic relations on $\mathbf{M}$ which determines the clone of term functions on $\mathbf{M}$ will not necessarily yield a duality on $\boldsymbol{\mathcal{A}}$. This is illustrated in [4, p.102] in case $\boldsymbol{\mathcal{A}}$ is the variety $\boldsymbol{\mathcal{K}}$ of Kleene algebras; for a more extended discussion we refer to [25, Section 5] or [19].

Our semantic solution to the Entailment Problem in [17] was carried out in two stages. Firstly, we showed that the second dual $ED(\mathbf{s})$ of an algebraic relation s can be *concretely* constructed from $G \cup H \cup R$, whether or not $G \cup H \cup R$ entails s (for details again see [17] or [2, 2.4.5 and 9.2.1]). Secondly, we showed that if $G \cup H \cup R$ entails s then s can be obtained from this second dual $ED(\mathbf{s})$ by a retractive projection, which is a bijective projection in case $G \cup H \cup R$ yields a duality on $\mathbf{s}$.

To explain the latter concepts, given an m-ary algebraic relation r on M and an injective mapping $\eta : \{1, \dots, n\} \to \{1, \dots, m\}$ $(n \leq m)$ we define the relation

$$r_\eta = \{\, (c_1, \dots, c_n) \in M^n \mid (\exists d_1 \dots d_m \in M)\ (d_1, \dots, d_m) \in r \text{ and } c_i = d_{\eta(i)}\ (1 \leq i \leq n) \,\}$$

(it can be alternatively denoted as the projection $P_{\eta(1),\ldots,\eta(n)}(r)$ of r into its coordinates $\eta(1),\ldots,\eta(n)$). Then we say that the relation $s := r_\eta$ is a *retractive projection of* r if the natural projection map $p : \mathbf{r} \to \mathbf{s}$ is a retraction, that is, there is a homomorphism $q : \mathbf{s} \to \mathbf{r}$ such that $p \circ q = \mathrm{id}_s$. It is called a *bijective projection* (as introduced by L. Zadori [45]) if moreover $q \circ p = \mathrm{id}_r$.

Consider G, H and R as before and let now $Z = \{z_1,\ldots,z_k\}$ be a finite substructure of M^T, for some non-empty set T. By the *graph of* $E(Z)$ (with respect to $G \cup H \cup R$) we mean the relation

$$G[E(Z)] := \{\, (u(z_1),\ldots,u(z_k)) \in M^k \mid u : Z \to M \text{ preserves } G \cup H \cup R \,\}.$$

Thus the graph of $E(Z)$ is simply $E(Z)$, given a fixed labelling of Z. We showed that if Z is a finite subset of M^T for some non-empty set T which is *hom-closed* (for details see [2, p. 66]), then the relation $G[E(Z)]$ can be concretely constructed from $G \cup H \cup R$.

For an n-ary algebraic relation s we take $Z := D(\mathbf{s})$ to be the dual of the algebra $\mathbf{s}$ and enumerate its elements as $\{\rho_1,\ldots,\rho_n,\mathcal{T}_1,\ldots,\mathcal{T}_m\}$. We then assume that

$$G[\mathbf{s}] := \{\, (\rho_1(a),\ldots,\rho_n(a),\mathcal{T}_1(a),\ldots,\mathcal{T}_m(a)) \in M^{n+m} \mid a \in s \,\}$$

encode the evaluation maps from $D(\mathbf{s})$ to M. It is evident that $G[\mathbf{s}]$ is in bijective correspondence with s itself. Now we have that if $G \cup H \cup R$ yields a duality on $\mathbf{s}$ then $G[ED(\mathbf{s})]$ necessarily coincides with $G[\mathbf{s}]$. It is helpful to employ the intuition that the relation $G[ED(\mathbf{s})] \setminus G[\mathbf{s}]$ can be thought of as a measure of how far $G \cup H \cup R$ is from yielding a duality on $D(\mathbf{s})$.

Since by the Test Algebra Theorem we have that an algebraic relation s is the retractive projection of $G[ED(\mathbf{s})]$ onto its first n coordinates, where the dual $D(\mathbf{s})$ of s is labelled as above, we immediately have:

Lemma 3.5. Let $\mathbf{s} \leq \mathbf{M}^n$ and $G \cup H \cup R$ entail s. Then s is a retractive projection of the graph $G[ED(\mathbf{s})]$ of $ED(\mathbf{s})$.

A number of consequences can be deduced. The first is the desired Semantic Entailment Theorem of [17]:

Theorem 3.6. (Semantic Entailment Theorem) Let R be a set of algebraic relations on a finite set M, let s be an algebraic relation on M and let $R \vdash s$. Then s can be obtained from R by a finite number of applications of product, intersection, trivial relations and repetition removal, followed by one application of retractive projection.

If a set R of algebraic relations on a finite set M is such that $R \vdash s$ for every algebraic relation s on M, then we say that R is *entailment-dense.* The following result, that can be derived from our semantic solution, was (independently to our investigations) discovered by L. Zádori [45]:

Theorem 3.7. (Special Semantic Entailment Theorem) Let R be a set of algebraic relations on a finite set M and let s be an algebraic relation on M.

(a) If R yields a duality on $\mathbf{s}$, then s can be constructed from R by a finite number of applications of product, intersection, trivial relations, repetition removal and bijective projection.

(b) The following are equivalent:

  (i) R yields a duality on every finite algebra in $\boldsymbol{\mathcal{A}}$;

(ii) R is entailment-dense;

(iii) every algebraic relation s on M can be constructed from R by a finite number of applications of product, intersection, trivial relations, repetition removal and bijective projection.

4 Endoprimality and endodualisability in theory and practice

The relationship between duality entailment and clone-entailment is rather complex. It is known that it is possible for $G \cup H \cup R$ to clone-entail every finite algebraic relation on $\mathbf{M}$ but to fail to dualise $\mathbf{M}$, but the circumstances under which this phenomenon occurs, and what it signifies, are still obscure. In particular, we may ask what it means for $\mathbf{M}$ to be *endoprimal* but not *endodualisable* (we refer to definitions of these concepts below). More explicitly, we may ask what it means for some finitary algebraic relation r on $\mathbf{M}$ to be clone-entailed but not entailed by (the graphs of) the endomorphisms of $\mathbf{M}$. From a semantic viewpoint, a clear difference can be seen: clone-entailment allows all relational products, whereas duality entailment allows only *homomorphic relational products* (for details see [17] or [2, 9.2.1]). Thus one may expect relational products appearing in the construction of r from the endomorphisms of $\mathbf{M}$ to be non-homomorphic relational products. Exactly how this behaviour happens in general is not clear.

4.1 Endoprimality versus endodualisability

In [19] we showed that the relationship between the two entailment concepts also lies at the heart of the relationship between endoprimality and endodualisability. This was nicely demonstrated by the Kleene algebra examples. We note that Kleene algebras were already known to illustrate the distinction between entailment in the clone sense and in the duality sense - we refer to [4, p. 87], [25, Section 5] and [2, pp. 272–273]. In [19] we gave a complete description of endodualisable and endoprimal finite Kleene algebras from the quasi-variety $\mathbb{ISP}(\mathbf{4})$ and showed that there was a plentiful supply of finite Kleene algebras which were endoprimal but not endodualisable.

Let $\mathbf{M} = (M; F)$ be any algebra. The algebra $\mathbf{M}$ is called *k-endoprimal* ($k \geq 1$) if every k-ary End($\mathbf{M}$)-preserving function on $\mathbf{M}$ is a term function of $\mathbf{M}$. Algebras which are k-endoprimal for every $k \geq 1$ are called *endoprimal.* A finite algebra $\mathbf{M}$ is *endodualisable* if End($\mathbf{M}$) yields a duality on the quasivariety $\mathbb{ISP}(\mathbf{M})$.

The relationship between endodualisability on one hand, and endoprimality and k-endoprimality on the other hand, was explored, successively, in [18], [5], [23], [32] and [19]. It was shown that in many quasivarieties a finite algebra is endoprimal if and only if it is endodualisable (we refer to [23], [33] and the papers cited therein).

In [18] we started an intensive study of a general relationship between endodualisability and endoprimality by the following result:

Theorem 4.1. (Endoprimality versus endodualisability for distributive lattices) Let $\mathbf{L} = (L; \vee, \wedge)$ be a finite non-trivial distributive lattice. The following are equivalent:

(1) $\mathbf{L}$ is 3-endoprimal;

(2) $\mathbf{L}$ is endoprimal;

(3) $\mathbf{L}$ is endodualisable;

(4) the retractions of $\mathbf{L}$ onto $\{0, 1\}$ together with the constants $0, 1$ yield a duality on $\mathbb{ISP}(\mathbf{L})$;

(5) $\mathbf{L}$ is not a Boolean lattice.

In case of bounded distributive lattices we obtained a similar result, the only difference is in Condition (1):

Theorem 4.2. (Endoprimality vs endodualisability for bounded distributive lattices) Let $\mathbf{L} = (L; \vee, \wedge, 0, 1)$ be a finite non-trivial bounded distributive lattice. The following are equivalent:

(1) $\mathbf{L}$ is 1-endoprimal;

(2) $\mathbf{L}$ is endoprimal;

(3) $\mathbf{L}$ is endodualisable;

(4) the retractions of $\mathbf{L}$ onto $\{0, 1\}$ together with the constants $0, 1$ yield a duality on $\mathbb{ISP}(\mathbf{L})$;

(5) $\mathbf{L}$ is not a Boolean lattice.

The first examples of finite algebras which are endoprimal but not endodualisable were found by B.A. Davey and J.G. Pitkethly in their paper [23], among algebras with a semilattice reduct. Many other such examples have been found among Kleene algebras in our paper [19].

4.2 A criterion for a finite endoprimal algebra to be endodualisable

In the paper [32] the strategy for finding endoprimal algebras due to B.A. Davey and J.G. Pitkethly [23] is further explored in the finite case. A new theoretical tool, called the *Retraction Test Algebra Lemma*, is used to show that, in many quasivarieties, endoprimality is equivalent to endodualisability for finite algebras which are suitably related to finitely generated free algebras. The main result of [32] is the following theorem.

Theorem 4.3. (Retraction Test Algebra Lemma) Let a finite algebra $\mathbf{D}$ be dualisable via the structure

$$\underset{\sim}{D} = (D; \mathrm{End}(\mathbf{D}), s_1, \ldots, s_m, \mathcal{T})$$

where $m \geq 1$ and $s_1, \ldots, s_m$ are finitary algebraic relations on $\mathbf{D}$. Let the algebras $\mathbf{s}_1, \ldots, \mathbf{s}_m$ be retracts of the k-generated free algebra $\mathbf{F}_{\mathfrak{D}}(k) \in \mathfrak{D}$ where $\mathfrak{D} = \mathbb{ISP}(\mathbf{D})$.

Then for any finite algebra $\mathbf{M} \in \mathfrak{D}$ which has $\mathbf{D}$ as a retract the following are equivalent:

(1) $\mathbf{M}$ is endoprimal;

(2) $\mathbf{M}$ is k-endoprimal;

(3) $\mathbf{M}$ is endodualisable.

The result can be applied to the (quasi-)varieties of distributive lattices (with $k = 3$), bounded distributive lattices ($k = 1$), finite vector spaces of dimension greater than one ($k = 2$), Stone algebras ($k = 2$), abelian groups ($k = 2$), sets ($k = 3$), semilattices ($k = 3$), lower-bounded semilattices ($k = 2$) and median algebras ($k = 3$), which have not been considered before as regards endoprimality.

We explain the applications of our theorem above in several selected cases:

Distributive lattices

The class $\mathfrak{D}$ of distributive lattices is the quasi-variety $\mathbb{ISP}(\mathbf{2})$ generated by the 2-element lattice $\mathbf{2} = (\{0, 1\}; \vee, \wedge)$. It is well-known (by *Priestley duality* presented in [41], [42]) that $\mathbf{2}$ is dualisable via the structure $\underset{\sim}{2} = (\{0, 1\}, 0, 1, \leq, \mathcal{T})$ where $\leq$ is the usual order on $\{0, 1\}$ and the constants 0 and 1 replace the usual unary constant endomorphisms onto 0 and 1, respectively. It is said that $\mathbf{2}$ is *almost endodualisable* with $\leq$ as the extra relation to the endomorphisms in the dualising structure. We notice that $\leq$ is, as a distributive lattice, isomorphic to the 3-element chain $\mathbf{3}$.

It is easy to check that the free algebras $\mathbf{F}_{\mathcal{D}}(1) \cong \mathbf{1}$ and $\mathbf{F}_{\mathcal{D}}(2) \cong \mathbf{2}^2$ do not have $\mathbf{3}$ as a retract while the free algebra $\mathbf{F}_{\mathcal{D}}(3)$ does have $\mathbf{3}$ as a retract. All non-trivial distributive lattices $\mathbf{L} \in \mathcal{D}$ have evidently $\mathbf{2}$ as their retracts. From our theorem above it therefore follows that a finite non-trivial distributive lattice $\mathbf{L}$ is endoprimal iff $\mathbf{L}$ is 3-endoprimal iff L is endodualisable.

Stone algebras

The class of Stone algebras is the quasi-variety $\mathbb{ISP}(\mathbf{3})$ generated by the 3-element Stone algebra $\mathbf{3} = (\{0, a, 1\}; \vee, \wedge, ^\star, 0, 1)$ where $\{0, a, 1\}$ is the 3-element chain, $0^\star = 1$, and $a^\star = 1^\star = 0$. It is well known that the structure $\underset{\sim}{3} = (\{0, a, 1\}, d, \preccurlyeq, \mathcal{T})$ yields a duality on the variety of Stone algebras (cf. e.g. [2, p. 105]) where $\preccurlyeq$ is the order $\{(0, 0), (a, a), (1, 1), (1, a)\}$ and $\text{graph}(d) = \{(0, 0), (1, 1), (a, 1)\}$. It means that $\mathbf{3}$ is almost endodualisable with the extra relation $\preccurlyeq$ which is isomorphic to the 4-element chain algebra $\mathbf{4}$ in $\mathcal{S}$. Now the smallest k-generated free algebra in $\mathcal{S}$ having $\mathbf{4}$ as a retract is known to be $\mathbf{F}_{\mathcal{S}}(2)$ (we refer to [29]). Our theorem can be applied to Stone algebras having $\mathbf{3}$ as a retract. The only Stone algebras which do not have $\mathbf{3}$ as a retract are the Boolean algebras (and these are endodualisable). It follows that a finite non-Boolean Stone algebra $\mathbf{L}$ is endoprimal iff $\mathbf{L}$ is 2-endoprimal iff $\mathbf{L}$ is endodualisable.

Median algebras

The class of median algebras is the quasi-variety $\mathcal{M} = \mathbb{ISP}(\mathbf{M})$ generated by the 2-element median algebra $\mathbf{M} = (\{0, 1\}; m)$ in which the ternary (median) operation m satisfies the equations

$$m(x, y, z) = m(y, x, z) = m(y, z, x),\ m(x, x, y) = x$$

and

$$m(m(x, y, z), u, v) = m(x, m(y, u, v), m(z, u, v)).$$

The duality for $\mathcal{M}$ is given by the structure $\underset{\sim}{M} = (\{0, 1\}; ^*, 0, 1, \leq, \mathcal{T})$, where * is the automorphism reversing 0 and 1 and $\leq$ is the usual order on $\{0, 1\}$ (we refer, for example, to [2, p. 103]). It follows that $\mathbf{M}$ is almost endodualisable with the extra relation $\leq$ which can be considered as a median algebra, say $\mathbf{s}$. In our paper [32] we present a verification in terms of natural duals of the fact that the smallest k-generated free algebra in $\mathcal{M}$ which has the algebra $\mathbf{s}$ as a retract is $\mathbf{F}_{\mathcal{M}}(3)$. Because any non-trivial median algebra $\mathbf{L} \in \mathcal{M}$ has $\mathbf{M}$ as a retract it immediately follows from our theorem that a finite non-trivial median algebra $\mathbf{L} \in \mathcal{M}$ is endoprimal iff $\mathbf{L}$ is 3-endoprimal iff $\mathbf{L}$ is endodualisable.

Abelian groups

Our method allows us to identify also the finite endoprimal abelian groups. Starting from a finite abelian group $\mathbf{A}$, one can choose $\mathcal{D}$ and the generator $\mathbf{D}$ of $\mathcal{D}$ in such a way that $\mathbf{A} \in \mathcal{D}$ and $\mathbf{D}$ is a retract of $\mathbf{A}$. This enables us to apply our theorem.

It is well-known that for any finite abelian group $\mathbf{A}$ there is a cyclic group $\mathbf{Z}_m$ such that $\mathbf{A} \in \mathcal{A}_m$ where $\mathcal{A}_m = \mathbb{ISP}(\mathbf{Z}_m)$ and $\mathbf{Z}_m$ is a direct factor, and hence a retract, of $\mathbf{A}$. It was shown in [26] (we also refer to [2, p. 114]) that the structure $\underset{\sim}{Z}_m = (Z_m; +, ^-, 0, \mathcal{T})$ yields a duality on the quasi-variety $\mathcal{A}_m$. This means that $\mathbf{Z}_m$ is almost endodualisable with graph(+) as the extra relation, which is, as an algebra, isomorphic to $\mathbf{Z}_m^2$. We have $\mathbf{F}_{\mathcal{A}_m}(2) \cong \mathbf{Z}_m^2$. Hence for the finite abelian group $\mathbf{A}$ and the associated quasivariety $\mathcal{A}_m = \mathbb{ISP}(\mathbf{Z}_m)$ we could apply our theorem with $k = 2$. It follows that a finite abelian group $\mathbf{A}$ is endoprimal iff it is 2-endoprimal iff it is endodualisable.

4.3 Endodualisable and endoprimal finite double Stone algebras

In the paper [33] we give a complete characterisation of the endoprimal finite double Stone algebras. In particular, we have shown that all of these algebras are endodualisable, and found in every case the minimum value of k for which k-endoprimality forces endoprimality. Much more work was involved in completing this analysis than that for the other examples considered in the paper [32], and further duality techniques were required.

Let us present a brief outline of the results. An algebra $\mathbf{L} = (L; \vee, \wedge, ^\star, ^+, 0, 1)$ is called a *double Stone algebra* if $(L; \vee, \wedge, ^\star, 0, 1)$ and $(L; \wedge, \vee, ^+, 1, 0)$ are Stone algebras. The double Stone algebras form a variety $\mathfrak{DS} = \mathbb{ISP}(\mathbf{4})$ which is generated by the 4-element chain algebra $\mathbf{4} = (\{0, a, b, 1\}; \vee, \wedge, ^\star, ^+, 0, 1)$ where $0 < a < b < 1$ and

$$1^\star = b^\star = a^\star = 0,\ 0^\star = 1,\ 0^+ = a^+ = b^+ = 1,\ 1^+ = 0.$$

The proper non-trivial subvarieties of $\mathfrak{DS}$ are generated by the subdirectly irreducible subalgebras $\mathbf{2} = \{0, 1\}$ and $\mathbf{3} = \{0, a, 1\}$. The variety $\mathbb{ISP}(\mathbf{2})$ is just the class of Boolean algebras, while $\mathbb{ISP}(\mathbf{3})$ is the variety of regular double Stone algebras, *alias* three-valued Lukasiewicz algebras. An algebra is *proper* precisely when it has $\mathbf{4}$ as a retract. We have to consider separately the algebras in $\mathbb{ISP}(\mathbf{4}) \setminus \mathbb{ISP}(\mathbf{3})$, which we call proper double Stone algebras, and algebras in $\mathbb{ISP}(\mathbf{3})$. Also, a further splitting into cases is necessary, into algebras with non-empty core and algebras with empty core. The *core* of an algebra $\mathbf{L}$ in $\mathfrak{DS}$ is defined to be $K(\mathbf{L}) = \{\, x \in L \mid x^\star = 0,\ x^+ = 1 \,\}$. A finite algebra $\mathbf{L}$ has empty core if and only if $\mathbf{L}$ has $\mathbf{2}$ as a direct factor. It is easily shown that this occurs if and only if $\mathbf{L} \in \mathbb{ISP}(\mathbf{4} \times \mathbf{2})$. Every k-generated free algebra $\mathbf{F}_{\mathfrak{DS}}(k)$ lies in the subquasivariety $\mathbb{ISP}(\mathbf{4} \times \mathbf{2})$.

The finite non-Boolean algebras in the variety $\mathbb{ISP}(\mathbf{3})$ are exactly those of the form $\mathbf{3}^m \times \mathbf{2}^\ell$ $(m \geq 1,\ \ell \geq 0)$. We could set up a duality for $\mathbb{ISP}(\mathbf{3} \times \mathbf{2})$ in which the only non-endomorphism was isomorphic to $\mathbf{3} \times \mathbf{2}^2$.

We proved the following result:

Theorem 4.4. (Endodualisable finite double Stone algebras) Let $\mathbf{L}$ be a finite non-trivial double Stone algebra and express $\mathbf{L}$ as $\mathbf{J} \times \mathbf{2}^\ell$ where $\mathbf{J}$ does not have $\mathbf{2}$ as a factor and $\ell \geq 0$.

Then $\mathbf{L}$ is endodualisable when $\mathbf{L}$ takes one of the forms described below.

(1) $\mathbf{L}$ has non-empty core and $\mathbf{L}$ satisfies the following equivalent conditions:

   (i) $\mathbf{L}$ has $\mathbf{5}$ as a retract;
   (ii) $K(\mathbf{L})$ is a non-Boolean lattice.

(2) $\mathbf{L}$ is proper, $\mathbf{J}$ has $\mathbf{5}$ as a retract and $\ell \geq 2$.

(3) $\mathbf{L}$ is not proper and takes the form $\mathbf{3}^m \times \mathbf{2}^\ell$ where $m \geq 1$ and $\ell \geq 2$.

(4) $\mathbf{L}$ is Boolean.

Let $\mathbf{L}$ be a finite non-trivial and non-Boolean double Stone algebra which is not shown by above theorem to be endodualisable and assume that $\mathbf{L}$ is expressed as $\mathbf{J} \times \mathbf{2}^\ell$ where $\mathbf{J}$ does not have $\mathbf{2}$ as a factor. The following cases arise:

(A) $\mathbf{L}$ is a Post algebra of order 3 (that is, $\mathbf{L}$ is not proper and $\ell = 0$);

(B) $\mathbf{L}$ has a single factor $\mathbf{2}$ (that is, $\ell = 1$);

(C) $\mathbf{L}$ is proper, $K(\mathbf{L}) \neq \emptyset$ (that is, $\ell = 0$), and $\mathbf{J}$ does not have $\mathbf{5}$ as a retract;

(D) $\mathbf{L}$ is proper, $\mathbf{J}$ does not have $\mathbf{5}$ as a retract and $\ell \geq 2$.

