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An Algebraic Calculation Method for Describing Time–Dependent Processes in Electrochemistry – Expansion of Existing Procedures

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ABSTRACT

In this paper an alternative model allowing the extension of the Debye-Hückel Theory (DHT) considering time dependence explicitly is presented. From the Electro-Quasistatic approach (EQS) introduced in earlier studies time dependent potentials are suitable to describe several phenomena especially conducting media as well as the behaviour of charged particles (ions) in electrolytes. This leads to a reformulation of the meaning of the nonlinear Poisson-Boltzmann Equation (PBE). If a concentration and/or flux gradient of particles is considered the original structure of the PBE will be modified leading to a nonlinear partial differential equation (nPDE) of the third order. It is shown how one can derive classes of solutions for the potential function analytically by application of pure algebraic steps. The benefit of the mathematical tools used here is the fact that closed-form solutions can be calculated and thus, numerical methods are not necessary. The important outcome of the present study is meaningful twofold: **(i)** The model equation allows the description of time dependent problems in the theory of ions, and **(ii)** the mathematical procedure can be used to derive classes of solutions of arbitrary nPDEs, especially those of higher order.

1 INTRODUCTION

Many problems of physical/chemical interest are described by nPDEs with appropriate side conditions. These can be suitable chosen initial and/or boundary

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conditions. If the equations are linear, widely used methods for solving PDEs are known (e.g. the Fourier and/or Green's method) and the superposition principle generates further solutions by known of a pair of solutions. For nPDEs, however, the linear superposition principle can not be applied to generate new classes of solutions.

> **Note:** We stress the existence of a nonlinear superposition principle known as the Bäcklund transformation which means a special contact transformation [1]. The nPDE under consideration is not of Painlevé type, e.g. [2], [3], [4] and therefore a suitable Bäcklund system can not be associated. Apart from this a Bäcklund system is only (in the most cases) derivable for 'simple strutured' nPDEs. Thus this fact justifies the use of algebraic methods for deriving analytical solutions and often represents the only suitable way for a successful solution procedure.

Because most of the of solution methods for linear equations fail, there is no general method of finding analytical classes of solutions for nPDEs and numerical techniques are usually required. Sometimes special transformations can be done to transform a nPDE into a linear PDE, or some other 'ad hoc' methods (and/or assumptions) can be used to derive classes of solutions of a particular nonlinear equation.

> **Note:** We arrange that we suppress the item 'classes of solutions', so we will simply understood 'solutions' instead of classes of solutions (although classes of solutions is the correct notation). Since time occurs in the derivation(s) explicitly such types of nPDEs are called evolution equations (EVEs) since they allow the study of time-dependent processes. Any nPDE may not have the outer form $u_t = K[u, u_x, u_{xx}, \dots]$ necessarily being an EVE where $u_t = K[u, u_x, u_{xx}, \dots]$ is a nonlinear operator in general. Equations containing mixed higher derivations like $u_{xt} = K[u]$ and/or $u_{xxt} = K[u]$ are also called EVEs.

Techniques of finding solutions represent only one aspect in dealing with nPDEs. Like linear equations, questions of existence, uniqueness, and stability of solutions are also of fundamental importance.

1.1. HISTORICAL DEVELOPMENTS – A SHORT OVERVIEW

There is a good historical reason to deal the subject. When the developments of interfacial electrochemistry along modern lines became restricted by the over thermodynamics attitude of its adherents in the pre-1950 days, much attention was diverted to what had seemed previously to some extent the accompanying side issues, i.e. the physical chemistry of the bulk solution adjoining the double layer.

This had concentrated upon an interest in the deviations in the behaviour of solutions from laws derived upon the assumption that interactions between particles are negligible. The properties of electrolyte solutions can significantly deviate from the laws used to derive the chemical potential of solutions. In non-electrolyte solutions the intermolecular forces are mostly comprised of weak Van der Waals interactions, which have a $\propto r^{-7}$ dependence (in principle), and for practical purposes this can be considered as ideal. In ionic solutions, however, there are significant electrostatic interactions between solute-solvent as well as solute-solute molecules. These electrostatic forces are governed by Coulomb's law which has a $\propto r^{-7}$ dependence. Consequently, the behaviour of an electrolyte solution deviates considerably from that an ideal solution. Thus the DHT of such interactions attracted the attention of electrochemists away from the blocked interface studies [5]. The DHT was proposed as a theoretical explanation for departures from ideality in solutions of electrolytes [6]. From about 1920 to 1950 the majority of research in this domain were occupied with determining activity coefficients of salts in dilute aqueous solutions, the electrical conductance of molten salts, or electrostatic effects of the dissociation constant of acids or bases in aqueous solutions [7], [8]. Note that by applying the DHT restrictions have taken into account, like much diluted solutions, completely dissociation and more [9]. Contemporaneously, Helmholtz considered a double-layer model wherein he proposed a simple charge separation at the interface [10].

Gouy [11], [12] developed an electric double-layer model that includes the effects both of the electric potential and ionic concentration with the aid of the Boltzmann distribution [7], [9].

A further contribution was done by Chapman [13]. He established the steady-state governing equation for the diffuse layer, the Poisson-Boltzmann Equation [11]. This equation is based upon the combination of the electrostatic basic equation, the Poisson Equation [14], and the Boltzmann distribution [15]. The model is referred to as the Gouy-Chapman model.

Further, Stern [16] improved the Gouy-Chapman model by assuming a finite ion size and by dividing the electrolyte into two layers, specified to as the Stern layer and the diffuse layer. Later on Grahame [17] revised the Stern model using three layers: The **I**nner Helmholtz layer (IHL), the **O**uter Helmholtz layer (OHL) and the diffuse layer. The difference between the Grahame model and the Stern model is due to the existence of a specific adsorption [11].

A transient version [11] is referred to as the Nernst-Planck-Poisson-modified Stern model or simply the Nernst-Planck-Poisson model (NPP) if there is no modified Stern layer.

During the past 90 decades several well-known scientists did their contributions in this domain, and, unfortunately only a small number are mentioned here like Bjerrum [18], Gronwall/La Mer/Sandved [19], Onsager [20], Kirkwood [21], Falkenhagen [6], [9], Ghosh [22], Smoluchowski [23], Parker [24], Walden [25], Planck [26], Fuoss [27], Kortüm [28], [29], and extensive developments are not finalized up to now.

1.2. ELECTROMAGNETICS FROM A QUASISTATIC PERSPECTIVE

The general theoretical considerations can be found in [30–32]. Here only the essentials are cited.

The quasistatic limit of the Maxwell Equations (MEs) is a kind of $c \to \infty$ limit (the fields propagate at once) obtained by neglecting time retardation. EQS has important applications modelling transient phenomena in approximating theories for materials with low conductivity (or the low-frequency approximation). The crucial step is the fact that a time dependent electric field may derived from a scalar potential which is, in our case the solution of a certain nPDE of the third order [33–37]. General transient electrodynamical problems are not easy to solve, e.g. by occurring solutions depending upon roots one has to take into account branch points. In media with a finite conductivity a static field is not possible and the pertinent relaxations time is given by $\tau = \varepsilon_0 \varepsilon \sigma^{-1}$ [38], where ε is the relative permittivity (of the material) and σ is the conductivity. For the most metals (e.g. copper) the relaxation time is in the range of 10^{-18}s. New developments in material sciences produce materials with a relative dielectric constant in the range of $2 < \varepsilon < 4$ and a conductivity of about $10^{-9} sm^{-1}$. Then the decay rate is approximately $\tau \approx 10^{-3}$s and this is long compared to other time constants of the system (e.g. if an electromagnetic field passes through a panel).

This is exactly the case where EQS can be applied [32], [38] and only pure capacitive effects are of interest. In further studies considering both capacitive and inductive effects the Darwin model will be used. Note that statics is just a particular case of the general MEs but quasistatics works as an approximation.

1.3. THE MODEL EQUATION UNDER CONSIDERATION

The starting point is an expanded version of the PBE, a special nPDE of the third order

$$\sigma \Delta u + \varepsilon_0 \varepsilon \frac{\partial}{\partial t} \Delta u + \frac{\partial}{\partial t} \left(- z_i F D \frac{c}{kT} \vec{\nabla} u \right) - \frac{\partial}{\partial t} \left(\sum_{i=1}^{N} z_i e_0 N_i^0 \exp \left[- \frac{z_i e_0 u}{kT} \right] \right) = 0 \quad (1)$$

where F is the Faraday constant, D the diffusion constant and k is the Boltzmann constant.

One assumes the conversion: Let $N_i^0 \times 1000 = N_A c_i$, c_i is the molar concentration and the ion strength is defined by $I = 1/2 \sum_i c_i z_i^2$. Introducing further per definition

$$\beta^2 = \frac{e_0^2 N_A}{1000\, kT} \frac{1}{2} \sum_i c_i z_i^2 \;\rightarrow\; \beta^2 = \frac{2 e_0^2 N_A}{1000\; kT} I \quad , \eta = \frac{z_i e_0}{kT}, \; \alpha^2 = \frac{DFc}{kT}, \tag{2}$$

one derives a third-order nPDE for the time-dependent potential function $u = u(x,t)$:

$$\varepsilon \varepsilon_0 \frac{\partial^3 u}{\partial x^2 \partial t} + \sigma \frac{\partial^2 u}{\partial x^2} - \alpha^2 \frac{\partial^2 u}{\partial x \partial t} - \beta^2 \frac{\partial u}{\partial t} e^{-\eta u} = 0 . \tag{3}$$

At this stage one formally imposes boundary conditions (BCs) so that $\lim_{x\to\infty} u_0 = u_L$ and $\lim_{x\to\infty} \frac{du}{dx} = 0$ holds; they are necessary conditions later for the function $u = u(x,t)$. Note that BCs may depend upon actual problems. We find it useful to split up the potential so that u_0 is the potential at any surfaces and u_L is the potential in the electrolyte far away from a reference ion, thus $\Delta u = u_0 - u_L$ (not to be changed with the Laplacian).

One seek solutions for the nPDE, Equation (3) for which $u = F(x,t)$, $F \in C^3(D)$, $D \subset R^2$ is an open set and

$$D := \left\{ u(x,t) \in \tilde{D} : u = 0,\, u_x = 0,\, u_t = 0, ... \right\}$$

is excluded with $t > 0$. Suitable solutions are $u \in I$, I an interval so that $I \subseteq D$ and $u : I \rightarrow R^2$. It is not an easy task to solve nPDEs (especially of higher order) exactly but here we wish to solve the Equation (3) analytically by using algebraic methods without numeric's. A mean value for the charge density is used in Equation (3) and one-valued ions are assumed so that $z_i = z = 1$. In later considerations the case of many-valued ions will be considered. The potential function $u(\vec{x},t) \equiv u$ represents the ion's potential surrounded by the 'ion cloud'. In further meaning this function describes the time-dependent potential of an arbitrary metal electrode dipping in an (liquid) electrolyte (due to the restrictions imposed by EQS not all metals can be considered). Note that a standard concentration of $c = 0{,}01 mol/l$, resp. c_i for the concentration of the i-th ion at a standard temperature of $T = 293{,}15\ K$ is assumed. In the following we shortly present the basics.

1.4. THE ALGEBRAIC SOLUTION PROCEDURE

Consider a given nPDE in its two independent variables x and t

$$P\left(u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial u}{\partial x}\frac{\partial u}{\partial t}, ..., \frac{\partial^{n-1} u}{\partial x^{n-1}}, \frac{\partial^n u}{\partial x^n}\right) = 0. \qquad \text{(a)}$$

Firstly the nPDE converts into a nODE by using a frame of reference $u(x,t) = f(\xi)$, where $\xi = \delta x - \lambda t$; δ and λ are constants to be determined. Thus one has

$$Q\left(f(\xi), f'(\xi), f''(\xi), ...\right) = 0. \qquad \text{(b)}$$

The next step is that the solutions we are looking for can be expressed in terms of a finite series representation such that

$$u(x,t) = f(\xi) = \sum_{i=0}^{n} a_i \, cn^i(\xi,k) \quad \text{and} \quad f^{(n)}(\xi) = \sum_{i=0}^{n} \frac{\partial^n}{\partial \xi^n}\left(a_i \, cn^i(\xi,k)\right) \qquad \text{(c)}$$

holds where $cn(\xi,k)$ means the cosine amplitude and k is the modulus. The parameter *n* in Equation (c) is found by balancing the highest derivative with the nonlinear terms in the reduced nODE Equation (b). This parameter must be a positive integer since it represents the number of terms in the series (c). In the case of fractions one can take suitable transformations as shown later. The substitution of Equation (c) into the relevant nODE Equation (b) will yield a system of nonlinear algebraic equations with respect to the unknowns $a_0, a_1, \ldots, k, \lambda$ and δ.

2. CALCULATION OF SOLUTIONS

We convert the Eq. (3) by $u(x,t) = f(\xi)$, $\xi = \delta x - \lambda t$ to derive the nODE of the third-order

$$\delta^2\lambda \frac{d^3 f}{d\xi^3} - \delta^2 \frac{d^2 f}{d\xi^2} + \alpha^2\delta\lambda \frac{d^2 f}{d\xi^2} + \beta^2\lambda \frac{df}{d\xi}\exp[-\eta f] = 0, \; f = f(\xi), -\infty < \xi < \infty \qquad (4)$$

> **Note:** The similarity transformation is called the travelling wave reduction describing any wave propagation and λ means the velocity. One of the new aspects here is the introduction of the quantity δ to generalize the method.

We seek for solutions for which $f = F(\xi)$, $F \in R^3$ and $D \subset R^2$ is an open set excluding

$$D := \left\{(f, \xi) \in \tilde{D} : f(\xi) = 0, \partial_t \neq 0\right\}.$$

Suitable solutions are $f \in I$, I an interval so that $I \subseteq D$ and $f : I \to R^2$. Since the l.h.s of Equation (4) is a continuous function we ensure at least existence locally and due to the lemmas from Peano and Picard-Lindelöf we assume uniqueness (also at least locally) in a given domain.

The question now is: Can we integrate the nODE Equation (4) directly so that we can rewrite the nODE (4) in a complete differential form? Indeed, one has

$$\frac{d}{d\xi}\left\{\delta^2\lambda\eta\frac{d^2f}{d\xi^2}-\delta^2\eta-\frac{df}{d\xi}+\alpha^2\delta\lambda\eta\frac{df}{d\xi}\right\}+\frac{d}{d\xi}\left\{\beta^2\lambda e^{-\eta f}\right\}=0\,. \tag{5}$$

Integrating once with c_1 as an arbitrary constant of integration gives a second-order nODE

$$\delta^2\lambda\eta\frac{d^2f}{d\xi^2}-\delta^2\eta\frac{df}{d\xi}+\alpha^2\delta\lambda\eta\frac{df}{d\xi}+\beta^2\lambda e^{-\eta f}=c_1\,. \tag{6}$$

Then the transformation $f(\xi)=1/\eta\ln[w(\xi)]$ will remove the exponential function yielding a further second-order nODE for the new dependent variable $w(\xi)$:

$$\delta^2\lambda w\frac{d^2w}{d\xi^2}-\delta^2\lambda\left(\frac{dw}{d\xi}\right)^2+\alpha^2\delta\lambda\, w\frac{dw}{d\xi}-\delta^2 w\frac{dw}{d\xi}-c_1w^2+\beta^2\lambda\, w=0\,,\ w=w(\xi) \tag{7}$$

To apply the algorithm performed in Section 1(d) above it is necessary to know the quantity n in the series Equation (c). It can be shown that two values exist: $n_1=-1$ and $n_2=-2$.

This is not possible since this quantity must be $n\in Z^+$. Introducing a new variable $p(\xi)$ by the transformations $w_1(\xi)=p(\xi)^{-1}$ and $w_2(\xi)=p(\xi)^{-2}$ will give two second-order nODEs (balancing now leads to $n_1=1$ and $n_2=2$) for the function $p(\xi)$:

$$2\delta^2\lambda\, p\frac{d^2p}{d\xi^2}-2\delta^2\lambda\left(\frac{dp}{d\xi}\right)^2+2\alpha^2\delta\lambda\, p\frac{dp}{d\xi}-2\delta^2 p\frac{dp}{d\xi}-\beta^2\lambda\, p^4+c_1p^2=0\text{, for } n_1=1 \tag{7a}$$

$$\delta^2\lambda\, p\frac{d^2p}{d\xi^2}-\delta^2\lambda\left(\frac{dp}{d\xi}\right)^2+\alpha^2\delta\lambda\, p\frac{dp}{d\xi}-\delta^2 p\frac{dp}{d\xi}-\beta^2\lambda\, p^3+c_1p^2=0\text{, for } n_2=2 \tag{7b}$$

Thus, from the Equation (c) the following solutions for the functions $p(\xi)$ are possible:

$$p_1(\xi)=a_0+a_1cn(\xi,k)\text{, for } n=1 \tag{8a}$$

$$p_2(\xi)=a_0+a_1cn(\xi,k)+a_2cn^2(\xi,k)\text{, for } n=2 \tag{8b}$$

Putting together the Equations (c), (8a), (8b) into the nODEs (7a), (7b) two systems of nonlinear algebraic equations appear. For control purposes we only stress the first and the last equation.

1st case, $n=1$:

$$\begin{aligned} &2a_0^2\beta^2\lambda - c_1 + 2a_1^2\beta^2\lambda + \delta^2\lambda = 0, \\ &a_1^2 + 2k\delta^2 = 0. \end{aligned} \tag{9}$$

2nd case, $n=2$:

$$\begin{aligned} &2a_0c_1 + 2a_2c_1 - 3a_0^3\beta^2\lambda - a_0^2\beta^2\lambda - 6a_0a_2\beta^2\lambda - 3a_2^2\beta^2\lambda - 3a_2\delta^2\lambda = 0, \\ &a_0^2c_1 + a_1^2c_1 + 2a_0a_2c_1 + a_2^2c_1 - a_0^2\beta^2\lambda - 3a_0a_1^2\beta^2\lambda - 3a_0^2a_2\beta^2\lambda - 3a_1^2a_2\beta^2\lambda - \\ &- 3a_0a_2^2\beta^2\lambda - a_2^3\beta^2\lambda - a_1^2\delta^2\lambda - 2a_0a_2\delta^2\lambda - 2a_2^2\delta^2\lambda = 0. \end{aligned} \tag{9a}$$

Solving these systems the following solutions are possible (the trivial solution is always a solution but meaningless for our purposes; the constants α and β are predetermined quantities and should not work as unknowns):

1st case:

(i) $a_0 = 0$, $c_1 = \delta^2\lambda\left(3-2\sqrt{3}\right)$, $k = \frac{1}{2}\left(\sqrt{3}-1\right) \approx 0{,}366$, $\delta \neq 0$, $\lambda \neq 0$, a_1 arbitrary, (10)

(ii) $a_0 = \pm\frac{1}{2}\sqrt{\frac{23}{6}}a_1$, $c_1 = -\frac{45\delta^2\lambda}{2}$, $k = 3$, $\delta \neq 0$, $\lambda \neq 0$, a_1 arbitrary, (10a)

(iii) $a_0 = 0$, $c_1 = \delta^2\lambda\left(3+2\sqrt{3}\right)$, $k = -\frac{1}{2}\left(1+\sqrt{3}\right) \approx -1{,}366$, $\delta \neq 0$, $\lambda \neq 0$, a_1 arbitrary (10b)

2nd case:

(i) $a_0 = 3a_2$, $a_1 = 0$, $c_1 = -\frac{7\delta^2\lambda}{2}$, $k = \frac{1}{2}$, $\delta \neq 0$, $\lambda \neq 0$. (10c)

An interesting role plays the constant c_1: It relates the parameters δ and λ in the similarity variable ξ if one sets $c_1 = 1$ and thus we exclude $c_1 = 0$ in the Equation (6). By using the Equations (8a) to (10c) one derives the following expressions for the functions $f(\xi)$ and therefore for the functions $u(x,t)$:

$$f_1(\xi) = \frac{1}{\eta}\ln\left[\frac{1}{a_1 cn(\xi,k)}\right] = -\frac{1}{\eta}\ln\left[a_1 cn(\xi,k)\right],\ k = \frac{1}{2}\left(\sqrt{3}-1\right),$$

$$\xi = \delta x - \frac{\lambda t}{\delta^2\left(3-2\sqrt{3}\right)}, \tag{11}$$

$$f_2(\xi) = -\frac{1}{\eta}\ln\left[a_1\left(\sqrt{\frac{23}{24}} + dn\left(3\sqrt{3}\xi, \frac{1}{3}\right)\right)\right],\ \xi = \delta x + \frac{2\lambda t}{45\delta^2},\ a_1 \text{ arbitrary},\ a_1 \neq 0, \tag{11a}$$

$$f_3(\xi) = -\frac{1}{\eta}\ln\left[a_1 dn\left(\sqrt{\frac{1}{2}\left(\sqrt{3}-1\right)}\xi, \frac{2}{3}\right)\right], \quad \xi = \delta x - \frac{\lambda t}{\delta^2\left(3+2\sqrt{3}\right)}, \; a_1 \text{ arbitrary},$$

$$a_1 \neq 0, \tag{11b}$$

and for the 2nd case

$$f_4(\xi) = -\frac{1}{\eta}\ln\left[a_2\left(3 + cn^2\left(\xi, \frac{1}{2}\right)\right)\right], \; \xi = \delta x - \frac{2\lambda t}{7\delta^2}, \; a_2 \text{ arbitrary}, \; a_2 \neq 0. \tag{11c}$$

Note: To derive this solutions the basic properties of the elliptic functions (and the logarithm) was used, especially the relation for the modulus $k^2 + k'^2 = 1$, the Jacobi's real transformation for negative modulus and the transformation for imaginary arguments, e.g. [39]. Thus, for example, one has the relation $cn(u,-k) := cd(\nu,\mu)$ for the cosine amplitude. Elliptic functions with the special modulus $k = 1/2$, e.g. in case of the function $f_4(\xi)$ are sometimes called lemniscate functions. For the following discussions it is only necessary to consider the functions in the form $f_i(\xi)$, $i = 1,...,4$. For the constant η we have $\eta^{-1} = 0{,}0253JC^{-1}$ and this is material independent. We assume the following domains of definition: $-1 \leq \left(sn(u), cn(u)\right) \leq 1$, $k' \leq dn(u) \leq 1$ and $-\infty \leq tn(u) \leq \infty$.

3. SOME SPECIAL PROPERTIES

In all cases a travelling character is observed, but for all functions the argument of the logarithm may not be the unity, since in this case the solutions take infinity or become a singularity, apart from that the expressions have singularities if the denominators take zero. All functions are continuously and differentiable at least two-fold in the domain $0 < \xi < 1$, the first, the second and all higher derivatives exist and have the same behaviors as above. Some special values are summarized in the following table.