We showed that $\mathbf{L}$ is not endodualisable in each of cases (A)–(D), treating these in turn.

Proposition 4.5. (Non-endodualisable finite double Stone algebras, Case A) Let $\mathbf{L}$ be a finite Post algebra of order 3. Then

(1) $\mathbf{L}$ is not endodualisable, with $\mathbf{2}$ serving as a test algebra;

(2) $\mathbf{L}$ is not 1-endoprimal.

Proposition 4.6. (Non-endodualisable finite double Stone algebras, Case B) Let $\mathbf{L} = \mathbf{J} \times \mathbf{2}$ be a finite non-Boolean double Stone algebra with exactly one factor $\mathbf{2}$. Then

(1) $\mathbf{L}$ is not endodualisable, with $\mathbf{2}^2$ serving as a test algebra;

(2) $\mathbf{L}$ is not 1-endoprimal.

For case (C) we showed that the algebra $\mathbf{L}$ is the retract of a power of a finite indecomposable algebra which is not 3-endoprimal.

Proposition 4.7. (Non-endodualisable finite double Stone algebras, Case C) Let $\mathbf{L}$ be a finite proper double Stone algebra with a non-empty core $K(\mathbf{L}) = [a, b]$ $(a < b)$ which is a Boolean lattice. Then $\mathbf{L}$ is not 3-endoprimal (and hence not endodualisable).

Finally we need to consider algebras which have $\mathbf{2}^\ell$ as a factor, where $\ell \geq 2$ (case (D)).

Proposition 4.8. (Non-endodualisable finite double Stone algebras, Case D) Let $\mathbf{L} = \mathbf{J} \times \mathbf{2}^\ell$, where $\mathbf{J} \in \mathbb{ISP}(\mathbf{4}) \setminus \mathbb{ISP}(\mathbf{3})$ is a finite double Stone algebra with a non-trivial Boolean core and $\ell \geq 2$. Then $\mathbf{L}$ is not 3-endoprimal (and so not endodualisable).

To summarise, we identified firstly various endodualisable finite double Stone algebras and then we showed, considering in turn four cases (A)–(D), that there are no other endodualisable finite double Stone algebras. Here we bring our results together.

Theorem 4.9. (Endodualisability for finite double Stone algebras, Summary) Assume that $\mathbf{L} = (L; \vee, \wedge, ^\star, ^+, 0, 1)$ is a finite proper double Stone algebra with a non-empty core $K(\mathbf{L}) = [a, b]$ $(a < b)$. Then the following are equivalent:

(1) $\mathbf{L}$ is endodualisable;

(2) $\mathbf{L}$ is endoprimal;

(3) $\mathbf{L}$ is 3-endoprimal;

(4) $\mathbf{5}$ is a retract of $\mathbf{L}$;

(5) the core $K(\mathbf{L})$ is a non-Boolean lattice.

For proper double Stone algebras with empty core we have the following theorem.

Theorem 4.10. Let $\mathbf{L} = (L; \vee, \wedge, ^\star, ^+, 0, 1)$ be a finite proper double Stone algebra with empty core. Then the following are equivalent:

(1) $\mathbf{L}$ is endodualisable;

(2) $\mathbf{L}$ is endoprimal;

(3) $\mathbf{L}$ is 3-endoprimal;

(4) $\mathbf{5} \times \mathbf{2}^2$ is a retract of $\mathbf{L}$.

For algebras in $\mathbb{ISP}(\mathbf{3})$ we have, likewise, the following result.

Theorem 4.11. Let $\mathbf{L}$ belong to the variety $\mathcal{R} = \mathbb{ISP}(\mathbf{3})$ of regular double Stone algebras and assume that $\mathbf{L}$ is not Boolean. Then the following are equivalent:

(1) $\mathbf{L}$ is endodualisable;

(2) $\mathbf{L}$ is endoprimal;

(3) $\mathbf{L}$ is 1-endoprimal;

(4) $\mathbf{3} \times \mathbf{2}^2$ is a retract of $\mathbf{L}$.

We record explicitly the following theorem, which is a corollary of our preceding results.

Corollary 4.12. A finite double Stone algebra is endoprimal if and only if it is endodualisable.

5 Full versus Strong Problem in the theory of natural dualities

Every quasi-variety of the form $\mathcal{A} = \mathbb{ISP}(M)$, where $\mathbf{M}$ is a finite lattice-based algebra, has a natural duality. In the case that M is distributive-lattice based, it is possible to use the *restricted Priestley duality* and the natural duality for $\mathcal{A}$ simultaneously. In tandem, these dualities can provide an extremely powerful tool for the study of $\mathcal{A}$: see Clark and Davey [2, Chapter 7]. As well as being a natural area of application of natural duality theory, distributive-lattice-based algebras in general, and distributive lattices in particular, have provided deep insights into the general theory. Important examples have been Heyting algebras, particularly the finite Heyting chains, and Kleene algebras; but here we firstly concentrate on the three-element bounded distributive lattice

$$\mathbf{3} = (\{0, d, 1\}; \vee, \wedge, 0, 1),$$

which was seminal in developments that led to the solution of the *Full versus Strong Problem*, one of the most tantalizing problems in the theory of natural dualities.

5.1 The seminal example of the three-element chain

For a natural-duality viewpoint, Priestley duality for the class $\mathcal{D}$ of bounded distributive lattices is obtained via homsets based on the two-element chain $\mathbf{2}$ and uses the fact that $\mathcal{D} = \mathbb{ISP}(\mathbf{2})$. By using the fact that $\mathcal{D} = \mathbb{ISP}(\mathbf{3})$, in [18] we introduced the following modified Priestley duality for $\mathcal{D}$ as a natural duality based on $\mathbf{3}$. Let f, g be the non-identity endomorphisms of 3 (see Figure 1) and let

$$\underset{\sim}{3} = (\{0, d, 1\}; f, g, \mathcal{T}),$$

where $\mathcal{T}$ is the discrete topology $\mathcal{T}$.

Let $\mathcal{X} = \mathbb{IS}_c\mathbb{P}^+(\underset{\sim}{3})$ be the class of all isomorphic copies of closed substructures of non-zero powers of $\underset{\sim}{3}$.

In [18] we showed that such a modified Priestley duality for $\mathcal{D}$, in which the order is replaced by endomorphisms, can be based on any finite non-boolean distributive lattice $\mathbf{M}$. We also showed that, while the order relation cannot be removed in the boolean case, it can at least be replaced by any finitary relation on $\mathbf{M}$, which itself, like the order on $\mathbf{2}$, forms a non-boolean lattice.

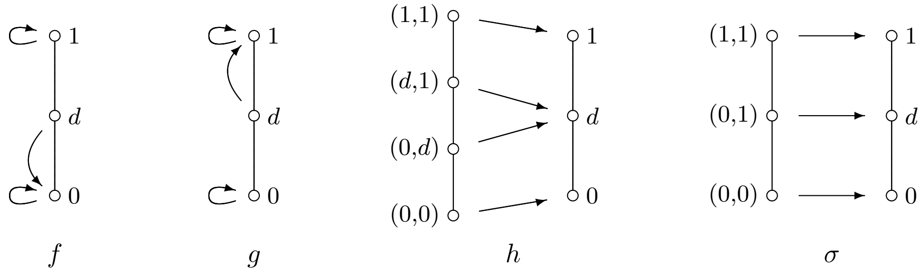

Figure 1. The (partial) operations f, g, h and σ on 3

In [9] we studied the enrichment of $\underset{\sim}{3}$ given by

$$\underset{\sim}{3}_\sigma := (\{0, d, 1\}; f, g, \sigma, \mathcal{T}),$$

and in [21] we explored deeply the enrichments $\underset{\sim}{3}_\sigma$ and

$$\underset{\sim}{3}_h := (\{0, d, 1\}; f, g, h, \mathcal{T}).$$

(The binary partial operations h and σ are also given in Figure 1.) If in the above scheme for the modified Priestley duality for $\mathfrak{D}$ based on $\mathbf{3}$ the alter ego $\underset{\sim}{3}$ of $\mathbf{3}$ is replaced with the alter ego $\underset{\sim}{3}_\sigma$, then not only the map $e_A : \mathbf{A} \to ED(\mathbf{A})$ is an isomorphism, for all $\mathbf{A} \in \mathfrak{D}$, establishing a duality between $\mathfrak{D} = \mathbb{ISP}(\mathbf{3})$ and $\mathfrak{X}_\sigma = \mathbb{IS}_c\mathbb{P}^+(\underset{\sim}{3}_\sigma)$, but moreover the map $\varepsilon_X : \mathbf{X} \to DE(\mathbf{X})$ is an isomorphism, for all $\mathbf{X} \in \mathfrak{X}_\sigma$, establishing a full duality between $\mathfrak{D}$ and $\mathfrak{X}_\sigma$. If the hom-functors D, E are restricted to the categories $\mathcal{A}_{\text{fin}}$ and $\mathfrak{X}_{\text{fin}}$ of finite members of $\mathcal{A}$ and $\mathfrak{X}$ only, then the concepts of a *finite-level* duality, full duality or strong duality are obtained.

The properties of the modified Priestley dualites for $\mathfrak{D}$ based on 3 given by the alter egos $\underset{\sim}{3}$, $\underset{\sim}{3}_h$ and $\underset{\sim}{3}_\sigma$ are summarized in the following theorem.

Theorem 5.1. Let $\underset{\sim}{3}$, $\underset{\sim}{3}_h$ and $\underset{\sim}{3}_\sigma$ be the alter egos of $\mathbf{3}$ defined above.

(i) $\underset{\sim}{3}$ yields a duality on $\mathfrak{D}$. (Davey, Haviar, Priestley [18])

(ii) $\underset{\sim}{3}_h$ yields a full duality, which is not strong, on the category $\mathfrak{D}_{\text{fin}}$ and yields a duality, which is not full, on the category $\mathfrak{D}$. (Davey, Haviar, Willard [21])

(iii) $\underset{\sim}{3}_\sigma$ yields a strong duality for $\mathfrak{D}$. (Davey, Haviar [9])

(iv) Every full duality on $\mathfrak{D}$ based on $\mathbf{3}$ is strong. (Davey, Haviar, Willard [21])

5.2 Full versus Strong Problem: its local versions and when full implies strong

Since the Full versus Strong Problem in its global version had remained open for twenty-five years, we introduced in [13] local versions of this problem that could prove more tractable and fruitful.

Problem 5.2. For an arbitrary finite algebra $\mathbf{M}$ in your favourite class $\mathfrak{C}$ of algebras, is every full duality based on $\mathbf{M}$ necessarily strong?

We also posed the finite-level version of Problem 5.2.

Problem 5.3. For an arbitrary finite algebra $\mathbf{M}$ in your favourite class $\mathfrak{C}$ of algebras, is every duality based on $\mathbf{M}$ that is full at the finite level necessarily strong at the finite level?

The first solutions to these local versions of the Full versus Strong Problem were given for full dualities based on the three-element chain in the variety of bounded distributive lattices in our paper [21] (as shown in the previous subsection). The answer was shown to be affirmative to Problem 5.2 and negative to Problem 5.3. In [13] we provided affirmative answers to Problems 5.2 and 5.3 for full dualities based on an arbitrary finite algebra in three varieties of algebras: abelian groups, semilattices (with or without bounds) and relative Stone Heyting algebras. We also developed some general conditions under which 'full implies strong' that had the potential to add to the list of solutions. Finally, we answered Problem 5.2 in the affirmative for full dualities based on an arbitrary finite lattice in the variety of bounded distributive lattices.

There is a further, weaker version of Problem 5.2, which deserves to be recorded here.

Problem 5.4. In your favourite class $\mathfrak{C}$ of algebras, is every fully dualisable finite algebra necessarily strongly dualisable?

It should be noted that the finite-level variant of this question makes no sense since every finite algebra $\mathbf{M}$ is strongly dualised at the finite level by the alter ego $\underset{\sim}{M} = \langle M; H, \mathfrak{T}\rangle$, where H consists of all finitary algebraic partial operation on $\mathbf{M}$. We found in [13] several sufficient conditions for full to imply strong:

Theorem 5.5. Let $\mathbf{D}$ be a finite algebra, let $\mathbf{M}$ be a finite algebra in $\boldsymbol{\mathcal{A}} := \mathbb{ISP}(\mathbf{D})$ such that $\mathbf{D}$ is a subalgebra of $\mathbf{M}$. Assume that $\underset{\sim}{D} = \langle D; G^D, H^D, R^D, \mathfrak{T}\rangle$ strongly dualises $\mathbf{D}$ [at the finite level] and that D, each relation $r \in R^D$, and $\mathrm{dom}(h)$, for all $h \in H^D$, is an intersection of equalizers of pairs of algebraic total operations on $\mathbf{M}$. Then any alter ego $\underset{\sim}{M}$ that fully dualises $\mathbf{M}$ [at the finite level] strongly dualises $\mathbf{M}$ [at the finite level].

When $R^D = \varnothing$ there is a particularly satisfying simplification of this result that involves assumptions on $\mathbf{D}$ only. We say that $\mathbf{D}$ is a *subretract* of $\mathbf{M}$ if $\mathbf{D}$ is a subalgebra of $\mathbf{M}$ and there is a *retraction* of $\mathbf{M}$ onto $\mathbf{D}$, that is, a homomorphism $\omega : \mathbf{M} \to \mathbf{D}$ with $\omega \restriction D = \mathrm{id}_D$.

Theorem 5.6. Let $\mathbf{D}$ be a finite algebra and let $\boldsymbol{\mathcal{A}} := \mathbb{ISP}(\mathbf{D})$. Assume that $\underset{\sim}{D} = \langle D; G^D, H^D, \mathfrak{T}\rangle$ strongly dualises $\mathbf{D}$ [at the finite level] and that, for all $h \in H^D$, the set $\mathrm{dom}(h)$ is an intersection of equalizers of pairs of algebraic total operations on $\mathbf{D}$. Let $\mathbf{M}$ be a finite algebra in $\boldsymbol{\mathcal{A}}$ such that $\mathbf{D}$ is a subretract of $\mathbf{M}$. Then any alter ego $\underset{\sim}{M}$ that fully dualises $\mathbf{M}$ [at the finite level] strongly dualises $\mathbf{M}$ [at the finite level].

The version of Theorem 5.6 that applies when $\underset{\sim}{D}$ is a total algebra turned out to be so striking that we stated it as a separate result:

Theorem 5.7. Let $\mathbf{D}$ be a finite algebra, let $\boldsymbol{\mathcal{A}} := \mathbb{ISP}(\mathbf{D})$ and let $\mathbf{M}$ be a finite algebra in $\boldsymbol{\mathcal{A}}$ that has $\mathbf{D}$ as a subalgebra. Assume that $\underset{\sim}{D} = \langle D; G^D, \mathfrak{T}\rangle$ is a total algebra that strongly dualises $\mathbf{D}$ [at the finite level]. If $\underset{\sim}{M}$ is an alter ego of $\mathbf{M}$ that fully dualises $\mathbf{M}$ [at the finite level], then $\underset{\sim}{M}$ strongly dualises $\mathbf{M}$ [at the finite level].

Also we presented the following special case of Theorem 5.5:

Theorem 5.8. Let $\mathbf{D}$ be a finite algebra. Assume that $\underset{\sim}{D} = \langle D; G^D, H^D, R^D, \mathfrak{T}\rangle$ strongly dualises $\mathbf{D}$ [at the finite level] and that each relation $r \in R^D$, and $\mathrm{dom}(h)$, for all $h \in H^D$, is an intersection of equalizers of pairs of algebraic total operations on $\mathbf{D}$. Then any alter ego that fully dualises $\mathbf{D}$ [at the finite level], strongly dualises $\mathbf{D}$ [at the finite level].

We then applied Theorem 5.7 to show that Questions 5.2 and 5.3 have affirmative answers for arbitrary finite algebras in the varieties of abelian groups and semilattices.

Abelian groups Let $\mathbf{M} = \langle M; +, ^{-}, 0\rangle$ be a finite non-trivial abelian group. Then there is a cyclic subgroup $\mathbf{D}$ of $\mathbf{M}$ such that $\mathbf{D}$ is a direct factor of $\mathbf{M}$ and such that $\mathbf{D}$ and $\mathbf{M}$ generate the same quasi-variety $\boldsymbol{\mathcal{A}}$. Since the total algebra $\underset{\sim}{D} = \langle D; +, ^{-}, 0, \mathcal{T}\rangle$ yields a strong duality on $\boldsymbol{\mathcal{A}}$ based on $\mathbf{D}$ (see [2, 4.4.2]), we may apply Theorem 5.7 to obtain that every alter ego $\underset{\sim}{M}$ that fully dualises the finite abelian group $\mathbf{M}$ [at the finite level] also strongly dualises $\mathbf{M}$ [at the finite level]. Hence the answers to Questions 5.2 and 5.3 in the variety of abelian groups are always in the affirmative.

Semilattices Let $\mathbf{D}_K = \langle\{0,1\}; \vee, K\rangle$ be the two-element semilattice with possible bounds $K \subseteq \{0,1\}$, let $\mathcal{S}_K := \mathbb{ISP}(\mathbf{D}_K)$ and let $\mathbf{S}$ be a finite non-trivial semilattice in $\mathcal{S}_K$. We have the following strong dualities on $\mathcal{S}_K := \mathbb{ISP}(\mathbf{D}_K)$ based on $\mathbf{D}_K$ given by total algebras.

(i) $\underset{\sim}{D} := \langle\{0,1\}; \vee, 0, 1, \mathcal{T}\rangle$ yields a strong duality on $\mathcal{S}$ based on the (unbounded) semilattice $\mathbf{D} = \langle\{0,1\}; \vee\rangle$.

(ii) $\underset{\sim}{D}_0 = \langle\{0,1\}; \vee, 0, \mathcal{T}\rangle$ yields a strong duality on $\mathcal{S}_0$ based on the semilattice with zero $\mathbf{D}_0 = \langle\{0,1\}; \vee, 0\rangle$.

(iii) $\underset{\sim}{D}_1 = \langle\{0,1\}; \vee, 1, \mathcal{T}\rangle$ yields a strong duality on $\mathcal{S}_1$ based on the semilattice with one $\mathbf{D}_1 = \langle\{0,1\}; \vee, 1\rangle$.

(iv) $\underset{\sim}{D}_{01} = \langle\{0,1\}; \vee, \mathcal{T})$ yields a strong duality on $\mathcal{S}_{01}$ based on the bounded semilattice $\mathbf{D}_{01} = \langle\{0,1\}; \vee, 0, 1\rangle$.

According to Theorem 5.7, if $\underset{\sim}{M}$ is an alter ego of $\mathbf{S}$ that fully dualises the finite semilattice $\mathbf{S}$ [at the finite level], then $\underset{\sim}{M}$ also strongly dualises $\mathbf{M}$ [at the finite level]. So Questions 5.2 and 5.3 have affirmative answers for arbitrary finite algebras in these varieties of semilattices (with bounds).

Bounded distributive lattices

Let $\mathfrak{D}$ be the variety of bounded distributive lattices. We proved in [13] the following theorem, thereby showing that Question 5.2 has an affirmative answer for an arbitrary finite algebra in the variety of bounded distributive lattices.

Theorem 5.9. Let $\mathbf{M}$ be a finite non-trivial bounded distributive lattice. If $\underset{\sim}{M}$ is an alter ego of $\mathbf{M}$ that yields a full duality on $\mathfrak{D}$ (based on $\mathbf{M}$), then $\underset{\sim}{M}$ yields a strong duality on $\mathfrak{D}$.

5.3 Full versus Strong Problem: related developments and the solution

The realm of natural dualities that were known to be full but not strong at the finite level was for some time a very small one, consisting of a single example. This example, based on the three-element bounded distributive lattice, was presented in our paper [21]. In our other developments, we extended this realm to the class of all natural dualities based on an arbitrary finite non-boolean bounded distributive lattice [14].

The results in [21] raised new questions and opened up new research paths within the field of natural dualities. More precisely, we were led to ask the following questions (cf. [14]):

(a) Could it be that, for a finite algebra that is strongly dualisable, every full duality on the quasi-variety it generates is strong?

(b) What is it about a finite algebra that allows its full dualities at the finite level to behave so differently from its full dualities at the infinite level?

(c) Which finite algebras generate a quasi-variety for which every duality that is full [at the finite level] is necessarily strong?

(d) Which finite algebras have an alter ego that yields a full but not strong duality at the finite level?

As already mentioned, in [13] we proved that, for each finite abelian group, semilattice and relative-Stone Heyting algebra, every duality that is full [at the finite level] is strong [at the finite level], and, for each finite bounded distributive lattice, every full duality is strong. This provided a partial answer to Question (c) and thereby provided examples with which to study Question (b). While Question (a) could be regarded as wild speculation, it was supported by the limited evidence available to us. In order to make headway on questions such as these, we felt we needed a range of examples of finite algebras that possess a full but not strong duality at the finite level.

In the paper [14] we addressed Question (d). More precisely, we proved the following result:

Theorem 5.10. Let $\mathbf{M}$ be a finite non-boolean bounded distributive lattice. Then there is an alter ego $\underset{\sim}{M}$ of $\mathbf{M}$ such that

(a) $\underset{\sim}{M}$ yields a duality that is not full on the class $\mathfrak{D}$ of all bounded distributive lattices, yet

(b) $\underset{\sim}{M}$ yields a duality that is full but not strong on the class of finite bounded distributive lattices.

Hence our Problem 5.3 was shown to have a negative answer in the variety of bounded distributive lattices by producing full but not strong dualities at the finite level based on an arbitrary finite non-boolean lattice.

The authors had hoped to find a conceptual proof of this last theorem that would indicate possible generalizations beyond distributive lattices. A natural approach would be to proceed as follows: let $\mathbf{M}$ be a finite non-boolean bounded distributive lattice; then $\mathbf{M}$ has the three-element chain $\mathbf{3}$ as a retract; in [21] an alter ego $\underset{\sim}{3}$ for $\mathbf{3}$ was given that yields a full but not strong duality at the finite level; use the retraction from $\mathbf{M}$ onto $\mathbf{3}$ to lift the alter ego $\underset{\sim}{3}$ up to an appropriate alter ego $\underset{\sim}{M}$ for $\mathbf{M}$. Unfortunately, this turned out to be too simple minded. We pursued this and many other approaches but to no avail. The hoped-for conceptual proof eluded us and we were left with the direct computational proof presented in [14]. Nevertheless, our result provided an infinite number of desired examples where previously there was only one.