Now we are interested in further quantities. We assume an electrical field $\vec{E}_i$ and this field will be generated by a given charge distribution. Such an electric field can then be derived from the potential by application of the gradient operator $\vec{E}_i = -\nabla f_i(\xi)$ to give the following expressions and without loss of generality one can also set $a_1 = a_2 = 1$; the modulus are given by the Equations (11) to (11c):

$$\vec{E}_1(\xi) = -\frac{1}{\eta} sn\left(\xi, k\right) dc\left(\xi, k\right), \quad \xi \neq 1{,}7546, \tag{12}$$

$$\vec{E}_2(\xi) = -\frac{1}{\eta}\frac{\sqrt{3}\,cn\left(3\sqrt{3}\,\xi,\frac{1}{3}\right)sn\left(3\sqrt{3}\,\xi,\frac{1}{3}\right)}{\sqrt{\frac{23}{24}+dn\left(3\sqrt{3}\,\xi,\frac{1}{3}\right)}}, \tag{12a}$$

$$\vec{E}_3(\xi) = -\frac{\sqrt{2\left(\sqrt{3}-1\right)}}{3\eta}cn\left(a\xi,\frac{2}{3}\right)sd\left(a\xi,\frac{2}{3}\right),\quad a=\sqrt{\frac{1}{2}\left(\sqrt{3}-1\right)}, \tag{12b}$$

$$\vec{E}_4(\xi) = -\frac{1}{\eta}\frac{2\,cn(\xi,k)\,dn(\xi,k)\,sn(\xi,k)}{3+cn^2(\xi,k)}. \tag{12c}$$

$f_i(\xi)$	$\partial_\xi f_i(\xi)\|_0$	$\partial_\xi f_i(\xi)\|_1$	$\partial_{\xi\xi} f_i(\xi)\|_0$	$\partial_{\xi\xi} f_i(\xi)\|_1$	$\lim_{\xi\to 0} f_i(\xi)$	$\lim_{\xi\to 1} f_i(\xi)$
$f_1(\xi)$	0	1,2182	1	1,9993	0	0,5423
$f_2(\xi)$	0	0,0005	0	-0,0041	-0,6826	-0,5853
$f_3(\xi)$	0	0,2073	0,2440	0,1394	0	0,1126
$f_4(\xi)$	0	0,2348	0,5	-0,1301	-1,3863	-1,2105

Table 1. Some selected properties of the functions Equation (11) to Equation (11c), here $a_1 = a_2 = 1$ is considered, $i = 1,...,4$.

Note: We stress that the first expression is not defined at those points where the denominator vanishes, e.g. at the points as $cn(\xi,k) = 0$. This is equivalent with the task to look for solutions of the equation $cn(\xi,k) = 0$. The first real zero is given explicitly and the same is true for the remaining denominators.

Now we show that the fields have a conservative character since by considering Cartesian coordinates, e.g. $\xi = (\xi_x, \xi_y, \xi_z)$ the relation $rot\,\vec{E}_i(\xi) = 0$ holds (the field is irrotational or equivalently, the existence of the potential is secured since the curl of the field vanishes).

To show that the fields are really solenoidal one introduces Cartesian coordinates in the Equations (12) to (12c) so that $\vec{E}_i(\xi) = (E_x, E_y, E_z)$. Here also $a_1 = a_2 = 1$ is assumed and we suppress the factor η^{-1} and dropping all

arguments. The calculation is performed only for the first component $\vec{E}_1(\xi)$, the remaining are similar. With a unit vector $\vec{e}_i$ one has:

$$rot\vec{E}_1 = \vec{\nabla}\times\vec{E}_1 = \begin{vmatrix} \vec{e}_x & \vec{e}_y & \vec{e}_z \\ \partial_x & \partial_y & \partial_z \\ E_x & E_y & E_z \end{vmatrix} = \vec{e}_x \begin{vmatrix} \partial_y & \partial_z \\ E_y & E_z \end{vmatrix} - \vec{e}_y \begin{vmatrix} \partial_x & \partial_z \\ E_x & E_z \end{vmatrix} + \vec{e}_z \begin{vmatrix} \partial_x & \partial_y \\ E_x & E_y \end{vmatrix}. \quad (13)$$

Now it follows that

$$rot\,\vec{E}_{1,x} = \left| \partial_y\left(\frac{sn(z,k)\,dn(z,k)}{cn(z,k)}\right) - \partial_z\left(\frac{sn(y,k)\,dn(y,k)}{cn(y,k)}\right)\right| + ... = 0,\ x \neq 0,\ y \neq 0,\ z \neq 0 \quad (13a)$$

All the individual terms disappear and therefore the rotation is zero and thus the field is solenoidal.

To derive the charge density one has to apply the divergence operator upon the electric field (ξ acts as a local coordinate once again) so that $\rho_i(\xi) = 1/(4\pi)\vec{\nabla}\cdot\vec{E}_i(\xi)$. This yields complicate expressions with elliptic functions; one can assume these as a kind of superposition. One has:

$$\rho_1(\xi) = \frac{1}{4\pi\eta}\left\{ dn^2(\xi,k) - k^2 sn^2(\xi,k) + dn^2(\xi,k)\,tn^2(\xi,k)\right\}, \quad (14)$$

$$\rho_2(\xi) = \frac{\left\{27\,dn(\xi,k)\,sn^2(\xi,k)\left(\sqrt{138}+12\,dn(\xi,k)\right) + cn^2(\xi,k)\times\right.}{\pi\eta\left(\sqrt{138}+12\,dn(\xi,k)\right)}$$
$$\frac{\left.\times\,dn(\xi,k)\left(\sqrt{138}+12\,dn(\xi,k)\right) + 4\,sn^2(\xi,k)\right\}}{\pi\eta\left(\sqrt{138}+12\,dn(\xi,k)\right)}, \quad (14a)$$

$$\rho_3(\xi) = \frac{1}{12}\left(\sqrt{3}-1\right)\left(-\frac{1}{\pi\eta}sn^2(a\xi,k) + \frac{1}{3\,\pi\eta}cd^2(a\xi,k)\right)\times$$
$$\times\left(\frac{1}{12\,\pi\eta} + \frac{1}{8}sd^2(a\xi,k)\right),\ a = \sqrt{\frac{1}{2}\left(\sqrt{3}-1\right)}, \quad (14b)$$

$$\rho_4(\xi) = \frac{1}{4\,\pi\eta\left(3+cn^2(\xi,k)\right)^2}\times\left(-6\,dn^2(\xi,k)\,sn^2(\xi,k) + cn^4(\xi,k)\times\right.$$
$$\left.\times\left(2\,dn^2(\xi,k) - sn^2(\xi,k)\right) + cn^2(\xi,k)\right)\left(-3\,sn^2(\xi,k) + 2\,dn^2(\xi,k)\left(3+sn^2(\xi,k)\right)\right). \quad (14c)$$

Let a be a specific distance e.g. from the electrode surface to the centre of the (hydrated) ion in the OHL. The total charge $q_{i,tot}$ contained in the OHL is obtained by integrating the charge densities $\rho_i(\xi)$ from the electrode surface with the reference point taken at infinity. Therefore one has to integrate once the expressions for the charge densities given in the Equations (14) to (14c). For the first density $\rho_1(\xi)$ one has:

$$q_{1,tot} = \int_a^\infty \rho_1(\xi) d\xi = \frac{1}{4\pi\eta}\left\{ \int_a^\infty dn^2(\xi,k) d\xi - k^2 \int_a^\infty sn^2(\xi,k) d\xi + \int_a^\infty dn^2(\xi,k)\, tn^2(\xi,k) d\xi \right\}. \tag{15}$$

The first and the second integration can be done exactly but the third term causes troubles and can be handled only numerically. This is a standard procedure for any numerical integration processes and will not be performed here. An alternative way is, since all the elliptic functions are continuous functions to consider known series representations by changing integration and sums. Otherwise the Weierstrass expansions [40], [41] of the involved elliptic functions can be made. This reflects, among other things, the immense difficulties in dealing such problems (convergence of the considered integrals is assumed). To reach the goal faster we suggest another possibility: Determining the first and the second integrals exactly and signing the last term by

$$\int_a^\infty dn^2(\xi,k)\, tn^2(\xi,k)\, d\xi \equiv \int_a^\infty R(\xi,k) d\zeta \ .$$

Then, integrating once, one has, in principle

$$q_{1.tot} = \frac{1}{4\pi\eta}\left\{ ak - \frac{k\, E\big(am(a,k),k\big)}{dn(a,k)\sqrt{1-k\, sn^2(a,k)}} - \frac{dn(a,k) E\big(am(a,k),k\big)}{\sqrt{1-k\, sn^2(a,k)}} + \right.$$
$$\left. + \frac{k^2 sn^2(a,k) E\big(am(a,k),k\big)}{dn(a,k)\sqrt{1-k\, sn^2(a,k)}} + \int_a^\infty R(\xi,k) d\xi + C \right\}, \tag{15a}$$

in which $E(.,.)$ is the elliptic integral of the second kind and $am(.,.)$ is the Jacobian amplitude. Taking the limit of each term, that is $a \to 0$ the terms approaches to zero except the third. This guarantees charge conservation so that charge cannot disappears anywhere. Here it is amplified how fast mathematical problems can grow up making problems unsolvable (at least analytically). In Equation (15a) the special case $k = 1$ yields:

$$q_{1,tot} = \frac{a + 2\coth(a)\,E\left(-gd\left(a\right),1\right)}{4\pi\eta} + \int_a^\infty \tanh^2(\xi)d\xi\,, \tag{15b}$$

in which the argument of the elliptic integral of the second order the Guderman function (or hyperbolic amplitude) occurs defined by $\frac{\pi}{2} - 2\arctan\left(e^a\right) =: -gd(a)$. In principle one also can consider the case $k = 0$ which gives a linear connection explicitly

$$q_{1,tot} = -\frac{a}{4\pi\eta} + \int_a^\infty \tan^2(\xi)d\xi\,. \tag{15c}$$

However one should bear in mind that the first, the second and the fourth term vanishes leading to the fact that essential contributions to the charge density could be lost. In fact, the expressions (15b) and (15c) represent the classical result known from electrostatics. For comparative purposes we show a graphical representation of these functions in Figure 6 (remember that $E(\varphi,0) = \varphi$ and $E(\varphi,1) = \sin\varphi$).

Note: It is possible to handle the expression $R(\xi,k)$ such that one assumes also special values for the modulus, e.g. $k = 0,1$. Then the elliptic functions degenerate to the usual circular and hyperbolic functions, resp., leading to integrals of the general form

$$R(u,0) = \int_a^\infty \tan^2(u)du \text{ and } R(u,1) = \int_a^\infty \tanh^2(u)du\,.$$

However one has to specify appropriate conditions to handle the divergence of these integrals. Otherwise an anti derivative of $R(\xi,k)$ exists in general and one has the expression

$$\int R(\xi,k)d\xi = \int dn^2(\xi,k)tn^2(\xi,k)d\xi = \xi - 2E(\xi) + dn(\xi,k)tn(\xi,k) + C\,.$$

If necessary one can make use of the formula for the double argument, in detail

$$dn^2(\xi,k)\,tn^2(\xi,k) = \left((1 - cn(2\xi)/((1 + cn(2\xi)\right)^2.$$

For the Gudermann function one has $gd(x) = 2\arctan(e^x) - \pi/2$. To prove this one has to show that both sides of the last relation vanishes as $x = 0$. Left side: $gd(0) = \arctan(\sinh(0)) = \arctan(0) = 0$, right side: $2\arctan(e^0) - \pi/2 = 1 - \pi/2 = 2\frac{\pi}{4} - \frac{\pi}{2} = 0.$

As a last remark we stress the possibility to express the cosine amplitude by theta- and sigma-functions; to give an example the solution Equation (11) reads, once again with $a_1 = 1$ as

$$f_1(\xi) = \frac{1}{\eta}\ln\left[\frac{1}{cn(\xi,k)}\right] \equiv \frac{1}{\eta}\ln\left[\frac{\sigma_3(\xi,k)}{\sigma_1(\xi,k)}\right] \equiv -\frac{1}{2\eta}\ln\left[\frac{\vartheta_2(v)}{\vartheta_4(v)}\frac{k'}{k}\right]. \tag{16}$$

Note: We want to show up here different ways to express solutions, the user can then apply a preferred representation. It is also possible to express these solutions in terms of the Weierstrassian $\wp$-function. Thus one has, in principle, the relation

$$\wp(u; g_2, g_3) = e_3 + (e_1 - e_3)\,ns^2(u\sqrt{e_1 - e_3}, k)$$

where u means a general argument of the ns-function, g_2, g_3 are the invariants of the $\wp$-function and e_1 and e_3 are the roots of the equation $4t^3 - g_2 t - g_3 = 0$ which are all different. To complete, the modulus of the ns-function is expressed by $k^2 = (e_2 - e_3)/(e_1 - e_3)$ for known values of the e_i .The involved functions are meromorphic and double-periodic, the σ_i are odd and entire functions; the ϑ_i are even and entire. To clarify the relationship we present the connection between σ_1 and ϑ_1, one has in detail $\sigma_1(u) = C_1 \exp\left[(\gamma u^2)/(2\omega)\right]\vartheta_1\left(\frac{1}{2} - v\right)$, [39], [46]. Also one has to take care the regularity of the arguments of the logarithm.

4. A NUMERICAL STATEMENT – PRACTICAL FUNCTION SERIES REPRESENTATIONS

For fast numerical calculations it is convenient to have series representations, therefore we calculate some ascending power series formulas for the solution functions Equation (11) to Equation (11c). The functions, derived from the transformation of the log-function are valid up to the given order valid at $\xi > 0$:

$$f_1(\xi) = \frac{1}{2\eta}\xi^2 - \frac{(-2+\sqrt{3})}{12\eta}\xi^4 + \frac{(5+2\sqrt{3})}{90\,\eta}\xi^6 + \frac{(23+12\sqrt{3})}{1260\,\eta}\xi^8 + ... + O[\xi]^{10}, \tag{17}$$

$$f_2(\xi) = \frac{1}{\eta}\ln\left[\frac{12}{12+\sqrt{138}}\right] + \frac{54}{\eta(12+\sqrt{138})}\xi^2 + \frac{81(120+13\sqrt{138})}{2\eta\left(12+\sqrt{138}\right)^2}\xi^4 + ... + O[\xi]^6, \tag{17a}$$

$$f_3(\xi) = \frac{1}{3\eta\sqrt{2}}\xi^2 - \frac{1}{27\eta}\xi^4 + \frac{7}{1215\sqrt{2}\,\eta}\xi^6 + \ldots + O[\xi]^8 \tag{17b}$$

$$f_4(\xi) = -\frac{\ln 4}{\eta} + \frac{1}{4\eta}\xi^2 - \frac{3}{32\eta}\xi^4 + \frac{23}{960\eta}\xi^6 - \ldots + O[\xi]^8. \tag{17c}$$

Note: Consider the first function series $f_1(\xi)$, where the necessary condition $\lim_{\xi\to 0} f_i(\xi) = 0$ holds. The terms thus form a sequence of zeros and also for the function $f_3(\xi)$. Since the function $f_1(\xi)$ is continuous (at least in the considered domain), the sum function is also a continuous function. In principle one has series of the general form $f_i(\xi) = a\xi^2 + b\xi^4 + c\xi^6 + \ldots = \Sigma d\xi^n$. Although the terms form a null sequence, such series are divergent. For practical calculations, only the first terms (row fractionation after the quadratic term) are important. The series $f_2(\xi)$ and $f_4(\xi)$ are divergent anyway since they do not form a null sequence. If one needs series for great arguments, asymptotic formulas are necessary. But here one has to be careful because the limit $\xi \to \infty$ does not exist. By using asymptotic series the divergence does not play any role.

Similar formulas can also be derived for the electric fields and charge densities (the convergence should be checked by appropriate methods). Another useful series representation in terms of circular functions (in the sense of a Fourier series) is given by the following formula; we only present the first function $f_1(\xi)$, Equation (11), similar expressions could be obtained for the remaining:

$$f_1(\xi) = -\frac{1}{\eta}\left\{\ln\left[\cos\left(\frac{\pi\xi}{2K}\right)\right] - 4\sum_{n=1}^{\infty}\frac{1}{n}\,\frac{q^n}{1+(-1)^n q^n}\sin^2\left(\frac{\pi n\xi}{2K}\right)\right\} \tag{18}$$

where $q = \exp[-\pi K'/K]$ and K, K' are the complete elliptic integrals $K = K(k)$. Here the expansion is valid in every strip of the form $\left|\operatorname{Im}\pi\xi/(2K)\right| < 1/2\pi\,\ln\tau$ with τ as a parameter with positive imaginary part [39,40].

From the Table 1, it is seen that the limiting values $\lim_{\xi\to 0} f_i(\xi)$ vanish for the functions $f_1(\xi)$ and $f_3(\xi)$, the functions $f_2(\xi)$ and $f_4(\xi)$ remain finite and real. Otherwise taking $\lim_{\xi\to\infty} f_i(\xi)$ it is seen that these limits do not exist. From this standpoint one can say that these functions are not stable in the sense of the stability of solutions which require that the function(s) must vanish as $\xi \to \infty$ (thus the limits must exist). This might cause troubles in quantum-mechanical considerations in which the potential functions must "behave well" but such types of functions are known and can be used by suitable assumptions (no square

integrability). Also for a fast overview one can solve the Equations (7a) and (7b) in terms of a power series representation; here we give formulas valid up to order two with arbitrary coefficients $a_i \neq 0$ and $\lambda = \delta = c_1 = 1$. Due to the similar structure of these nODEs the series hardly differ; and one gets, for the eq.(7a)

$$p_1(\xi) = a_0 + a_1\xi + \frac{1}{4}\left(a_0^3\beta^2 - a_0 - 2\left(\alpha^2 - 1\right)a_1 + \frac{2a_1^2}{a_0}\right)\xi^2 + O[\xi]^3, \tag{19}$$

and similar for the Equation (7b)

$$p_2(\xi) = a_0 + a_1\xi + \frac{1}{2}\left(a_0^2\beta^2 - a_0 - \left(\alpha^2 - 1\right)a_1 + \frac{a_1^2}{a_0}\right)\xi^2 + O[\xi]^3. \tag{19a}$$

5. SUMMARY – BENEFITS AND DISADVANTAGES – OPEN PROBLEMS

I. Transient electrodynamical (and electrochemical) problems are notoriously difficult to solve (in the general case one needs Green's tensors and/or vector potentials) and uniqueness is not always given (solutions depending upon roots are involved so that branch cuts must be taken into account).

II. In this study we showed that a nPDE, the Equation (1) which has the meaning of a modified Poisson-Boltzmann Equation can be solved analytically by application of pure algebraic steps. The highly nonlinear equation was introduced by the author recently [33] to describe time depending electrochemical processes and/or charge transfer upon electrodes.

III. We applied an algebraic approach containing elliptic functions explicitly. It is remarkable that classes of solutions derived by this special method differ completely from solutions of the DHT in their behaviour. It is a special hallmark of algebraic methods that one cannot predict appropriate solutions in the sense of the solubility of the nonlinear algebraic system of polynomial equations. Several other approaches are used but none of them leads to useful results.

IV. The success and/or failure strongly depends upon the solubility of the nonlinear algebraic system. Due to the experience of the author such systems are often over determined and the number of equations n_e is greater than the number of unknowns n_u. The ideal case is therefore $n_e = n_u$ and by

skillful considerations in combination with the physical reality the outer form of the nonlinear algebraic system can be controlled. Thus we expand the original similarity variable $\xi = x - \lambda t$ to $\xi = \delta x - \lambda t$. The purpose of the similarity variable is twofold: It reduces a given nPDE to a nODE – this always works, and, if one seeks for, due to the physical situation, a traveling wave solution. One cannot, in general predict the solution manifold; that means that by use of the traveling wave reduction one has no guarantee to generate a traveling motion. In each case one has at least to check whether the solution represents a traveling wave motion or not.

V. A further important fact is given by the integration constant c_1 in the Equations (7a) and (7b), respectively. Only in the context of soliton theory one can set $c_i = 0$ (in view of a localized wave). Generally it is not allowed to set it zero as happen in several papers. Otherwise an interesting feature can be observed here: The constant c_1 relates the parameters δ and λ.

VI. The difference of the method used here to other algebraic methods is enormous. Most algebraic methods are based upon the fact that the unknown solution function satisfies a nODE of the first order [42], [43], [44], and [45] to mention some examples. Thus the name of the (algebraic) method comes from the used nODE, e.g. the hyperbolic tangent method (including the Riccati Equation as the cornerstone), the exponential transform method, the Weierstrass transform method, the Lambert function transform method and so on. Here, in our analysis the unknown solution function (the cosine amplitude function, Equation (c) and its derivatives can be used independently from any nODEs. Of course, the function and their derivatives have to satisfy general mathematical properties such like continuity, differentiability and existence in a given domain.

Note: For all scientists and engineers who are dealing with elliptic functions we recommend the excellent formula collection from Byrd and Friedmann, [46]. This attractive and unique treatment as well as the classical Abramowitz/Stegun [39] should be a standard equipment for all mathematical considerations.

VII. In fact, the algorithm works efficiently and solutions of the highly nPDE, the Equation (1) and the Equation (3) respectively can be derived without

any problems. Problems may appear by further using of the solution functions, e.g. the analytic determination of the total charge, the Equation (15). Here only a numerical procedure is possible. Also the solution procedure of the nonlinear algebraic system, the Equations (9) and (9a), respectively may cause troubles. If one is interested in dealing higher order nPDEs, the degree of the system will increase rapidly and long computing time is expected. Due to the experience of the author many of such systems are satisfied only by the trivial solution and the algebraic solution process will fail.

VIII. In the present analysis the EQS approximation was used and no magnetic effect were considered. To handle this case a further extensions will be done in future. Another aspect is the fact that the particles involved have quantum-like properties and another theory is necessary. Thus a quantum mechanical approach will be considered as a next task.

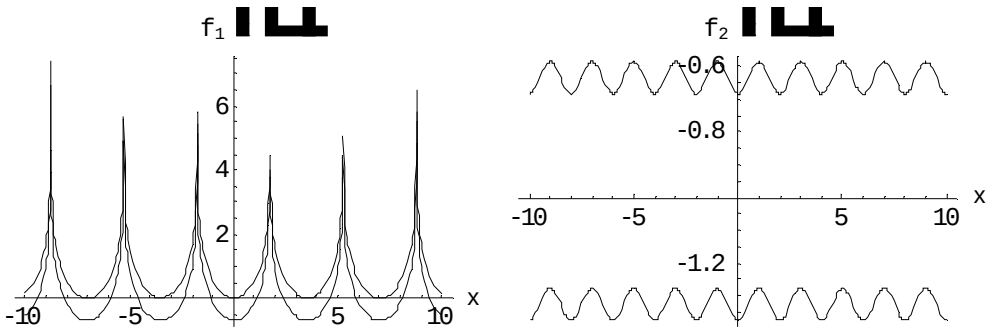

Figure 1. The solution function $f_1(\xi)$, Equation (11), left and the solution function $f_2(\xi)$, Equation (11a), right. Both functions show a travelling character. The graphs are generated by using the constant $a_1 = \pm 1$. The influence of the constant $\eta^{-1} = 0{,}0253$ (numerically) is such that it shifts the graphs upon the vertical axis and this true for all further graphics.

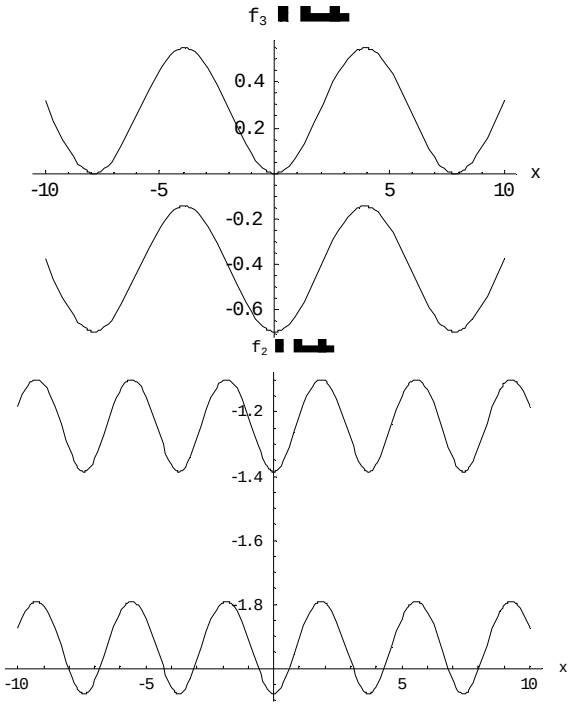

Figure 2. The solution function $f_3(\xi)$, Equation (11b), left and the solution function $f_4(\xi)$, Equation (11c), right. Also both functions show a travelling character. The functions are generated by using the constant $a_1 = \pm 1$ and $a_2 = \pm 1$.