Now, at last, we briefly present the much-seeked solution to the Full versus Strong Problem that was presented by D. M. Clark, B. A. Davey and R. Willard [3].

Let $\mathbf{R} := (\{0, a, b, 1\}; t, \vee, \wedge, 0, 1)$ be the four-element chain with $0 < a < b < 1$ enriched with the ternary discriminator function t. Let u be the partial endomorphism of $\mathbf{R}$ with domain $\{0, a, 1\}$ given by $u(a) = b$. In [3] the authors showed (via three slightly different approaches, found gradually by each of them) that the algebra $\mathbf{R}$ provides a negative solution to the Full versus Strong Problem of the theory of natural dualities:

Theorem 5.11. The alter ego $\underset{\sim}{R}_{\perp} = (\{0, a, b, 1\}; \mathrm{graph}(u), \mathcal{T})$ yields a full but not strong duality on $\mathbb{ISP}(\mathbf{R})$. (Clark, Davey, Willard [3])

In general, a finite algebra $\mathbf{M}$ admits essentially only one finite-level strong duality, but can admit many different finite-level full dualities. The alter egos $\underset{\sim}{M}$ yielding the finite-level full dualities for $\mathbb{ISP}_{\mathrm{fin}}(\mathbf{M})$ form a doubly algebraic lattice $\mathfrak{F}(\widetilde{M})$ introduced and studied in B. A. Davey, J. G. Pitkethly and R. Willard [24]. The following theorem summarises results in this direction.

Theorem 5.12.

(i) $|\mathfrak{F}(\mathbf{M})| = 1$ for any finite semilattice, abelian group or relative Stone Heyting algebra $\mathbf{M}$. (Davey, Haviar, Niven [13])

(ii) $\mathfrak{F}(\mathbf{M})$ is finite for any finite quasi-primal algebra $\mathbf{M}$; in particular, for the algebra $\mathbf{R}$ defined above, $|\mathfrak{F}(\mathbf{R})| = 17$. (Davey, Pitkethly, Willard [24])

(iii) The lattice $\mathfrak{F}(\mathbf{3})$ is non-modular and has size $2^{\aleph_0}$. (Davey, Haviar and Pitkethly [16]).

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Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 51–61, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

Polynomials, sign patterns and Descartes' rule

Vladimir P. Kostov
Université Côte d'Azur, CNRS, LJAD, Parc Valrose, 06108 Nice Cedex 2, France
vladimir.kostov@unice.fr

Boris Z. Shapiro
Department of Mathematics, Stockholm University, SE-106 91 Stockholm, Sweden
shapiro@math.su.se

Abstract
The famous Descartes' rule of signs from 1637 giving an upper bound on the number of positive roots of a real univariate polynomial in terms of the number of sign changes of its coefficients, has been an indispensable source of inspiration for generations of mathematicians. Trying to extend and sharpen this rule, we consider below the set of all real univariate polynomials of a given degree, a given collection of signs of their coefficients, and given numbers of positive and negative roots. In spite of the elementary definition of the main object of our study, it is a non-trivial question for which sign patterns and numbers of positive and negative roots the corresponding set is non-empty. The main result of the present paper is a discovery of a new infinite family of non-realizable combinations of sign patterns and the numbers of positive and negative roots.

Received 15 March 2019
Revised 1 October 2019
Accepted in final form 7 October 2019
Communicated with Miroslav Haviar.

Keywords standard discriminant, Descartes' rule of signs, sign pattern.
MSC(2010) Primary: 26C10, Secondary: 30C15.

1 Introduction

This paper continues the line of study of Descartes' rule of signs initiated in [4]. The basic set-up under consideration is as follows.

Consider the affine space Pol_d of all real monic univariate polynomials of degree d. Below we concentrate on polynomials from Pol_d with all coefficients non-vanishing. An arbitrary ordered sequence $\overline{\sigma} = (\sigma_0, \sigma_1, \ldots, \sigma_d)$ of $\pm$-signs is called a *sign pattern.* When working with monic polynomials we will use their *shortened sign patterns* $\widehat{\sigma}$ representing the signs of all coefficients except the leading term which equals 1. For the actual sign pattern $\overline{\sigma}$, we write $\overline{\sigma} = (1, \widehat{\sigma})$ to emphasise that we consider monic polynomials.

Given a shortened sign pattern $\widehat{\sigma}$, we say that its *Descartes pair* $(p_{\widehat{\sigma}}, n_{\widehat{\sigma}})$ is the pair of non-negative integers counting sign changes and sign preservations of $\overline{\sigma} = (1, \widehat{\sigma})$. By Descartes' rule of signs, $p_{\widehat{\sigma}}$ (resp. $n_{\widehat{\sigma}}$) gives the upper bound on the number of positive (resp. negative) roots of any monic polynomial from $Pol_d(\widehat{\sigma})$. (Observe that, for any $\widehat{\sigma}$, $p_{\widehat{\sigma}}+n_{\widehat{\sigma}} = d$.) To any monic polynomial $q(x)$ with the sign pattern $\overline{\sigma} = (1, \widehat{\sigma})$, we associate the pair (pos_q, neg_q) giving the numbers of its positive and negative roots counted with multiplicities. Obviously the pair (pos_q, neg_q) satisfies the standard restrictions

$$pos_q \leq p_{\overline{\sigma}},\ pos_q \equiv p_{\overline{\sigma}} \pmod 2,\ neg_q \leq n_{\overline{\sigma}},\ neg_q \equiv n_{\overline{\sigma}} \pmod 2. \tag{1.1}$$

We call pairs (pos, neg) satisfying (1.1) *admissible* for $\overline{\sigma}$. Conversely, for a given pair (pos, neg), we call a sign pattern $\overline{\sigma}$ such that (1.1) is satisfied *admitting* the latter pair. It turns out that there exist couples $(\overline{\sigma}, (pos, neg))$, where $\overline{\sigma}$ is a sign pattern and (pos, neg) is a pair admissible for $\overline{\sigma}$, which are not realizable by polynomials. Namely, D. J. Grabiner [5] found the first example of non-realizable combination for polynomials of degree 4. He has shown that the sign pattern $(+,-,-,-,+)$ does not allow to realize the pair $(0,2)$ and the sign pattern $(+,+,-,+,+)$ does not allow to realize $(2,0)$. Observe that their Descartes pairs equal $(2,2)$.

His argument is very simple. (Due to symmetry induced by $x \mapsto -x$ it suffices to consider only the first case.) Observe that a fourth-degree polynomial with only two negative roots for which the sum of roots is positive could be factored as $a(x^2+bx+c)(x^2-sx+t)$ with $a,b,c,s,t>0$, $s^2<4t$, and $b^2 \geq 4c$.

The product of these factors equals $a(x^4+(b-s)x^3+(t+c-bs)x^2+(bt-cs)x+ct)$. To get the correct sign pattern, we need $b<s$ and $bt<cs$, which gives $b^2t<s^2c$ and thus $b^2/c<s^2/t$. But we have $b^2/c \geq 4 > s^2/t$.

The following basic question and related conjecture were formulated in [4]. (Apparently for the first time Problem 1 was mentioned in [3].)

Problem 1. *For a given sign pattern $\overline{\sigma}$, which admissible pairs (pos, neg) are realizable by polynomials whose signs of coefficients are given by $\overline{\sigma}$?*

Observe that we have the natural $\mathbb{Z}_2 \times \mathbb{Z}_2$-action on the space of monic polynomials and on the set of all sign patterns respectively. The first generator acts by reverting the signs of all monomials in second, fourth etc. position (which for polynomials means $P(x) \to (-1)^d P(-x)$); the second generator acts by reading the pattern backwards (which for polynomials means $P(x) \to x^d P(1/x)$). If one wants to preserve the set of monic polynomials one has to divide $x^d P(1/x)$ by its leading term. We will refer to the latter action as the *standard* $\mathbb{Z}_2 \times \mathbb{Z}_2$*-action*. Up to some trivialities, the properties we will study below are invariant under this action. The following initial results were partially proven in [3, 1] and in complete generality in [4].

Theorem 1.

(i) *Up to degree $d \leq 3$, for any sign pattern $\overline{\sigma}$, all admissible pairs (pos, neg) are realizable.*

(ii) *For $d=4$, (up to the standard $\mathbb{Z}_2 \times \mathbb{Z}_2$-action) the only non-realizable combination is $(1,-,-,-,+)$ with the pair $(0,2)$;*

(iii) *For $d=5$, (up to the standard $\mathbb{Z}_2 \times \mathbb{Z}_2$-action) the only non-realizable combination is $(1,-,-,-,-,+)$ with the pair $(0,3)$;*

(iv) *For $d=6$, (up to the standard $\mathbb{Z}_2 \times \mathbb{Z}_2$-action) the only non-realizable combinations are $(1,-,-,-,-,-,+)$ with $(0,2)$ and $(0,4)$; $(1,+,+,+,-,+,+)$ with $(2,0)$; $(1,+,-,-,-,-,+)$ with $(0,4)$.*

The next two results can be found in [4] and [8].

Theorem 2. *For $d=7$, among the 1472 possible combinations of a sign pattern and a pair (up to the standard $\mathbb{Z}_2 \times \mathbb{Z}_2$-action), there exist exactly 6 which are non-realizable. They are:*

$$(1,+,-,-,-,-,-,+) \quad \textit{with} \quad (0,5); \quad (1,+,-,-,-,-,+,+) \quad \textit{with} \quad (0,5);$$

$$(1,+,-,+,-,-,-,-) \quad \textit{with} \quad (3,0); \quad (1,+,+,-,-,-,-,+) \quad \textit{with} \quad (0,5);$$
$$\textit{and,} \quad (1,-,-,-,-,-,-,+) \quad \textit{with}\ (0,3)\ \textit{and}\ (0,5).$$

Theorem 3. *For $d = 8$, among the 3648 possible combinations of a sign pattern and a pair (up to the standard $\mathbb{Z}_2 \times \mathbb{Z}_2$-action), there exist exactly 13 which are non-realizable. They are:*

$$(1,+,-,-,-,-,-,+,+) \quad \textit{with} \quad (0,6); \quad (1,-,-,-,-,-,-,+,+) \quad \textit{with} \quad (0,6);$$
$$(1,+,+,+,-,-,-,-,+) \quad \textit{with} \quad (0,6); \quad (1,+,+,-,-,-,-,-,+) \quad \textit{with} \quad (0,6);$$
$$(1,+,+,+,-,+,+,+,+) \quad \textit{with} \quad (2,0); \quad (1,+,+,+,+,+,-,+,+) \quad \textit{with} \quad (2,0);$$
$$(1,+,+,+,-,+,-,+,+) \quad \textit{with}\ (2,0)\ \textit{and}\ (4,0)\ ; \quad (1,-,-,-,+,-,-,-,+) \quad \textit{with}$$
$$(0,2)\ \textit{and}\ (0,4); \quad (1,-,-,-,-,-,-,-,+) \quad \textit{with}\ (0,2), (0,4),\ \textit{and}\ (0,6).$$

Finally, it was shown in [9] that for $d = 11$, the sign pattern

$$(+,-,-,-,-,-,+,+,+,+,+,-)$$

is not realizable with the admissible pair $(1,8)$. This is the first example found of non-realizability in which both components of the admissible pair are nonzero.

The first goal of the present paper is to present a new infinite series of non-realizable patterns, defined for odd degrees, this is why we call it *the odd series.* (Two other series can be found in [4]; one of them, defined for even degrees, is called *the even series.*) Namely, for a fixed odd degree $d \geq 5$ and $1 \leq k \leq (d-3)/2$, denote by σ_k the sign pattern beginning with two pluses followed by k pairs "$-,+$" and then by $d-2k-1$ minuses. Its Descartes pair equals $(2k+1, d-2k-1)$.

Theorem 4.

(i) *The sign pattern σ_k is not realizable with any of the pairs $(3,0)$, $(5,0)$, $\ldots$, $(2k+1,0)$;*

(ii) *the sign pattern σ_k is realizable with the pair $(1,0)$;*

(iii) *the sign pattern σ_k is realizable with any of the pairs $(2\ell+1, 2r)$, $\ell = 0, 1, \ldots, k$, $r = 1, 2, \ldots, (d-2k-1)/2$.*

Theorem 4 is proved in § 2. Notice that Cases (i), (ii) and (iii) exhaust all possible admissible pairs (pos, neg). It is also worth mentioning that Theorem 4 covers the only non-realizable case for degree 5 (up to the $\mathbb{Z}_2 \times \mathbb{Z}_2$-action) and the third and the last two non-realizable cases for degree 7 mentioned above. Indeed,

1) for $d = 5$, the sign pattern $\sigma^\bullet := (+,-,-,-,-,+)$ is not realizable with the admissible pair $(0,3)$ if and only if the sign pattern $\sigma^\circ := (+,+,-,+,-,-)$ is not realizable with the pair $(3,0)$ (should the couple $(\sigma^\bullet, (0,3))$ be realizable by some polynomial $P(x)$, then $(\sigma^\circ, (3,0))$ should be realizable by the polynomial $-P(-x)$); see part (iii) of Theorem 1;

2) for $d = 7$, the third example of Theorem 2 is exactly the case of σ_1 with the pair $(3,0)$ of Theorem 4;

3) by analogy with 1), the sign pattern $(+,-,-,-,-,-,-,+)$ is not realizable with the admissible pair $(0,3)$ or $(0,5)$ (see the last case in Theorem 2) if and only if the sign pattern $(+,+,-,+,-,+,-,-)$ is not realizable with the pair $(3,0)$ or $(5,0)$ (this is the case of σ_2, see Theorem 4).

The second aim of this paper is to present discriminant loci for families of polynomials of degree $d \leq 4$, see § 3. These loci and the coordinate hyperplanes partition the space of coefficients of monic degree d polynomials into open domains in each of which one and the same couple (sign pattern, admissible pair) is realized. We explain the correspondence between the couples and the domains and for degree 4, we explain the non-realizability of the case mentioned in part (ii) of Theorem 1 by the absence of the corresponding domain.

2 Proofs

Proof of Theorem 4. Part (i): Suppose that a polynomial $P := \sum_{j=0}^{d} a_j x^{d-j}$ has the sign pattern σ_k and realizes the pair $(2s+1, 0)$, $1 \leq s \leq k$. Denote by

$$P_e := \sum_{\nu=0}^{(d-1)/2} a_{2\nu+1} x^{d-2\nu-1} \quad \text{and} \quad P_o := \sum_{\nu=0}^{(d-1)/2} a_{2\nu} x^{d-2\nu}$$

its even and odd parts respectively. In each of the sequences $\{a_{2\nu+1}\}_{\nu=0}^{(d-1)/2}$ and $\{a_{2\nu}\}_{\nu=0}^{(d-1)/2}$ there is exactly one sign change. Therefore by Descartes' rule of signs each of the polynomials P_e and P_o has exactly one real positive root (denoted by x_e and x_o respectively) which is simple.

Remarks 5.

(i) The polynomial P_e (resp. P_o) is positive and increasing on (x_e, ∞) (resp. on (x_o, ∞)) and negative on $[0, x_e)$ (resp. on $(0, x_o)$).

(ii) One has $x_o \neq x_e$, otherwise $P(-x_o) = 0$, i.e. P has a negative root which is a contradiction.

Without loss of generality we assume all positive roots of P to be distinct. Indeed, if P has a positive root h of multiplicity $\kappa > 1$, then P is of the form $P = (x-h)^{\kappa} P^{\sharp}$, where $P^{\sharp}(h) \neq 0$. Then for $\varepsilon > 0$ small enough, the polynomial $(x-h)^{\kappa-1}(x-h-\varepsilon)P^{\sharp}$ realizes the same sign pattern as P, with the same admissible pair $(2s+1, 0)$, but has one simple positive root more than P. Continuing like this one can obtain after $\leq 2s$ steps a polynomial with $2s+1$ simple positive roots, defining the same sign pattern as P and realizing the admissible pair $(2s+1, 0)$

Denote the smallest three of the positive roots of P by $0 < \xi_1 < \xi_2 < \xi_3$. Hence at any point $\zeta \in (\xi_1, \xi_2)$ one has the $P(\zeta) > 0$; clearly P is negative on (ξ_2, ξ_3). One can choose $\zeta \neq x_e$ and $\zeta \neq x_o$. Hence it is impossible to have $P_e(\zeta) \leq 0$ and $P_o(\zeta) \leq 0$ (with at most one equality, see part (ii) of Remarks 5). It is also impossible to have $P_e(\zeta) \geq 0$ and $P_o(\zeta) \geq 0$. Indeed, this would imply that $x_e \leq \zeta$ and $x_o \leq \zeta$. Thus one would get $P_e(x) \geq 0$ and $P_o(x) \geq 0$, i.e. $P(x) > 0$, for $x \in (\xi_2, \xi_3)$ – a contradiction.

The two remaining possibilities are (one can skip the possibilities to have equalities, they were already taken into account):

a) $P_e(\zeta) > 0$, $P_o(\zeta) < 0$;

b) $P_e(\zeta) < 0$, $P_o(\zeta) > 0$.

The first one is impossible because it would imply that

$$P(-\zeta) = P_e(\zeta) - P_o(\zeta) > 0 \ ,$$

and since $P(0) < 0$ and $P(x) \to -\infty$ for $x \to -\infty$, the polynomial P would have at least one negative root in $(-\infty, -\zeta)$ and at least one in $(-\zeta, 0)$ – a contradiction.

So suppose that possibility b) takes place. In this case one must have $x_o < \zeta < x_e$. Without loss of generality one can assume that $\xi_1 = 1$; this can be achieved by a rescaling $x \mapsto \xi_1 x$. Hence $P_o(1) = \beta > 0$ and $P_e(1) = -\beta$. Considering the polynomial P/β instead of P, one can assume that $\beta = 1$. Lemma 6 below immediately implies that there are no real roots of P larger than 1 (one can use the Taylor series of P at 1) which is a contradiction finishing the proof of Part (i).

Lemma 6. *Under the above assumptions, $P^{(m)}(1) > 0$, for any $m = 1, 2, \dots, d$.*

Proof of Lemma 6. In the proof we use minimization arguments which can be applied to compact sets, so we allow zero values of the coefficients as well. For any $m = 1$, 2, $\dots$, d, it is true that if the sum of the coefficients $\delta := a_2 + a_4 + \cdots + a_{d-1}$ is fixed (recall that all these coefficients are negative), then $P_o^{(m)}(1)$ is minimal for $a_2 = \delta$, $a_4 = a_6 = \cdots = a_{d-1} = 0$. Indeed, when taking derivatives and computing their values at $x = 1$, monomials of larger degree in x are multiplied by larger factors (equal to these degrees); we apply $(d-3)/2$ times the fact that if $A \geq 0$, $B \geq 0$ and $\lambda > \mu > 0$, then for $A + B$ fixed, the sum $\lambda A + \mu B$ is maximal when $B = 0$. Therefore in what follows we assume that $a_4 = a_6 = \cdots = a_{d-1} = 0$, and hence $a_2 = 1 - a_0 < 0$.

Similarly, consider $P_e^{(m)}(1)$. Recall that $a_1 > 0$, $a_3 > 0$, $\dots$, $a_{2k+1} > 0$, $a_{2k+3} < 0$, $a_{2k+5} < 0$, $\dots$, $a_d < 0$. Hence for fixed sums $\delta_* := a_1 + a_3 + \cdots + a_{2k+1}$ and $\delta_{**} := a_{2k+3} + a_{2k+5} + \cdots + a_d$, the value of $P_e^{(m)}(1)$ is minimal if

$$\begin{cases} a_1 = \cdots = a_{2k-1} = 0 \ , \ a_{2k+1} = \delta_* \\ a_{2k+5} = \cdots = a_d = 0 \ , \ a_{2k+3} = \delta_{**}. \end{cases} \tag{2.1}$$

Let us now assume that conditions (2.1) are valid. Thus $P_e = a_{2k+1}x^{d-2k-1} + a_{2k+3}x^{d-2k-3}$ and $a_{2k+1} + a_{2k+3} = -1$. One can further decrease $P_e^{(m)}(1)$ by assuming that $a_{2k+1} = 0$, $a_{2k+3} = -1$. Thus $P(x) = a_0x^d + a_2x^{d-2} - x^{d-2k-3}$ and $a_0 + a_2 = 1$.

But then $P^{(m)}(x) = u_m a_0 x^{d-m} + v_m a_2 x^{d-2-m} - w_m x^{d-2k-3-m}$ and $P^{(m)}(1) = u_m a_0 + v_m a_2 - w_m$ for some numbers $0 \leq w_m \leq v_m < u_m$. Therefore

$$\begin{aligned} P^{(m)}(1) &= w_m(a_0 + a_2 - 1) + (v_m - w_m)(a_0 + a_2) + (u_m - v_m)a_0 \\ &= (v_m - w_m)(a_0 + a_2) + (u_m - v_m)a_0 > 0 \ . \end{aligned}$$

□

Proof of Part (ii): The polynomial $x^d - 1$ has the necessary signs of the leading coefficient and of the constant term. It has a single real simple root at 1. One can construct a polynomial of the form $S := x^d - 1 + \varepsilon \sum_{j=1}^{d-1} c_j x^j$, where $c_j = 1$ (resp. $c_j = -1$) if the sign at the corresponding position of σ_k is + (resp. −). For a small enough $\varepsilon > 0$, the polynomial S has a single simple real root close to 1, and its coefficients have the sign pattern σ.

Finally, our approach to settling Part (iii) is based on the following lemma borrowed from [4].

Lemma 7 (See Lemma 14 in [4])**.** *Suppose that the monic polynomials P_1 and P_2 of degrees d_1 and d_2 with sign patterns $\bar{\sigma}_1 = (1, \hat{\sigma}_1)$ and $\bar{\sigma}_2 = (1, \hat{\sigma}_2)$, respectively, realize the pairs (pos_1, neg_1) and (pos_2, neg_2).*

Then

(i) *if the last position of* $\hat{\sigma}_1$ *is* $+$, *then for any small enough* $\varepsilon > 0$, *the polynomial* $\varepsilon^{d_2} P_1(x) P_2(x/\varepsilon)$ *realizes the sign pattern* $(1, \hat{\sigma}_1, \hat{\sigma}_2)$ *and the pair* $(pos_1 + pos_2, neg_1 + neg_2)$.