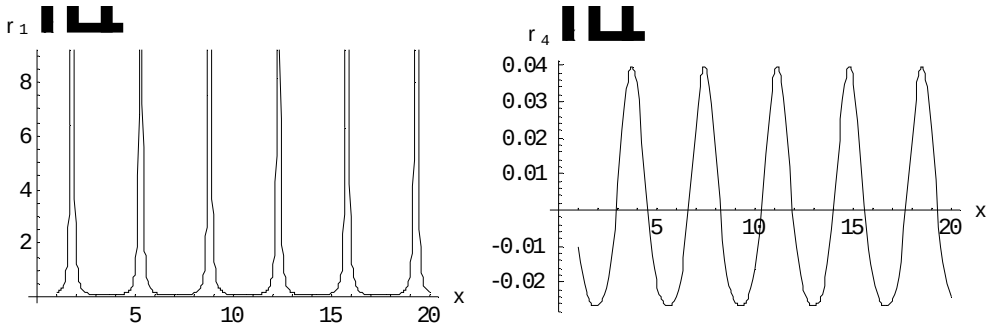

Figure 3. A planar sketch of the charge densities $\rho_1(\xi)$, left and $\rho_4(\xi)$, right. Here, also $a_1 = a_2 = 1$ was used. The functions show periodic behaviour once again. The periodic peaks left may be interpreted as a charge distribution near a charged particle (e.g. analogously in a crystal lattice).

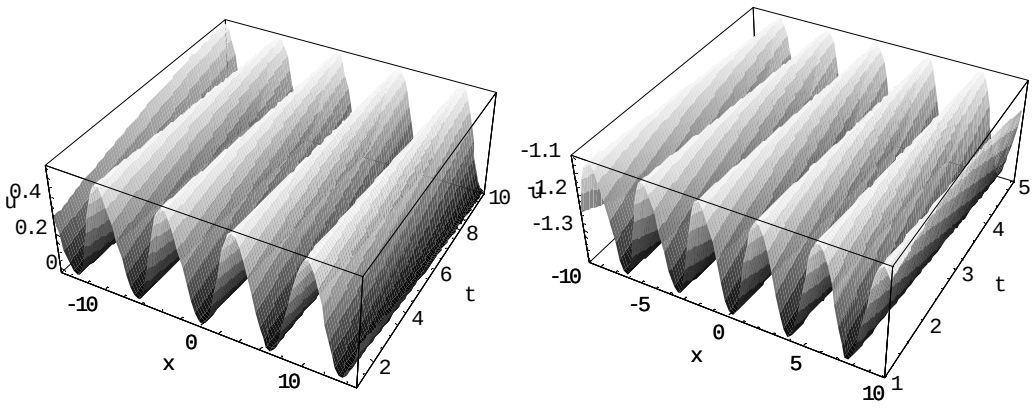

Figure 4. A three-dimensional plot of the functions $u_4(x,t)$, left and $u_3(x,t)$ right. The functions have the modulus $k = 1/2$ and $k = 2/3$ respectively and the values $\delta = \lambda = 1$ were used.

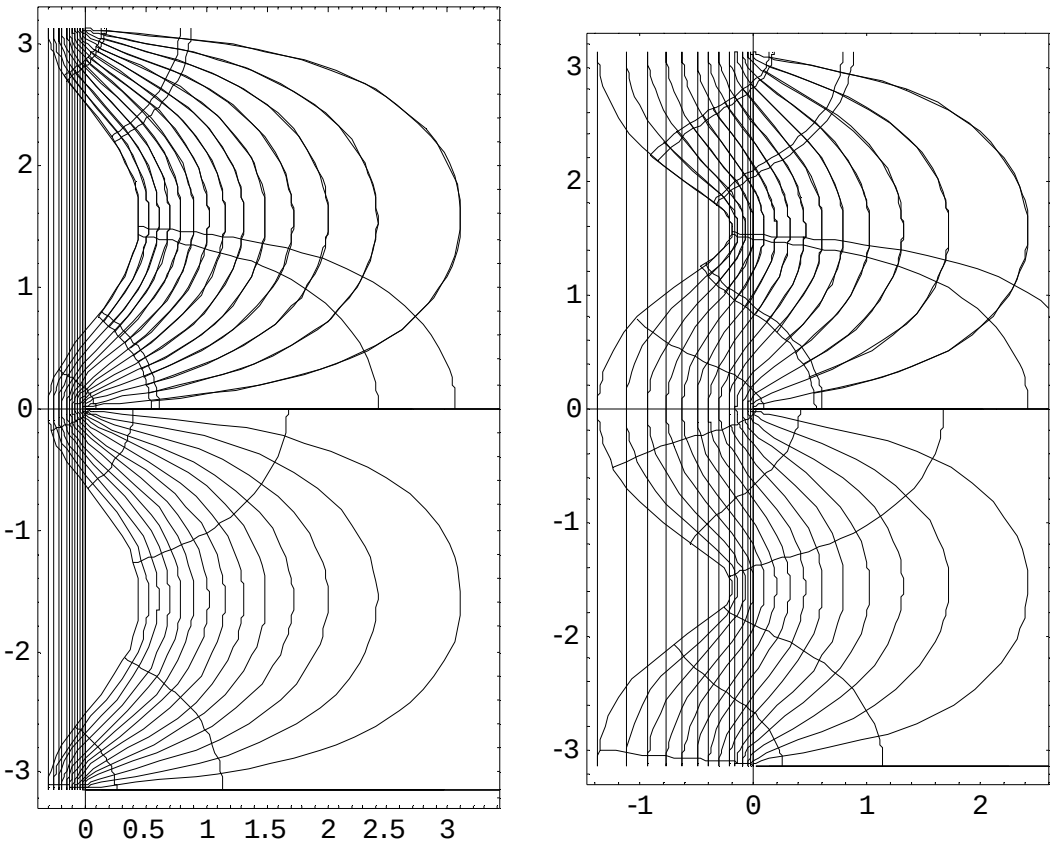

Figure 5. A graphical representation of the function Equation (11) in the principal form $\approx -\ln[cn(\xi,k)]$ with the modulus $k = 0{,}3660$ and for $0 < \xi < \pi/4$ left and $0 < \xi < \pi/2$ right without the influence of the constant η. One can see the poles in the given domain surrounded by symmetrical 'field line distribution'.

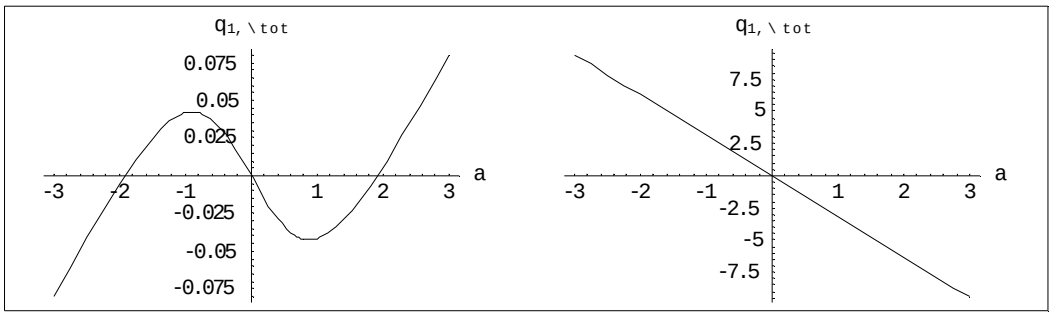

Figure 6. A planar sketch of the charge densities, the Equations (15b) left and (15c) right without the integral contributions. If one interprets the distance "a" as the seat of a charge generating size, then, on both sides of a charge accumulation is lockable). In this model the central ion is thought to be located in the centre. The increasing (decreasing) part up to the maximum (minimum) matches domains of higher concentrated charged areas.

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The Irregularity and Total Irregularity of Eulerian Graphs

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ABSTRACT

For an arbitrary graph G, the irregularity and total irregularity of G are defined as $irr(G) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)|$ and $irr_t(G) = 1/2 \sum_{u,v\in V(G)} |d_G(u) - d_G(v)|$, respectively, where $d_G(u)$ is the degree of vertex u. In this paper, we characterize all connected Eulerian graphs with the second minimum irregularity, the second and third minimum total irregularity, respectively.

1. INTRODUCTION

Throughout this paper, G is a simple and connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively. For a graph G, there is a novel notion named ***third Zagreb polynomial***, defined as $M_3(G,x) = \sum_{uv\in E(G)} x^{|d_G(u)-d_G(v)|}$. Astaneh-Asl et al. [7] studied $M_3(G,x)$ of Cartesian product of two graphs and a type of dendrimers. In special case, the value of derivative of this polynomial at point $x = 1$ is well known as the ***irregularity*** of G and denoted by $irr(G)$, which was already proposed by Albertson [6]. In the other words

$$irr(G) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)| \qquad (1)$$

In [6], Albertson gave some upper bounds on irregularity for trees, bipartite, and triangle-free graphs. Recall that the ***first Zagreb index*** M_1 and the ***second Zagreb index*** M_2 of G are defined as $M_1(G) = \sum_{u\in V(G)} d_G^2(u)$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u).d_G(v)$, respectively. These indices were introduced in [16] and reflect the extent of branching of the molecular carbon-atom skeleton and can be viewed as molecular structure-descriptors [8,25]. Moreover, the values of these indices are computed for a class of nanostar dendrimers in [26]. Fath-Tabar

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[14] named the sum in (1) the ***third Zagreb index,*** and established new bounds on the first and second Zagrab indices that depend on $irr(G)$. Zhou and Luo obtained the relationship between irregularity and first Zagreb index of graphs, and also they determined the graphs with maximum irregularity among trees and unicyclic graphs with given matching number and number of pendent vertices [19, 29]. Hansen and Melot determined the maximum irregularity of graphs with n vertices and m edges [17]. Moreover, Abdo and Dimitrov considered the irregularity of graphs under several graph operations [5]. Previously, we characterized all graphs with the second minimum of the irregularity in [20]. Also, we studied in [15, 21], trees and unicyclic graphs whose irregularity is extremal. More works about this graph invariant have been reported in [2, 9, 18, 22–24].

Recently, Abdo et al. [1] introduced a new measure of irregularity of a graph, so-called the ***total irregularity***, as $irr_t(G) = 1/2\sum_{u,v\in V(G)}|d_G(u) - d_G(v)|$. For a connected graph G, the irregularity indices irr and irr_t were compared in [12], where it was shown that $irr_t(G) \leq n^2/4irr(G)$. Furthermore, they proved that if G is a tree, then $irr_t(G) \leq (n-2) \times irr(G)$. Abdo and Dimitrov [4] gave the upper bounds on irr_t of graphs under several graph operations including lexicographic, Cartesian, strong, direct, and corona products, also join, disjunction and symmetric difference. In [1], graphs with maximal total irregularity were characterized and the upper bound on the total irregularity of graphs was obtained. In special classes of graphs, such as trees, unicyclic and bicyclic graphs, this invariant has been studied in [13, 27, 28].

An ***Eulerian circuit*** is a closed walk in a graph that visits every edge of the graph once and only once. A graph containing an Eulerian circuit is called an ***Eulerian graph***. The study of these graphs was initiated in 1736. Their study is a very fertile field of research for graph theorists. Although, in the graph theory, the term Eulerian graph has two common meanings, i.e. a graph with an Eulerian circuit, or a graph with every vertex of even degree. Note that in the case of connected graph, these definitions are equivalent [10].

The aim of this paper is to study the irregularity and total irregularity of connected Eulerian graphs. In Section 2, we show that the irregularity of an Eulerian graph is a multiple of 4, and by using it, we characterize all Eulerian graphs with the second minimum irregularity value. Finally in Section 3, we determine graphs with the second and third minimum of total irregularity value over the class of all connected Eulerian graphs.

2. THE SECOND MINIMUM IRREGULARITY OF EULERIAN GRAPHS

In this section,we first restate a proven result in [10], which is needful for proving that the irregularity of Eulerian graphs is divisible by 4. Afterwards, we would able to determine the Eulerian graphs with the second minimum irregularity value.

Lemma 2.1. [*10*] *A connected graph is Eulerian if and only if each of its vertices has even degree.*

Theorem 2.2. *Let G be an Eulerian graph with n vertices, then $irr(G) = 4k$, for some non-negative integer k.*

Proof. We prove the theorem by induction on n. Obviously, for $n = 1$, we have $irr(K_1) = 0$. Suppose that for any Eulerian graph H on less than n vertices, $irr(H) = 4k$, for some non-negative integer k. Now, we shall show that if G is an Eulerian graph on n vertices, then there exists a non-negative integer k' with $irr(G) = 4k'$. To show this, we shall use induction on the number of edges. For $m = 0$, it is obvious that $irr(\overline{K_n}) = 0$. By induction on m, suppose that for any n-vertex Eulerian graph H, which has less than m edges, we have $irr(H) = 4k$, for some non-negative integer k. Let G be an n-vertex Eulerian graph with m edges. Let $C_q = v_1v_2 \cdots v_qv_1$ be the smallest simple cycle in G, and $H = G - E(C_q)$. If $H = \overline{K_n}$, then $G = C_q$, and therefore $irr(G) = 0$. If $H \neq \overline{K_n}$, then either H is an n-vertex Eulerian graph with less than m edges, or each of connected components of H is an Eulerian graph on less than n vertices. Therefore, by inductions' hypotheses, there is some $k \geq 0$ such that $irr(H) = 4k$. For convenience, we use the following notations:

$$E' = \{xv \in E(H) : v \in V(C_q) \,\&\, x \in V(G) \setminus V(C_q)\},$$

$$d_l(v) = |\{xv \in E' : d_H(x) \leq d_H(v)\}|,$$

$$d_g(v) = |\{xv \in E' : d_H(x) > d_H(v)\}|,$$

$$sign(s) = \begin{cases} 1 & ; s = l \\ -1 & ; s = g \end{cases}.$$

Assume that $v_{q+1} = v_1$. With above notations, one can immediately see that for any vertex v_i of C_q, $d_H(v_i) = d_l(v_i) + d_g(v_i)$. Note that by the choice of C_q, there is no non-consecutive indices i and j such that $v_iv_j \in E(G)$. Moreover, for any edge $xv \in E'$, if $d_H(x) \leq d_H(v)$, then

$$|d_G(x) - d_G(v)| - |d_H(x) - d_H(v)| = 2 = 2\,sign(l).$$

Moreover, if $d_H(x) > d_H(v)$ then

$$|d_G(x) - d_G(v)| - |d_H(x) - d_H(v)| = -2 = 2\,sign(g).$$

Now, we have:

$$irr(G) - irr(H) = \sum_{uv \in E(C_q)} |d_G(u) - d_G(v)| + \sum_{xv \in E'} (|d_G(x) - d_G(v)| - |d_H(x) - d_H(v)|)$$

$$= \sum_{uv \in E(C_q)} |d_G(u) - d_G(v)| + 2\sum_{v \in V(C_q)} \left(d_l(v) - d_g(v)\right)$$

$$= \sum_{uv \in E(C_q)} \left(|d_G(u) - d_G(v)| + d_l(u) - d_g(u) + d_l(v) - d_g(v)\right) = \sum_{i=1}^{q} r_i.$$

such that for any $i = 1,2,\dots,q$,

$$r_i = |d_G(v_i) - d_G(v_{i+1})| + d_l(v_i) - d_g(v_i) + d_l(v_{i+1}) - d_g(v_{i+1}).$$

One can easily check that if $d_G(v_{i+1}) \leq d_G(v_i)$, then

$$r_i = 2d_l(v_i) - 2\,d_g(v_{i+1}) = 2\,\mathrm{sign}(l)d_l(v_i) + 2\,\mathrm{sign}(g)d_g(v_{i+1}),$$

and if $d_G(v_{i+1}) > d_G(v_i)$, then

$$r_i = -2\,d_g(v_i) + 2d_l(v_{i+1}) = 2\,\mathrm{sign}(g)d_g(v_i) + 2\,\mathrm{sign}(l)d_l(v_{i+1}).$$

Hence, for some suitable $s_i, s_i' \in \{l, g\}$, where $1 \leq i \leq q$, we can write the following:

$$\begin{aligned}
irr(G) - irr(H) = \sum_{i=1}^{q} r_i &= \left(2\,\mathrm{sign}(s_1)d_{s_1}(v_1) + 2\,\mathrm{sign}(s_2')d_{s_2'}(v_2)\right) \\
&\quad + \left(2\,\mathrm{sign}(s_2)d_{s_2}(v_2) + 2\,\mathrm{sign}(s_3')d_{s_3'}(v_3)\right) + \cdots \\
&\quad + \left(2\,\mathrm{sign}(s_q)d_{s_q}(v_q) + 2\,\mathrm{sign}(s_1')d_{s_1'}(v_1)\right) \\
&= \sum_{i=1}^{q}\left(2\,\mathrm{sign}(s_i)d_{s_i}(v_i) + 2\,\mathrm{sign}(s_i')d_{s_i'}(v_i)\right) \\
&= 2\sum_{i=1}^{q}\left(\mathrm{sign}(s_i)d_{s_i}(v_i) + \mathrm{sign}(s_i')d_{s_i'}(v_i)\right) \\
&= 2\sum_{i=1}^{q} t_i.
\end{aligned}$$

For each $i = 1,2,\dots,q$, there exist three cases as follow:

1) If $s_i = s_i' = l$, then $t_i = 2\,d_l(v_i)$.
2) If $s_i = s_i' = g$, then $t_i = -2\,d_g(v_i)$.
3) If $s_i \neq s_i'$, then $t_i = d_l(v_i) - d_g(v_i)$.

Since $d_G(v_i) = d_l(v_i) + d_g(v_i)$ is even, $d_l(v_i) - d_g(v_i)$ is even, too. Therefore, in all of the above cases, t_i is even. Thus,

$$irr(G) - irr(H) = 2\sum_{i=1}^{q} t_i = 4\sum_{i=1}^{q}\left(\frac{1}{2}\right)t_i = 4k''$$

where k'' is an integer. Hence, the theorem is proved by induction. □

Obviously, for a connected graph G, $irr(G) = 0$ if and only if it is a regular graph. Therefore, we have the following result:

Corollary 2.3. *For a non-regular connected Eulerian graph G of order n, $irr(G) \geq 4$.*

We know that the minimal irregularity of graphs is zero. Obviously, the irregularity of a graph is zero if and only if all of its connected components are regular. Since for each positive integer $r \geq 1$, each connected $2r$-regular graph is an Eulerian graph, hence the first minimum irregularity of Eulerian graphs is zero; and by Theorem 2.2, we conclude that the

second minimum of the irregularity of Eulerian graphs is 4. In the following theorem we characterize connected Eulerian graphs with the second minimum irregularity.

Theorem 2.4. *There are* 12 *types of connected Eulerian graphs with irregularity value 4, where* the *general forms and examples of them are shown in Figure 1 and Table 1, respectively.*

Proof. Let G be a connected Eulerian graph with $irr(G) = 4$. For each edge uv of G, set $irr(uv) = |d_G(u) - d_G(v)|$, so we can write $irr(G) = \sum_{uv \in E(G)} irr(uv)$. The proof continues in three separate cases as follows:

Case 1. Let xy be an edge of G such that $irr(xy) = 4$. Since G is a connected Eulerian graph, there is a cycle $xyv_1v_2 \cdots v_kx$ in G containing edge xy. Clearly, since $irr(G) = irr(xy) = 4$, then $irr(yv_1) = irr(v_1v_2) = \cdots = irr(v_kx) = 0$ and we deduce that $d_G(y) = d_G(v_1) = d_G(v_2) = \cdots = d_G(v_k) = d_G(x)$, which is a contradiction. Therefore, this case does not occur.

Case 2. There are two edges xy and xz such that $irr(xy) = irr(xz) = 2$. It is clear that yxz is a path from vertex y to vertex z. Suppose $U = \{u_1, u_2, \ldots, u_s\}$ and $V = \{v_1, v_2, \ldots, v_r\}$ are subsets of vertices of G such that $x, y, z \notin U, V$. Also assume that $yu_1u_2 \cdots u_sxz$ and $yxv_1v_2 \cdots v_rz$ are two paths in G from vertex y to vertex z containing vertex x. Since $irr(G) = irr(xy) + irr(xz)$, then

$$irr(yu_1) = irr(u_1u_2) = \cdots = irr(u_sx) = irr(xv_1) = irr(v_1v_2) = \cdots = irr(v_rz) = 0.$$

Consequently, $d_G(x) = d_G(y) = d_G(z)$, which is a contradiction . Thus, two subcases will be considered as:

(**I**) There are two paths from vertex y to vertex z such that vertex x belongs to only one of them. Assume that $yu_1u_2 \cdots u_sz$ is a path in G, so $d_G(y) = d_G(z)$. Therefore, G is constructed of two separated components G_1 and G_2 that are connected by edges xy and xz, which $x \in V(G_1)$ and $y, z \in V(G_2)$. Let $|V(G_1)| = k$ and $|V(G_2)| = n - k$. Thus, we may consider two different parts as follows:

(i) $d_G(x) = a, d_G(y) = d_G(z) = a - 2$;

(ii) $d_G(x) = a, d_G(y) = d_G(z) = a + 2$.

In part(i), for any u in $V(G_1)\backslash\{x\}$, $d_{G_1}(u) = a$, $d_{G_1}(x) = a - 2$, and for any vertex u in $V(G_2)\backslash\{y,z\}$, $d_{G_2}(u) = a - 2$, $d_{G_2}(y) = d_{G_2}(z) = a - 3$. Therefore, $2|E(G_1)| = ka - 2$, $2|E(G_2)| = n(a - 2) - ka + 2(k - 1)$, G_1 is a $(2t + 2)$-regular graph, and G_2 is a $2t$-regular graph, for some $t \geq 1$. Consequently, ka and $n(a - 2)$ are even. Since a is even, k and n can be odd or even. Thus, four types will occur (see Table 1, types 1-4).

In part(ii), we have $2|E(G_1)| = ka - 2$, $2|E(G_2)| = (n - k)(a + 2) - 2$. Consequently, k and n can be odd or even. Thus, we have four further types (see Table 1,

types 5–8). Note that in these types, G_1 is a $2t$-regular graph and G_2 is a $(2t+2)$-regular graph, for some $t \geq 1$.

(II) There is only one path, say yxz, joining vertices y and z which contains vertex x. Suppose $xu_1u_2\cdots u_sy$ and $xv_1v_2\cdots v_rz$ are two paths in G, where $u_1 \neq z$ and $v_1 \neq y$. Since $irr(G) = irr(xy) + irr(xz)$, then by above assumptions, $d_G(x) = d_G(y) = d_G(z)$, which is a contradiction to $irr(xy) = irr(xz) = 2$. Therefore, G is composed of three separate components G_1, G_2 and G_3 where G_1 and G_2 are connected by edge xy, G_1 and G_3 are connected by edge xz, $x \in V(G_1), y \in V(G_2), z \in V(G_3), V(G) = V(G_1) \cup V(G_2) \cup V(G_3)$ and $E(G) = E(G_1) \cup E(G_2) \cup E(G_3) \cup \{xy, xz\}$. Obviously, $2|E(G_2)| + 1 = \sum_{u\in V(G_2)} d_G(u)$ but $d_G(u)$ is even, for any vertex u of G. Therefore, this subcase does not occur.

Case 3. There are two distinct edges xy and uv such that $irr(xy) = irr(uv) = 2$. As case 2, we may again check this case in two subcases as follows:

(I) vertices y and u belong to all paths from vertex x to vertex v;

(II) There are two paths from vertex x to vertex v such that vertices y and u belong to only one of them.

Similar to case 2, in subcase **(I)**, G is constructed of three separate components G_1, G_2 and G_3, where $G_1$and $G_2$are connected by edge xy, and G_2, G_3 are connected by edge uv, $x \in V(G_1), y, u \in V(G_2), v \in V(G_3), V(G) = V(G_1) \cup V(G_2) \cup V(G_3)$ and $E(G) = E(G_1) \cup E(G_2) \cup E(G_3) \cup \{xy, uv\}$. Obviously, $2|E(G_1)| + 1 = \sum_{w\in V(G_1)} d_G(w)$ but $d_G(w)$ is even, for any vertex w of G. Therefore, this case does not occur.

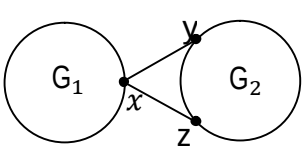
In subcase **(II)**, we can see that G is composed of two separate components G_1, G_2 where G_1 and G_2 are connected by edges xy and uv, also $x, v \in V(G_1)$ and $y, u \in V(G_2)$. Let $d_G(x) = a, |V(G_1)| = k$ and $|V(G_2)| = n - k$. Without loss of generality, in the case **(II)**, we can consider following two parts:

(i) $d_G(x) = d_G(v) = a, d_G(y) = d_G(u) = a + 2$;

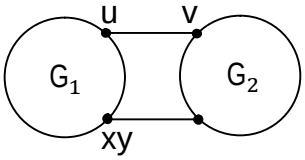
(ii) $d_G(x) = d_G(v) = a, d_G(y) = d_G(u) = a - 2$.

A similar argument as case 2, in part(i), k and n can be odd or even . Thus we have another four types (see Table.1, types 9–12). Note that, the graphs in parts(ii) and (i) are identical, where G_1 is $2t$-regular, and G_2 is $(2t+2)$-regular, for some $t \geq 1$. □

Note that, in generally, the irregularity of a graph is equal to the summation of its connected components' irregularities. Therefore, if G is an n-vertex (not necessary connected) Eulerian graph with $irr(G) = 4$, then Theorem 2.2 implies that $G \cong G' \cup \overline{K_s}$, where G' is a connected Eulerian graph on $n - s$ vertices with $irr(G') = 4$.



General form of types 1−8



General form of types 9−12

Figure 1. General forms of Eulerian graphs with the second minimum irregularity.

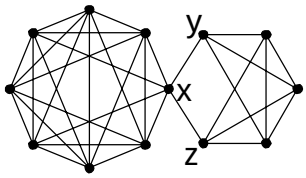
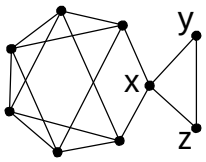
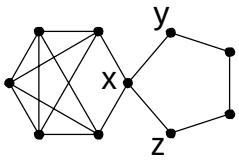
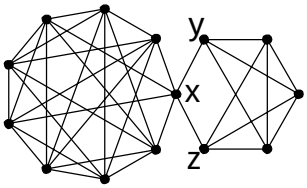
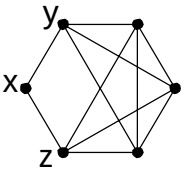
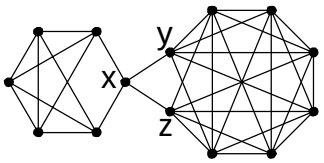
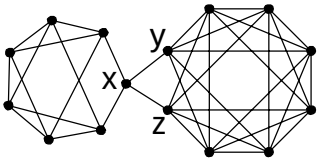
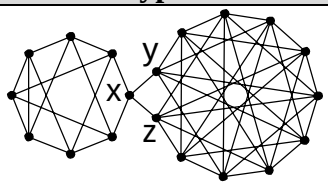
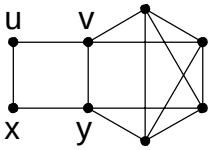
Type 1	**Type 2**	**Type 3**
		
n=13,k=8,a=6,t=2 G_1: (2t + 2)-regular G_2: 2t-regular	n=9,k=7,a=4,t=1 G_1: (2t + 2)-regular G_2: 2t-regular	n=10,k=6,a=4,t=1 G_1: (2t + 2)-regular G_2: 2t-regular
Type 4	**Type 5**	**Type 6**
		
n=14,k=9,a=6,t=2 G_1: (2t + 2)-regular G_2: 2t-regular	n=6,k=1,a=2,t=1 G_1: 2t-regular G_2: (2t + 2)-regular	n=14,k=6,a=4,t=2 G_1: 2t-regular G_2: (2t + 2)-regular
Type 7	**Type 8**	**Type 9**
		
n=15,k=7,a=4,t=2 G_1: 2t-regular G_2: (2t + 2)-regular	n=19,k=8,a=4,t=2 G_1: 2t-regular G_2: (2t + 2)-regular	n=8,k=2,a=2,t=1 G_1: 2t-regular G_2: (2t + 2)-regular

Table 1. Examples of Eulerian graphs with the second minimum irregularity.

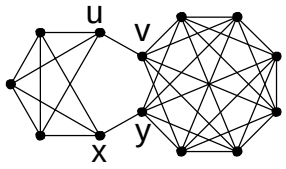
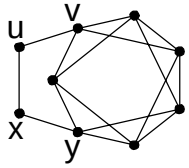
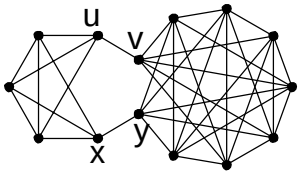
Type 10	Type 11	Type 12
		
$n=13,k=5,a=4,t=2$	$n=9,k=2,a=2,t=1$	$n=14,k=5,a=4,t=2$
G_1: $2t$-regular	G_1: $2t$-regular	G_1: $2t$-regular
G_2: $(2t+2)$-regular	G_2: $(2t+2)$-regular	G_2: $(2t+2)$-regular

Table 1. (Continued).

3. THE SECOND AND THIRD MINIMUM TOTAL IRREGULARITY FOR EULERIAN GRAPHS

In this section, first we express some initially basic definitions and a prominent proved result of [3], and then investigate the second and third minimum total irregularity of connected Eulerian graphs.

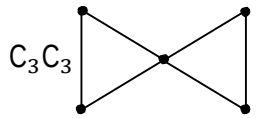
If $V(G) = \{v_1, v_2, \ldots, v_n\}$, then the sequence $(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$ is called a ***degree sequence*** of G [11]. Without loss of generality, we may assume that $d_G(v_1) \geq d_G(v_2) \geq \ldots \geq d_G(v_n)$. A ***bicyclic graph*** is a simple connected graph in which the number of edges equals to $n + 1$. A ***basic bicyclic ∞-graph***, denoted by $\infty(p, q, l)$, is obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex of C_p and one of C_q with a path P_l of length $l - 1$ (in the case of $l = 1$, identifying the above two vertices) where $p, q \geq 3$ and $l \geq 1$.

Clearly, a graph G has total irregularity zero if and only if G is a regular graph. Note that the connected $2r$-regular graph, is an Eulerian graph with $irr_t = 0$. Hence,the first minimum total irregularity of Eulerian graphs is zero. Moreover the corresponding extremal Eulerian graphs with total irregularity 0 are exactly all $2r$-regular Eulerian graphs, where $r \geq 0$, and if $r > 0$ then the graph is connected. In [3], the authors characterized the non-regular graphs with the second and the third smallest total irregularity.

Lemma 3.1. [3] *Let G be a simple connected graph with n vertices. If G is a non-regular graph, then $irr_t(G) \geq 2n - 4$.*

In the following result, we show that the second minimum of the total irregularity of Eulerian graphs is 8 and determine the unique Eulerian graph with $irr_t = 8$.

Theorem 3.2. *Let G be a connected non-regular Eulerian graph of ordern, then* $irr_t(G) \geq 8$*, and the equality holds if and only if* $G \cong \infty(3,3,1)$*, where the bicyclic graph* $\infty(3,3,1)$ *is shown in Figure 2.*

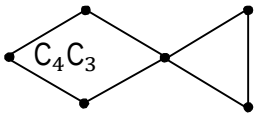


$\infty(3,3,1)$

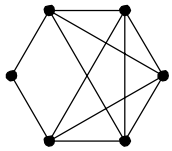
Figure 2. Unique Eulerian graph with the second minimum total irregularity.

Proof. By Lemma 3.1, if $n \geq 7$, then $irr_t > 8$. If $n = 6$, then the degree sequence of G can be one of the following cases: $(4,4,4,4,4,2), (4,4,4,4,2,2), (4,4,4,2,2,2), (4,4,2,2,2,2)$, and $(4,2,2,2,2,2)$. By a simple calculation, one can easily see that in these cases, $irr_t(G) > 8$. If $n = 5$, then the degree sequence of G may be either $(4,4,2,2,2)$ or $(4,2,2,2,2)$. Note that the cases $(4,4,4,4,2)$ and $(4,4,4,2,2)$ do not occur. Also, the total irregularity of graph G with degree sequence $(4,4,2,2,2)$ is equal to 12 and with degree sequence $(4,2,2,2,2)$ is equal to 8. Additionally, the graph G with degree sequence $(4,2,2,2,2)$ is the bicyclic graph $\infty(3,3,1)$. Clearly, regular graphs C_3 and C_4 are the only Eulerian graphs with 3 and 4 vertices, which have total irregularity 0. □

Theorem 3.3. *Let* $G \ncong \infty(3,3,1)$ *be a connected non-regular Eulerian graph of order n, then* $irr_t(G) \geq 10$*, and the equality holds if and only if* $G \cong \infty(4,3,1)$ *or H, where graphs* $\infty(4,3,1)$ *and H are shown in Figure 3.*



$\infty(4,3,1)$



H

Figure 3. Eulerian graphs with the third minimum total irregularity.

Proof. By Lemma 3.1, if $n \geq 8$ then $irr_t > 10$. If $n = 7$, then the degree sequence of G may be the following cases:

$(6,6,6,6,6,6,4), (6,6,6,6,6,6,2), (6,6,6,6,6,4,4), (6,6,6,6,6,4,2), (6,6,6,6,6,2,2),$
$(6,6,6,6,4,4,4), (6,6,6,6,4,4,2), (6,6,6,6,4,2,2), (6,6,6,6,2,2,2), (6,6,6,4,4,4,4),$
$(6,6,6,4,4,4,2), (6,6,6,4,4,2,2), (6,6,6,4,2,2,2), (6,6,6,2,2,2,2), (6,6,4,4,4,4,4),$
$(6,6,4,4,4,4,2), (6,6,4,4,4,2,2), (6,6,4,4,2,2,2), (6,6,4,2,2,2,2), (6,6,2,2,2,2,2),$
$(6,4,4,4,4,4,4), (6,4,4,4,4,4,2), (6,4,4,4,4,2,2), (6,4,4,4,2,2,2), (6,4,4,2,2,2,2),$
$(6,4,2,2,2,2,2), (6,2,2,2,2,2,2), (4,4,4,4,4,4,2), (4,4,4,4,4,2,2), (4,4,4,4,2,2,2),$
$(4,4,4,2,2,2,2), (4,4,2,2,2,2,2), (4,2,2,2,2,2,2).$

By a simple calculation, one can easily see that in these cases, $irr_t(G) > 10$. If $n = 6$, then the degree sequence of G can be the following cases:

$$(4,4,4,4,4,2), (4,4,4,4,2,2), (4,4,4,2,2,2), (4,4,2,2,2,2), (4,2,2,2,2,2).$$

The total irregularity of graph G with degree sequence $(4,4,4,4,4,2)$ or $(4,2,2,2,2,2)$ is equal to 10 and with the other degree sequences is more than 10. Note that if $(4,4,4,4,4,2)$ is degree sequence of graph G, then $G \cong H$, and if $(4,2,2,2,2,2)$ is degree sequence of graph G, then $G \cong \infty(4,3,1)$. Finally, if $n \leq 5$, then by referring to the proof of Theorem 3.2, we see that the total irregularity value of G is not equal to 10. □

Corollary 3.4. *The second and third minimum value of the total irregularity of Eulerian graphs are* 8 *and* 10*, respectively.*

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Some Remarks on the Arithmetic–Geometric Index

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ABSTRACT

Using an identity for effective resistances, we find a relationship between the arithmetic-geometric index and the global cyclicity index. Also, with the help of majorization, we find tight upper and lower bounds for the arithmetic-geometric index.

1. INTRODUCTION

Let G=(V,E) be a finite simple graph with vertex set V={1, 2, ..., n}, edge set E and degrees $d_1 \geq d_2 \geq \cdots \geq d_n$. The arithmetic-geometric index of a graph, proposed by Vukičević and Furtula (see[19]), is defined by

$$GA(G) = \sum_{(i,j)\in E} \frac{2\sqrt{d_i d_j}}{d_i + d_j} \qquad (1)$$

This index has attracted considerable attention and, through a variety of inequalities, it has been compared to a number of other indices, such as the ABC index, the first and second Zagreb indices, the general Randić index, the modified Narumi-Katayama index and the harmonic and sum-connectivity indices, among others. Different upper and lower bounds have been found for *GA*(*G*) either through the connections to these other indices, or from first principles, see [5 – 8, 12, 15 – 18] for details.

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In this note we present two additional contributions to the study of *GA*(*G*). First, we use notions of electric circuits in order to prove a relationship, to the best of our knowledge not explored yet, between *GA*(*G*) and the global cyclicity index, introduced by Klein and Ivanciuc (see [10]) and defined by

$$C(G) = \sum_{(i,j)\in E} \frac{1}{R_{ij}} - |E| \tag{2}$$

where R_{ij} denote the effective resistance between the vertices *i* and *j*, that is, the voltage drop between vertices *i* and *j* when a battery is installed between those two vertices such that a unit current flows between them. This index has further been studied in [2, 21–23].

We also apply majorization techniques in order to find tight upper and lower bounds for *GA*(*G*). Majorization has been applied extensively to find bounds and extremal values for a variety of descriptors .We point out the book chapters [1] and [3] and the recent articles [9, 13, 21] for a sample of the variety of scenarios covered with this approach.

Here is a brief summary of majorization (for more details the reader is referred to [11]): given two n-tuples $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ with $x_1 \geq x_2 \geq \cdots \geq x_n$ and $y_1 \geq y_2 \geq \cdots \geq y_n$, we say that x majorizes y and write $x \succ y$ in case

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \tag{3}$$

for $1 \leq k \leq n-1$ and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i. \tag{4}$$

A Schur-convex function $\Phi : R \to R$ keeps the majorization inequality, that is, if Φ is Schur-convex then $x \succ y$ implies $\Phi(x) \geq \Phi(y)$. Likewise, a Schur-concave function reverses the inequality: for this type of function $x \succ y$ implies $\Phi(x) \leq \Phi(y)$. A simple way to construct a Schur-convex (resp. Schur-concave) function is to consider $\Phi(x) = \sum_{i=1}^{n} f(x_i)$, where $f: \mathbb{R} \to \mathbb{R}$ is a convex (resp. concave) one-dimensional real function.

The main idea for finding bounds through majorization for a molecular index is to express such index as a Schur-convex or Schur-concave function, and then to identify maximal and minimal elements, x^* and x_* respectively, that is, elements in the subspace of interest of the n-dimensional real space (which can be a set of n-tuples of degrees of vertices, or eigenvalues, or effective resistances, etc.) such that $x^* \succ x \succ x_*$, for all n-tuples x in the subspace of interest, and then if Φ is Schur-convex we will have $\Phi(x^*) \geq \Phi(x) \geq \Phi(x_*)$, for all x, having thus found the upper and lower bounds of interest, $\Phi(x^*)$ and $\Phi(x_*)$, respectively. A similar conclusion follows, exchanging the words “upper” and “lower”, if Φ is Schur-concave.

2. EFFECTIVE RESISTANCES AND THE GEOMETRIC-ARITHMETIC INDEX

The following lemma is fundamental for what follows.

Lemma 1. For any G and (i,j) ∈ E we have

$$R_{ij} \geq \frac{\delta}{\delta+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{5}$$

Proof. We prove that

$$\frac{d_i+d_j-2}{d_i d_j-1} \geq \frac{\delta}{\delta+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{6}$$

Without loss of generality, let us assume that $d_i = \max\{d_i,d_j\}$ and $d_j = \min\{d_i,d_j\}$. Then $\delta \leq d_j$ and since the real function $f(x) = \frac{x}{x+1}$ is increasing, in order to prove (6) it is enough to prove that

$$\frac{d_i+d_j-2}{d_i d_j-1} \geq \frac{d_j}{d_j+1}\left(\frac{1}{d_i}+\frac{1}{d_j}\right) \tag{7}$$

But it is an easy computation to see that the truth of (7) is equivalent to the statement $(d_i-1)(d_i-d_j) \geq 0$. And now we can apply a result in [14] stating that for (i,j) ∈ E $R_{ij} \geq \frac{d_i+d_j-2}{d_i d_j-1}$ finishing the proof .With this lemma we can prove now the following

Proposition 2. For any graph G we have

$$GA(G) \geq \frac{2\delta}{\Delta(\delta+1)}\left(C(G)+|E|\right) \tag{8}$$

Proof. For any G we have

$$GA(G) = \sum_{(i,j)\in E} \frac{2\sqrt{d_i d_j}}{d_i+d_j} \geq \frac{2}{\Delta}\sum_{(i,j)\in E}\left(\frac{1}{d_i}+\frac{1}{d_j}\right)^{-1}$$
$$\geq \frac{2\delta}{\Delta(\delta+1)}\sum_{(i,j)\in E}\frac{1}{R_{ij}} = \frac{2\delta}{\Delta(\delta+1)}(\mathrm{C(G)+|E|}).$$

The previous proposition yields as corollaries many lower bounds for GA(G) and upper bounds for C(G). For example,

Corollary 3. For any G with n ≥ 3 we have

$$GA(G) \geq \frac{2\delta|E|^2}{\Delta(\delta+1)(n-1)} \tag{9}$$

For any d-regular G we have

$$C(G) \leq \frac{nd(d-1)}{4} \tag{10}$$

Proof. It is shown in [21] that, for n ≥ 3, $C(G) \geq \frac{|E|(|E|-n+1)}{n-1}$. Inserting into (8) finishes the proof of (a). For (b), it is immediate from the definition that if G is regular, then GA(G) = |E| and inserting this into (8) gives us the desired result .

Remarks4. The inequality (9) attains the equality for K_n, but not for other regular graphs, and it is not comparable to the bound found in [5]:

$$GA(G) \geq \frac{2|E|\sqrt{\Delta\delta}}{\Delta+\delta} \tag{11}$$

as can be seen taking G to be K_{n-1} together with an extra vertex attached with a single edge to any of the vertices of the K_{n-1} . For this graph the bound (11) is of order $n^{3/2}$ whereas (9) is of order n^2 . We will improve slightly the bound (9) below. Also, the bound (10) recovers a result in [21], with a totally different proof.

3. MAJORIZATION AND THE GEOMETRIC-ARITHMETIC INDEX

We present the following results, found in Section 2.3 of [1] (Corollary 2.3.2 and Theorem 2.3.2) as a lemma which will be used below.

Lemma 1. Let Σ_a be the set of real n – tuples $x = (x_1, x_2, \dots, x_n)$ such that $x_1 \geq x_2 \geq \dots \geq x_n$ and $\sum_{i=1}^{n} x_i = a$. Let S_a be the set of n-tuples belonging to Σ_a which additionally satisfy $M \geq x_i \geq m$. Then

(i) The minimal element of Σ_a is $(\frac{a}{n}, \dots, \frac{a}{n})$

(ii) If the minimal element in (i) belongs to S_a , then it is also the minimal element of S_a;

(iii) the maximal element of S_a is (M,M,...,M,θ,m,m,...,m), where M appears k times, m appears $n - k - 1$ times, $k = [\frac{a-nm}{M-m}]$ and $\theta = a - Mk - m(n - k - 1)$.

Lemma 2. For all G we have

$$\frac{2}{\Delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}} \leq GA(G) \leq \frac{2}{\delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}} \ , \tag{12}$$

where $A_{ij} = \frac{1}{d_i} + \frac{1}{d_j}$.

Proof. Write

$$\sum_{(i,j)\in E}\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{2}{\Delta}\sum_{(i,j)\in E}\frac{d_i d_j}{d_i + d_j} = \frac{2}{\Delta}\sum_{(i,j)\in E}\frac{1}{A_{ij}}$$

The other inequality proceeds similarly. Now we will apply majorization to the summation $\sum_{(i,j)\in E}\frac{1}{A_{ij}}$, by looking at the function $\Phi(x) = \sum_{i=1}^{|E|}\frac{1}{x_i}$ on the set of |E|-tuples $x = (x_1, x_2, \dots, x_n)$. Specifically we will show the following:

Proposition 3. For any G we have

$$\frac{2}{\Delta}\frac{|E|^2}{n} \leq GA(G) \leq \frac{2}{\delta}\left(\frac{2k}{3} + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2}\right) \tag{13}$$

where

$$k = \left[\frac{n-|E|\frac{2}{n-1}}{\frac{3}{2}-\frac{2}{n-1}}\right], \theta = n - \frac{3}{2}k - \frac{2}{n-1}(|E| - k - 1).$$

The lower bound is attained by any regular graph. The upper bound is attained by the complete graph.

Proof. We notice that the numbers A_{ij} satisfy

$$\frac{2}{n-1} \leq A_{ij} \leq \frac{3}{2} \tag{14}$$

And

$$\sum_{(i,j)\in E} A_{ij} = \sum_{i=1}^{n} \frac{d_i}{d_i} = n \tag{15}$$

The right inequality in (14) is clear because in any edge (i,j) of a connected graph G with n > 2, if $d_i = 1$ then $d_j \geq 2$.

Let us consider the subset of $\mathbb{R}^{|E|}$ defined as

$$\Sigma_n = \{x \in \mathbb{R}^{|E|} : x_1 \geq x_2 \geq \cdots \geq x_{|E|}\,;\, \sum_{j=1}^{|E|} x_j = n\}$$

and S_n the subset of Σ_n such that its |E|-tuples satisfy $\frac{3}{2} \geq x_i \geq \frac{2}{n-1}$ for $1 \leq i \leq |E|$. By Lemma 1 we can find explicitly the minimal element of S_n, that is, an |E|-tuple x_* such that $x \succ x_*$ for $x \in S_n$, indeed $x_* = \left(\frac{n}{|E|}, \frac{n}{|E|}, \ldots, \frac{n}{|E|}\right)$.

Notice that x_* belongs to S_n because the coordinates of x_*, which are all equal to $\frac{n}{|E|}$ Satisfy $m = \frac{1}{2(n-1)} \leq \frac{n}{|E|} \leq \frac{n}{n-1} \leq \frac{3}{2} = M$, as long as $n \geq 3$. Also, since $f(x) = \frac{1}{x}$, for $x > 0$, is convex, then $\Phi(x) = \sum_{i=1}^{|E|} \frac{1}{x_i}$is Schur-convex, and $\Phi(x) \geq \Phi(x_*) = \frac{|E|^2}{n}$, and since the |E|-tuple of numbers A_{ij} over the edges of the graph, properly arranged in decreasing order, belongs to the set S_n on account of facts (14) and (15), we have that $\sum_{(i,j)\in E} A_{ij} \geq \frac{|E|^2}{n}$, and this together with (12) of lemma 2 ends the proof of the lower bound in (13).