(ii) *if the last position of* $\hat{\sigma}_1$ *is* $-$, *then for any* $\varepsilon > 0$ *small enough, the polynomial* $\varepsilon^{d_2} P_1(x) P_2(x/\varepsilon)$ *realizes the sign pattern* $(1, \hat{\sigma}_1, -\hat{\sigma}_2)$ *and the pair* $(pos_1 + pos_2, neg_1 + neg_2)$. *(Here* $-\hat{\sigma}$ *is the sign pattern obtained from* $\hat{\sigma}$ *by changing each* $+$ *by* $-$ *and vice versa.)*

Remark 8. Example 15 in [4] explains some of the possible applications of Lemma 7. We present and extend this example below. If

$$P_2 = x - 1 \ , \ x + 1 \ , \ x^2 + 2x + 2 \ , \ x^2 + 2x + 0.5 \ , \ x^2 - 2x + 2 \quad \text{or} \quad x^2 - 2x + 0.5 \ ,$$

then $(pos_2, neg_2) = (1, 0)$, $(0, 1)$, $(0, 0)$, $(0, 2)$, $(0, 0)$ and $(2, 0)$ respectively. Denote by τ the last entry of $\hat{\sigma}_1$. When $\tau = +$, then one has respectively $\hat{\sigma}_2 = (-)$, $(+)$, $(+, +)$, $(+, +)$, $(-, +)$ and $(-, +)$ and the sign pattern of $\varepsilon^{d_2} P_1(x) P_2(x/\varepsilon)$ equals

$$(1, \hat{\sigma}_1, -) \ , \ (1, \hat{\sigma}_1, +) \ , \ (1, \hat{\sigma}_1, +, +) \ , \ (1, \hat{\sigma}_1, +, +) \ , \ (1, \hat{\sigma}_1, -, +) \quad \text{or} \quad (1, \hat{\sigma}_1, -, +) \ .$$

If $\tau = -$, then $-\hat{\sigma}_2 = (+)$, $(-)$, $(-, -)$, $(-, -)$, $(+, -)$ and $(+, -)$ and the sign pattern of $\varepsilon^{d_2} P_1(x) P_2(x/\varepsilon)$ equals

$$(1, \hat{\sigma}_1, +) \ , \ (1, \hat{\sigma}_1, -) \ , \ (1, \hat{\sigma}_1, -, -) \ , \ (1, \hat{\sigma}_1, -, -) \ , \ (1, \hat{\sigma}_1, +, -) \quad \text{or} \quad (1, \hat{\sigma}_1, +, -) \ .$$

Proof of Part (iii): Recall that the sign pattern σ_k ends with $d - 2k - 1$ minuses. Set $\sigma_k = (+, +, \sigma^*, \sigma^\dagger)$, where the sign patterns σ^* (resp. $\sigma^\dagger$) consist of a minus followed by k pairs $(+, -)$ (resp. of $d - 2k - 2$ minuses).

The sign pattern $(+, +)$ is realizable by the polynomial $x + 1$ (hence with the pair $(0, 1)$). To obtain a polynomial realizing the sign pattern $(+, +, \sigma^*)$ with the pair $(2\ell + 1, 1)$ one applies Lemma 7, first $k - \ell$ times with $P_2 = x^2 - 2x + 2$, and then $2\ell + 1$ times with $P_2 = x - 1$. After this one applies Lemma 7, first $2r - 1$ times with $P_2 = x + 1$, and then $(d - 2k - 1)/2 - r$ times with $P_2 = x^2 + 2x + 2$ to realize the sign pattern σ_k with the pair $(2\ell + 1, 2r)$. □

3 Discriminant loci of cubic and quartic polynomials under a microscope

The goal of this section is mainly pedagogical. For the convenience of our readers, we present below detailed descriptions and illustrations of cases of (non)realizability of sign patterns and admissible pairs for polynomials of degree up to 4.

Define the *standard real discriminant locus* $\mathcal{D}_d \subset Pol_d$ as the subset of all polynomials having a real multiple root. (Detailed information about a natural stratification of $\mathcal{D}_d$ can be found in e.g., [6].) It is a well-known and simple fact that $Pol_d \setminus \mathcal{D}_d$ consists of $\left[\frac{d}{2}\right] + 1$ components distinguished by the number of real simple roots. Moreover, each such component is contractible in Pol_d. Obviously, the number of real roots in a family of monic polynomials changes if and only if this family crosses the discriminant locus $\mathcal{D}_d$.

3.1 Degrees 1 and 2

Clearly, a polynomial $x + u$ has a single real root $-u$ whose sign is opposite to the sign of the constant term. For degrees 2, 3 and 4 we will use the invariance of the zero set of the family of polynomials $x^n + a_1 x^{n-1} + \cdots + a_n$ with respect to the group of quasi-homogeneous dilatations $x \mapsto tx$, $a_j \mapsto t^j a_j$, to set the subdominant coefficient to 1. Namely, for $a_1 \neq 0$, if we set $x \mapsto a_1 x$, then this changes the family of polynomials

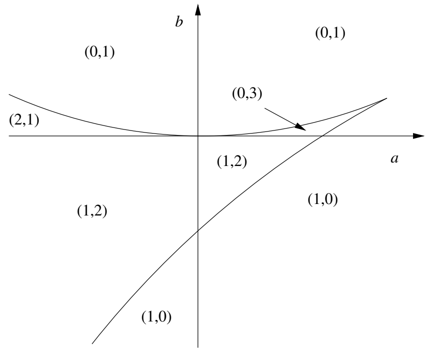

Figure 1. The discriminant locus of the family $x^3 + x^2 + ax + b$.

into $(a_1)^n(x^n + x^{n-1} + \cdots)$ which upon division by $(a_1)^n$ (which preserves the zero set) gives $x^n + x^{n-1} + \cdots$. Thus for $n = 2$, we consider the family $P_2 := x^2 + x + a$. For $a \leq 1/4$, it has two real roots; for $a < 1/4$, these are distinct. For $a \in (0, 1/4)$, they are both negative while for $a < 0$, they are of opposite signs.

3.2 Degree 3

For $n = 3$, we consider the family $P_3 := x^3 + x^2 + ax + b$. Its discriminant locus Σ is defined by the equation $4a^3 - a^2 + 4b - 18ab + 27b^2 = 0$. This is a curve shown in Fig. 1. It has an ordinary cusp for $(a, b) = (1/3, 1/27)$ and an ordinary tangency to the a-axis at the origin. In the eight regions of the complement to its union with the coordinate axes, the polynomial has roots as indicated in Fig. 1. (Here $(0, 1)$ means 0 positive and 1 negative real roots hence there exists a complex conjugate pair as well.) The point of the cusp corresponds to a triple root at $-1/3$, the upper arc corresponds to the case of one double real root to the right and a simple one to the left (and vice versa for the lower arc).

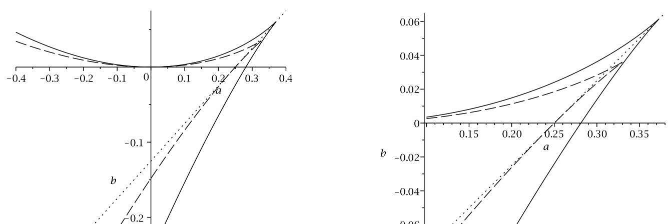

Figure 2. The projection of the discriminant locus of $x^4 + x^3 + ax^2 + bx + c$ to the plane of parameters (a, b). (Picture on the right shows the enlarged portion of the projection near the cusp point.)

3.3 Degree 4

For $n = 4$, we consider the family $P_4 := x^4 + x^3 + ax^2 + bx + c$. In Fig. 2 we show the projection $\tilde{\Phi}$ of its discriminant locus Φ in the (a, b)-plane. (For the other sets their projections in (a, b) are denoted by the same letters with tilde.) By the dashed line we show the set Σ for the family P_3. One has

$$\Phi \cap \{c = 0\} = \Sigma \cup \{b = c = 0\}.$$

By the solid line we represent the projection

$$\tilde{\Lambda} \ : \ 64a^3 - 18a^2 + 54b - 216ab + 216b^2 = 0$$

of the subset $\Lambda \subset \Phi$ for which the polynomial P_4 has a real root of multiplicity at least 3. The ordinary cusp point of $\tilde{\Lambda}$ is the projection of the point $(3/8, 1/16, 1/256)$ which defines the polynomial $x^4 + x^3 + 3x^2/8 + x/16 + 1/256 = (x + 1/4)^4$ to the plane (a, b).

At this point the set Φ has a swallowtail singularity, see e.g. [2]. On the upper arc of Λ the polynomial P_4 has one triple root to the right and a simple one to the left (and vice versa for the lower arc). The upper arc of $\tilde{\Lambda}$ has an ordinary tangency to the a-axis at the origin. Along the curve Λ the intersections of the hypersurface Φ with planes transversal to Λ have cusp points.

The cusp point of Σ belongs to Λ. At this point Λ intersects the (a, b)-plane. The tangent line $\tilde{L} : b = a/2 - 1/8$ to $\tilde{\Lambda}$ at its cusp at $(3/8, 1/16)$ is tangent to the curve Σ at $(1/4, 0)$. ($\tilde{L}$ is shown by the dotted line.) The set L corresponds to polynomials having two double roots. For $a < 3/8$, these roots are real, and for $a > 3/8$, they are complex conjugate. The curve L is tangent to the (a, b)-plane at the point $(1/4, 0, 0)$. It belongs to the half-space $\{c \geq 0\}$.

Now we consider the intersections of Φ with the planes parallel to the (b, c)-plane. For $a < 3/8$, they have two ordinary cusps (which are the points of Λ) and a transversal self-intersection point (which belongs to L). The first three pictures in Fig. 3 show this intersection with the plane $a = -0.1$ in different scales. The curves are tangent to the a-axis. Inside the curvilinear triangle (denoted by H_4) the polynomial has four distinct real roots. In the domain H_2 which surrounds H_4, the polynomial P_4 has two distinct real roots and a complex conjugate pair. In the domain H_0 above the self-intersection point it has two complex conjugate pairs. These domains are defined in the same way for all $a < 3/8$. For $a > 3/8$, the domain H_4 does not exist.

The set $\Phi \cap \{a < 0, b < 0, c > 0\}$ divides the set $\{a < 0, b < 0, c > 0\}$ into four sectors, see the first picture in Fig. 3. The intersection $\{a < 0, b < 0, c > 0\} \cap H_2$ consists of two contractible components. They correspond to the two cases $(0, 2)$ (the right sector, bordering $\{a < 0, b > 0, c > 0\}$) and $(2, 0)$ (the left sector) realizable with the sign pattern $(+, +, -, -, +)$. The other two cases realizable in $\{a < 0, b < 0, c > 0\}$ are $(2, 2)$ (the sector below) and $(0, 0)$ (the sector above).

For $a < 0$, $b > 0$, $c > 0$, and when the polynomial P_4 belongs respectively to H_4, H_2 or H_0, it realizes the cases $(2, 2)$, $(0, 2)$ and $(0, 0)$. The set $\{a < 0, b > 0, c > 0\} \cap H_2$ is contractible, so only one of the cases $(0, 2)$ and $(2, 0)$ (namely, $(0, 2)$) is realizable with the sign pattern $(+, +, -, +, +)$ (see the first picture in Fig. 3).

In $\{a < 0, b < 0, c < 0\}$ one can realize the cases $(1, 3)$ and $(1, 1)$. They correspond to the domains $\{a < 0, b < 0, c < 0\} \cap H_4$ (the curvilinear triangle) and $\{a < 0, b < 0, c < 0\} \cap H_2$ (its complement).

In $\{a < 0, b > 0, c < 0\}$ one can similarly realize the cases $(3, 1)$ (the curvilinear triangle) and $(1, 1)$ (its complement).

On the fourth and fifth pictures in Fig. 3 we present the intersection of Φ with the plane $\{a = 0.15\}$. The figures are quite similar to the first three pictures in Fig. 3, and the realizable pairs are the same with one exception. Namely, for $a > 0$, $b > 0$, $c > 0$ in the domain H_4 it is the pair $(0, 4)$ which is realized. And, clearly, the third component of the sign patterns changes from $-$ to $+$.

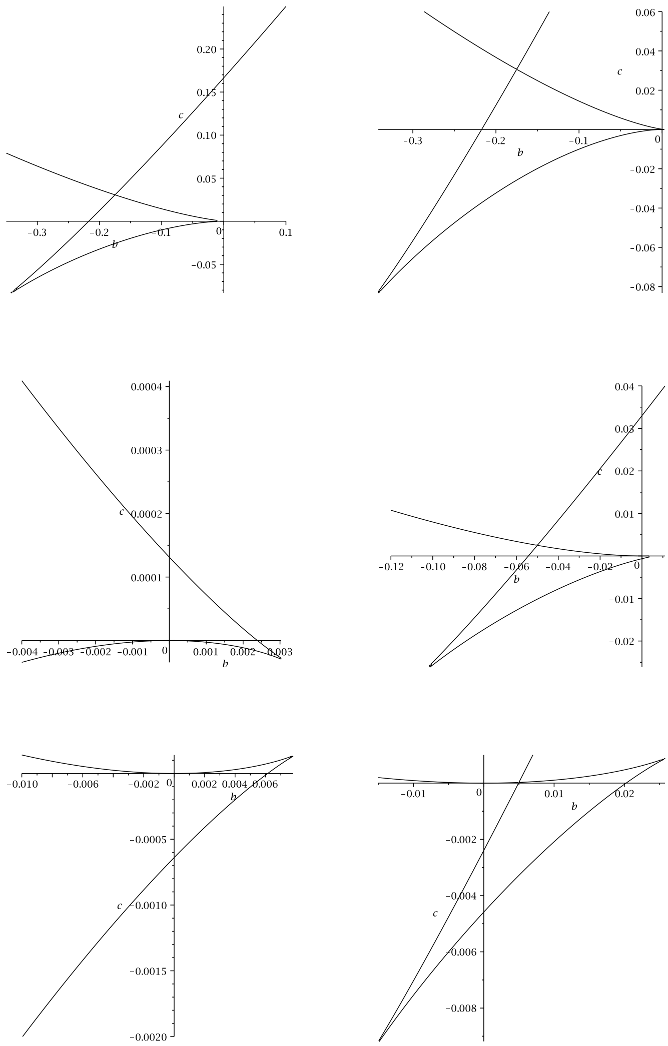

Figure 3. Intersections of the discriminant locus of $x^4 + x^3 + ax^2 + bx + c$ with the planes $a = -0.1$ (the first three pictures); $a = 0.15$ (the fourth and the fifth pictures); and $a = 0.26$ (the last picture).

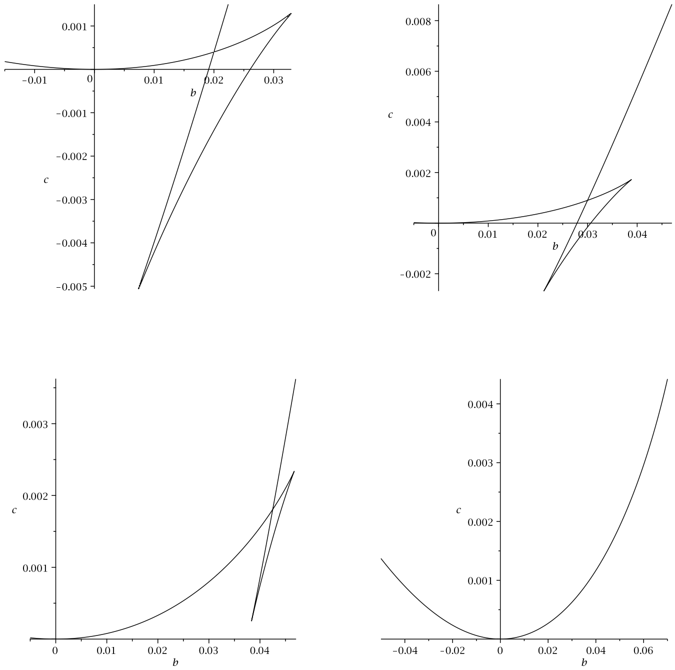

Figure 4. The intersection of the discriminant locus of $x^4 + x^3 + ax^2 + bx + c$ with the planes $a = 0.29; 0.31; 0.335; 0.4$.

The intersections of Φ with the planes $\{a = 0.26\}$, $\{a = 0.29\}$, $\{a = 0.31\}$ and $\{a = 0.335\}$ are shown on the last picture in Fig. 3 and in Fig. 4. For $a_0 > 0.375$, the intersections of Φ with the planes $\{a = a_0\}$ resemble the lower right picture in Fig. 4.

4 Final Remarks

The following important questions closely related to the main topic of the present paper remained unaddressed above.

Problem 2. *Is the set of all polynomials realizing a given pair (pos, neg) and having a sign pattern $\overline{\sigma}$ path-connected (if non-empty)?*

Given a real polynomial p of degree d with all non-vanishing coefficients, consider the sequence of pairs

$$\{(pos_0(p), neg_0(p)), (pos_1(p), neg_1(p)), (pos_2(p), neg_2(p)), \ldots, (pos_{d-1}(p), neg_{d-1}(p))\},$$

where $(pos_j(p), neg_j(p))$ is the numbers of positive and negative roots of $p^{(j)}$ respectively. Observe that if one is given the above sequence of pairs, then one knows the sign pattern of a polynomial p which is assumed to be monic. Additionally it is easy to construct examples when the converse fails.

Problem 3. *Which sequences of pairs are realizable by real polynomials of degree d with all non-vanishing coefficients?*

Notice that a similar problem for the sequence of pairs of real roots (without division into positive and negative) was considered in [7]. One can easily find examples of non-realizable sequences $\{(pos_j(p), neg_j(p))\}_{j=0}^{d-1}$. E. g. for $d = 4$ this is the sequence $(2, 0)$,

$(2, 1)$, $(1, 1)$, $(0, 1)$. Indeed, the sign pattern must be $(+, +, -, +, +)$ about which we know that it is not realizable with the pair $(2, 0)$. However it is not self-evident that all non-realizable sequences are obtained in this way.

Our final question is as follows.

Problem 4. *Is the set of all polynomials realizing a given sequence of pairs as above path-connected (if non-empty)?*

Acknowledgements

The first author is grateful to the Mathematics Department of Stockholm University for their hospitality.

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Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 63–82, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

Modified Chromatic Schultz Polynomial of Some Cycle Related Graphs

Rohith Raja M*
Department of Mathematics
CHRIST (Deemed to be University)
Bangalore, Karnataka, INDIA.
rohith.m@res.christuniversity.in

Sudev Naduvath
Department of Mathematics
CHRIST (Deemed to be University)
Bangalore, Karnataka, INDIA.
sudev.nk@christuniversity.in

Charles Dominic
Department of Mathematics
CHRIST (Deemed to be University)
Bangalore, Karnataka, INDIA.
charles.dominic@christuniversity.in

Abstract

Let $\mathcal{C} = c_1, c_2, \ldots, , c_\ell$ be a proper colouring of a connected graph G with chromatic number ℓ. Then, the chromatic Schultz polynomial $S(G,x)$ of G is defined as $S(G,x) = \sum\limits_{v_i,v_j \in V(G)} (\zeta(v_i) + \zeta(v_j))x^{d(u,v)}$, where $\zeta(v_i) = s$, when the vertex v_i has the colour c_s under $\mathcal{C}$. In this paper, we study the chromatic Schultz polynomials of certain cycle related graph classes.

Received 19 November 2018
Accepted in final form 14 October 2019
Communicated with Ján Karabáš.

Keywords graph colouring, χ^--colouring, χ^+-colouring, chromatic Schultz polynomial, modified chromatic Schultz polynomial.
MSC(2010) 05C31, 05C15, 05C12.

1 Introduction

For all terms and definitions, not defined specifically in this paper, we refer to [1, 5, 12, 13] and for graph classes, we refer to [2, 4]. Further, for graph colouring, see [3, 6, 9]. Unless mentioned otherwise, all graphs considered here are undirected, simple, finite and connected.

A *vertex colouring* is an assignment $c : V(G) \to \mathcal{C}$ which assigns the vertices of G, to a set of colours (or labels or weights) $\mathcal{C} = \{c_1, c_2, c_3, \ldots, c_\ell\}$. The vertex colouring c is said to be *proper* if no two adjacent vertices of G have same colours with respect to that colouring. The number of colours required in a minimum proper colouring of G is called the *chromatic number* of G and is denoted $\chi(G)$. A colour class of G is the set

*corresponding author

of all vertices of G which have the same colour. The cardinality of the colour class of a colour c_i is said to be the *strength* of that colour in G and is denoted by $\theta(c_i)$. We can also define a function $\zeta : V(G) \to \{1, 2, 3, \ldots, \ell\}$ such that $\zeta(v_i) = s$ if and only if $c(v_i) = c_s, c_s \in \mathcal{C}$.

If we colour the vertices of G in such a way that c_1 is assigned to maximum possible number of vertices, then c_2 is assigned to maximum possible number of remaining uncoloured vertices and proceed in this manner until all vertices are coloured, then such a colouring is called a χ^--*colouring* of G (see [7]). In a similar manner, if c_ℓ is assigned to maximum possible number of vertices, then $c_{\ell-1}$ is assigned to maximum possible number of remaining uncoloured vertices and proceed in this manner until all vertices are coloured, then such a colouring is called a χ^+-*colouring* of G (see [7, 8].

With respect to a proper colouring $c : V(G) \to \mathcal{C}$, a function $\zeta : V(G) \to \mathbb{N}_0$ is defined in [10] as $\zeta(v) = s$ if $c(v) = c_s \in \mathcal{C}$.

The chromatic version of Schultz polynomial was introduced in [10] as follows:

Definition 1 (Chromatic Schultz Polynomial of Graphs)**.** [10] Let G be a connected graph with chromatic number $\chi(G)$. Then, the *chromatic Schultz polynomial* of G denoted by $S_\chi(G, x)$ is defined as

$$S\chi(G, x) = \sum_{u,v \in V(G)} (\zeta(u) + \zeta(v))x^{d(u,v)}.$$

A modified version of the chromatic Schultz polynomial was also introduced in [10] as given below:

Definition 2 (Modified Chromatic Schultz Polynomial of Graphs)**.** [10] Let G be a connected graph with chromatic number $\chi(G)$. Then, the chromatic Schultz polynomial of G denoted by $S_\chi(G, x)$ is defined as

$$S\chi(G, x) = \sum_{u,v \in V(G)} (\zeta(u) \cdot \zeta(v))x^{d(u,v)}.$$

The two versions of chromatic Schultz polynomials of some fundamental graph classes were determined in [10]. Following that article, in this paper, we investigate the chromatic Schultz polynomials of certain related graph classes.