Analogously for the upper bound, by Lemma 2 we can identify explicitly the maximal element of S_n, that is, the |E|-tuple x^* such that $x^* \succ x$ for all $x \in S_n$, indeed $x^* = \left(\frac{3}{2}, \frac{3}{2}, \ldots, \frac{3}{2}, \theta, \frac{2}{n-1}, \frac{2}{n-1}, \ldots, \frac{2}{n-1}\right)$, where $\frac{3}{2}$ appears k times, $\frac{2}{n-1}$ appears $|E| - k - 1$ times and $k = \left[\frac{n-|E|\frac{2}{n-1}}{\frac{3}{2}-\frac{2}{n-1}}\right], \theta = n - \frac{3}{2}k - \frac{2}{n-1}(|E| - k - 1)$. Therefore

$$\sum_{(i,j)\in E} A_{ij} \leq \Phi(x^*) = \left(\frac{2k}{3} + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2}\right),$$

and this together with (12) gives us the upper bound in (13).

For any Δ-regular graph G the lower bound becomes |E|, which coincides with the value of GA(G). For the complete graph K_n , k = 0, $\theta = \frac{2}{n-1}$ and the upper bound becomes $\frac{n(n-1)}{2}$, which is precisely the value of GA(K_n) = |E|.

Remarks 4. The versatility of majorization can be seen in this theorem, where the quantities to be majorized are neither degrees, nor eigenvalues, nor effective resistances, as is usually the case in the literature, but the numbers A_{ij} , which perhaps do not have a clear-cut graph significance. The lower bound in (13) is always better than (8) on account of the fact that $\delta \leq n - 1$. We point out that this lower bound could have been obtained without majorization, by using the harmonic mean-arithmetic mean inequality. The real strength of the method in this case seems to be in the upper bound, which can be improved if we restrict somewhat the degrees of the vertices in the graph, as in the following three propositions.

Proposition 5. For any G without pendent vertices we have

$$GA(G) \leq \frac{2}{\delta}\left(k + \frac{1}{\theta} + (|E| - k - 1)\frac{n-1}{2}\right)$$

Where $k = \left[\frac{n(n-1)-2|E|}{n-1}\right]$,$\theta = n - k - \frac{2}{n-1}(|E| - k - 1)$. The equality is attained by the cycle graph C_n and the complete graph K_n .

Proof. In the absence of pendent vertices we can get the upper bound $A_{ij} \leq 1$ and the proof in the previous proposition applies, replacing everywhere 3/2 with 1. For the complete graph we obtain k = 0, $\theta = \frac{2}{n-1}$ and the upper bound becomes $\frac{n(n-1)}{2}$, which is the precise value of GA(K_n) = |E|. For the cycle graph, where |E| = n, we get k = n and $\theta = \frac{2}{n-1}$, and the upper bound becomes n, which is the value GA(C_n) = |E|.

Recall that a chemical graph is one where $d_i \leq 4$ for all i. For this sort of graph we can prove the following.

Proposition 6. For any chemical graph G we have

$$GA(G) \leq \frac{2}{\delta}\left(\frac{2k}{3} + \frac{1}{\theta} + 2(|E| \pm k - 1)\right),$$

Where $k = [n - \frac{|E|}{2}]$, $\theta = n - \frac{3}{2}k - \frac{1}{2}(|E| - k - 1)$. The equality is attained by any 4-regular graph.

Proof. In this case we can get the lower bound $A_{ij} \geq \frac{1}{2}$ and the proof in proposition 2 applies, replacing everywhere $\frac{2}{n-1}$ with $\frac{1}{2}$. For any 4-regular graph we have k = 0 and $\theta = \frac{1}{2}$, and thus the upper bound becomes 2n, which is precisely the value of GA(G) = |E|. Combining the two hypotheses, we obtain a more compact statement in the following

Proposition 7. For any chemical graph G without pendent vertices we have

$$GA(G) \leq \frac{2}{\delta}(3|E| - 2n)$$

The equality is attained by the cycle graph C_n and any 4-regular graph.

Proof. In this case we obtain that k = 2n−|E| and $\theta = \frac{1}{2}$, making the computations, similar to those in the previous propositions, very simple .

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Novel Atom–Type–Based Topological Descriptors for Simultaneous Prediction of Gas Chromatographic Retention Indices of Saturated Alcohols on Different Stationary Phases

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ABSTRACT

In this work, novel atom-type-based topological indices, named *AT* indices, were presented as descriptors to encode structural information of a molecule at the atomic level. The descriptors were successfully used for simultaneous quantitative structure-retention relationship (QSRR) modeling of saturated alcohols on different stationary phases (SE-30, OV-3, OV-7, OV-11, OV-17 and OV-25). At first, multiple linear regression models for Kovats retention index (*RI*) of alcohols on each stationary phase were separately developed using *AT* and Randic's first-order molecular connectivity ($^1\chi$) indices. Adjusted correlation coefficient (R^2_{adj}) and standard error (*SE*) for the models were in the range of 0.994-0.999 and 4.40-8.90, respectively. Statistical validity of the models were verified by leave-one-out cross validation ($R^2_{cv} > 0.99$). In the next step, whole *RI* values on the stationary phases were combined to generate a new data set. Then, a unified model, added McReynolds polarity term as a descriptor, was developed for the new data set and the results were satisfactory (R^2_{adj}=0.995 and *SE*=8.55). External validation of the model resulted in the average values of 8.29 and 8.69 for standard errors of calibration and prediction, respectively. The topological indices well covered the molecular properties known to be relevant for retention indices of the model compounds.

1. INTRODUCTION

QSRR modeling as a branch of quantitative structure–property relationship (*QSPR*) studies, is one of the most effective approaches to provide significant information on retention

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mechanism as well as the effect of molecular structure on retention behavior of various classes of compounds [1,2]. The first important step in QSPR studies is to quantify chemical structures of the molecules by descriptors that can show structural similarity and diversity of the molecules. Among the different types of descriptors, ***topological indices*** have found major popularity in QSRR studies since they can be rapidly obtained using only two dimensional structure of molecules. These descriptors are exact numbers without uncertainty that offer a simple way of measuring molecular branching, shape, size, cyclicity, symmetry, centricity and complexity [3].

A current trend in QSPR studies is the use of the ***atomic level topological indices*** that unlike classical topological indices that characterize a molecule as a whole, code the structural environment of each atom type in the molecule and describe the structural information of a molecule at the atomic level. Ren [4] proposed a set of ***atomic-based AI topological indices*** that along with modified ***Xu*** index were successfully used in estimation of different physical and chemical properties. The topological indices showed good correlations with normal boiling points, molar volumes, molar refractions, and molecular total surface areas of alcohols [5]. Combination of *Xu* and *AI* indices was also used to develop high quality QSPR models for physical properties of alkanes including normal boiling points, heats of vaporization, molar volumes, molar refractions, van der Waals' constants, and Pitzer's eccentric factors [6]. Panneerselvam *et al*. [7] developed a linear regression model based on *AI* indices for normal boiling point of trialkyl phosphates. In a previous paper, QSPR study of standard formation enthalpies of acyclic alkanes using atom-type-based *AI* topological indices was reported by our group [8]. Nevertheless, *AI* indices have not found widespread application in QSRR studies and there is only one report in which gas chromatographic retention index (***RI***) values of a data set consisting of 33 aldehydes and ketones on four different polar stationary phases were separately correlated with *AI* atom-type-based indices [9].

The main aim of this study was to introduce novel atom-type-based topological indices that can be effectively used in QSRR modeling. The other goal was to demonstrate the role of structural features on the molecular mechanism of chromatographic retention on different stationary phases. In this paper, ***novel atom-type-based AT topological indices*** along with the most-used ***Randić's first-order molecular connectivity index*** as a classical topological index were used for simultaneous prediction of gas chromatographic Kovats retention index of saturated alcohols on low to medium polar stationary phases (SE-30, OV-3, OV-7, OV-11, OV-17 and OV-25). The model satisfactorily accounted for the influence of molecular size and each atom-type or group on retention indices of alcohols on different stationary phases. As far as I am aware, this is the first time use of the atomic level topological indices for simultaneous prediction of *RI* data on the stationary phases of different polarity.

2. COMPUTATIONAL DETAILS

2.1 DATA SET

The data sets of Kovats retention indices of 25 saturated alcohols on six stationary phases of different polarity (SE-30, OV-3, OV-7, OV-11, OV-17 and OV-25) were taken from the report of Pias and Gasco [10]. The *RI* values of the model compounds fall in the range of 544-1156 on different stationary phases. Table 1 shows the data sets of Kovats retention indices of 25 model compounds on six stationary phases of different polarity.

Table 1. Kovats retention indices of saturated alcohols on different stationary phases.

No	Compound	Stationary phases					
		SE-30 (53)[a]	OV-3 (86)[a]	OV-7 (113)[a]	OV-11 (142)[a]	OV-17 (158)[a]	OV-25 (204)[a]
1	1-Butanol	650	672	702	725	748	792
2	1-Hexanol	856	881	907	935	959	1003
3	1-Heptanol	960	985	1010	1038	1062	1104
4	2-Butanol	586	607	633	656	675	711
5	2-Pentanol	689	711	735	756	777	811
6	3-Pentanol	689	708	733	756	777	808
7	3-Hexanol	785	807	830	853	878	904
8	3-Heptanol	886	909	929	955	975	1008
9	4-Heptanol	880	904	924	946	968	999
10	4-Methyl-2-Butanol	628	652	674	692	709	738
11	2-Methyl-2-Hexanol	822	848	862	884	904	930
12	2-Methyl-2-Heptanol	920	944	961	982	1001	1026
13	2-Methyl-3-Hexanol	858	876	897	920	939	969
14	3-Methyl-1-Butanol	725	747	771	798	817	855
15	4-Methyl-1-Pentanol	827	849	876	902	923	960
16	2-Ethyl-1-Hexanol	1019	1046	1067	1092	1116	1156
17	3-Ethyl-3-Pentanol	853	876	898	920	939	974
18	2,2-Dimethyl-3-Pentanol	814	834	855	874	890	919
19	2,2-Dimethyl-3-Hexanol	906	926	944	962	977	1004
20	1-Propanol	544	574	-	-	-	-
21	1-Pentanol	751	777	-	806	856	900
22	2-Hexanol	787	811	835	-	878	914
23	2-Methyl-1-Propanol	612	641	654	-	680	740
24	2-Methyl-2-Pentanol	726	748	767	-	801	827
25	2-Ethyl-1-Butanol	834	857	-	907	928	-

[a] McReynolds polarity

2.2 DEFINITION OF *AT* TOPOLOGICAL INDEX

Novel atom-type-based *AT* topological indices were derived from the molecular topological graph in the same manner of Ren [11] with some modifications. As known, a molecular graph G = {*V*, *E*} consists of the vertex V(*G*) and edge E(*G*) sets, where vertices correspond to individual atoms in the graph and the edges correspond to chemical bonds between them. The graph G can be characterized by the distance matrix, $\mathbf{D} = [d_{ij}]_{n\times n}$, whose elements are the length of the shortest distance between the vertices *i* and *j* in a molecular graph with n vertices. Clearly, the sum over the row *i* (or column *j*) of the distance matrix gives the distance sum vector, $\mathbf{S} = [s_i]_{n\times 1}$, for the graph. The molecular graph can also be coded by a vertex degree vector $\mathbf{V} = [v_i]_{n\times 1}$ whose elements are the number of connections (edges) of the vertex i in the graph. For heteroatoms and multiple bonds in the graph, the new degree of vertex introduced by Ren [6], v^m, can be used to replace the v_i values. This novel degree of vertex is derived from the valence connectivity δ^v of Kier-Hall [12] and is defined as:

$$v^m = \delta + k \tag{1}$$

$$k = 1 / [(2/N)^2 \delta^v + 1] \tag{2}$$

where δ is the number of connections of that atom and parameter *k* is a perturbing term reflecting the effect of heteroatom. *N* is the principal quantum number of the valence shell.

According to the above definitions, for any atom *i* that belongs to the *j*-th atom-type in the graph, the $AT_i(j)$ is defined as follows:

$$AT_i(j) = n \times \frac{s_i v_i}{\sum_{i=1}^{n} s_i v_i} \tag{3}$$

Clearly, for *j*-th atom-type in a graph, the corresponding *AT*(*j*) index is the sum of all $AT_i(j)$ values of the same atom type.

$$AT(j) = \sum_{i}^{n} AT_i(j) \tag{4}$$

As an illustration, Figure 1 depicts the labeled molecular graph of 3-methyl-1-butanol.

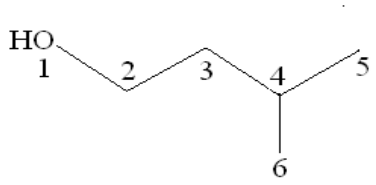

Figure 1. Labeled molecular graph of 3-methyl-1-butanol.

The distance matrix **D** is expressed as follows:

$$D = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 4 \\ 1 & 0 & 1 & 2 & 3 & 3 \\ 2 & 1 & 0 & 1 & 2 & 2 \\ 3 & 2 & 1 & 0 & 1 & 1 \\ 4 & 3 & 2 & 1 & 0 & 2 \\ 4 & 3 & 2 & 1 & 2 & 0 \end{bmatrix}$$

The distance sum vector and vertex degree vector are readily obtained as

$$\mathbf{S} = [\ 14 \quad 10 \quad 8 \quad 8 \quad 12 \quad 12\ ]$$

$$\mathbf{V} = [\ 1.167 \quad 2 \quad 2 \quad 3 \quad 1 \quad 1\ ]$$

where the elements of the vector **V**, are the modified vertex-degree ν^m. According to the above definitions, the *AT* indices are calculated as follows:

$$AT(-CH_3) = AT(5) + AT(6) = \left(6\times\frac{1\times12}{100.338}\right)+\left(6\times\frac{1\times12}{100.338}\right)=1.4351.$$

$$AT(-CH_2-) = AT(2) + AT(3) = \left(6\times\frac{2\times10}{100.338}\right)+\left(6\times\frac{2\times8}{100.338}\right)=2.1527.$$

$$AT(-CH-) = AT(4) = \left(6\times\frac{3\times8}{100.338}\right)=1.4351.$$

$$AT(-OH) = AT(1) = \left(6\times\frac{14\times1.167}{100.338}\right)=0.9770.$$

2.3 Regression Analysis and Model Validation

Multiple linear regression (MLR) analyses were performed using SPSS/PC software package [13]. Criteria for selection of the best models were the statistics of coefficient of multiple determination (R^2), adjusted correlation coefficient, Fisher-ratio and *SE*. Validity and stability of the individual models obtained for the stationary phases was tested using leave-one-out cross-validation (LOO-CV) method [14]. External stability of the unified model generated for simultaneous prediction of *RI* data of saturated alcohols on different stationary phases was tested by external validation method. Standard error of calibration (*SEC*) and standard error of prediction (*SEP*) were used for evaluating quality of the unified MLR model [15].

3. RESULTS AND DISCUSSIONS

3.1 INDIVIDUAL AND COMBINED LINEAR REGRESSION MODELS FOR DIFFERENT STATIONARY PHASES

In the first step of the study, a combination of $^{1}\chi$ and *AT* topological indices were used to develop individual QSRR models for saturated alcohols on different stationary phases. Specifications of the best models found for describing the *RI* values of saturated alcohols on the stationary phases are given in Table 2. It can be seen that the equations represent excellent QSRR models judging from R^2_{adj} and *SE* values in the range of 0.994-0.999 and 4.40-8.90, respectively. Also, *F* values show a high degree of statistical credibility and are indicative of an excellent fit of the models to experimental retention data. Table 3 shows the values of topological descriptors entered in the individual MLR models.

To validate the models, LOO-CV test was performed and cross-validated correlation coefficient (R^2_{cv}) values were in the range of 0.993-0.999 (Table 2) which indicate that the models are robust and reliable over the sample space. As shown, in all cases, cross-validated correlation coefficient is only slightly less than the corresponding value of the full model indicating the models are robust and reliable over the sample space. Table 4 gives the cross-validated predicted values of *RI* and corresponding relative errors resulted from the individual models developed for the stationary phases. It can be easily seen that relative errors for predicted retention indices are less than 3% and only one case with a slightly large error was found on OV-17 column (4.3% for 2-Methyl-1-Propanol).

In the next step of the study, to generate a unified QSRR model for simultaneous prediction of Kovats retention indices of saturated alcohols on the stationary phases of different polarity, whole retention data for saturated alcohols were combined and used as a new data set including 140 *RI* data points. As known, generation of a single QSRR model for simultaneous prediction of retention data on different stationary phases requires a parameter that reflects the contribution of the stationary phase to chromatographic retention. The contribution may be reflected by the polarity which is the most representative chromatographic property of the stationary phase. In this work, system of the stationary phase selectivity constant of McReynolds was used and the polarity value compared to butanol (y') was employed [16] as additional parameter in QSRR modeling. McReynolds polarity parameter values (*M*) are given in Table 1.

Table 2. Characteristics of the best individual QSRR models found for saturated alcohols on different stationary phases.

Parameter	Coefficients (standardized coefficients)					
	SE-30	OV-3	OV-7	OV-11	OV-17	OV-25
Constant	-78.658	-61.020	-24.207	-32.319	23.379	23.473
$^1\chi$	212.539 (1.109)	212.954 (1.114)	211.921 (1.094)	213.848 (1.096)	216.928 (1.098)	216.654 (1.113)
AT(–OH)	236.651 (0.172)	244.899 (0.179)	237.995 (0.176)	266.654 (0.204)	233.514 (0.175)	283.435 (0.213)
AT(–CH₃)	-13.586 (-0.068)	-15.149 (-0.076)	-18.715 (-0.094)	-18.006 (-0.099)	-28.620 (-0.147)	-32.403 (-0.169)
	Statistics					
R^2	0.998	0.999	0.998	0.995	0.995	0.995
R^2_{adj}	o.998	0.999	0.997	0.995	0.994	0.994
R^2_{cv}	0.998	0.999	0.997	0.994	0.993	0.993
SE	5.39	4.40	6.20	8.34	8.83	8.90
F	4079.5	6082.8	2514.8	1225.3	1311.3	1251.9
n^a	25	25	22	21	24	23

[a] Number of molecules in the data set.

Table 3. Values of the topological descriptors entered in the individual QSRR models.

No	$^1\chi$	*AT* (*–CH₃*)	*AT* (*–OH*)	No	$^1\chi$	*AT* (*–CH₃*)	*AT* (*–OH*)
1	2.4142	0.8108	0.9462	14	2.770	1.4351	0.9770
2	3.4142	0.7924	0.9248	15	3.270	1.4055	0.9648
3	3.9142	0.7869	0.9183	16	4.346	1.5273	0.8459
4	2.2701	1.5937	0.8752	17	3.682	2.3684	0.737
5	2.7701	1.5599	0.8402	18	3.481	2.8968	0.7982
6	2.8081	1.6278	0.8037	19	3.981	2.8547	0.7364
7	3.3081	1.6137	0.7634	20	1.914	0.8275	0.9657
8	3.8081	1.5915	0.7429	21	2.914	0.8000	0.9336
9	3.8081	1.6183	0.7177	22	3.270	1.5340	0.8225
10	2.5607	2.2947	0.8369	23	2.270	1.4952	0.9815
11	3.5607	2.1802	0.7673	24	3.063	2.2309	0.7923
12	4.0607	2.1455	0.7541	25	3.346	1.5572	0.9086
13	3.6807	2.2554	0.7403				

Table 4. Prediction results of the individual QSRR models for saturated alcohols on six stationary phases using leave-one-out cross validation method.

No	Predicted retention indices (relative error%)					
	SE-30	OV-3	OV-7	OV-11	OV-17	OV-25
1	647 (-0.5)	673 (0.1)	696 (-0.9)	721 (-0.6)	745 (-0.4)	788 (-0.5)
2	855 (-0.1)	880 (-0.1)	904 (-0.3)	929 (-0.6)	957 (-0.2)	999 (-0.4)
3	960 (0.0)	986 (0.1)	1009 (-0.1)	1034 (-0.4)	1065 (0.3)	1107 (0.3)
4	590 (0.7)	614 (1.2)	636 (0.5)	658 (0.3)	674 (-0.1)	712 (0.1)
5	688 (-0.1)	711 (0.0)	733 (-0.3)	756 (0.0)	776 (-0.1)	811 (0.0)
6	686 (-0.4)	709 (0.1)	731 (-0.3)	753 (-0.4)	773 (-0.5)	807 (-0.1)
7	783 (-0.3)	806 (-0.1)	828 (-0.2)	849 (-0.5)	872 (-0.7)	904 (0.0)
8	885 (-0.1)	908 (-0.1)	930 (0.1)	951 (-0.4)	978 (0.3)	1007 (-0.1)
9	878 (-0.2)	900 (-0.4)	923 (-0.1)	944 (-0.2)	972 (0.4)	1000 (0.1)
10	633 (0.8)	655 (0.5)	675 (0.1)	699 (1.0)	709 (0.0)	742 (0.5)
11	831 (1.1)	852 (0.5)	873 (1.3)	895 (1.2)	913 (1.0)	943 (1.4)
12	936 (1.7)	957 (1.4)	978 (1.8)	1001 (1.9)	1022 (2.1)	1051 (2.4)
13	847 (-1.3)	869 (-0.8)	889 (-0.9)	911 (-1.0)	929 (-1.1)	956 (-1.3)
14	721 (-0.6)	746 (-0.1)	768 (-0.4)	794 (-0.5)	810 (-0.9)	854 (-0.1)
15	825 (-0.2)	851 (0.2)	871 (-0.6)	898 (-0.4)	917 (-0.7)	960 (0.0)
16	1028 (0.9)	1049 (0.3)	1071 (0.4)	1096 (0.4)	1121 (0.4)	1155 (-0.1)
17	845 (-0.9)	867 (-1.0)	886 (-1.3)	907 (-1.4)	925 (-1.5)	953 (-2.2)
18	810 (-0.5)	831 (-0.4)	847 (-0.9)	872 (-0.2)	879 (-1.2)	906 (-1.4)
19	902 (-0.4)	923 (-0.3)	940 (-0.4)	965 (0.3)	977 (0.0)	1002 (-0.2)
20	546 (0.4)	569 (-0.9)	-	-	-	-
21	751 (0.0)	776 (-0.1)	-	829 (2.9)	850 (-0.7)	892 (-0.9)
22	790 (0.4)	814 (0.4)	836 (0.1)	-	881 (0.3)	915 (0.1)
23	617 (0.8)	640 (-0.2)	665 (1.7)	-	709 (4.3)	747 (0.9)
24	730 (0.6)	752 (0.5)	772 (0.7)	-	810 (1.1)	841 (1.7)
25	826 (-1.0)	850 (-0.8)	-	896 (-1.2)	916 (-1.3)	-

Specifications of the unified QSRR model found for simultaneous prediction of Kovats retention indices of saturated alcohols on the six stationary phases are given in Equation 5. As can be easily found, addition of the McReynolds polarity parameter to the descriptors entered in the individual models resulted in a unified model for all *RI* data with R^2_{adj} value of 0.995 and *SE* of 8.55. Based on the results, regression explained by the model is significant at 99% confidence level and the combined model explains 99.5% of the variance in the retention data.

$$RI = -130.088 + 214.334\ {}^{1}\chi + 250.597\ AT(-OH) - 35.750\ AT(-CH_3) + 0.828\ M \quad (5)$$

$n = 140$ $R^2 = 0.995$ $R^2_{adj} = 0.995$ $SE = 8.55$ $F = 7334.2$

To prove the external stability of the combined model and to further demonstrate the absence of chance correlation, external validation method was employed. In the method, the whole data set divided into five subsets and each subset was predicted by the other four subsets as the training set. In this procedure, the same descriptors were retained in the correlation equation but the coefficients were allowed to vary. Calculated values of *SEC* and *SEP* for different subsets are given in Table 5. Good agreement between average values of 8.29 for *SEC* and 8.69 for *SEP* with standard error of the full model shows good efficiency of the topological indices in simultaneous modeling of *RI* data for saturated alcohols on different stationary phases. Average values of training and predicting qualities (R^2_{train}=R^2_{pred}=0.995) also indicate high statistical stability and validity of the combined model. Graphical indication of the quality of the combined model can be seen in Figure 2 through the correlation between the experimental and calculated retention indices for different prediction sets. Figure 3 is the plot of residuals versus experimental retention indices for the prediction sets. As shown, all residuals values fall within a horizontal band centered around zero showing absence of systematic error in development of the combined QSRR model.

Table 5. Verification of statistical validity of the combined model based on the external validation method.

Training set[a]	Prediction set[a]	R^2_{train}	*SEC*	R^2_{pred}	*SEP*
2-5	1	0.995	8.35	0.993	8.84
1 & 3-5	2	0.996	8.07	0.994	8.45
1,2 & 4,5	3	0.996	8.31	0.995	8.67
1-3 & 5	4	0.995	8.28	0.995	8.79
1-4	5	0.995	8.38	0.997	8.70
Average		0.995	8.29	0.995	8.69

[a] Number of molecules in the training and prediction sets are 112 and 28, respectively.

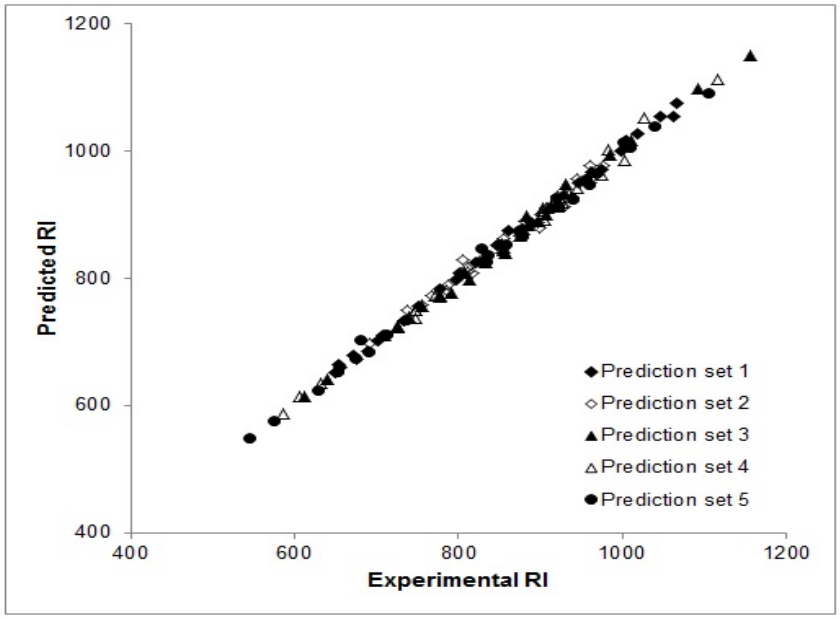

Figure 2. Plot of the predicted versus experimental retention indices for different prediction sets used in the external validation test.

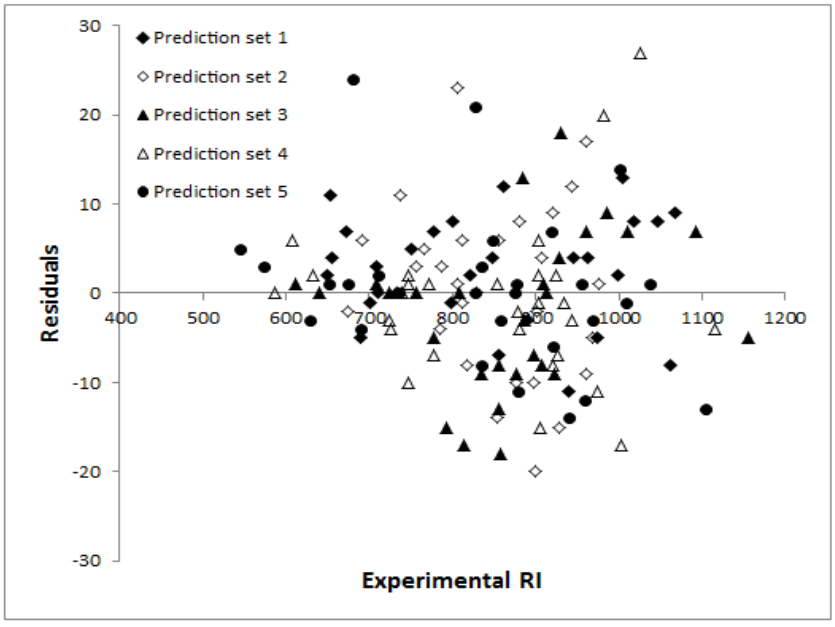

Figure 3. Plot of residuals versus experimental retention indices for different prediction sets used in the external validation test.

To assess the performance of the *AT* topological indices in retention prediction of saturated alcohols, the obtained results were compared with previously reported topological based QSRR models developed for the same data set. Figure 4 shows a comparison between standard errors of the present MLR models and those of the models reported by Liu et al. [17] and Guo et al. [18] for predicting retention indices of saturated alcohols. Clearly, the *AT* based individual models are significantly better than the other two models. As shown, standard errors of the *AT* based individual models are 35.1 to 60.7% less than the model developed by Liu et al. and are 16.9 to 51.3% less than the other model. Moreover, a decrease of about 18% is observed in the standard error of the combined QSRR model presented in this work relative to the model generated by Guo et al. Better results obtained in the present study provide good evidence for high potential of the *AT* topological indices in QSRR modeling of saturated alcohols.

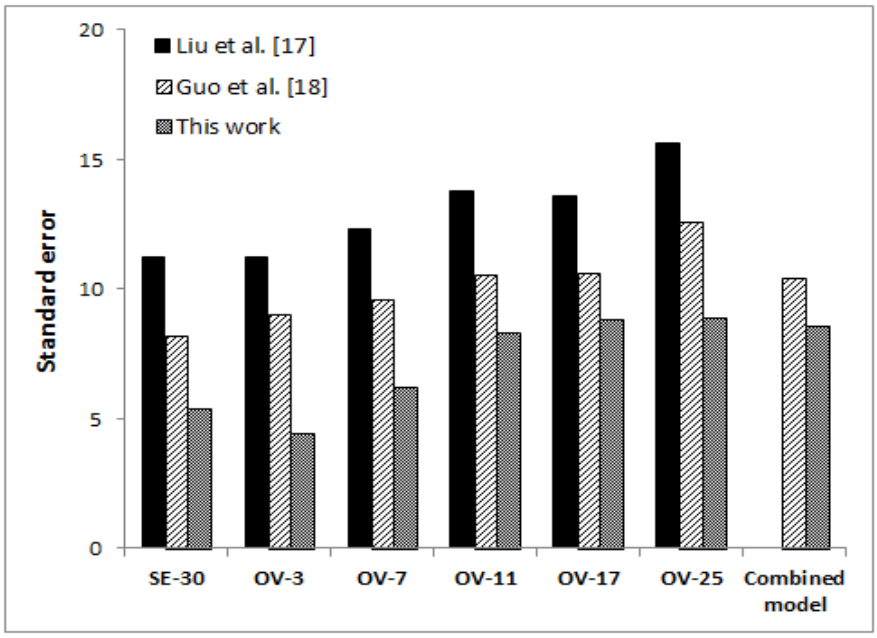

Figure 4. Comparison between standard errors of the presented and previous linear models for prediction of retention indices of saturated alcohols on different stationary phases.

3.2 Contribution of the Individual Indices to Retention Index of Saturated Alcohols

Gas chromatographic retention indices strongly depend on the solute-stationary phase interactions and QSRR studies provide useful information on the mechanism of these interactions [19]. To explore the role of the topological features of the model compounds in

determining their retention indices on each stationary phase, the standardized regression coefficients for the individual QSRR models were used (Table 2). Furthermore, precise contributions of the parameters entered in the combined QSRR model to *RI* values were determined using calculation of the relative contribution (Ψ_r) and fraction contribution (Ψ_f) as follows [20]:

$$\Psi_r\,(\mathrm{i}) = c_i\,\overline{TI}_i \tag{6}$$

$$\Psi_f\,(\mathrm{i}) = [\,R^2 \times |\Psi_r\,(\mathrm{i})| \,/\, \sum_i |\Psi_r\,(\mathrm{i})|\,] \times 100\% \tag{7}$$

where c_i and $\overline{TI}_i$ are the coefficient and the average value of the *i*-th topological index entered in the model. The sum is over all indices in the model.

According to the results, standardized regression coefficients of the descriptors decreased in the order of $AT(^1\chi) > AT(\text{–}OH) > AT(\text{–}CH_3)$ for all the stationary phases. The $^1\chi$ index encodes information about the bulkiness and branching of molecules and its value increases with molecular size but decreases with molecular branching [21]. Positive standardized coefficient for $^1\chi$ index indicates that the molecule with higher $^1\chi$ value will have higher *RI* value due to larger molecular size or less branching. This relationship suggests that the main interaction force contributing to the chromatographic behavior of saturated alcohols on the stationary phases is dispersive. As known, the magnitude of this type of intermolecular solute-stationary phase interaction is related to molecular size as well as degree of branching [22].

The topological index $AT(\text{–}OH)$ had smaller standardized coefficient than $^1\chi$ for all the stationary phases. The descriptor that is a measure of solute polarity showed positive standardized coefficients for all the stationary phases as the hydroxyl group of the alcohol molecule makes the intermolecular interaction between solute and stationary phase stronger and increases the *RI* value. The $AT(\text{–}CH_3)$ topological index with minimum value of the standardized coefficient indicates the role of branching in determining *RI* of saturated alcohols, because $AI(\text{–}CH_3)$ index is clearly related to the number of methyl groups which is a crude measure of branching [20]. As shown, standardized coefficient for the descriptor is negative that indicates the larger the number of the branches of molecule is, the smaller its *RI* value because branching prevents solutes from close contact with stationary phase and reduces the interactions between the solutes and the stationary phase. Consequently, retention indices of the solutes decrease.

Relative contributions of the topological indices entered in the combined model to *RI* data showed the same trend as the standardized regression coefficients of the individual QSRR models. The obtained Ψ_r values for $^1\chi$, $AT(\text{–}OH)$ and $AT(\text{–}CH_3)$ were 701.58, 210.07 and -35.75, respectively. Moreover, McReynold polarity had much larger contribution (Ψ_r=103.07) than $AT(\text{–}CH_3)$ indicating the important role of the stationary phase polarity in determining retention indices of the model compounds. Positive sign of the parameter

shows that *RI* of saturated alcohols increases with increasing polarity of the stationary phase. Based on the obtained results, fraction contributions of bulkiness and polarity of the solutes to the retention indices were 66.45% and 19.90%, respectively. Furthermore, stationary phase polarity (Ψ_f = 9.76%) and methyl groups of the alcohol molecules (Ψ_f = 3.39%) showed smaller contributions to *RI* values. Results of the study showed that the topological descriptors included in the regression models provide useful information about structural features important in determining retention indices of saturated alcohols on the stationary phases of different polarity.

4. CONCLUSION

In the present study, preliminary individual and combined QSRR models for predicting Kovats retention indices of saturated alcohols on the stationary phases of different polarity were developed using a combination of $^1\chi$ index and the novel atom-type-based *AT* topological indices. According to the results, $^1\chi$ and *AT(–OH)* indices were the most important descriptors affecting *RI* of saturated alcohols showing important role of size, branching and polarity of the solutes molecules in determining their retention indices. In addition, polarity of the stationary phases showed relatively large contribution in the unified QSRR model developed for simultaneous prediction of retention indices of saturated alcohols on the stationary phases. Satisfactory prediction results evidently suggest efficiency of the *AT* based QSRR models for accurate estimation of the retention indices for similar compounds using only two dimensional structures of the molecules. This work can be a good starting point to provide a simple procedure for QSRR study of other heteroatom containing aliphatic compounds.

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A Note on the Bounds of Laplacian–Energy–Like Invariant

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ABSTRACT

The Laplacian-energy-like of a simple connected graph G is defined as $\mathrm{LEL} = \mathrm{LEL(G)} = \sum_{i=1}^{n} \sqrt{\mu_i}$, where $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ are the Laplacian eigenvalues of the graph G. In this paper, some upper and lower bounds for LEL, as well as, some lower bounds for the spectral radius of graph are obtained.

1 INTRODUCTION

The graph energy is a graph-spectrum-based quantity, initiated in the 1970s. After a latent period of 20-30 years, it became a well-liked topic of research both in mathematical chemistry and in "pure" spectral graph theory, resulting in over 600 published papers. Considering the applications of graph energies, one can see them in entropy [5, 15], modeling the properties of proteins (especially those of biological relevance) in [6, 24, 28], applying them in the search for the genetic causes of Alzheimer disease [3] and also for modeling of the spread of epidemics [26].

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Suppose $G = (V, E)$ is a simple graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \cdots, n$. The maximum and minimum degree of G are denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively. Let $A(G)$ and $D(G) = \mathrm{diag}(d_1, d_2, \cdots, d_n)$ be the (0,1)-adjacency matrix of G and the diagonal matrix of vertex degrees, respectively. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. This matrix has nonnegative eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. Assume that $\mathrm{Spec}(G) = \{\mu_1, \mu_2, \cdots, \mu_n\}$ stands for the spectrum of $L(G)$, i.e., the Laplacian spectrum of G. As well-known [20], the Laplacian spectrum obeys the relations $\sum_{i=1}^{n} \mu_i = 2m$ and $\sum_{i=1}^{n} {\mu_i}^2 = 2m + \sum_{i=1}^{n} {d_i}^2$.

In 2008, Liu and Liu [18] considered a new Laplacian-spectrum-based graph invariant $LEL = LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$, and named it *Laplacian-energy-like invariant* (LEL for short). The motivation for initiating LEL is in its analogy [12] to the earlier much studied graph energy [10, 11, 16]. We refer to [17,18] for more details on LEL and encourage the interested readers to consult papers [4, 9, 12, 14, 25, 27, 29, 31] for mathematical properties of this graph invariant.

2. AN UPPER BOUND FOR LAPLACIAN–ENERGY–LIKE INVARIANT

In order to arrive at one of our main results, we begin by recalling a crucial lemma as follows.

Lemma 1 ([20]). Let G be a graph on n vertices with at least one edge. Then $\mu_1 \geq \Delta + 1$. Moreover, if G is connected, then the equality holds if and only if $\Delta = n - 1$.

We are now in a position to formulate the lower and upper bounds on LEL in terms of n, m and d_i, $i = 1, 2, \cdots, n$.

Theorem 1. Suppose that G is a simple connected graph on $n > 1$ vertices and m edges. Then the inequality

$$LEL \leq \sqrt{\Delta + 1} + (n-2)^{3/4} \sqrt[4]{2m - (\Delta + 1)^2 + \sum_{i=1}^{n} {d_i}^2} \qquad (1)$$

holds.

Proof. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be the eigenvalues of the Laplacian matrix with respect to the graph G. Then, as is well-known, we have $\mu_1 \geq \Delta + 1$ (see also Lemma 1). Moreover, since

$$\sum_{i=1}^{n} {\mu_i}^2 = 2m + \sum_{i=1}^{n} {d_i}^2 \tag{2}$$

must hold, we get $\sum_{i=2}^{n-1} {\mu_i}^2 = 2m - {\mu_1}^2 + \sum_{i=1}^{n} {d_i}^2$. Using this together with the Cauchy-Schwarz inequality for twice, applied to the vectors $(\sqrt{\mu_2}, \sqrt{\mu_3}, \cdots, \sqrt{\mu_{n-1}})$ and $(1, 1, \cdots, 1)$ with $n-2$ entries, we derive the inequality

$$\begin{aligned}\sum_{i=2}^{n-1} \sqrt{\mu_i} &\leq \sqrt{(n-2)\sum_{i=2}^{n-1} \mu_i} \leq (n-2)^{3/4} \sqrt[4]{\sum_{i=2}^{n-1} {\mu_i}^2} \\ &= (n-2)^{3/4} \sqrt[4]{2m - {\mu_1}^2 + \sum_{i=1}^{n} {d_i}^2}. \end{aligned} \tag{3}$$

Hence, we must have

$$LEL \leq \sqrt{\mu_1} + (n-2)^{3/4} \sqrt[4]{2m - {\mu_1}^2 + \sum_{i=1}^{n} {d_i}^2}. \tag{4}$$

Now, consider the real function $f(x) = \sqrt{x} + A\sqrt[4]{B - x^2}$, where $A = (n-2)^{3/4}$ and $B = 2m + \sum_{i=1}^{n} {d_i}^2$. It is obvious that f is decreasing on the interval

$$I = \left[\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}, \sqrt{B}\right).$$

On the other hand, we claim $\sqrt{\frac{B}{A^{\frac{4}{3}}+1}} \leq \Delta + 1$. Since $\Delta \leq n-1$,

$$\begin{aligned} B = 2m + \sum_{i=1}^{n} {d_i}^2 &= \sum_{i=1}^{n} d_i(d_i + 1) \leq n\Delta(\Delta + 1) \\ &\leq (n-1)(\Delta + 1)^2 = (A^{\frac{4}{3}} + 1)(\Delta + 1)^2 \end{aligned}$$

which proves our claim. Moreover, in view of Lemma 1 and Equations (2) and (4), we see that $\Delta + 1 \leq \mu_1 \leq \sqrt{B}$, and hence

$$LEL \leq f(\mu_1) \leq f(\Delta + 1) \leq f\left(\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}\right). \tag{5}$$

Remark 1. In virtue of the proof of Theorem 1, we can analyze the growth of the obtained bounds, i.e., (5), which can be fruitful for the investigation on the energy of hyperstructures, that is, the models with large size.

$$\begin{aligned} LEL \leq f\left(\sqrt{\frac{B}{A^{\frac{4}{3}}+1}}\right) &= \frac{\sqrt[4]{B}}{\sqrt{n-1}} + \frac{\sqrt[4]{B}\cdot(n-2)}{\sqrt[4]{n-1}} \\ &\leq \frac{\sqrt[4]{n\Delta(\Delta+1)}}{\sqrt{n-1}} + \frac{\sqrt[4]{n\Delta(\Delta+1)}\cdot(n-2)}{\sqrt[4]{n-1}} \sim \sqrt[4]{n\Delta(\Delta+1)}.O(n) \end{aligned}$$

which yields an upper bound for LEL related to the graphs with high order and Δ as a fixed parameter. We note that a same fashion with using (1) implies the same result:

$$LEL \leq f(\Delta+1) \leq \sqrt{\Delta+1} + (n-2)^{3/4}\sqrt[4]{n\Delta(\Delta+1)-(\Delta+1)^2} \sim \sqrt[4]{\Delta(\Delta+1)}.O(n).$$

3. BOUNDS OF SPECTRAL RADIUS OF GRAPHS IN TERMS OF THE NUMBER OF TRIANGLES

For a given graph G, let us suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the corresponding eigenvalues of the adjacency matrix A which are called A-eigenvalues and also let Δ_G be the number of triangles in G. Throughout this section, we give upper and lower bounds for λ_1 such that each edge of G belongs to at least Δ_G triangles. The goal is to utilize the upper bound obtained in order to result a lower bound for Laplacian-energy-like invariant.

Theorem 2. Assume G is a simple graph with n vertices and m edges. If each edge of G belongs to at least Δ_G triangles, $\Delta_G \geq 1$, then

$$|\lambda_1| \leq \sqrt{2m-\delta-\Delta_G(\delta-1)}. \quad (6)$$

Proof. Suppose that A_i stands for the i-th row of A. Clearly, d_i is its row sum. Without loss of generality, let $\boldsymbol{u} = (u_1, u_2, \cdots, u_n)^T$ be a unit eigenvector of $A(G)$ corresponding to $\lambda_1 = \lambda_1(G)$. Assume $\boldsymbol{u}(i)$ indicates the vector obtained from $\boldsymbol{u}$ by replacing u_j with 0 if v_i is not adjacent to v_j where $1 \leq j \leq n$. Since $A(G)\boldsymbol{u} = \lambda_1\boldsymbol{u}$, considering the $i-$th component of the vectors in both sides of recent equality, we derive $\lambda_1 u_i = A_i\boldsymbol{u} = A_i\boldsymbol{u}(i)$. Therefore, by taking the $|\cdot|^2$, applying the well-known Lagrange identity and simplifying the right hand side we see for each i that

$$\begin{aligned}\lambda_1{}^2 u_i{}^2 = |A_i\boldsymbol{u}(i)|^2 &= |A_i|^2 \cdot |\boldsymbol{u}(i)|^2 - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2 \\ &= d_i \sum_{\substack{1\leq j\leq n \\ a_{ij}\neq 0}} u_j{}^2 - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2 \\ &= d_i\left(1-\sum_{\substack{1\leq j\leq n \\ a_{ij}=0}} u_j{}^2\right) - \sum_{\substack{1\leq j<k\leq n \\ a_{ij}=a_{ik}=1}} (u_j-u_k)^2.\end{aligned}$$

Summing over $1 \leq i \leq n$ in both sides we obtain,

$$\lambda_1{}^2 = 2m - \sum_{i=1}^{n} d_i \left(\sum_{\substack{1\le j\le n \\ a_{ij}=0}} u_j{}^2 \right) - \sum_{i=1}^{n} \sum_{\substack{1\le j<k\le n \\ a_{ij}=a_{ik}=1}} (u_j - u_k)^2. \qquad (7)$$

On the other hand, one can notice that

$$\sum_{i=1}^{n} d_i \left(\sum_{\substack{1\le j\le n \\ a_{ij}=0}} u_j{}^2 \right) \ge \sum_{i=1}^{n} d_i \, u_i{}^2 \ge \delta.$$

Moving forward, since each edge belongs to at least Δ_G triangles, then applying Cauchy-Schwarz inequality we derive the following

$$\begin{aligned} \sum_{i=1}^{n} \sum_{\substack{1\le j<k\le n \\ a_{ij}=a_{ik}=1}} (u_j - u_k)^2 &\ge \Delta_G \sum_{\substack{1\le j<k\le n \\ a_{jk}=1}} (u_j - u_k)^2 \\ &= \Delta_G \sum_{i=1}^{n} d_i \, u_i{}^2 - 2\Delta_G \sum_{\substack{1\le j<k\le n \\ a_{jk}=1}} u_j u_k \\ &\ge \Delta_G \delta - \Delta_G \sum_{j\ne k} |u_j u_k| \\ &\ge \Delta_G (\delta - 1). \end{aligned}$$

Now, viewing the equality (7) yields the following

$$|\lambda_1| \le \sqrt{2m - \delta - \Delta_G(\delta - 1)}.$$

3.1. CLOSED WALKS IN GRAPH

Throughout this subsection, we aim to derive some results related to lower bound of spectral radius of graph by using the term of Δ_G which may be useful in further investigations. Before present the next result, we need some preliminaries. We recall that a *closed walk* in G is a walk that ends where it begins. The number of closed walks in G of length ℓ starting at v_i is thus given by $(A(G)^\ell)_{ii}$, so the total number $f_G(\ell)$ of closed walks of length ℓ is given by

$$f_G(\ell) = \sum_{i=1}^{n} (A(G)^\ell)_{ii} = \mathrm{tr}(A(G)^\ell)$$

where tr denotes the trace (sum of the main diagonal entries). From the theory of matrices, we know that if the matrix A has eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$ then A^ℓ has eigenvalues $\lambda_1^\ell, \lambda_2^\ell, \cdots, \lambda_n^\ell$. Therefore,

$$f_G(\ell) = \sum_{i=1}^{n} \lambda_i^\ell. \qquad (8)$$

Some immediate consequences of (8) are as follows:

i. For $\ell = 1$,$\sum_{i=1}^{n} \lambda_i = 0$ which is deduced by noting that the sum of the eigenvalues is the trace of the adjacency matrix which is 0 since A is 0 on the diagonal.

ii. For $\ell = 2$, $\sum_{i=1}^{n} \lambda_i^2 = 2m$ which is followed by the fact that the sum of the squares of the eigenvalues is the same as the trace of A^2. The diagonal entries of A^2 count the number of closed walks of length 2 (a closed walk is a walk that starts and ends at the same vertex; since we are on the diagonal the starting and ending vertices are the same), for which each edge is counted exactly twice.

iii. For $\ell = 3$, $\sum_{i=1}^{n} \lambda_i^3 = 6\Delta_G$. This is obeyed by the fact that the sum of the cubes of the eigenvalues is the same as the trace of A^3, i.e., the same as the number of closed walks of length 3. Each triangle will be counted exactly six times (i.e., a choice of 3 initial vertices and 2 directions for each triangle).