Definition 3. Let G be a connected graph with chromatic number $\chi(G)$. Then, the *modified chromatic Schultz polynomial* of G, denoted by $S^*_\chi(G, x)$, is defined as

$$S^*_\chi(G, x) = \sum_{u,v \in V(G)} (\zeta(u)\zeta(v))x^{d(u,v)}$$

Definition 4. Let G be a connected graph with chromatic number φ^- and φ^+ be the minimal and maximal parameter colouring of G. Then,

(i) the *modified* χ^--*chromatic Schultz polynomial* of G, denoted by $S^*_{\chi^-}$, is defined as

$$S^*_{\chi^-}(G, x) = \sum_{u,v \in V(G)} (\zeta_{\varphi^-}(u) \cdot \zeta_{\varphi^-}(v))x^{d(u,v)};$$

and

(ii) the χ^+-*chromatic Schultz polynomial* of G, denoted by $S^*_{\chi^-}$, is defined as

$$S^*_{\chi^+}(G,x) = \sum_{u,v \in V(G)} (\zeta_{\varphi^+}(u) \cdot \zeta_{\varphi^+}(v)) x^{d(u,v)}.$$

The two versions of chromatic Schultz polynomials of some fundamental graph classes namely paths, cycles and complete graphs were determined in [10]. The chromatic Schultz polynomial of certain other graph classes namely wheel graphs, helm graphs, closed helm graphs, sunflower graphs, flower graphs and sunflower graphs were determined in [11]. Following those articles, in this paper, we investigate the modified chromatic Schultz polynomials of certain cycle related graph classes.

2 Discussion and New Results

2.1 The Modified Chromatic Schultz Polynomial of Wheel Graphs

A *wheel graph, denoted by* W_n, is a graph obtained by joining all vertices of a cycle C_{n-1} to an external vertex. That is, $W_n = C_{n-1} + K_1$. The vertices on the cycle of W_n is called its rim vertices and the vertex K_1 is called the central vertex. The wheel graph on 9 vertices is shown in Figure 1.

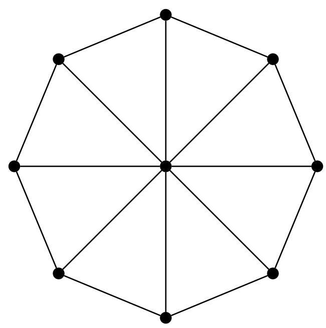

Figure 1. The wheel graph W_9.

The following theorem discusses the modified chromatic Schultz polynomial of wheel graphs.

Theorem 5. *Let W_n be a wheel graph on n vertices. Then, we have*

$$S^*_{\chi^-}(W_n,x) = \begin{cases} \frac{1}{8}(9n^2 - 44n + 35)x^2 + \frac{1}{2}(13n-13)x + \frac{1}{2}(5n+13); & \text{if } n \text{ is odd};\\ \frac{1}{8}(7n^2 - 6n - 88)x^2 + (8n+3)x + \frac{5}{2}(n+8); & \text{if } n \text{ is even.} \end{cases}$$

Proof. Let $V = \{v_1, v_2, \dots, v_n\}$ be the vertex set of W_n, where the rim vertices are labelled consecutively from v_1 to v_{n-1} and v_n is the central vertex. We note that the diameter of W_n is 2. Hence, the power of the variable x varies from 0 to 2 in the modified Schultz polynomial of W_n. Here, we need to consider the following two cases:

Note that if n is odd and $\chi(W_n) = 4$ if n is even. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring W_n.

Case-1: Let n be odd. In this case, $\chi(W_n) = 3$. Let c_1, c_2, c_3 be the three colours we use for colouring the vertices of W_n. Then, with respect to a χ^--colouring, the vertices $v_1, v_3, v_5, \dots v_{n-2}$ get the colour c_1, the vertices $v_2, v_4, v_6, \dots v_{n-1}$ get the colour c_2 and v_n gets the colour c_3. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 1.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1,c_1)	$\frac{n-1}{2}$
	(c_2,c_2)	$\frac{n-1}{2}$
	(c_3,c_3)	1
1	(c_1,c_2)	$n-1$
	(c_1,c_3)	$\frac{n-1}{2}$
	(c_2,c_3)	$\frac{n-1}{2}$
2	(c_1,c_1)	$\frac{(n-3)(n-1)}{8}$
	(c_2,c_2)	$\frac{(n-3)(n-1)}{8}$
	(c_1,c_2)	$\frac{(n-5)(n-1)}{4}$

Table 1

In Table 1, the possible distances between different pairs of vertices are written in the first column, the different colour pairs with respect to each distance is written in the second column and the number of corresponding colour pairs with respect to each distance is written in the third column.

From Table 1, we have the modified chromatic Schultz polynomial of the wheel graph W_n when number of vertices n is odd, is given by

$$\begin{aligned} S^*_{\chi^-}(W_n,x) &= [1(\frac{n-1}{2})+4(\frac{n-1}{2})+9]x^0+[2(n-1)+3(\frac{n-1}{2})+6(\frac{n-1}{2})]x^1 \\ &\quad +[1(\frac{(n-3)(n-1)}{8})+4(\frac{(n-3)(n-1)}{8})+2(\frac{(n-5)(n-1)}{8})]x^2 \\ &= \frac{1}{8}(9n^2-44n+35)x^2+\frac{13}{2}(n-1)x+\frac{1}{2}(5n+13) \end{aligned}$$

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1,c_1)	$\frac{n-2}{2}$
	(c_2,c_2)	$\frac{n-2}{2}$
	(c_3,c_3)	1
	(c_4,c_4)	1
1	(c_1,c_2)	$n-3$
	(c_1,c_4)	$\frac{n-2}{2}$
	(c_2,c_4)	$\frac{n-2}{2}$
	(c_1,c_3)	1
	(c_2,c_3)	1
	(c_3,c_4)	1
2	(c_1,c_1)	$\frac{(n-4)(n-2)}{8}$
	(c_2,c_2)	$\frac{(n-4)(n-2)}{8}$
	(c_1,c_2)	$\frac{(n-4)(n-2)}{8}$
	(c_2,c_3)	$\frac{n-4}{2}$
	(c_1,c_3)	$\frac{n-4}{2}$

Table 2

Case-2: Let n be even. In this case, $\chi(W_n)=4$. Let c_1,c_2,c_3,c_4 be the four colours we use for colouring the vertices of W_n. Then, with respect to a given χ^--colouring, the vertices $v_1, v_3, v_5, \dots v_{n-3}$ get the colour c_1, the vertices $v_2, v_4, v_6, \dots v_{n-2}$ get the colour c_2, the vertex v_3 gets the colour c_3 and the vertex v_4 gets the colour c_4. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 2.

From Table 2, we have the modified chromatic Schultz polynomial of the Wheel graph W_n when the number of vertices, n is even, is given by

$$\begin{aligned}
S^*_{\chi^-}(W_n, x) &= [1(\frac{n-2}{2}) + 4(\frac{n-2}{2}) + 9(1) + 16(1)]x^0 + [2(n-3) + 4(\frac{n-2}{2}) + \\
&\quad 8(\frac{n-2}{2}) + 3(1) + 6(1) + 12(1)]x^1 + [1\frac{(n-4)(n-2)}{8} \\
&\quad +4\frac{(n-4)(n-2)}{8} + 2\frac{(n-4)(n-2)}{8} + 6(\frac{n-4}{2}) + 3(\frac{n-4}{2})]x^2 \\
&= \frac{1}{8}(7n^2 - 6n - 88)x^2 + (8n+3)x + \frac{5}{2}(n+8)
\end{aligned}$$

Therefore,

$$S^*_{\chi^-}(W_n, x) = \begin{cases} \frac{1}{8}(9n^2 - 44n + 35)x^2 + \frac{1}{2}(13n - 13)x + \frac{1}{2}(5n + 13); & \text{if } n \text{ is odd;} \\ \frac{1}{8}(7n^2 - 6n - 88)x^2 + (8n+3)x + \frac{5}{2}(n+8); & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

Since χ^+-colouring can be obtained by reversing the colouring pattern, the modified chromatic Schultz polynomial of a wheel graph with respect to its χ^+-colouring can be determined as follows:

Theorem 6. *Let W_n be a wheel with n vertices. Then, we have*

$$S^*_{\chi^+}(W_n, x) = \begin{cases} \frac{1}{8}(25n^2 - 144n + 99)x^2 + \frac{1}{2}(17n - 17)x + \frac{1}{2}(13n - 11); & \textit{if } n \textit{ is odd;} \\ \frac{1}{8}(26n^2 - 100n - 40)x^2 + \frac{1}{2}(31n - 54)x + \frac{1}{2}(25n - 40); & \textit{if } n \textit{ is even.} \end{cases}$$

2.2 The Modified Chromatic Schultz Polynomial of Helm Graphs

A helm graph consists of wheel graphs consisting of n rim vertices and each rim vertex has an extra (pendant) vertex attached to it. Therefore, a helm graph consists of $2n+1$ vertices where n is the number of rim vertices. The helm graph on 17 vertices is depicted in Figure 2.

When n is odd, H_n is 4-colourable and when n is even, H_n is 3-colourable. The modified chromatic Schultz polynomial of the helm graph with respect to χ^- colouring, can be determined as n the following theorem.

Theorem 7. *Let H_n be a helm graph with $2n+1$ vertices. Then, we have*

$$S^*_{\chi^-}(H_n, x) = \begin{cases} \frac{1}{2}(n^2 - 3n)x^4 + \frac{1}{2}(5n^2 - 15n - 24)x^3 \\ +\frac{1}{8}(25n^2 + 128n - 241)x^2 + (11n + 11)x + \frac{5}{2}(3n+1); & \textit{if } n \textit{ is odd;} \\ \frac{1}{2}(n^2 - 3n)x^4 + \frac{1}{2}(27n)x^3 + \frac{1}{4}(25n^2 - 74n + 96)x^2 + \\ 11nx + \frac{1}{2}(15n + 2); & \textit{if } n \textit{ is even.} \end{cases}$$

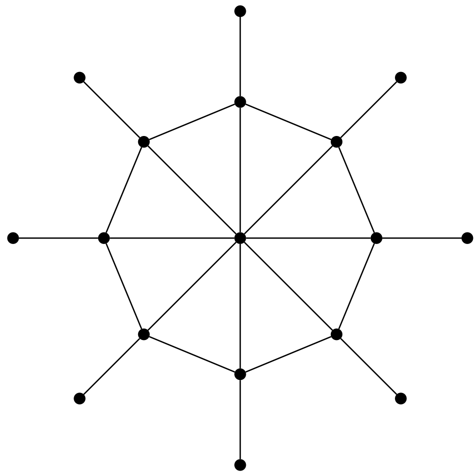

Figure 2. The helm graph H_8.

Proof. Let $V = \{v_1, v_2, \ldots, v_{2n+1}$ be the vertex set of H_n, where the rim vertices are labelled consecutively from v_1 to v_n, the corresponding extra vertices are labelled from v_{n+1} to v_{2n} and v_{2n+1} is the central vertex. We note that the diameter of H_n is 4. Hence, the power of the variable x varies from 0 to 4 in the modified Schultz polynomial of H_n. Here, we need to consider the following two cases:

Note that $\chi(H_n) = 4$ if the number of rim vertices n is odd and $\chi(H_n) = 3$ if n is even. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring H_n.

Case-1: Let n be odd. In this case, $\chi(H_n) = 4$. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring the vertices of H_n. Then, with respect to a χ^--colouring, the vertices $v_n, v_{n+1}, v_{n+2}, \ldots v_{2n}$ and v_{2n+1} get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-2}$ get the colour c_2, $v_2, v_4, v_6, \ldots v_{n-1}$ get the colour c_3, and v_n gets the colour c_4. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 3.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	$n+1$
	(c_2, c_2)	$\frac{n-1}{2}$
	(c_3, c_3)	$\frac{n-1}{2}$
	(c_4, c_4)	1
1	(c_1, c_2)	$n-1$
	(c_1, c_3)	$n-1$
	(c_1, c_4)	2
	(c_2, c_3)	$n-2$
	(c_2, c_4)	1
	(c_3, c_4)	1
2	(c_1, c_1)	n
	(c_2, c_2)	$\frac{(n-1)(n+1)}{8}$
	(c_3, c_3)	$\frac{(n-1)(n+1)}{8}$
	(c_1, c_2)	$n-1$
	(c_1, c_3)	$n-1$
	(c_2, c_3)	$\frac{(n-1)(n+1)}{4}$

	(c_1, c_4)	2
	(c_2, c_4)	$\frac{n-3}{2}$
	(c_3, c_4)	$\frac{n-3}{2}$
3	(c_1, c_1)	n
	(c_1, c_2)	$\frac{n(n-5)}{2}$
	(c_1, c_3)	$\frac{n(n-5)}{2}$
	(c_1, c_4)	$n-3$
4	(c_1, c_1)	$\frac{n(n-3)}{2}$

Table 3

In Table 3, the possible distances between different pairs of vertices are written in the first column, the different colour pairs with respect to each distance is written in the second column and the number of corresponding colour pairs with respect to each distance is written in the third column.

From Table 3, we have the chromatic Schultz polynomial of the helm graph H_n when number of rim vertices n is odd, is given by

$$\begin{aligned} S^*_{\chi^-}(H_n, x) &= [n+1+13(\frac{n-1}{2})+16]x^0 + [5(n-1)+6(n-2)+28]x^1 \\ &\quad +[n+13\frac{(n^2-1)}{8}+5(n-1)+6\frac{(n^2-1)}{4}+8+20\frac{n-3}{2}]x^2 + \\ &\quad [n+5\frac{n(n-5)}{2}+4(n-3)]x^3+[1(\frac{(n-3)n}{2})]x^4 \\ &= \frac{1}{2}(n^2-3n)x^4+\frac{1}{2}(5n^2-15n-24)x^3+\frac{1}{8}(25n^2+128n-241)x^2 \\ &\quad +(11n+11)x+\frac{5}{2}(3n+1). \end{aligned}$$

Distance $d(u, v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	$n+1$
	(c_2, c_2)	$\frac{n}{2}$
	(c_3, c_3)	$\frac{n}{2}$
1	(c_1, c_2)	n
	(c_1, c_3)	n
	(c_2, c_3)	n
2	(c_1, c_1)	n
	(c_2, c_2)	$\frac{n(n-2)}{4}$
	(c_1, c_2)	n
	(c_1, c_3)	n
	(c_2, c_3)	$\frac{(n-4)(n-2)}{2}$
	(c_3, c_3)	$\frac{n(n-2)}{4}$
3	(c_1, c_1)	n
	(c_1, c_2)	$\frac{5n}{2}$
	(c_1, c_3)	$\frac{5n}{2}$
4	(c_1, c_1)	$\frac{n(n-3)}{2}$

Table 4

Case-2: Let n be even. In this case, $\chi(H_n) = 3$. Let c_1, c_2, c_3 be the three colours we use for colouring the vertices of H_n. Then, with respect to a χ^- colouring, the vertices $v_{n+1}, v_{n+2}, v_{n+3}, \ldots v_{2n}$ and v_{2n+1} get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-1}$ get the colour c_2, and the vertices $v_2, v_4, v_6, \ldots v_n$ the colour c_3. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 4.

From Table 4, we have the modified chromatic Schultz polynomial of the helm graph H_n when the number of rim vertices n is even, is given by

$$\begin{aligned} S^*_{\chi^-}(H_n, x) &= [1(n+1) + 4(\frac{n}{2}) + 9(\frac{n}{2})]x^0 + [2(n) + 3(n) + 6(n)]x^1 \\ &\quad + [1(n) + 4\frac{n(n-2)}{4} + 2(n) + 3(n) + 6\frac{(n-4)(n-2)}{2} + 9\frac{n(n-2)}{4}]x^2 \\ &\quad + [1(n) + 2(\frac{5n}{2}) + 3(\frac{5n}{2}]x^3 + [\frac{(n-3)n}{2}]x^4 \\ &= \frac{1}{2}(n^2 - 3n)x^4 + \frac{27}{2}nx^3 + \frac{1}{4}(25n^2 - 74n + 96)x^2 + 11nx + \frac{1}{2}(15n + 2). \end{aligned}$$

Therefore,

$$S^*_{\chi^-}(H_n, x) = \begin{cases} \frac{1}{2}(n^2 - 3n)x^4 + \frac{1}{2}(5n^2 - 15n - 24)x^3 \\ +\frac{1}{8}(25n^2 + 128n - 241)x^2 + (11n + 11)x + \frac{5}{2}(3n + 1); & \text{if } n \text{ is odd;} \\ \frac{1}{2}(n^2 - 3n)x^4 + \frac{1}{2}(27n)x^3 + \frac{1}{4}(25n^2 - 74n + 96)x^2 + \\ (11n)x + \frac{1}{2}(15n + 2); & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

Using a similar argument, we get the modified chromatic Schultz polynomial of a helm graph, with regard to a χ^+-colouring, as follows:

Theorem 8. *Let H_n be a helm graph with n rim vertices. Then, with respect to χ^+ colouring, we have*

$$S^*_{\chi^+}(H_n, x) = \begin{cases} 8(n^2 - 3n)x^4 + (10n^2 - 30n - 12)x^3 + \frac{1}{8}(19n^2 + \\ 308n - 181)x^2 + (26n - 19)x + \frac{1}{2}(45n + 20); & \textit{if } n \textit{ is odd;} \\ \frac{9}{2}(n^2 - 3n)x^4 + \frac{1}{2}(63n)x^3 + \frac{1}{4}(9n^2 + 38n + 32)x^2 + \\ 11nx + \frac{1}{2}(23n + 18); & \textit{if } n \textit{ is even.} \end{cases}$$

2.3 The Modified Chromatic Schultz Polynomial of Closed Helm Graphs

A *closed helm graph* consists of helm graphs with each attached extra vertex connected to its neighbouring extra vertices by edges. Therefore, a closed helm graph H_n^* consists of $2n+1$ vertices where n is the number of rim vertices. When n is odd, H_n^* is 4-colourable and when n is even, H_n^* is 3-colourable. The closed helm graph on 17 vertices is depicted in Figure 3.

The modified chromatic Schultz polynomial of the helm graph with respect to χ^- colouring, can be determined as in the following theorem.

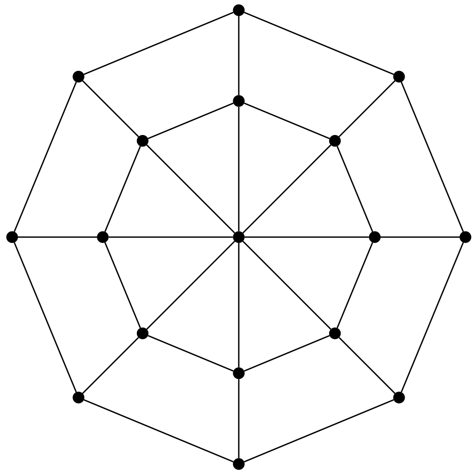

Figure 3. The closed helm graph H_8^*.

Theorem 9. *Let H_n^* be a closed helm graph with $2n+1$ vertices. Then, we have*

$$S^*_{\chi^-}(H_n^*, x) = \begin{cases} \frac{1}{8}(5n^2-4n-177)x^4 + \frac{1}{4}(9n^2-2n-3)x^3 \\ +\frac{1}{4}(2n^2+56n+10)x^2 + \frac{1}{2}(24n+42)x + (5n+29); & \text{if } n \text{ is odd;} \\ \\ \frac{1}{4}(n^2-10n+24)x^4 + (11n)x^3 + \frac{1}{8}(2n^2+92n)x^2 \\ +\frac{1}{2}(21n)x + (5n+9); & \text{if } n \text{ is even.} \end{cases}$$

Proof. Let $V = \{v_1, v_2, \dots, v_{2n+1}\}$ be the vertex set of H_n^*, where the rim vertices are labelled consecutively from v_1 to v_n, the corresponding extra vertices are labelled from v_{n+1} to v_{2n} and v_{2n+1} is the central vertex. We note that the diameter of H_n^* is 4. Hence, the power of the variable x varies from 0 to 4 in the modified Schultz polynomial of H_n^*. Here, we need to consider the following two cases:

Note that $\chi(H_n^*) = 4$ if the number of rim vertices n is odd and $\chi(H_n^*) = 3$ if n is even. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring H_n^*.

Case-1: Let n be odd. In this case, $\chi(H_n^*) = 4$. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring the vertices of H_n^*. Then, with respect to a χ^--colouring, the vertices $v_1, v_3, v_5, \dots v_{n-2}$ and the vertices $v_{n+2}, v_{n+4}, v_{n+6}, \dots v_{2n}$ get the colour c_1, the vertices $v_2, v_4, v_6, \dots v_{n-1}$ and the vertices $v_{n+3}, vn+5, v_{n+7}, \dots v_{2n-1}$ get the colour c_2, the vertices v_n and v_{n+1} gets the colour c_3 and the vertex v_{2n+1} gets the colour c_4. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 5.

In Table 5, the possible distances between different pairs of vertices are written in the first column, the different colour pairs with respect to each distance is written in the second column and the number of corresponding colour pairs with respect to each distance is written in the third column.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	$n-1$
	(c_2, c_2)	$n-1$
	(c_3, c_3)	2
	(c_4, c_4)	1

1	(c_1, c_2)	$3n-6$
	(c_1, c_3)	3
	(c_1, c_4)	$\frac{n-1}{2}$
	(c_2, c_3)	3
	(c_2, c_4)	$\frac{n-1}{2}$
	(c_3, c_4)	1
2	(c_1, c_1)	$\frac{3n-7}{2}$
	(c_2, c_2)	$\frac{3n-7}{2}$
	(c_3, c_3)	1
	(c_1, c_2)	$1+\frac{(n-5)(n-3)}{4}$
	(c_1, c_3)	$\frac{n-1}{2}$
	(c_2, c_3)	$\frac{(n-1)}{2}$
	(c_1, c_4)	$\frac{n-1}{2}$
	(c_2, c_4)	$\frac{n-1}{2}$
	(c_3, c_4)	1
3	(c_1, c_1)	$(\frac{n-3}{2})^2$
	(c_2, c_2)	$(\frac{n-3}{2})^2$
	(c_1, c_2)	$\frac{(n-3)(n+1)}{2}$
	(c_1, c_3)	$n-1$
	(c_2, c_3)	$n-1$
4	(c_1, c_1)	$\frac{(n-5)(n-3)}{8}$
	(c_2, c_2)	$\frac{(n-5)(n-3)}{8}$
	(c_1, c_3)	$\frac{n-7}{2}$
	(c_2, c_3)	$\frac{n-7}{2}$

Table 5

From Table 5, we have the modified chromatic Schultz polynomial of the closed helm graph H_n^* when number of rim vertices n is odd, is given by

$$\begin{aligned} S^*_{\chi^-}(H_n^*, x) &= [5(n-1)+34]x^0 + [2(3n-6)+9+12(\frac{n-1}{2})+30]x^1 \\ &\quad +[5(\frac{3n-7}{2})+9+2(\frac{n^2-8n+19}{4})+41(\frac{n-1}{2})+24]x^2 \\ &\quad +[5(\frac{n-3}{2})^2+2\frac{(n^2-2n-3)}{2}+9(n-1)]x^3+ \\ &\quad [5(\frac{(n^2-8n-15)}{4})+9(\frac{n-7}{2})]x^4 \\ &= \frac{1}{8}(5n^2-4n-177)x^4+\frac{1}{4}(9n^2-2n-3)x^3+\frac{1}{4}(2n^2+56n+10)x^2 \\ &\quad +\frac{1}{2}(24n+42)x+(5n+29). \end{aligned}$$

Case-2: Let n be even. In this case, $\chi(H_n^*)=3$. Then, with respect to a χ^- colouring, the vertices the vertices $v_1, v_3, v_5, \ldots v_{n-1}$ and the vertices $v_{n+2}, v_{n+4}, v_{n+6}, \ldots v_{2n}$ get the colour c_1, the vertices $v_2, v_4, v_6, \ldots v_n$ and the vertices $v_{n+1}, v_{n+3}, v_{n+5}, \ldots v_{2n-1}$ get the colour c_2, and the vertex v_{2n+1} get the colour c_3. The possible colour pairs and their numbers in G in terms of the distances between them are as given in Table 6.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1,c_1)	n
	(c_2,c_2)	n
	(c_3,c_3)	1
1	(c_1,c_2)	$3n$
	(c_1,c_3)	$\frac{n}{2}$
	(c_2,c_3)	$\frac{n}{2}$
2	(c_1,c_1)	$\frac{3n}{2}$
	(c_2,c_2)	$\frac{3n}{2}$
	(c_1,c_2)	$\frac{(n-4)(n+2)}{8}$
	(c_1,c_3)	$\frac{n}{2}$
	(c_2,c_3)	$\frac{n}{2}$
3	(c_1,c_1)	n
	(c_2,c_2)	n
	(c_1,c_2)	$3n$
4	(c_1,c_1)	$\frac{(n-6)(n-4)}{4}$
	(c_2,c_2)	$\frac{(n-6)(n-4)}{4}$

Table 6

From Table 6, we have the modified chromatic Schultz polynomial of H_n^*, when the number of rim vertices n is even, is given by

$$\begin{aligned} S^*_{\chi^-}(H_n^*,x) &= [5n+9]x^0+[6n+9(\frac{n}{2})]x^1+[5(\frac{3n}{2})+2(\frac{(n-4)(n+2)}{8})+9(\frac{n}{2})]x^2 \\ &\quad +11nx^3+[5(\frac{(n-6)(n-4)}{4})]x^4 \\ &= \frac{1}{4}(n^2-10n+24)x^4+11nx^3+\frac{1}{8}(2n^2+92n)x^2+\frac{21}{2}nx+(5n+9). \end{aligned}$$

Therefore,

$$S^*_{\chi^-}(H_n^*,x)=\begin{cases} \frac{1}{8}(5n^2-4n-177)x^4+\frac{1}{4}(9n^2-2n-3)x^3 \\ +\frac{1}{4}(2n^2+56n+10)x^2+\frac{1}{2}(24n+42)x+(5n+29); & \text{if } n \text{ is odd;} \\ \\ \frac{1}{4}(n^2-10n+24)x^4+(11n)x^3+\frac{1}{8}(2n^2+92n)x^2 \\ +\frac{1}{2}(21n)x+(5n+9); & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

Theorem 10. *Let H_n^* be a closed helm graph with n rim vertices. Then, with respect to χ^+ colouring, we have*

$$S^*_{\chi^+}(H_n^*,x)=\begin{cases} \frac{1}{8}(25n^2-144n-73)x^4+\frac{1}{4}(49n^2-216n+97)x^3+ \\ \frac{1}{4}(12^2+12n-28)x^2+\frac{1}{2}(79n-63)x+(25n-16); & \textit{if } n \textit{ is odd;} \\ \\ \frac{13}{4}(n^2-10n+24)x^4+(31n)x^3 \\ +\frac{1}{4}(3n^2+82n-24)x^2+\frac{1}{2}(41n)x+(13n+1); & \textit{if } n \textit{ is even.} \end{cases}$$

2.4 The Modified Chromatic Schultz Polynomial of Sunflower Graphs

A sunflower graph SF_n is a graph obtained by replacing each edge of the rim of a wheel graph W_n by a triangle such that two triangles share a common vertex if and only if the corresponding edges in W_n are adjacent in W_n. Therefore, a sunflower graph consists of $2n+1$ vertices where n is the number of rim vertices. The sunflower graph on 17 vertices is depicted in Figure 4.

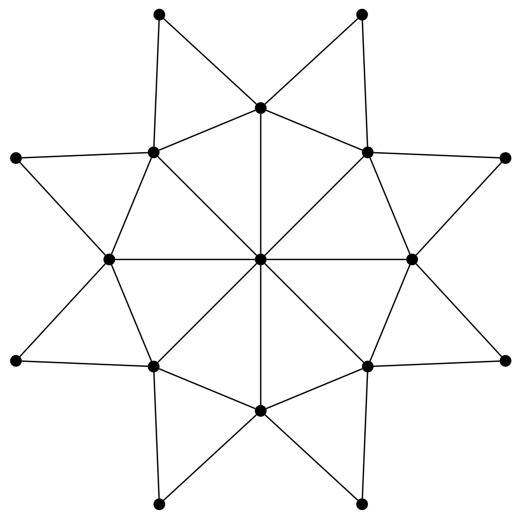

Figure 4. The sunflower graph SF_8.

When n is odd, SF_n is 4-colourable and when n is even, SF_n is 3-colourable. The modified chromatic Schultz polynomial of the sunflower graph with respect to χ^- colouring, can be determined as n the following theorem.

Theorem 11. *Let SF_n be a sunflower graph with $2n+1$ vertices. Then, we have*

$$S^*_{\chi^-}(SF_n, x) = \begin{cases} \frac{1}{2}(n^2-5n)x^4 + (15n-6)x^3 + \frac{1}{8}(24n^2+168n)x^2 \\ +\frac{1}{2}(27n+25)x + \frac{1}{2}(15n+5); & \text{if } n \text{ is odd;} \\ \\ \frac{1}{2}(n^2-5n)x^4 + \frac{3}{2}(n^2-6n)x^3 + \frac{1}{8}(19n^2+34n)x^2 \\ +\frac{21}{2}nx + \frac{1}{2}(15n+1); & \text{if } n \text{ is even.} \end{cases}$$

Proof. Let $V = \{v_1, v_2, \ldots, v_{2n+1}$ be the vertex set of SF_n, where the rim vertices of W_n are labelled consecutively from v_1 to v_n, the corresponding extra vertices of the triangle are labelled from v_{n+1} to v_{2n} and the central vertex is v_{2n+1}. We note that the diameter of SF_n is 4. Hence, the power of the variable x varies from 0 to 4 in the modified chromatic Schultz polynomial of SF_n. Here, we need to consider the following two cases:

Note that $\chi(SF_n) = 4$ if the number of rim vertices n is odd and $\chi(SF_n) = 3$ if n is even. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring SF_n.

Case-1: Let n be odd. In this case, $\chi(SF_n) = 4$. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring the vertices of SF_n. Then, with respect to a χ^--colouring, the vertices $v_{n+1}, v_{n+2}, v_{n+3}, \ldots v_{2n}$ and v_{2n+1} get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-2}$ get the colour c_2, $v_2, v_4, v_6, \ldots v_{n-1}$ get the colour c_3, and v_n gets the colour c_4. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 7.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1,c_1)	$n+1$
	(c_2,c_2)	$\frac{n-1}{2}$
	(c_3,c_3)	$\frac{n-1}{2}$
	(c_4,c_4)	1
1	(c_1,c_2)	$\frac{3n-3}{2}$
	(c_1,c_3)	$\frac{3n-3}{2}$
	(c_1,c_4)	3
	(c_2,c_3)	$n-2$
	(c_2,c_4)	1
	(c_3,c_4)	1
2	(c_1,c_1)	$2n$
	(c_1,c_2)	$n-1$
	(c_1,c_3)	$n-1$
	(c_1,c_4)	2
	(c_2,c_2)	$\frac{(n-3)(n-1)}{8}$
	(c_2,c_3)	$(\frac{(n-3)}{2})^2$
	(c_1,c_4)	$\frac{n-3}{2}$
	(c_2,c_4)	$\frac{(n-3)(n-1)}{8}$
	(c_3,c_4)	$\frac{n-3}{2}$
3	(c_1,c_1)	n
	(c_1,c_2)	$2n+2$
	(c_1,c_3)	$2n+2$
	(c_1,c_4)	$n-4$
4	(c_1,c_1)	$\frac{(n-5)n)}{2}$

Table 7

In Table 7, the possible distances between different pairs of vertices are written in the first column, the different colour pairs with respect to each distance is written in the second column and the number of corresponding colour pairs with respect to each distance is written in the third column.

From Table 7, we have the modified chromatic Schultz polynomial of the Sunflower graph SF_n when number of rim vertices n is odd, is given by

$$\begin{aligned} S_{\chi^-}(SF_n,x) &= [1(n+1)+4(\frac{n-1}{2})+9(\frac{n-1}{2})+16(1)]x^0 \\ &\quad +[2(\frac{3n-3}{2})+3(\frac{3n-3}{2})+4(3)+6(n-2)+8(1)+12(1)]x^1 \\ &\quad +[1(2n)+2(n-1)+3(n-1)+4(2)+4(\frac{(n-3)(n-1)}{2})+6(\frac{n-3}{2})^2 \\ &\quad +4(\frac{n-3}{2})+8(\frac{(n-3)(n-1)}{4})+12(\frac{n-3}{2})]x^2 \\ &\quad +[1(n)+2(2n+2)+3(2n+2)+4(n-4)]x^3+[1\frac{(n-5)n}{2}]x^4 \\ &= \frac{1}{2}(n^2-5n)x^4+(15n-6)x^3+\frac{1}{8}(24n^2+168)x^2 \\ &\quad +\frac{1}{2}(27n+25)x+\frac{1}{2}(15n+5). \end{aligned}$$

Case-2: Let n be even. In this case, $\chi(SF_n) = 3$. Let c_1, c_2, c_3 be the three colours we use for colouring the vertices of SF_n. Then, with respect to a χ^- colouring, the vertices $v_{n+1}, v_{n+2}, v_{n+3}, \ldots v_{2n}$ and v_{2n+1} get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-1}$ get the colour c_2, and the vertices $v_2, v_4, v_6, \ldots v_n$ the colour c_3. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 8

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	$n+1$
	(c_2, c_2)	$\frac{n}{2}$
	(c_3, c_3)	$\frac{n}{2}$
1	(c_1, c_2)	$\frac{3n}{2}$
	(c_1, c_3)	$\frac{3n}{2}$
	(c_2, c_3)	n
2	(c_1, c_1)	$2n$
	(c_1, c_2)	n
	(c_1, c_3)	n
	(c_2, c_2)	$\frac{n(n+2)}{8}$
	(c_2, c_3)	$\frac{n(n-2)}{8}$
	(c_3, c_3)	$\frac{n(n-2)}{8}$
3	(c_1, c_1)	n
	(c_1, c_2)	$\frac{(n-4)n}{2}$
	(c_1, c_3)	$\frac{(n-4)n}{2}$
4	(c_1, c_1)	$\frac{(n-5)n}{2}$

Table 8

From Table 8, we have the modified chromatic Schultz polynomial of the sunflower graph SF_n when the number of rim vertices n is even, is given by

$$\begin{aligned}
S^*_{\chi^-}(SF_n, x) &= [1(n+1) + 4(\frac{n}{2}) + 9(\frac{n}{2}]x^0 + [2(\frac{3n}{2}) + 3(\frac{3n}{2}) + 6(n)]x^1 \\
&\quad + [1(2n) + 2(n) + 3(n) + 4(\frac{n(n+2)}{8}) + 6(\frac{n(n-2)}{8}) + 9(\frac{n(n-2)}{8})]x^2 \\
&\quad + [n + 5(\frac{(n-4)n}{2})]x^3 + [\frac{(n-5)n}{2}]x^4 \\
&= \frac{1}{2}(n^2 - 5n)x^4 + \frac{3}{2}(n^2 - 6n)x^3 + \frac{1}{8}(19n^2 + 34n)x^2 + \frac{21}{2}nx + \frac{1}{2}(15n + 1).
\end{aligned}$$

Therefore,

$$S^*_{\chi^-}(SF_n, x) = \begin{cases} \frac{1}{2}(n^2 - 5n)x^4 + (15n - 6)x^3 + \frac{1}{8}(24n^2 + 168n)x^2 \\ + \frac{1}{2}(27n + 25)x + \frac{1}{2}(15n + 5); & \text{if } n \text{ is odd;} \\ \\ \frac{1}{2}(n^2 - 5n)x^4 + \frac{3}{2}(n^2 - 6n)x^3 + \frac{1}{8}(19n^2 + 34n)x^2 + \\ \frac{1}{2}(21n)x + \frac{1}{2}(15n + 1); & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

Theorem 12. *Let SF_n be a sunflower graph with n rim vertices. Then, with respect to χ^+ colouring, we have*

$$S_{\chi^+}(SF_n,x) = \begin{cases} 8(n^2-5n)x^4+(60n+24)x^3 \\ +\frac{1}{8}(18n^2+288n-24)x^2+(36n-25)x+\frac{1}{2}(45n+20); & \text{if } n \text{ is odd;} \\ \frac{9}{2}(n^2-5n)x^4+\frac{9}{2}(9n^2-2n)x^3+ \\ \frac{1}{8}(7n^2+218n)x^2+\frac{1}{2}(33n)x+\frac{1}{2}(23n+18); & \text{if } n \text{ is even.} \end{cases}$$

2.5 The Modified Chromatic Schultz Polynomial of Flower Graphs

A flower graph Fl_n is a graph which is obtained by joining the pendant vertices of a helm graph H_n to its central vertex. Therefore, a flower graph consists of $2n+1$ vertices where n is the number of rim vertices. The flower graph on 17 vertices is depicted in Figure 5.

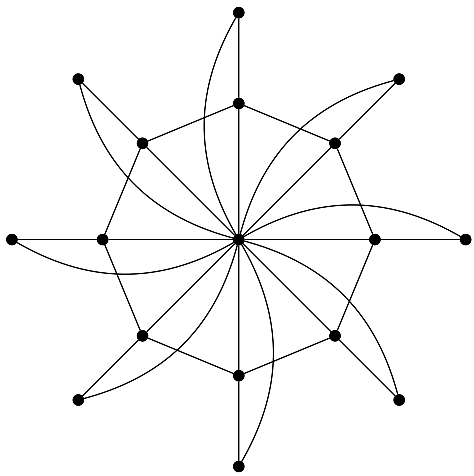

Figure 5. The flower graph Fl_8.

When n is odd, Fl_n is 5-colourable and when n is even, Fl_n is 4-colourable. The modified chromatic Schultz polynomial of the flower graph with respect to χ^- colouring, can be determined as n the following theorem.

Theorem 13. *Let Fl_n be a flower graph with $2n+1$ vertices. Then, we have*

$$S^*_{\chi^-}(Fl_n,x) = \begin{cases} \frac{3}{2}(2n^2-n-1)x^2+(21n+22)x+\frac{1}{2}(15n+69); & \text{if } n \text{ is odd;} \\ 3(n^2-n)x^2+\frac{1}{2}(45n)x+\frac{1}{2}(15n+32); & \text{if } n \text{ is even.} \end{cases}$$

Proof. Let $V = \{v_1, v_2, \dots, v_{2n+1}$ be the vertex set of Fl_n, where the rim vertices of W_n are labelled consecutively from v_1 to v_n, the corresponding extra vertices are labelled from v_{n+1} to v_{2n} and the central vertex is v_{2n+1}. We note that the diameter of Fl_n is 2. Hence, the power of the variable x varies from 0 to 2 in the modified chromatic Schultz polynomial of Fl_n. Here, we need to consider the following two cases:

Note that $\chi(Fl_n) = 5$ if the number of rim vertices n is odd and $\chi(Fl_n) = 4$ if n is even. Let c_1, c_2, c_3, c_4, c_5 be the five colours we use for colouring Fl_n.

Case-1: Let n be odd. In this case, $\chi(Fl_n) = 5$. Let c_1, c_2, c_3, c_4, c_5 be the five colours we use for colouring the vertices of Fl_n. Then, with respect to a χ^--colouring, the vertices $v_{n+1}, v_{n+2}, v_{n+3}, \ldots v_{2n}$ get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-2}$ get the colour c_2, $v_2, v_4, v_6, \ldots v_{n-1}$ get the colour c_3, v_n gets the colour c_4 and v_{2n+1} gets the colour c_5. The possible colour pairs and their numbers in G in terms of the distances between them are listed in the following table.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	n
	(c_2, c_2)	$\frac{n-1}{2}$
	(c_3, c_3)	$\frac{n-1}{2}$
	(c_4, c_4)	1
	(c_5, c_5)	1
1	(c_1, c_2)	$\frac{n-1}{2}$
	(c_1, c_3)	$\frac{n-1}{2}$
	(c_1, c_4)	1
	(c_1, c_5)	1
	(c_2, c_3)	$n-2$
	(c_2, c_4)	1
	(c_2, c_5)	$\frac{n-1}{2}$
	(c_3, c_4)	1
	(c_3, c_5)	$\frac{n-1}{2}$
	(c_4, c_5)	1
2	(c_1, c_1)	$\frac{(n-1)n}{2}$
	(c_1, c_2)	$\frac{(n-1)^2}{2}$
	(c_1, c_3)	$\frac{(n-1)^2}{2}$
	(c_1, c_4)	$n-1$

Table 9

In Table 9, the possible distances between different pairs of vertices are written in the first column, the different colour pairs with respect to each distance is written in the second column and the number of corresponding colour pairs with respect to each distance is written in the third column.

From Table 9, we have the modified chromatic Schultz polynomial of the flower graph Fl_n when number of rim vertices n is odd, is given by

$$\begin{aligned} S_{\chi^{-*}}(Fl_n, x) &= [1(n) + 4(\frac{n-1}{2}) + 9(\frac{n-1}{2}) + 16(1) + 25(1)]x^0 \\ &\quad +[2(\frac{n-1}{2}) + 3(\frac{n-1}{2}) + 4(1) + 5(1) \\ &\quad +6(n-2) + 8(1) + 10(\frac{n-1}{2}) + 12(1) + 15(\frac{n-1}{2}) + 20(1)]x^1 \\ &\quad +[1(\frac{n(n-1)}{2} + 2\frac{(n-1)^2}{2} + 3(\frac{(n-1)^2}{2}) + 4(n-1)]x^2 \\ &= \frac{3}{2}(2n^2 - n - 1)x^2 + (21n + 12)x + \frac{1}{2}(15n + 69). \end{aligned}$$

Case-2: Let n be even. In this case, $\chi(Fl_n) = 4$. Let c_1, c_2, c_3, c_4 be the four colours we use for colouring the vertices of Fl_n. Then, with respect to a χ^- colouring, the vertices $v_{n+1}, v_{n+2}, v_{n+3}, \ldots v_{2n}$ get the colour c_1, the vertices $v_1, v_3, v_5, \ldots v_{n-1}$ get the colour c_2, the vertices $v_2, v_4, v_6, \ldots v_n$ the colour c_3 and the vertex v_{2n+1} gets the colour c_4. The possible colour pairs and their numbers in G in terms of the distances between them are listed in Table 10.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	n
	(c_2, c_2)	$\frac{n}{2}$
	(c_3, c_3)	$\frac{n}{2}$
	(c_4, c_4)	1
1	(c_1, c_2)	$\frac{n}{2}$
	(c_1, c_3)	$\frac{n}{2}$
	(c_1, c_4)	n
	(c_2, c_3)	n
	(c_2, c_4)	$\frac{n}{2}$
	(c_3, c_4)	$\frac{n}{2}$
2	(c_1, c_1)	$\frac{n(n-1)}{2}$
	(c_1, c_2)	$\frac{n(n-1)}{2}$
	(c_1, c_3)	$\frac{n(n-1)}{2}$

Table 10

From Table 10, we have the modified chromatic Schultz polynomial of the helm graph Fl_n when the number of rim vertices n is even, is given by

$$\begin{aligned} S^*_{\chi^-}(Fl_n, x) &= [1(n) + 4(\frac{n}{2}) + 9(\frac{n}{2} + 16(1)]x^0 \\ &\quad +[2(\frac{n}{2}) + 3(\frac{n}{2}) + 4(n) + 6(n) + 8(\frac{n}{2} + 12(\frac{n}{2})]x^1 \\ &\quad +[1(\frac{n(n-1)}{2}) + 2(\frac{n-1)^2}{2}) + 3(\frac{n-1)^2}{2})] \\ &= 3(n^2 - n)x^2 + \frac{45}{2}nx + \frac{1}{2}(15n + 32). \end{aligned}$$

Therefore,

$$S^*_{\chi^-}(Fl_n, x) = \begin{cases} \frac{3}{2}(2n^2 - n - 1)x^2 + (21n + 22)x + \frac{1}{2}(15n + 69); & \text{if } n \text{ is odd;} \\ 3(n^2 - n)x^2 + \frac{1}{2}(45n)x + \frac{1}{2}(15n + 32); & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

The following theorem provides the modified chromatic Schultz polynomial of a flower graph Fl_n with respect to its χ^+-colouring.