One can continue this process but it becomes impractical to get some effective information about a graph. Next, using (iii) we study on bounds of Δ_G and then spectral radius of graph. Let the A-eigenvalues of G be in form of $\lambda_1 \geq \cdots \geq \lambda_k \geq 0 > \lambda_{k+1} \geq \cdots \geq \lambda_n$ and $\Lambda_+ = \sum_{i=1}^{k} \lambda_i^3 > 0$, $\Lambda_- = \sum_{i=k+1}^{n} \lambda_i^3 < 0$, $\Lambda = \sum_{i=1}^{n} |\lambda_i|^3$. This implies that $\Lambda_+ + \Lambda_- = 6\Delta_G$, $\Lambda_+ - \Lambda_- = \Lambda$, which yields that $36\Delta_G^2 = \Lambda^2 + 4\Lambda_+ \cdot \Lambda_-$. Therefore,

$$\Lambda = \sqrt{36\Delta_G^2 - 4\Lambda_+ \cdot \Lambda_-} \leq 6\Delta_G + 2\sqrt{-\Lambda_+ \cdot \Lambda_-} \leq 6\Delta_G + 2n|\lambda_1\lambda_n|^{\frac{3}{2}}. \tag{9}$$

On the other hand, by Hölder inequality one can see that

$$\sum_{i=1}^{n} |\lambda_i|^2 \leq \Lambda^{\frac{2}{3}} \cdot \sqrt[3]{n}$$

which means that

$$\sqrt{\frac{8m^3}{n}} \leq \Lambda. \tag{10}$$

Equations (9) and (10) derive the following relation

$$\sqrt{\frac{2m^3}{n}} \leq \frac{\Lambda}{2} \leq 3\Delta_G + n|\lambda_1\lambda_n|^{\frac{3}{2}}$$

which shows Δ_G is bounded below by

$$\frac{1}{3}\left(\sqrt{\frac{2m^3}{n}} - n|\lambda_1\lambda_n|^{\frac{3}{2}}\right).$$

The recent bound seems good for the graph with big size, i.e., $m \to \infty$. Now, to obtain a lower bound for the spectral radius of G, inspired by (iii), we easily see that

$$\lambda_1 \geq \sqrt[3]{\frac{6\Delta_G}{n}}. \qquad (11)$$

With the help of inequality (11), one can make some lower bounds only in terms of m, n following some well-known results.

$\Delta_G \geq *$(Results in previous)	Hypotheses	$\lambda_1 \geq *$
$\Delta_G \geq \frac{(4m-n^2)m}{3n}$(Nordhaus et al. [22])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{2(4m-n^2)m}{n^2}}$
$\Delta_G \geq \frac{9mn-2n^3-2(n^2-3m)^{\frac{3}{2}}}{27}$(Fisher [8])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{2(9mn-2n^3-2(n^2-3m)^{\frac{3}{2}})}{9n}}$
$\Delta_G = (m - \lfloor \frac{n^2}{4} \rfloor) \lfloor \frac{n}{2} \rfloor$(Nikiforov et al. [21], Lovász et al. [19])	$\lfloor \frac{n^2}{4} \rfloor \leq m \leq \lfloor \frac{n^2}{4} \rfloor + \lfloor \frac{n}{2} \rfloor$	$\lambda_1 \geq \sqrt[3]{\frac{6(m - \lfloor \frac{n^2}{4} \rfloor) \lfloor \frac{n}{2} \rfloor}{n}}$
$\Delta_G \geq \frac{(4m-n^2)n}{9}$(Bollobás [2])	$\frac{n^2}{4} \leq m \leq \frac{n^2}{3}$	$\lambda_1 \geq \sqrt[3]{\frac{8m-2n^2}{3}}$

Table 1: A list of lower bounds of spectral radius

Remark 2. Concentrating on Table 1, we observe that since the lower bound of Δ_G obtained by Fisher [8] is the best bound in comparison with the others in the list above, hence the corresponding lower bound of spectral radius is the best in the list.

4. Lower Bound on Laplacian–Energy–Like Invariant

Throughout this section, applying a crucial lemma we derive a lower bound for Laplacian-energy-like invariant.

The following result which is known as Weyl's inequalities, is concerned with the eigenvalues of sum of Hermitian matrices (see Theorem III.2.1, [1]).

Lemma 2. Let $A, B \in M_n$ be Hermitian matrices and assume that A and $A + B$ are arranged in non-increasing order. Then

$$\lambda_k(A) + \lambda_n(B) \leq \lambda_k(A + B) \leq \lambda_k(A) + \lambda_1(B), \quad k = 1, 2, \cdots, n. \qquad (12)$$

Let us recall that algebraic connectivity of G (called by Fiedler [7]) is denoted by μ_{n-1}. Obviously, since G is connected, $\mu_{n-1} \neq 0$. Using the terms of

algebraic connectivity and edge connectivity of G, i.e., $\eta = \eta(G)$, we obtain a lower bound for Laplacian-energy-like invariant as follows:

Theorem 3. Assume G is a simple connected graph with n vertices and m edges. Then, the following inequality holds

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}} \tag{13}$$

where λ_1 is the spectral radius of G and

$$\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}.$$

Proof. Since $D(G) = A(G) + L(G)$ and A, B are Hermitian matrices, by Lemma 2 we get

$$\lambda_k(L) + \lambda_n(A) \leq \lambda_k(D) \leq \lambda_k(L) + \lambda_1(A), \quad k = 1, 2, \cdots, n$$

which is simplified as

$$\mu_k + \lambda_n \leq d_k \leq \mu_k + \lambda_1, \quad k = 1, 2, \cdots, n.$$

Let $\mu_k + \lambda_1 \leq \alpha\lambda_1\mu_k$ for a proper constant α large enough such that $\alpha \geq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$. Indeed, for $k = 1, 2, \cdots, n-1$ we see

$$\sqrt{\frac{n}{2m}} + \frac{1}{\mu_k} \leq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}} \leq \alpha \iff \frac{\mu_k + \sqrt{\frac{2m}{n}}}{\mu_k\sqrt{\frac{2m}{n}}} \leq \alpha \iff \frac{\mu_k}{\alpha\mu_k - 1} \leq \sqrt{\frac{2m}{n}} \leq \lambda_1.$$

Moving forward, $\sqrt{d_k} \leq \sqrt{\mu_k + \lambda_1} \leq \sqrt{\alpha\lambda_1\mu_k}$ which shows that

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}}$$

for any $\alpha \geq \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$.

Thus we get the required result by the value $\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{\mu_{n-1}}$ in recent inequality.

In the following we give some immediate consequences.

Corollary 1. Suppose that G is a simple connected graph with n vertices and m edges. Then, the following inequality holds

$$LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\lambda_1}}$$

where

$$\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{2\eta(1-\cos\frac{\pi}{n})}.$$

Following the formula mentioned in Theorem 2 and the bounds below we have the following immediate consequences:

a) $\lambda_1 \leq \sqrt{2m-n+1}$, (see Hong [13])

b) $\lambda_1 \leq \frac{\sqrt{1+8m}-1}{2}$, (see Stanley [23])

c) $\lambda_1 \leq \sqrt{2m-\delta-\Delta_G(\delta-1)}$, (Equation (6)).

Theorem 4. Assume G is a simple connected graph with n vertices and m edges. Then, the following inequalities hold

i) $LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\sqrt{2m-n+1}}}$

ii) $LEL \geq \sum_{k=1}^{n} \sqrt{\frac{2d_k}{\alpha(\sqrt{1+8m}-1)}}$

iii) $LEL \geq \sum_{k=1}^{n} \sqrt{\frac{d_k}{\alpha\sqrt{2m-\delta-\Delta_G(\delta-1)}}}$

where

$$\alpha = \sqrt{\frac{n}{2m}} + \frac{1}{2\eta(1-\cos\frac{\pi}{n})}.$$

Proof. Viewing (a)−(c) and Corollary 1, the results (i)−(iii) are clear.

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On the Eigenvalues of some Matrices Based on Vertex Degree

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ABSTRACT

The aim of this paper is to first compute some bounds for forgotten index and then to present spectral properties of this topological index. In continuing, we define a new version of energy namely ISI energy corresponding to the ISI index. Finally, we determine some bounds for this new graph invariant.

1. INTRODUCTION

All graphs considered in this paper are connected, undirected and finite without loops and multiple edges. Denoted by $V(G)$ and $E(G)$, we mean the set of vertices and the set of edges of graph G, respectively.

A topological index is a kind of molecular descriptor which anticipates some properties of chemical compound. Many topological indices were defined and many properties are discovered. Furtula and Gutman[2] introduced the forgotten index which is a special case of **general first Zagreb index** and studied its basic properties. In this paper some application of forgotten index in chemistry is also presented and the authors proved that this index can significantly enhance the physico-chemical applicability of the first Zagreb index. We refer to [3] for more information about this graph invariant.

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The real number $\lambda$is called the eigenvalue of a graph Γ with adjacency matrix Aif the equation $Ax=\lambda x$has a nonzero solution. A solution $v$for this equation is called eigenvector corresponding to the eigenvalue λ. The characteristic polynomial of the matrix A is defined as$\chi_\lambda(G) = det(A - \lambda I)$. It is easy to see that the eigenvalues of A are roots of$\chi_\lambda(G)$.

2. NOTATION AND DEFINITIONS

There are two types of Zagreb indices introduced by Gutman and Trinajestic[12]: the first Zagreb index M_1 and the second Zagreb index M_2 defined as follows:

$$M_1 = M_1(G) = \sum_{u\in V(G)} d(u)^2 \text{ and } M_2 = M_2(G) = \sum_{uv\in E(G)} d(u)d(v),$$

where d_u denotes the degree of vertex u, see [1,4,7,9]. The first Zagreb index can be rewritten also as $M_1 = M_1(G) = \sum_{uv\in E(G)}[d(u) + d(v)]$. For more details on these topological indices we refer to [7, 14–16, 18]. With this notation, the F- index is defined as [2,3,11,13]

$$F = F(G) = \sum_{u\in V(G)} d(u)^3 = \sum_{uv\in E(G)}[d(u)^2 + d(v)^2].$$

In [5] the following three topological indices are proposed:

$$TI_1 = TI_1(G) = \sum_{v\in V(G)} F_1(v), TI_1 = TI_1(G) = \sum_{uv\in E(G)} F_2(u.v),$$
$$TI_1 = TI_1(G) = \sum_{u\neq v.\{u.v\}\subseteq V(G)} F_3(u.v) \quad (1)$$

where F_1, F_2 and F_3 are functions dependent of a vertex or on a pair of vertices of the molecular graph G and forgotten index is of the form *Equation* 1.

3. BOUNDS OF FORGOTTEN INDEX

Let G be a graph on n vertices with maximum degree Δ, where $n \geq 3$. It is clear that $5m \leq d_u^2 + d_v^2 \leq 2\Delta^2$ and thus $5m \leq F(G) \leq 2\Delta^2 m$. The aim of this section is to compute some bounds for $F(G)$ and then we present some algebraic properties of this index. Let A be the adjacency matrix of G and B is a symmetric matrix with the following entries:

$$b_{uv} = \begin{cases} d(u)^2 + d(v)^2 & if\ uv \in E(G) \\ 0 & otherwise \end{cases}.$$

Lemma 2. We have

i) $F(G) \leq \sqrt{tr(A^2)m/2}$,

ii) $\sum_{uv\in E(G)} d_u^2 d_v^2 \geq M_1^2(G)/n$,

iii) $tr(B) = 2$ and $\sum_{uv\in E(G)}(d_u^2 + d_v^2)^2$,

iv) $F(G) \geq \sqrt{\frac{tr(B^2)}{2}}$,

v) If G is *r*-regular, then $F(G) = \frac{1}{4r^2} tr(B^2)$.

Proof.

i) It is not so difficult to see that

$$F(G) = \sum_{uv\in E(G)}\left[{d_u}^2 + {d_v}^2\right] \le \sqrt{\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)^2} \cdot m^{\frac{1}{2}} = \sqrt{tr(A^2)m/2},$$

as desired.

ii) According to geometrical-arithmetic inequality we have

$$M_1^2(G) = \left(\sum_{u\in V(G)} d_u^2\right)^2 \ge n\sum_{uv\in E(G)} d_u^2 d_v^2.$$

iii) Since every element in the main diagonal of *B* is 0, we obtain *tr*(*B*)=0 The *i*-th entry b_{ii} in the diagonal of B^2 is $b_{ii} = \sum_{v_iv_j\in E(G)}\left[{d_{v_i}}^2 + {d_{v_j}}^2\right]^2$. Thus, $tr(B^2) = \sum_{i=1}^n b_{ii} = \sum_{i=1}^n \sum_{u_iv_i\in E(G)}\left({d_{v_i}}^2 + {d_{v_j}}^2\right)^2 = 2\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)^2$.

iv) By Lemma 1, $tr(B^2) = 2\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)^2 \le 2\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right) \le 2F^2(G)$.

v) If *G* is *r*-regular, then $B = 2r^2A$ and $tr(B^2) = 4r^4 tr(A^2)$. Hence,

$$F(G) = 2r^2m = 2r^2 \times \frac{1}{2} tr(A^2) = \frac{1}{4r^2} tr(B^2).$$

Denote by σ^2 the variance of the sequence of the terms $\left\{{d_u}^2 + {d_v}^2\right\}$ appearing in the definition of *F*(*G*).

Lemma 3. For any graph *G*, $F(G) = \sqrt{m/2tr(B^2) - m^2\sigma^2}$.

Proof. Lemma 2 gives $\frac{1}{2} tr(B^2) = \sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)^2$. By the definition of σ^2, we have

$$\sigma^2 = \frac{1}{m}\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)^2 - \left(\frac{1}{m}\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)\right)^2 = \frac{1}{2m} tr(B^2) - \frac{1}{m^2}F(G)^2$$

and this equality yields the results.

Lemma 4. Let $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$ be all eigenvalues of *B*, then we have

i) $\sum_{i=1}^n \mu_i^2 \ge n\mu_1^2/(n-1)$.

ii) $\sqrt{\frac{n}{2(n-1)}}\mu_1 \le F(G) \le \frac{1}{2}\mu_1 n$.

Proof. Suppose $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$ are the eigenvalues of *B*.

i) Since $\sum_{i=1}^{n}\mu_i = tr(B) = 0$, we have $\mu_1 = -\sum_{i=2}^{n}\mu_i$ and Cauchy-Schwarz inequality gives

$$\mu_1^2 = (\sum_{i=2}^{n}\mu_i)^2 \leq (\sum_{i=2}^{n}\mu_i)^2(n-1).$$

Hence,

$$\sum_{i=1}^{n}\mu_i^2 = \mu_1^2 + \sum_{i=2}^{n}\mu_i^2 \geq \mu_1^2 + \frac{\mu_1^2}{n-1} = \frac{n\mu_1^2}{n-1}.$$

ii) Suppose j is the vector $j = (1.1.\ldots.1) \in R^n$. By Perron-Frobenius theorem we can conclude that $\mu_1 \geq |\mu_j|$, for every j, and then $\mu_1 \geq 0$. Hence, Rayleigh quotient yields

$$\mu_1 = max\frac{\langle Bx.x\rangle}{\|x\|^2} \geq \frac{\langle Bj.j\rangle}{\|j\|^2} = \frac{2F(G)}{n}.$$

According to Part (i), we have

$$F(G)^2 = \left(\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)\right)^2 \geq \sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right) \geq \frac{1}{2}\sum_{i=1}^{n}\mu_i^2$$
$$= \frac{1}{2}(\mu_1^2 + \sum_{i=2}^{n}\mu_i^2) \geq \frac{1}{2}\left(\mu_1^2 + \frac{\mu_1^2}{n-1}\right) = \frac{n\mu_1^2}{2(n-1)}.$$

Assume now that G is a Δ-regular graph. Then $B = 2\Delta^2 A$ and $\mu_i = 2\Delta^2\lambda_i$. It is well know that the greatest eigenvalue of a Δ-regular graph is Δ itself. Hence, $\mu_1 = 2\Delta^2\lambda_1$ and then $F(G) = 2\Delta^2 m = \Delta^2\Delta n = n\Delta^2\lambda_1 = \frac{n}{2}\mu_1$.

4. SPECTRAL PROPERTIES

For given graph G, if the maximum degree of every vertex reaches to four, then G is called a molecular graph. The first **inverse sum indeg index** (ISI index) defined as follows [17]:

$$ISI(G) = \sum_{uv\in E(G)}\frac{d_u d_v}{d_u + d_v}.$$

Let V(G)= {v_1,v_2,...,v_n} be the vertex set of graph G. For 1, 2, ...,n, let d_i be the degree of the vertex v_i. Then define the ISI adjacency matrix PA to be a matrix with entries b_{ij} as follows:

$$b_{ij} = \begin{cases} \frac{d_i d_j}{d_i + d_j} & v_i v_j \in E(G) \\ 0 & otherwise \end{cases}.$$

If the graph G is regular of degree r, then $PA(G) = \frac{r}{2}A(G)$ and

$$PA^2(G) = \frac{1}{4}r^2A^2(G). \quad (2)$$

Example 1. Let Gbean$r$-regular graph. Since $tr(A^2) = 2m$, we have $tr(A^2(G)) = nr$. This means that $tr(PA^2(G)) = nr^3/4$.

Example 2. By using Equation 2, we have $tr(PA^2(S_n)) = 2(n-1)^3/n^2$. Let P_n denote the path P_n, then

$$PA(P_n) = \begin{bmatrix} 0 & 2/3 & 0 & & & & \\ 2/3 & 0 & 1 & 0 & & 0 & \\ 0 & 1 & 0 & & & & \\ & 0 & & \ddots & & 0 & \\ & & & & 0 & 1 & 0 \\ & 0 & & 0 & 1 & 0 & 2/3 \\ & & & & 0 & 2/3 & 0 \end{bmatrix}.$$

The diagonal elements of PA^2 are $\frac{4}{9}.\frac{13}{9}.2.2.\ldots.2.\frac{13}{9}.\frac{4}{9}$. Therefore,

$$tr\big(PA^2(P_n)\big) = \frac{34}{9} + 2(n-4) = 2n - \frac{38}{9}.$$

Lemma 4. Let $PA(G) = \frac{r}{2}A(G)$, then $\chi_\lambda\big(PA(G)\big) = (\frac{r}{2})^n \chi_{\frac{2}{r}\lambda}\big(A(G)\big)$.

Proof. The proof is straightforward.

For an example, $PA(S_n) = \frac{n-1}{n}A(S_n)$ and by using Lemma 4,

$$\chi_\lambda\big(PA(S_n)\big) = (\frac{n-1}{n})^n \chi_{\frac{n\lambda}{n-1}}\big(A(S_n)\big).$$

It is not so difficult to see that $PA(K_{m.n}) = \frac{mn}{m+n}A(K_{m.n})$ and hence

$$\chi_\lambda\big(PA(K_{m.n})\big) = (\frac{mn}{m+n})^n \chi_{\frac{(m+n)\lambda}{mn}}\big(A(K_{m.n})\big).$$

Theorem 5. Let *G* be a graph with vertices set $\{1.2.\ldots.n\}$ and *ISI* matrix PA. Then

i) $tr(PA) = 0$

ii) $tr(PA^2) = 2\sum_{i\sim j}\left(\frac{d_i d_j}{d_i+d_j}\right)^2.(PA^2)_{jj} = d_i d_j \sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}$.

iii) $tr(PA^3) = 2\sum_{i\sim j}\frac{(d_i d_j)^2}{d_i+d_j}\left(\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)$.

iv) $tr(PA^4) = \sum_{i=1}^n\left(\sum_{i\sim l}\left(\frac{d_i d_l}{d_i+d_l}\right)^2\right)^2 + \sum_{i\neq j} d_i d_j\left(\sum_{.l\sim i.l\sim j}\frac{d_l^2}{(d_i+d_l)(d_j+d_l)}\right)^2$.

Proof. All parts can be proved as follows:

i) The Part (i) is clear.

ii) For $i=j$, $(PA^2)_{ii} = \sum_{k=1}^n PA_{ik}PA_{ki} = \sum_{k=1}^n (PA_{ik})^2 = \sum_{i\sim j}(PA_{ij})^2 = \sum_{i\sim j}\left(\frac{d_i d_j}{d_i+d_j}\right)^2$. Therefore, $tr(PA^2) = \sum_{i=1}^n\sum_{i\sim k}\left(\frac{d_i d_k}{d_i+d_k}\right)^2 = 2\sum_{i\sim j}\left(\frac{d_i d_j}{d_i+d_j}\right)^2$. Suppose $i\neq j$. Then, $(PA^2)_{ij} = \sum_{k=1}^n PA_{ik}PA_{kj} = \sum_{.k\sim i.k\sim j} PA_{ik}PA_{kj} = \sum_{.k\sim i.k\sim j}\left(\frac{d_i d_k}{d_i+d_k}\right)\left(\frac{d_j d_k}{d_j+d_k}\right) = d_i d_j \sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}$.

iii) For the matrix PA^3 we have $(PA^3)_{ii} = \sum_{j=1}^{n} PA_{ij}(PA^2)_{jk} = \sum_{i\sim j} \frac{d_i d_j}{d_i+d_j}(PA^2)_{jk} = \sum_{i\sim j}(\sum_{.k\sim i.k\sim j} \frac{d_k^2}{(d_i+d_k)(d_j+d_k)})$ and so we obtain

$$tr(PA^3) = \sum_{i=1}^{n}\sum_{i\sim j}\frac{(d_i d_j)^2}{d_i+d_j}\Big(\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\Big)$$
$$= 2\sum_{i\sim j}\frac{(d_i d_j)^2}{d_i+d_j}\Big(\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\Big).$$

iv) The trace of PA^4 is

$$tr(PA^4) = \sum_{i.j=1}^{n}(PA^2)_{ij}^2 = \sum_{i=j}(PA^2)_{ij}^2 + \sum_{i\neq j}(PA^2)_{ij}^2$$
$$= \sum_{i=1}^{n}\Big(\sum_{i\sim l}\Big(\frac{d_i d_l}{d_i+d_l}\Big)^2\Big)^2 + \sum_{i\neq j} d_i d_j\Big(\sum_{.l\sim i.l\sim j}\frac{d_l^2}{(d_i+d_l)(d_j+d_l)}\Big)^2.$$

This completes our argument.

5. ENERGY AND LAPLACIAN ENERGY

One of branches of graph theory which has many applications in chemistry is spectral theory based on the eigenvalues of the adjacency matrix [6,10]. Let G be a simple graph on n vertices and $\lambda_1.\lambda_2.\ldots.\lambda_n$ be the eigenvalues of its adjacency matrix. The energy $E(G)$ of the graph G is defined as the sum of the absolute values of its eigenvalues, i.e. $E = E(G) = \sum_{i=1}^{n}|\lambda_i|$. Here, we define the ISI energy as the sum of absolute values of the eigenvalues of the ISI matrix. More formally: Let $\rho_1.\rho_2.\ldots.\rho_n$ be the eigenvalues of the ISI matrix PA(G). It is not difficult to see that these eigenvalues are real numbers and their sum is zero. Hence, the ISI energy can be defined as [8] $PAE = PAE(G) = \sum_{i=1}^{n}|\rho_i|$. This definition is applicable to all graphs.