Theorem 14. *Let Fl_n be a flower graph with n rim vertices. Then, with respect to χ^+ colouring, we have*

$$S^*_{\chi^+}(Fl_n, x) = \begin{cases} \frac{1}{2}(60n^2 - 75n + 15)x^2 + \frac{1}{2}(18n + 46)x + \frac{1}{2}(75n - 15); & \textit{if } n \textit{ is odd;} \\ 20(n^2 - n)x^2 + \frac{1}{2}(39n)x + \frac{1}{2}(45n + 1); & \textit{if } n \textit{ is even.} \end{cases}$$

2.6 The Modified Chromatic Schultz Polynomial of Friendship Graphs

A *friendship graph* F_n consists of n triangles joined together by a single vertex. F_n consists of $2n+1$ vertices and $3n$ edges. F_n is 3-colourable. The friendship graph on 9 vertices is shown in Figure 6.

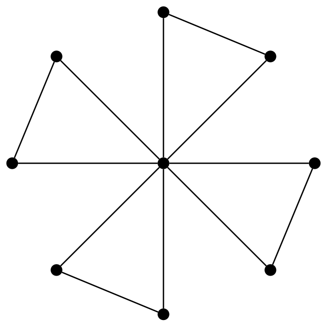

Figure 6. The friendship graph F_4.

The following theorem discusses the chromatic Schultz polynomial of friendship graphs:

Theorem 15. *Let F_n be a friendship graph with n triangles. Then, we have*

$$S_{\chi^-}(F_n, x) = \frac{9}{2}(n^2 - n)x^2 + (11n)x + (5n + 9)$$

Proof. Let $V = \{v_1, v_2, \ldots, v_{2n+1}\}$ be the vertex set of F_n. We note that the diameter of F_n is 2. Hence the power of the variable x varies from 0 to 2 in the modified chromatic Schultz polynomial of F_n. For Friendship graph, number of vertices is always odd. Now, $\chi(F_n) = 3$. Let c_1, c_2, c_3 be the three colours we use for colouring the vertices of F_n. Then, with respect to a χ^- colouring, one vertex each of the triangles are coloured c_1, the other is coloured c_2 and the common vertex is coloured c_3. The possible colour pairs and their numbers in F_n in terms of the distances between them are listed in Table 11.

Distance $d(u,v)$	Colour pairs	Number of pairs
0	(c_1, c_1)	n
	(c_2, c_2)	n
	(c_3, c_3)	1
1	(c_1, c_2)	n
	(c_1, c_3)	n
	(c_2, c_3)	n
2	(c_1, c_1)	$\frac{n(n-1)}{2}$
	(c_2, c_2)	$\frac{n(n-1)}{2}$
	(c_1, c_2)	$n(n-1)$

Table 11

From Table 11, the modified chromatic Schultz polynomial of F_n can be evaluated as follows:

$$S^*_{\chi^-}(F_n, x) = [1(n) + 4(n) + 9(1)]x^0 + [2(n) + 3(n) + 6(n)]x^1 +$$

$$[1(\frac{n(n-1)}{2}) + 4(\frac{n(n-1)}{2}) + 2(n(n-1))]x^2$$
$$= \frac{9}{2}(n^2 - n)x^2 + (11n)x + (5n + 9).$$

This completes the proof. □

In a similar way, the modified chromatic Schultz polynomial of a friendship graph with respect to its χ^+-colouring, can be determined as in the following theorem.

Theorem 16. *Let F_n be a friendship graph with n triangles. Then we have,*

$$S^*_{\chi^+}(F_n, x) = \frac{25}{2}(n^2 - n)x^2 + (11n)x + (13n + 1).$$

3 Conclusion

In this paper, we have discussed the modified chromatic Schultz polynomial of certain cycle related graphs. This polynomial can be determined for many other graph classes with finite diameter. Further investigations on the chromatic Schultz polynomial and modified chromatic Schultz polynomial of graph operations, graph products and graph powers are also promising. This study can be extended to other types of graph colouring such as injective colouring and equitable colouring. The concept can be extended to edge colouring and map colouring also. All these facts show a wide scope for further studies in this area.

Acknowledgements

Authors of the paper would like to acknowledge the anonymous referees, whose creative and constructive comments improved the content and presentation style of the paper significantly.

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Acta Universitatis Matthiae Belii, series Mathematics
Volume 27 (2019), 83–93, ISSN 1338-712X, ISBN 978-80-557-1690-9
Online version available at http://actamath.savbb.sk

Generalized $(\theta, \phi)-$derivations and Jordan ideals in prime rings

Gurninder S. Sandhu*
Patel Memorial National College, Department of Mathematics, Rajpura-140401, India
gurninder_ra@pbi.ac.in

Deepak Kumar
Punjabi University, Department of Mathematics, Patiala-147002, India
deep_math1@yahoo.com

Abstract
In this paper we prove some basic results on Jordan ideals of rings that make the study of derivations on Jordan ideals of (semi)prime rings parallel to the study of derivations on ideals of (semi)prime rings. More precisely, we prove a number of commutativity theorems with generalized $(\theta, \phi)-$derivations that act on Jordan ideals of prime rings. Consequently, many known results of this subject are unified or extended.

Received October 15, 2019
Accepted in final form January 22, 2020
Communicated with Miroslav Haviar.
Keywords Generalized $(\theta, \phi)-$derivations, Jordan ideals, prime rings, commutativity.
MSC(2010) 16W25, 16W20, 15A27.

1 Introduction

For any ring R, an additive subgroup J of R is said to be the Jordan ideal (resp. Lie ideal) of R if $J \circ R \subseteq J$ (resp. $[J, R] \subseteq J$), where the symbol $x \circ y$ (resp. $[x, y]$) denotes the Jordan product $xy + yx$ (resp. Lie product $xy - yx$). It is well-known that if J is a nonzero Jordan ideal of R then for any $j \in J$, $2[j^2, R] \subseteq J$, $4j^2R \subseteq J$, $4Rj^2 \subseteq J$ (see [[3], proof of Lemma 3]) and $4jRj \subseteq J$ (see [[3], proof of Theorem 3]). Moreover, $2J[R, R] \subseteq J$ and $2[R, R]J \subseteq J$ (see [[19], Lemma 2.4]). It is well-known that if union of two proper subgroups G_1 and G_2 of a group G is whole of G, then either $G_1 = G$ or $G_2 = G$, provided $G_1 \nsubseteq G_2$ and $G_2 \nsubseteq G_1$. This fact is known as *Brauer's trick.* Recall that a ring R is said to be prime (resp. semiprime) if for any $a, b \in R$, $aRb = (0)$ (resp. $aRa = (0)$) implies $a = 0$ or $b = 0$ (resp. $a = 0$) and an additive mapping $d : R \to R$ is called a derivation of R if $d(xy) = d(x)y + xd(y)$ for any $x, y \in R$. For a fixed $\alpha \in R$, a mapping $d_\alpha : R \to R$ such that $x \mapsto [\alpha, x]$ is a derivation, which is known as the inner derivation induced by α. For some fixed $a, b \in R$, a mapping $F_{a,b} : R \to R$ such that $x \mapsto ax + xb$ is called the generalized inner derivation of R. Immediately it follows that, if $F_{a,b}$ is generalized inner derivation, then we have $F_{a,b}(xy) = F_{a,b}(x)y + xd_{-b}(y)$, where d_{-b} is inner derivation associated with the element $(-b)$. This observation of Brešar [5] gave rise to the notion of generalized derivation. Accordingly, if d is a derivation of R and $F : R \to R$ is an additive map such that $F(xy) = F(x)y + xd(y)$ for all

*ORCID iD: 0000-0001-8618-6325

$x, y \in R$, then F is called a generalized derivation of R. The familiar examples of these mappings are derivations, left multipliers (i.e., an additive mapping $T : R \to R$ such that $T(xy) = T(x)y$ for all $x, y \in R$). For any ring endomorphisms θ and ϕ, a $(\theta, \phi)-$derivation is an additive mapping $d : R \to R$ such that $d(xy) = d(x)\theta(y) + \phi(x)d(y)$ for all $x, y \in R$. Such mappings appeared first time in the classic text [10] by Jacobson. Of course, a derivation is an $(1_R, 1_R)-$derivation, where 1_R is the identity map on R. A mapping $d_\alpha : R \to R$ such that $x \mapsto \alpha\theta(x) - \phi(x)\alpha$ is called the $(\theta, \phi)-$ inner derivation of R, where $\alpha \in R$ is a fixed element. Intuitively, a generalized $(\theta, \phi)-$ inner derivation of R is a mapping $F_{a,b} : R \to R$ such that $x \mapsto a\theta(x) + \phi(x)b$, where a, b are fixed elements of R. Similarly, if $F_{a,b}$ is a generalized $(\theta, \phi)-$inner derivation of R, then we have $F_{a,b}(xy) = F_{a,b}(x)\theta(y) + \phi(x)d_{-b}(y)$, where d_{-b} is $(\theta, \phi)-$inner derivation of R. This computation naturally extends the notion of generalized derivation to generalized $(\theta, \phi)-$derivation. More specifically, an additive mapping $F : R \to R$ is said to be a generalized $(\theta, \phi)-$derivation of R if $F(xy) = F(x)\theta(y) + \phi(x)d(y)$ for all $x, y \in R$, where d is a $(\theta, \phi)-$ derivation of R. We denote the $(\theta, \phi)-$commutator and $(\theta, \phi)-$anticommutator by $[x, y]_{\theta,\phi} = x\theta(y) - \phi(y)x$ and $(x \circ y)_{\theta,\phi} = x\theta(y) + \phi(y)x$ respectively. In order to prevent any confusion, note that a generalized $(\theta, \phi)-$derivation has also been used by many authors as generalized $(\alpha, \beta)-$derivation or generalized $(\sigma, \tau)-$derivation. We use the following commutator and anti-commutator identities without mentioning them specifically:

- $[x, yz] = y[x, z] + [x, y]z$,
- $[xy, z] = x[y, z] + [x, z]y$,
- $(x \circ yz) = (x \circ y)z - y[x, z] = y(x \circ z) + [x, y]z$ and
- $(xy \circ z) = x(y \circ z) - [x, z]y = (x \circ z)y + x[y, z]$.

The study of certain types of conditions (e.g. polynomial conditions and differential conditions) that finally imply commutativity of rings is very natural in the noncommutative ring theory. For instance the famous Wedderburn's theorem can be taken as the first precedent. In this line of investigation the initial results are mainly due to the work of Jacobson, Herstein and Posner (see [12]). Since then several authors investigated the commutativity of (semi)prime rings admitting various types of derivations which satisfy appropriate algebraic identities on suitable subsets of the rings. For example, we refer the reader to [1], [2], [6], [7], [13], [14], [15], [17], [18] with further references therein).

A classical result of Herstein [8] states that if d is a nonzero derivation of a 2-torsion free prime ring R such that $[d(x), d(y)] = 0$ for all $x, y \in R$, then R is commutative. Inspired by this, Bell and Daif [4] proved that: *If d is a nonzero derivation of a prime ring R and $d([x, y]) = 0$ for all $x, y \in I$, where I is nonzero ideal of R, then R is commutative.* In 2002, Ashraf and Rehman [2] extended this result by proving it for $(\sigma, \tau)-$derivations of 2-torsion free prime rings. Moreover, at the same time Ashraf and Rehman [1] studied the derivation d of prime ring R satisfying the conditions $d([x, y]) = [x, y]$ and $d(x \circ y) = (x \circ y)$, and obtained the commutativity of R. In [18], Rehman et al. obtained many informative results by studying generalized $(\alpha, \beta)-$derivations of prime rings that satisfy several conditions on Lie ideals. In the same direction, Marubayashi et al. [13] examined all these above mentioned conditions by replacing derivation and $(\sigma, \tau)-$derivation by generalized $(\alpha, \beta)-$derivation F. More precisely, they proved that every 2-torsion free prime ring is commutative if it satisfies any one of the identities: (i) $[F(x), x]_{\alpha,\beta} = 0$, (ii) $F([x, y]) = 0$, (iii) $F(x \circ y) = 0$, (iv) $F([x, y]) = [x, y]_{\alpha,\beta}$, (v) $F(x \circ y) = (x \circ y)_{\alpha,\beta}$, (vi) $F(xy) - \alpha(xy) \in Z(R)$, (vii) $F(x)F(y) - \alpha(xy) \in Z(R)$ for all $x, y \in R$. Recently, Dhara et al. [6] studied all these situations in semiprime rings admitting generalized $(\sigma, \tau)-$derivations.

On the other hand, Oukhtite and Mamouni [16] explored the commutativity of 2-torsion free prime ring R admitting a nonzero derivation d satisfying $d([x, y]) = 0$ on a nonzero Jordan ideal J of R. In addition, Oukhtite et al. [14] proved that a 2-torsion free prime ring R must be commutative if it admits a nonzero derivation d such that $d([x, y]) \in Z(R)$ for all $x, y \in J$, a nonzero Jordan ideal of R. Motivated by these commutativity theorems, we present some results which are the generalization and unification of the above-mentioned results. Precisely, we investigate the commutativity of 2-torsion free prime rings by taking the conditions: (i) $F([x, y]) = 0$, (ii) $F(x \circ y) = 0$, (iii) $F([x, y]) = [x, y]_{\theta,\phi}$, (iv) $F(x \circ y) = (x \circ y)_{\theta,\phi}$, (v)$F(xy) \pm \theta(xy) = 0$, (vi) $F(xy) \pm \phi(xy) \in Z(R)$, (vii) $[F(x), x]_{\theta,\phi} = 0$ for all $x, y \in J$; here F is a generalized $(\theta, \phi)-$derivation of R and J is a nonzero Jordan ideal of R.

The following lemmas are essential in the development of our main results.

Lemma 1. *[[7], Lemma 4] Let R be a 2-torsion free $*$-prime ring, J a nonzero $*$-Jordan ideal of R and d a nonzero (α, β)-derivation of R. If d commutes with $*$ and $d(J) = (0)$, then R is commutative.*

Lemma 2. *[[17], Lemma 3] Let R be a 2-torsion free $*$-prime ring and J a nonzero $*$-Jordan ideal of R. If $J \subseteq Z(R)$, then R is commutative.*

Lemma 3. *[[17], Theorem 1] Let $(R, *)$ be a 2-torsion free prime ring with involution. Let J be a nonzero $*$-Jordan ideal of R and d be a nonzero derivation centralizing on J. If R is $*$-prime, then R is commutative.*

Lemma 4. *[[19], Lemma 2.6] Let R be a 2-torsion free prime ring and J a nonzero Jordan ideal of R. If $aJb = (0)$, then $a = 0$ or $b = 0$.*

Lemma 5. *[[19], Lemma 2.7] Let R be a 2-torsion free prime ring and J a nonzero Jordan ideal of R. If J is a commutative Jordan ideal, then $J \subseteq Z(R)$.*

The following lemma will play a key role throughout.

Lemma 6. *Let R be a ring and J be a Jordan ideal of R. Then*

1. $2R[j^2, i] \subseteq J$ *for all* $i, j \in J$,
2. $2[j^2, i]R \subseteq J$ *for all* $i, j \in J$,
3. $2R[j^2, i]R \subseteq J$ *for all* $i, j \in J$.

Proof. (1) Let $r \in R$ and $x \in J$. Then we know that $2[r, x^2] \in J$ (see [3], proof of Lemma 3). That means

$$2(rx^2 - x^2r) \in J. \tag{1.1}$$

For any $y \in J$, we replace r by ry in (1.1) and find $2(ryx^2 - x^2ry) \in J$. But

$$\begin{aligned} 2(ryx^2 - x^2ry) &= 2(ryx^2 - x^2ry + rx^2y - rx^2y) \\ &= 2(ryx^2 - rx^2y) + 2(rx^2y - x^2ry) \\ &= 2r[y, x^2] + 2[r, x^2]y. \end{aligned}$$

Since $2[r, x^2]y \in J$ for all $r \in R$ and $x, y \in J$, it follows that $2r[y, x^2] \in J$ for each $x, y \in J$ and $r \in R$. In other words, $2R[J^2, J] \subseteq J$.

(2) We replace r by yr in order to find $2(yrx^2 - x^2yr) \in J$. But

$$\begin{aligned} 2(yrx^2 - x^2yr) &= 2(yrx^2 - x^2yr + yx^2r - yx^2r) \\ &= 2(yrx^2 - yx^2r) + 2(yx^2r - x^2yr) \\ &= 2y[r, x^2] + 2[y, x^2]r. \end{aligned}$$

Since $2y[r, x^2] \in J$ for all $r \in R$ and $x, y \in J$, it follows that $2[y, x^2]r \in J$ for all $x, y \in J$ and $r \in R$. In other words $2[J^2, J]R \subseteq J$.
(3) We have $2[y, x^2]r \in J$ for all $x, y \in J$ and $r \in R$. For any $s \in R$, we compute $2((x^2y - yx^2)r)s + 2s(x^2y - yx^2)r \in J$. That is $R[2J^2, J]R \subseteq J$ and we are done. □

Lemma 7. *Let R be a 2-torsion free prime ring and J be a nonzero Jordan ideal of R. If $[J, [R, R]] = (0)$ (i.e., $J \subseteq C_R([R, R])$), then R is commutative.*

Proof. For any $x \in J$, we have $[x, [R, R]] = (0)$. Assume that R is noncommutative. Then $[R, R]$ is a noncommutative Lie ideal of R. By Lemma 2 of [11], if R is not a PI-ring, then $[R, R]$ and R satisfy the same GPIs. Thus, by assumption, we have $[x, R] = (0)$ implies $x \in Z(R)$ for all $x \in J$. In the light of Lemma 2, R is commutative, which is a contradiction. □

2 The results on generalized $(\theta, \phi)-$derivations

In everything that follows, R denotes a prime ring with char(R) $\neq 2$, J is a nonzero Jordan ideal and θ, ϕ are the automorphisms of R, unless otherwise mentioned.

Proposition 8. *If $[x, y]_{\theta,\phi} = 0$ or $(x \circ y)_{\theta,\phi} = 0$ for all $x, y \in J$, then R is commutative.*

Proof. Let us consider

$$[x, y]_{\theta,\phi} = x\theta(y) - \phi(y)x = 0, \tag{2.1}$$

for all $x, y \in J$. When replacing x by $4xz^2$ in (2.1), we get

$$xz^2\theta(y) - \phi(y)xz^2 = 0. \tag{2.2}$$

Post-multiply (2.1) by z^2 and subtract from (2.2), we obtain $x[z, \theta(y)] = 0$, where $x, y, z \in J$. With the aid of Lemma 4, we get $[\theta(y), z^2] = 0$. On substituting $y = x \circ r$, we get $[\theta(x \circ r), z^2] = 0$ for all $x, z \in J$ and $r \in R$. Explicitly we have

$$\theta(x)[\theta(r), z^2] + [\theta(r), z^2]\theta(x) = 0. \tag{2.3}$$

Replacing x by $2x[p, q]$ in (2.3), we obtain $\theta(x)[[\theta(p), \theta(q)], [\theta(r), z^2]] = 0$ for all $p, q, r \in R$ and $x, z \in J$. Invoking Lemma 4 gives $[[\theta(p), \theta(q)], [\theta(r), z^2]] = 0$. That is $[[R, R], [R, z^2]] = (0)$. For any $a, b, c \in R$, we have $[[a, b], [c, z^2]] = 0$. Replacing b by ba, we obtain $[a, b][a, [c, z^2]] = 0$. Taking br in place of b, we get $[a, b]R[a, [c, z^2]] = (0)$ for all $a, b, c \in R$ and $z \in J$. It implies that either R is commutative or $[R, [R, z^2]] = 0$. In the latter case we have $[r, [s, z^2]] = 0$ for all $z \in J$ and $r, s \in R$. Replacing s by z^2s, we have $[r, z^2][s, z^2] = 0$. It implies that $[r, z^2]R[r, z^2] = (0)$ for all $z \in J$ and $r \in R$. It forces that $[r, z^2] = 0$. Hence R is commutative (see [[14], proof of Lemma 5]). □

Theorem 9. *Let $d : R \to R$ be a $(\theta, \phi)-$derivation such that $d(x^2) = 0$ for all $x \in J$. Then, $d = 0$.*

Proof. By hypothesis, we have $d(x^2) = 0$, where $x \in J$. By linearizing, we get

$$d(xy + yx) = 0 \text{ for all } x, y \in J. \tag{2.4}$$

Now, we have two cases, as follows:
Case 1. Let $J \subseteq Z(R)$. For any $r \in R$ and $u \in J$, we have $2ru = u \circ r$. Hence, equation (2.4) gives that $2d(xy) = 0$ which implies $d(xy) = 0$. Substitute $2yr$ for y, we get $\phi(x)\phi(y)d(r) = 0$ for all $x, y \in J$ and $r \in R$. That is, $xJ\phi^{-1}(d(r)) = 0$. Hence, $\phi^{-1}(d(r)) = 0$ for all $r \in R$. It forces that $d = 0$.
Case 2. Suppose $J \nsubseteq Z(R)$. With the aid of Lemma 6, we substitute $y = 2r[u^2, v]s$ (where $r, s \in R$ and $u, v \in J$) in (2.4). Thus we have

$$d(xr[u^2, v]s) + d(r[u^2, v]sx) = 0.$$

Replacing s by sx in the last expression, we get $d(xr[u^2, v]s)\theta(x) + \phi(xr[u^2, v]s)d(x) + d(r[u^2, v]sx)\theta(x) + \phi(r[u^2, v]sx)d(x) = 0$ for all $x, y \in J$ and $r, s \in R$. It reduces to $\phi(x \circ r[u^2, v]s)d(x) = 0$. For any $z \in J$, we take zr in place of r and obtain $\phi(z)\phi(x \circ r[u^2, v]s)d(x) + \phi([x, z])\phi(r)\phi([u^2, v]s)d(x) = 0$. It implies $\phi([x, z])R\phi([u^2, v]s)d(x) = 0$ for all $x, y, z \in J$ and $r, s \in R$. That means, for each $x \in J$, either $[x, z] = 0$ or $\phi([u^2, v]s)d(x) = 0$. We set

$$G_1 = \{x \in J : [x, z] = 0 \quad \text{for all } z \in J\} \text{ and}$$
$$G_2 = \{x \in J : \phi([u^2, v]s)d(x) = 0 \text{ for all } u, v \in J,\ s \in R\}.$$

It is easy to see that G_1 and G_2 are additive subgroups of J and $J = G_1 \cup G_2$. By Brauer's trick, we have either $J = G_1$ or $J = G_2$. If $J = G_1$, that means $[x, z] = 0$ for all $x, z \in J$. It easily implies that $J \subseteq Z(R)$, which is a contradiction. On the other hand, let $I = G_2$ i.e., for any $s \in R$ and $x, u, v \in J$, we have $\phi([u^2, v]s)d(x) = 0$. That is $\phi([u^2, v])Rd(x) = (0)$ for all $x, u, v \in J$. Since R is a prime ring, either $[u^2, v] = 0$ for all $u, v \in J$ or $d(J) = (0)$. In view of [[14], proof of Lemma 5], a contradiction follows. Finally, we suppose that $d(x) = 0$ for all $x \in J$. It forces that $d = 0$, by Lemma 7. Thus we have $d = 0$ in each case. □

Remark 10. Similarly, we can prove that: *Let R be a 2-torsion free prime ring and J a nonzero Jordan ideal of R. If R admits a nonzero $(\theta, \phi)-$derivation d such that $d([x, y]) = 0$ for all $x, y \in J$, then R is commutative.* Consequently, this result proves a complete form of Theorem 3 of [2].

Theorem 11. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d such that $F([x, y]) = 0$ for all $x, y \in J$. Then, R is commutative.*

Proof. By our hypothesis, we have $F(xy) - F(yx) = 0$ for all $x, y \in J$. That is

$$F(x)\theta(y) + \phi(x)d(y) - F(y)\theta(x) - \phi(y)d(x) = 0.$$

In view of Lemma 6, substitute $2r[u^2, v]s$ for y, where $u, v \in J$ and $r, s \in R$, then

$$F(x)\theta(r[u^2, v]s) + \phi(x)d(r[u^2, v]s) - F(r[u^2, v]s)\theta(x) - \phi(r[u^2, v]s)d(x) = 0. \tag{2.5}$$

Replace s by sx in (2.5), we get

$$\begin{aligned} F(x)\theta(r[u^2, v]s)\theta(x) + \phi(x)d(r[u^2, v]s)\theta(x) + \phi(x)\phi(r[u^2, v]s)d(x) - F(r[u^2, v]s) \\ \theta(x)\theta(x) - \phi(r[u^2, v]s)d(x)\theta(x) - \phi(r[u^2, v]s)\phi(x)d(x) = 0. \end{aligned} \tag{2.6}$$

Equation (2.5) reduces (2.6) to

$$\phi([x, r[u^2, v]s])d(x) = 0 \text{ for all } x, u, v \in J, \ r, s \in R. \tag{2.7}$$

Taking qr instead of r in (2.7), where $q \in R$, we get $\phi([x, q])\phi(r[u^2, v]s)d(x) = 0$. It implies that

$$[x, q]r[u^2, v]R\phi^{-1}d(x) = 0 \text{ for all } x, u, v \in J, \ r, q \in R.$$

Applying Brauer's trick, we get that either $[x, q]r[u^2, v] = 0$ for all $x, u, v \in J$ and $r, q \in R$ or $d(x) = 0$ for all $x \in J$. The second case forces R commutative. Now the first case gives $[x, q]R[u^2, v] = 0$ for all $x, u, v \in J$ and $q \in R$. It implies that either $J \subseteq Z(R)$ or $[u^2, v] = 0$ for all $u, v \in J$. In both of these cases, we get R is commutative (see Lemma 2 and [[14], proof of Lemma 5] respectively). □

Using similar techniques as we used in the proof of Theorem 11 with necessary variations, we can obtain the following result:

Theorem 12. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d such that $F(x \circ y) = (0)$ for all $x, y \in J$. Then, R is commutative.*

Theorem 13. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d such that $F([x, y]) = [x, y]_{\theta,\phi}$ for all $x, y \in J$. Then, R is commutative.*

Proof. By hypothesis, we have $F(xy) - F(yx) = x\theta(y) - \phi(y)x$ for all $x, y \in J$. Taking $y = 2r[u^2, v]s$ in particular, where $r, s \in R$ and $u, v \in J$, we find

$$F(x2r[u^2, v]s) - F(2r[u^2, v]sx) = x\theta(2r[u^2, v]s) - \phi(2r[u^2, v]s)x.$$

Replace s by sx, we obtain

$$F(x.2r[u^2, v]s)\theta(x) + \phi(x.2r[u^2, v]s)d(x) - F(2r[u^2, v]s.x)\theta(x) - \phi(2r[u^2, v]s.x)d(x) = x\theta(2r[u^2, v]s)\theta(x) - \phi(2r[u^2, v]s)\phi(x)x.$$

Our hypothesis reduces it to

$$\phi([x, r[u^2, v]s])d(x) = \phi(r[u^2, v]s)[x, x]_{\theta,\phi}. \tag{2.8}$$

Substituting pr instead of r in (2.8) and using it, we get $\phi([x, p])\phi(r[u^2, v]s)d(x) = 0$ for all $x, u, v \in J$ and $r, s, p \in R$. It implies that

$$[x, p]R[u^2, v]s\phi^{-1}(d(x)) = 0.$$

Since R is prime ring, we find that for each $x \in J$, either $[x, p] = 0$ for all $p \in R$ or $[u^2, v]s\phi^{-1}(d(x)) = 0$ for all $u, v \in J$ and $s \in R$. Application of Brauer's trick yields that either $J \subseteq Z(R)$ (and hence R is commutative by Lemma 2) or $[u^2, v]s\phi^{-1}(d(x)) = 0$. In the latter case we get that either $[u^2, v] = 0$ for all $u, v \in J$ or $d(x) = 0$ for all $x \in J$. The prior case implies that R is commutative (see the proof of Lemma 5 in [14]). Assume that $d(x) = 0$ for all $x \in J$. In view of Lemma 1, we get the commutativity of R. □

Using similar techniques as we used in the proof of Theorem 13 with necessary variations, we can obtain the following result:

Theorem 14. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a (θ, ϕ)-derivation d such that $F(x \circ y) = (x \circ y)_{\theta,\phi}$ for all $x, y \in J$. Then, R is commutative.*

Theorem 15. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d such that $F(xy) \in Z(R)$ for all $x, y \in J$. Then, R is commutative.*

Proof. By our hypothesis, we have $F(xy) \in Z(R)$ for any $x, y \in J$. Let us put $y = 2r[u^2, v]s$, where $r, s \in R$ and $u, v \in J$, that is

$$F(x)\theta(r[u^2, v]s) + \phi(x)d(r[u^2, v]s) \in Z(R). \tag{2.9}$$

Replace s by sq, where $q \in R$, we get

$$F(x)\theta(r[u^2, v]s)\theta(q) + \phi(x)d(r[u^2, v]s)\theta(q) + \phi(x)\phi(r[u^2, v]s)d(q) \in Z(R).$$

Commuting with $\theta(q)$ and using (2.9), we get

$$[\phi(x)\phi(r[u^2, v]s)d(q), \theta(q)] = 0 \text{ for all } x, u, v \in J, \; r, s, q \in R. \tag{2.10}$$

Replace x by $2[m, n]x$ (2.10), where $m, n \in R$, we get

$$[\phi([m, n]), \theta(q)]\phi(r[u^2, v]s)d(q) = 0.$$

That is

$$[[m, n], \phi^{-1}(\theta(q))]R[u^2, v]s\phi^{-1}(d(q)) = (0)$$

for all $u, v \in J$ and $s, q, m, n \in R$. It implies that either $[[m, n], \phi^{-1}(\theta(q))] = 0$ or $[u^2, v]s\phi^{-1}(d(q)) = 0$. Using Brauer's trick, we get either $[\phi([m, n]), \theta(q)] = 0$ for all $m, n, q \in R$ or $[u^2, v]s\phi^{-1}(d(q)) = 0$ for all $u, v \in J$ and $s, q \in R$. Clearly first assertion implies commutativity of R. Thus we consider the latter case i.e., $[u^2, v]R\phi^{-1}(d(q)) = (0)$ for all $u, v \in J$ and $q \in R$. Since R is prime ring and d is a nonzero $(\theta, \phi)-$derivation, we get $[u^2, v] = 0$ for all $u, v \in J$. In view of [[14], proof of Lemma 5], R is commutative. □

By substituting $F + \theta$ and $F - \theta$ for F in Theorem 15, we have the following theorem:

Theorem 16. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d. If any one of the following holds,*

1. $F(xy) + \theta(xy) \in Z(R)$,
2. $F(xy) - \theta(xy) \in Z(R)$,

for all $x, y \in J$, then R is commutative.

Theorem 17. *Let $F : R \to R$ be a generalized (θ, ϕ)-derivation of R associated with a nonzero (θ, ϕ)-derivation d of R such that $[F(x), x]_{\theta,\phi} = 0$ for all $x \in J$. Then, R is commutative.*

Proof. By hypothesis, we have

$$[F(x), x]_{\theta,\phi} = 0 \text{ for all } x \in J. \tag{2.11}$$

It implies that

$$[F(x), y]_{\theta,\phi} + [F(y), x]_{\theta,\phi} = 0 \text{ for all } x \in J. \tag{2.12}$$

In view of Lemma 6, we take $2r[u^2, v]x$ in place of y in (2.12) in order to obtain

$$\begin{aligned}[F(x), 2r[u^2, v]]_{\theta,\phi}\theta(x) + \phi(2r[u^2, v])[F(x), x]_{\theta,\phi} + [F(2r[u^2, v])\theta(x), x]_{\theta,\phi} \\ +[\phi(2r[u^2, v])d(x), x]_{\theta,\phi} = 0.\end{aligned} \tag{2.13}$$

Re-writing it as

$$[F(x), 2r[u^2, v]]_{\theta,\phi}\theta(x) + \phi(2r[u^2, v])[F(x), x]_{\theta,\phi} + \Lambda(x, u, v, r) = 0$$

for all $x, u, v \in J,\ r \in R$, where

$$\begin{aligned}\Lambda(x, u, v, r) &= [F(2r[u^2, v])\theta(x), x]_{\theta,\phi} + [\phi(2r[u^2, v])d(x), x]_{\theta,\phi}\\ &= F(2r[u^2, v])\theta(x)\theta(x) - \phi(x)F(2r[u^2, v])\theta(x) + \phi(2r[u^2, v])d(x)\theta(x)\\ &\quad -\phi(2r[u^2, v])\phi(x)d(x) + \phi(2r[u^2, v])\phi(x)d(x) - \phi(x)\phi(2r[u^2, v])d(x)\\ &= [F(2r[u^2, v]), x]_{\theta,\phi}\theta(x) + \phi(2r[u^2, v])[d(x), x]_{\theta,\phi} + \phi([2r[u^2, v], x])d(x).\end{aligned}$$

Combining the last relation with (2.13) and using (2.11) and (2.12), we obtain

$$\phi(r[u^2, v])[d(x), x]_{\theta,\phi} + [\phi(r[u^2, v]), \phi(x)]d(x) = 0 \text{ for all } x, u, v \in J, r \in R. \quad (2.14)$$

Taking sr instead of r in (2.14), where $s \in R$, we obtain $[\phi(s), \phi(x)]R\phi([u^2, v])d(x) = 0$ for all $x, u, v \in J$ and $s \in R$. And hence primeness of R forces that for each $x \in J$, either $[\phi(s), \phi(x)] = 0$ or $\phi([u^2, v])d(x) = 0$. By Brauer's trick, we obtain that either $J \subseteq Z(R)$ or $\phi([u^2, v])d(x) = 0$ for all $x, u, v \in J$. The first case implies that R is commutative and we are done. Let us assume that $\phi([u^2, v])d(x) = 0$. Replacing v by $2[p, q]v$, where $p, q \in R$, we get $\phi([u^2, [p, q]])Jd(x) = 0$ for all $x, u \in J$. By Lemma 4, it follows that either $u^2 \in Z([R, R])$ or $d(J) = 0$. In light of lemma 2, latter case implies that R is commutative. Now, in case $u^2 \in Z([R, R])$, we get $u^2 \in Z(R)$ and hence R is commutative. □

3 The results on generalized $(1_R, \phi)-$derivations

Theorem 18. *Let $F : R \to R$ be a generalized $(1_R, \phi)$-derivation associated with an $(1_R, \phi) -$ derivation d. If for any $0 \neq \alpha \in R$, $\alpha(F(x)F(y) \pm xy) = 0$ for all $x, y \in J$, then either R is commutative or there exists $\lambda \in C$ such that $F(x) = \lambda x$ for all $x \in R$ and $\lambda^2 = \pm 1$.*

Proof. By hypothesis, we have

$$\alpha(F(x)F(y) \pm xy) = 0 \quad (3.1)$$

for all $x, y \in J$. Replace y by $4yz^2$, where $z \in J$. We get $\alpha(F(x)F(y) \pm xy)z^2 + \alpha F(x)\phi(y)d(z^2) = 0$. Our hypothesis reduces it to $\alpha F(x)\phi(y)d(z^2) = 0$ for all $x, y, z \in J$. That is, $\phi^{-1}(\alpha F(x))J\phi^{-1}(d(z^2)) = (0)$ for all $x, z \in J$. By Lemma 4, we have $\alpha F(x) = 0$ or $d(z^2) = 0$ for all $x, z \in J$. Firstly, let $\alpha F(J) = (0)$. Eq. (3.1) implies that $\alpha xy = 0$ for all $x, y \in J$. Since J is nonzero, we have $\alpha = 0$, which is a contradiction. Thus, we must have $d(z^2) = 0$ for all $z \in J$. In the light of Theorem 9, we obtain $d = 0$. Consequently $F(xy) = F(x)y$ for all $x, y \in R$. By Lemma 2 of [9], there exists $\lambda \in Q_{mr}(R_C)$ such that $F(x) = \lambda x$ for all $x \in R$. Since $2R[J^2, J]R \subseteq J$ (by Lemma 6), we replace x by $2r[u^2, v]y$ in (3.1) in order to obtain

$$\alpha(F(r[u^2, v])yF(y) \pm r[u^2, v]y^2) = 0 \text{ for all } u, v, y \in J \text{ and } r \in R. \quad (3.2)$$

By substituting $x = 2r[u^2, v]$ in (3.1), where $u, v \in J$ and $r \in R$, we obtain

$$\alpha(F(r[u^2, v])F(y) \pm r[u^2, v]y) = 0.$$

Post-multiplying the above relation by y, we get

$$\alpha(F(r[u^2, v])F(y)y \pm r[u^2, v]y^2) = 0. \quad (3.3)$$

Subtract (3.2) from (3.3), we have $\alpha F(r)[u^2, v][F(y), y] = 0$ for any $u, v, y \in J$ and $r \in R$. Replace r by rs, where $s \in R$, we get $\alpha F(r)s[u^2, v][F(y), y] = 0$. That is

$$\alpha F(r)R[u^2, v][F(y), y] = (0)$$

for all $u, v, y \in J$ and $r \in R$. Since R is prime ring, it follows that either $\alpha F(r) = 0$ or $[u^2, v][F(y), y] = 0$. The first case is not possible, thus we have $[u^2, v][F(y), y] = 0$ where $u, v, y \in J$. Replace v by $2[r, s]v$ in the last expression and using it, we find $[u^2, [r, s]]J[F(y), y] = (0)$ for all $u, y \in J$ and $r, s \in R$. Lemma 4 forces $[F(y), y] = 0$ or $[u^2, [r, s]] = 0$ for all $u, y \in J$ and $r, s \in R$. If $[u^2, [r, s]] = 0$ for all $u \in J$ and $r, s \in R$, then by Lemma 7, we find that $u^2 \in Z(R)$. Hence R is commutative, as we have already seen in the proof of Theorem 11.

Next, we consider $[F(y), y] = 0$ for all $y \in J$. It gives $[\lambda y, y] = 0$ for all $y \in J$. Linearizing w.r.t.y, we find $[\lambda, x]y + [\lambda, y]x = 0$ for all $x, y \in J$. Changing y by $2y[r, s]$, we find $[\lambda, x]y[r, s] + y[\lambda, [r, s]]x + [\lambda, y][r, s]x = 0$ for all $x, y \in J$ and $r, s \in R$. It implies

$$y[\lambda, [r, s]]x + [\lambda, y][[r, s], x] = 0. \tag{3.4}$$

Taking $2py^2$ in place of y in the last expression, where $p \in R$, we may infer that

$$p(2y^2)[\lambda, [r, s]] + p[\lambda, 2y^2][[r, s], x] + [\lambda, p]2y^2[[r, s], x] = 0.$$

Equation (3.1) reduces it to $[\lambda, p]2y^2[[r, s], x] = 0$ for all $x, y \in J$ and $r, s, p \in R$. It implies that $[\lambda, p]Ry^2[[r, s], x] = 0$. In view of our assumption, it yields that $[\lambda, p] = 0$ for all $p \in R$. It is a well known fact of theory of differential identities that a prime ring R and U (the Utumi quotient ring of R) satisfies the same GPI. Hence the first case implies that $\lambda \in C$, while it is easy to check that the latter case forces R to be commutative. □

Theorem 19. *Let $F : R \to R$ be a generalized $(1_R, \phi)$-derivation associated with an $(1_R, \phi)-$derivation d of R. If for any $0 \neq \alpha \in R$, $\alpha(F(x)F(y) \pm yx) = 0$ for all $x, y \in J$, then R is commutative or there exists $\lambda \in C$ such that $F(x) = \lambda x$ for all $x \in R$ and $\lambda^2 = \pm 1$.*

Proof. By the hypothesis, we have

$$\alpha(F(x)F(y) \pm yx) = 0 \text{ for all } x, y \in J. \tag{3.5}$$

In view of Lemma 6, we replace y by $2r[u^2, v]s$ (where $r, s \in R$ and $u, v \in J$) in (3.5) and get

$$\alpha(F(x)F(r[u^2, v]s) \pm r[u^2, v]sx) = 0. \tag{3.6}$$

Replacing s by sx, we obtain

$$\alpha(F(x)F(r[u^2, v]s)x + F(x)\phi(r[u^2, v]s)d(x) \pm r[u^2, v]sx^2) = 0.$$

Thus (3.6) reduces it to

$$\alpha(F(x)\phi(r)\phi([u^2, v]s)d(x)) = 0 \text{ for all } x, u, v \in J,\ r, s \in R.$$

That is $\alpha F(x)R\phi([u^2, v]s)d(x) = (0)$. It implies that for each $x \in J$, either $\alpha F(x) = 0$ or $\phi([u^2, v]s)d(x) = 0$. Applying Brauer's trick, we find that either $\alpha F(x) = 0$ for all $x \in J$ or $\phi([u^2, v]s)d(x) = 0$ for all $x, u, v \in J$ and $s \in R$. Now onwards, we split the proof into two parts.

First we assume that $\alpha F(x) = 0$ for all $x \in J$. In this view (3.5) implies $\alpha yx = 0$ for all $x, y \in J$. By Lemma 4, we get $\alpha = 0$, which is a contradiction. Thus, we have

$$\phi([u^2, v]s)d(x) = 0 \text{ for all } x, u, v \in J,\ s \in R.$$

It forces that either $d(x) = 0$ for all $x \in J$ or $[u^2, v] = 0$ for all $u, v \in J$. The latter subcase implies that R is commutative (see the proof of Lemma 5 in [14]). We now consider $d(x) = 0$ for all $x \in J$. In view of Lemma 1, it follows that either $d = 0$ or R is commutative.

Let us assume that $d = 0$. Consequently $F(xy) = F(x)y$ for all $x, y \in R$. By Lemma 2 of [9], there exists $\lambda \in Q_{mr}(R_C)$ such that $F(x) = \lambda x$ for all $x \in R$.

When replacing x by $4x^2r$ in (3.5), where $r \in R$, we get

$$\alpha(F(2x^2)rF(y) \pm 2yx^2r) = 0. \tag{3.7}$$

Replace x by $2x^2$ in (3.5), we find $\alpha(F(2x^2)F(y) \pm 2yx^2) = 0$. Post-multiply by r, we get

$$\alpha(F(2x^2)F(y)r \pm 2yx^2r) = 0. \tag{3.8}$$

Eq. (3.7) together with Eq. (3.8) gives $\alpha F(x^2)[F(y), r] = 0$, where $x, y \in J$ and $r \in R$. It easily follows that $\alpha F(x^2)R[F(y), r] = (0)$. Since R is a prime ring, we have either $\alpha F(x^2) = 0$ or $[F(y), r] = 0$. Let us consider $\alpha F(x^2) = 0$ for all $x \in J$. When linearizing, we obtain $\alpha F(x \circ y) = 0$ for any $x, y \in J$. Putting $4uy^2$ for y (where $u \in J$) in the last relation, we obtain

$$\begin{aligned} 0 &= \alpha F((x \circ u)y^2) - \alpha F(u[x, y^2]) \\ &= \alpha F((x \circ u))y^2 - \alpha F(u)[x, y^2] \\ &= -\alpha F(u)[x, y^2]. \end{aligned}$$

Replace u by $4uru$ in above expression, we obtain $\alpha F(u)Ru[x, y^2] = (0)$ for all $u, x, y \in J$. It follows that either $\alpha F(u) = 0$ or $u[x, y^2] = 0$. But according to our assumption $\alpha F(u) = 0$ is not the case, hence we have $u[x, y^2] = 0$ implies $[x, y^2] = 0$ for all $x, y \in J$. As above, it implies that R is commutative.

In the latter case, we assume that $[F(y), r] = 0$ for all $y \in J$ and $r \in R$. Thus by our hypothesis, we find

$$\alpha(F(y)F(x) \pm yx) = 0 \quad \text{for all } x, y \in J.$$

By repeating the same reasoning as in Theorem 18, there exists some $\lambda \in C$ such that $F(x) = \lambda x$ for all $x \in R$ and $\lambda^2 = \pm 1$. □

Acknowledgements

We would like to thank Prof. Abdellah Mamouni for reading the first draft of the manuscript and giving constructive comments. We are also grateful to the editor Prof. Miroslav Haviar and the referee(s) for many helpful suggestions.

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Title	Acta Universitatis Matthiae Belii Series Mathematics
Volume	27
First Edition	
Number of copies	110
Pages	93
Design and layout	Ján Karabáš
Published by	Belianum, vydavateľstvo UMB
Printed by	Equilibria, s.r.o., Košice
Typeset with LaTeX	
ISSN	1338-712X
ISBN	978-80-557-1690-9

Acta Universitatis Matthiae Belii

Series Mathematics Volume 27 2019

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