Theorem 6. Let G be a graph with n vertices. Then $PAE(G) \leq \sqrt{2n}ISI(G)$.

Proof. The variance of the numbers $|\rho_i|$, i=1,2,…,n is equal to

$$\frac{1}{n}\sum_{i=1}^{n}|\rho_i|^2 - \left(\frac{1}{n}\sum_{i=1}^{n}|\rho_i|\right)^2$$

which is greater than or equal to zero. Now, $\sum_{i=1}^{n}|\rho_i|^2 = \sum_{i=1}^{n}\rho_i{}^2 = tr(PA^2)$ and therefore $\frac{1}{n}tr(PA^2) - (\frac{1}{n}PAE)^2 \geq 0$. Hence,

$$PAE(G) \leq \sqrt{ntr(PA^2)} \leq \sqrt{2n(ISI(G))^2} = \sqrt{2n}ISI(G).$$

Theorem 7. Let G be a graph with n vertices and at least one edge. Then

$$PAE(G) \geq 2\sum_{i\sim j}\frac{d_i d_j}{d_i+d_j}\left(\frac{2\sum_{i\sim j}\frac{d_i d_j}{d_i+d_j}}{\sum_{i=1}^{n}\left(\sum_{i\sim j}\left(\frac{d_i d_j}{d_i+d_j}\right)^2\right)^2+\sum_{i\neq j}d_i d_j\left(\sum_{k\sim i,k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)^2}\right)^{\frac{1}{2}}.$$

Proof. The Hölder inequality implies that

$$\sum_{i=1}^{n}a_i b_i \leq \left(\sum_{i=1}^{n}a_i^p\right)^{1/p}\left(\sum_{i=1}^{n}a_i^q\right)^{1/q}$$

which holds for any non-negative real number a_i, $b_i (i = 1,2,\ldots,n)$. Put $a_i = |\rho_i|^{2/3}$, $b_i = |\rho_i|^{4/3}$, $p = 3/2$ and $q = 3$, thus we have

$$\sum_{i=1}^{n}|\rho_i|^2 = \sum_{i=1}^{n}|\rho_i|^{2/3}(|\rho_i|^4)^{1/3} \leq \left(\sum_{i=1}^{n}|\rho_i|\right)^{2/3}\left(\sum_{i=1}^{n}|\rho_i|^4\right)^{1/3}. \quad (3)$$

If G has at least one edge, then not all ρ_i's are equal to zero. Then $\sum_{i=1}^{n}|\rho_i^4| \neq 0$ and Equation 3 can be rewritten as

$$PAE(G) = \sum_{i=1}^{n}|\rho_i| \geq \frac{\left(\sum_{i=1}^{n}|\rho_i|^2\right)^{\frac{3}{2}}}{\left(\sum_{i=1}^{n}|\rho_i^4|\right)^{\frac{1}{2}}} = \frac{\left(\sum_{i=1}^{n}\rho_i^2\right)^{\frac{3}{2}}}{\left(\sum_{i=1}^{n}\rho_i^4\right)^{\frac{1}{2}}} = \sqrt{\frac{tr(PA^2)^3}{tr(PA^4)}}$$

$$= 2\sum_{i\sim j}\frac{d_i d_j}{d_i+d_j}\left(\frac{2\sum_{i\sim j}\frac{d_i d_j}{d_i+d_j}}{\sum_{i=1}^{n}\left(\sum_{i\sim j}\left(\frac{d_i d_j}{d_i+d_j}\right)^2\right)^2+\sum_{i\neq j}d_i d_j\left(\sum_{k\sim i,k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)^2}\right)^{\frac{1}{2}}.$$

Theorem 8. If G is a regular graph of degree r where $r>0$, then $PAE(G) = \frac{r}{2}E(G)$. If, in addition $r = 0$, then PA$E = 0$.

Proof. If $r = 0$, then G is a graph without edges. Then directly from the definition of matrix PA, it follows that $PA_{ij} = 0$, for all $i.j = 1.2.\ldots.n$ and consequently PA(G) = 0. Therefore, PAE(G) = 0. Suppose now that G is regular of degree $r \geq 0$ and $d_1 = d_2 = \cdots = d_n = r$. Then all none-zero terms in PA(G) are equal to r/2, implying that $PA(G) = \frac{r}{2}A(G)$. Therefore, $\rho_i = \frac{r}{2}\lambda_i$ for i=1,2,…n and hence $PAE(G) = \sum_{i=1}^{n}|\rho_i| = \frac{r}{2}\sum_{i=1}^{n}|\lambda_i| = \frac{r}{2}E(G)$, which completes the proof.

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Further Results on Betweenness Centrality of Graphs

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ABSTRACT

Betweenness centrality is a distance-based invariant of graphs. In this paper, we use link and lexicographic products to compute betweenness centrality of some important classes of graphs. Finally, we pose some open problems related to this topic.

1 INTRODUCTION

All graphs in this paper are finite and simple. A graph G is an ordered pair (V_G, E_G) consisting of a set V_G of vertices and a set E_G, disjoint from V_G, of edges, together with an incidence function f_G that associates with each edge of G an unordered pair of (not necessarily G distinct) vertices of G. A path in a graph is a finite or infinite sequence of edges which connect a sequence of vertices which are all distinct from one another. The distance $d_G(u, v)$ between the vertices u and v of a graph G is equal to the length of a shortest path that connects u and v.

The betweenness centrality, B_G, was first introduced by Bavelas [3] as the number of times a node acts as a bridge along the shortest path between two other nodes. In other words, for a vertex $v \in V_G$, $B_G(v) = \sum_{s \neq v \neq t \in V_G} \frac{\sigma_G^v(s,t)}{\sigma_G(s,t)}$, where $\sigma_G(s,t)$

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is total number of shortest paths from node s to node t and $\sigma_G^v(s,t)$ is the number of those paths that pass through v [7].

This invariant has important role in Psychology to study on mental illnesses. We encourage readers to see [6, 8, 9, 12 − 17] for the role of betweenness centrality in analysis of social networks, computer networks, and many other types of network data models.

The lexicographic product $G[H]$ of graphs G and H, studied first by Felix Hausdor in 1914, is the graph with vertex set $V_G \times V_H$ and (g_1, h_1) is adjacent with (g_2, h_2) whenever (g_1 is adjacent to g_2) or ($g_1 = g_2$ and h_1 is adjacent to h_2). We encourage the reader to consult the book Handbook of Product Graphs, written by Hammack, Imrich and Klavžar, for more information on results on this product.

Suppose G and H are graphs with disjoint vertex sets, $x \in V_G$ and $y \in V_H$. A link of G and H by vertices y and z is a graph operation defined as the graph $(G \sim H)(x; y)$ obtained by joining x and y by an edge in the union of these graphs, see [2, 5]. Let $V_G = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix $A(G) = [a_{ij}]$ is an $n \times n$ matrix for which $a_{ij}=1$ if $v_i v_j \in E_G$ and $a_{ij}=0$ otherwise [10].

The degree of a vertex v in G is denoted by $deg_G(v)$. We use $N_G[v]$ to denote the ball of radius one centered at the vertex v in G. Also, we use the notations P_n, C_n and K_n to denote the path, cycle, complete graph with n vertices, respectively. Our other notations are standard and taken mainly from the standard books of graph theory such as [4].

2. BETWEENNESS CENTRALITY UNDER LEXICOGRAPHIC AND LINK PRODUCTS

In this section, we compute the betweenness centrality of link and lexicographic products from the betweenness centrality of their initial factors.

Theorem 2.1. Let (g, h) be a vertex of $G[H]$. Then

$$B_{G[H]}((g,h)) = |V_H| B_G(g) + \frac{1}{|V_H|}\left(\binom{|V_H|}{2} - |E_H| - \sum_{1 \le i < j \le |V_H|} I(a_{ij}^{(2)})\right) \sum_{gg' \in E_G} \frac{1}{deg_G(g')} + \sum_{g' \in N_G[g], d_H(h',h'')=2} \frac{1}{|V_H| deg_G(g') + \sigma_H(h',h'')}$$

where $a_{ij}^{(2)}$ is ij-th entry of $A^2(G)$ and $I(x) = \begin{cases} 0 & \text{if } x = 0 \\ 1 & \text{otherwise} \end{cases}$.

Proof. Let (g, h), (g_1, h_1) and (g_2, h_2) be three different vertices of $G[H]$. Thus, there are four cases in which $\sigma_{G[H]}^{(g,h)}((g_1, h_1), (g_2, h_2)) \neq 0$, as follows:

1. $g_1 = g_2 = g$ and $d_H(h_1, h_2) = 2$. Then $\sigma_{G[H]}((g_1, h_1), (g_2, h_2)) = |V_H| deg_G(g) + \sigma_H(h_1, h_2)$ and $\sigma_{G[H]}^{(g,h)}((g_1, h_1), (g_2, h_2)) = 1$. Set
$$B_1 = \sum_{h_1,h_2 \in V_H, d_H(h_1,h_2)=2} \frac{1}{|V_H| deg_G(g) + \sigma_H(h_1,h_2)}.$$

2. $g_1 = g_2$, $gg_1 \in E_G$ and $d_H(h_1, h_2) = 2$. Then $\sigma_{G[H]}((g_1, h_1), (g_2, h_2)) = |V_H| deg_G(g_1) + \sigma_H(h_1, h_2)$ and $\sigma_{G[H]}^{(g,h)}((g_1, h_1), (g_2, h_2)) = 1$. Set
$$B_2 = \sum_{h_1,h_2 \in V_H, d_H(h_1,h_2)=2, gg' \in E_G} \frac{1}{|V_H| deg_G(g') + \sigma_H(h_1,h_2)}.$$

3. $g_1 = g_2$, $gg_1 \in E_G$ and $d_H(h_1, h_2) > 2$. Then $\sigma_{G[H]}((g_1, h_1), (g_2, h_2)) = |V_H| deg_G(g_1)$ and $\sigma_{G[H]}^{(g,h)}((g_1, h_1), (g_2, h_2)) = 1$. Set
$$B_3 = \sum_{h_1,h_2 \in V_H, d_H(h_1,h_2)>2, gg' \in E_G} \frac{1}{|V_H| deg_G(g')}$$
and so $B_3 = \frac{1}{|V_H|}\left(\binom{|V_H|}{2} - |E_H| - \sum_{1 \le i < j \le |V_H|} I(a_{ij}^{(2)})\right) \sum_{gg' \in E_G} \frac{1}{deg_G(g')}$.

4. $g_1 \neq g \neq g_2$ and $d_G(g_1, g_2) \geq 2$. Then
$\sigma_{G[H]}((g_1, h_1), (g_2, h_2)) = \sigma_G(g_1, g_2) |V_H|^{d_G(g_1,g_2)-1}$,
$\sigma_{G[H]}^{(g,h)}((g_1, h_1), (g_2, h_2)) = \sigma_G^g(g_1, g_2) |V_H|^{d_G(g_1,g_2)-2}$.
Set $B_4 = \sum_{\{h_1,h_2\} \subseteq V_H, d_G(g',g'') \geq 2} \frac{\sigma_G^g(g',g'') |V_H|^{d_G(g',g'')-2}}{\sigma_G(g',g'') |V_H|^{d_G(g',g'')-1}}$ and so $B_4 = |V_H| B_G(g)$.

Therefore, by summation of B_1, B_2, B_3 and B_4 , the result can be proved. □

Corollary 2.1. If (g, h) is a vertex of $G[C_n]$ and $n > 4$, then
$$B_{G[C_n]}((g, h)) = nB_G(g) + \frac{n-5}{2} \sum_{gg' \in E_G} \frac{1}{deg_G(g')} + n \sum_{g' \in N_G[g]} \frac{1}{n deg_G(g') + 1}.$$
Also, if G is a k-regular graph, we have
$$B_{G[C_n]}((g, h)) = nB_G(g) + \frac{n(k+1)}{nk+1} + \frac{n-5}{2}.$$

Corollary 2.2. Let (g, h) be a vertex of $G[C_4]$, then
$$B_{G[C_4]}((g, h)) = 4B_G(g) + 2 \sum_{g' \in N_G[g]} \frac{1}{4 \deg(g') + 2}.$$
Moreover, if G is a k-regular graph, then
$$B_{G[C_4]}((g, h)) = 4B_G(g) + \frac{k+1}{2k+1}.$$

Corollary 2.3. If (g, h) is a vertex of $G[C_3]$, then $B_{G[C_3]}((g, h)) = 3B_G(g)$.

Theorem 2.2. Let G and H be graphs with disjoint vertex sets, $x \in V_G$ and $y \in V_H$. Then

$$B_{(G\sim H)(x;y)}(u) = \begin{cases} B_G(u) + |V_H| \sum_{t\in V_G} \frac{\sigma_G^u(t,x)}{\sigma_G(t,x)} & if\ u \in V_G \\ B_H(u) + |V_G| \sum_{t\in V_H} \frac{\sigma_H^u(t,y)}{\sigma_H(t,y)} & if\ u \in V_H \end{cases}.$$

Proof. Supose *u*, *s* and *t* are three different vertices of (*G* ~ *H*)(*x*;*y*). There are two cases as follow:

1. $u \in V_G$. In this case, if $s,t \in V_G$, then

$$\sigma_{(G\sim H)(x;y)}(s,t) = \sigma_G(s,t) \quad \text{and } \sigma^u_{(G\sim H)(x;y)}(s,t) = \sigma^u_G(s,t)$$

and if $s \in V_G$ and $t \in V_H$, then

$$\sigma_{(G\sim H)(x;y)}(s,t) = \sigma_G(s,x)\sigma_H(y,t) \quad \text{and } \sigma^u_{(G\sim H)(x;y)}(s,t) = \sigma^u_G(s,x)\sigma_H(y,t).$$

Note that if $s,t \in V_H$, then $\sigma^u_{(G\sim H)(x;y)}(s,t) = 0$. Therefore,

$$B_{(G\sim H)(x;y)}(u) = B_G(u) + |V_H| \sum_{s\in V_G} \frac{\sigma_G^u(t,x)}{\sigma_G(t,x)}.$$

2. $u \in V_H$. Using a similar argument applied in the first case, we have

$$B_{(G\sim H)(x;y)}(u) = B_H(u) + |V_G| \sum_{t\in V_H} \frac{\sigma_H^u(t,y)}{\sigma_H(t,y)},$$

which completes our proof. □

3. APPLICATIONS

In this section, we apply our results to compute the betweenness centrality of some well-known graphs.

Example 3.1. Consider the Catlin graph $C_5[C_3]$ shown in Figure 1. Then $\sum_{1\le i\le j\le 3} I\left(a_{ij}^{(2)}\right) = 0$. On the other hand, by [20], $B_{C_n}(v) = \begin{cases} \frac{1}{8}(n-2)^2 & 2|n \\ \frac{1}{8}(n-1)(n-3) & 2\nmid n \end{cases}$. Therefore, by Corollary 1.1, we have $B_{C_5[C_3]}((g,h)) = 3$.

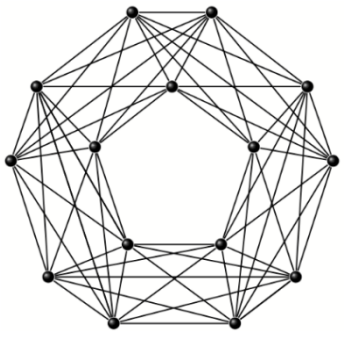

Figure 1. The Catlin graph.

Example 3.2. Let G be the closed fence graph shown in Figure 2. It is clear that the lexicographic product of C_n and P_2 is isomorphic to G. Then, by Theorem 1, we have

$$B_G(v) = B_{C_n[P_2]}(v) = \begin{cases} \frac{1}{4}(n-2)^2 & 2|n \\ \frac{1}{4}(n-1)(n-3) & 2 \nmid n \end{cases}.$$

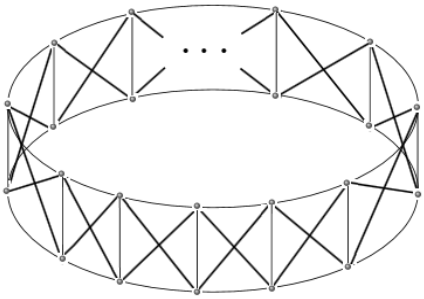

Figure 2. Closed fence graph.

Example 3.3. Let G be the open fence graph depicted in Figure 3. It is not difficult to check that $G \cong P_n[P_2]$ and $B_{P_n}(v_1) = (i-1)(n-i)$. Then, by Theorem 1, we have

$$B_G\left((g_i, h_j)\right) = B_{P_n[P_2]}\left((g_i, h_j)\right) = 2(n-i)(i-1).$$

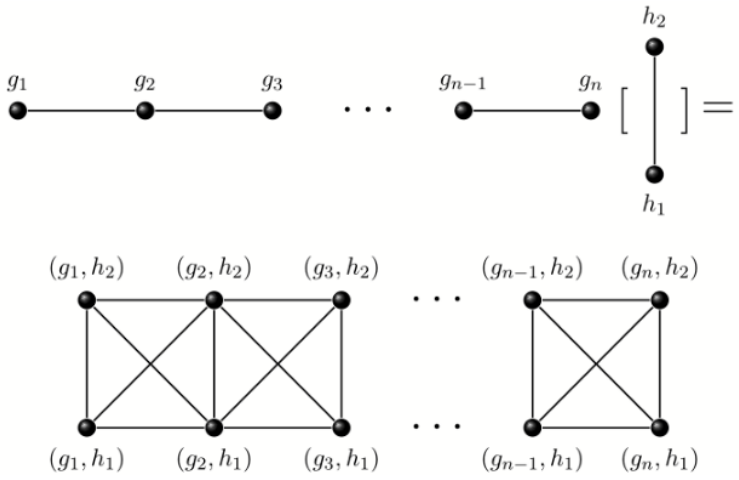

Figure 3. Open fence graph.

The Wiener index, W, is equal to the sum of the lengths of the shortest paths between all pairs of vertices. Kumar and Balakrishnan [11] gave the following relation between the Wiener index and the betweenness centrality index for a graph G:

$$W(G) = \sum_{v\in V_G} B_G(v) + \binom{|V_G|}{2}.$$

Thus, we can use betweenness centrality instade of Wiener index. Therefore, if $B(v) = B(u)$ for each $u,v \in V_G$, then $B_G(v) = \frac{W(G)-\binom{|V_G|}{2}}{|V_G|}$. For example, Since $B_{C_n}(v) = B_{C_n}(u)$ for each $u,v \in V_{C_n}$, then $B_{C_n}(v) = \frac{W(C_n)-\binom{n}{2}}{n}$.

Example 3.4. Consider the dendrimer D_1 shown in Figure 4. As one can see in this figure, $D_1 = (G \sim H)(x; y)$. On the other hand, if u is the vertex of G shown in Figure 4, it is not difficult to check that $B_G(u) = 2$ and $\sum_{s\in V_G} \frac{\sigma_G^u(t,x)}{\sigma_G(t,x)} = 0$. Therefore, by Theorem 2, we have $B_{D_1}(u) = B_{(G\sim H)(x;y)}(u) = 2$. Also, by the previous argument,

$$W(D_1)=\sum_{u\in V_{D_1}} B_{D_1}(u) + \binom{|V_{D_1}|}{2}.$$

Using a similar argument, $B_{D_n}(u) = 2$, where u is the vertex of D_n shown in Figure 4.

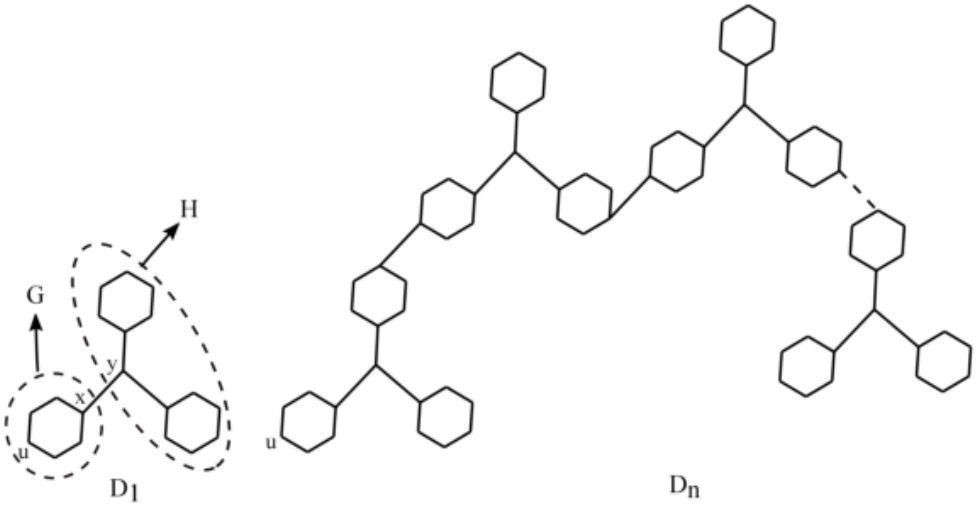

Figure 4. Dendrimers D_1 and D_n.

Example 3.5. A k-almost tree is a graph in which each biconnected component is obtained by adding at most k edges to a tree. Akutsu and Nagamochi [1] studied these graphs as an example of chemical graphs.

Consider graph G, graph H and the almost tree Γ shown in Figure 5. As one can see, $\Gamma = (G\sim H)(x;y)$. Then, by Theorem 2 and this fact that $B_G(u)=\frac{1}{2}$, we have

$$B_\Gamma(u)=B_{(G\sim H)(x;y)}(u)=\frac{1}{2}.$$

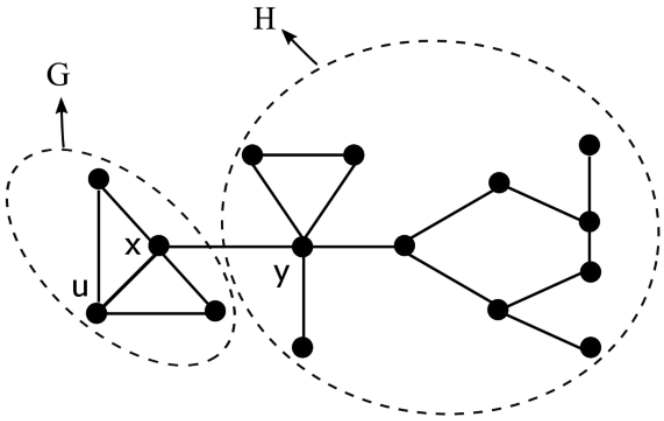

Figure 5. The almost tree Γ.

Example 3.6. For handcuffs graph $C_n \sim C_m$, we have

$$B_{(C_n \sim C_m)(x;y)}(u) = \begin{cases} \frac{1}{8}(n-2)^2+m \sum\limits_{t \in V_{C_n}} \frac{\sigma^u_{C_n}(t,x)}{\sigma_{C_n}(t,x)} & if\ u \in V_{C_n}\ \&\ 2|n \\ \frac{1}{8}(n-1)(n-3)+m \sum\limits_{t \in V_{C_n}} \frac{\sigma^u_{C_n}(t,y)}{\sigma_{C_n}(t,x)} & if\ u \in V_{C_n}\ \&\ 2 \nmid n \\ \frac{1}{8}(m-2)^2 + n \sum\limits_{t \in V_{C_m}} \frac{\sigma^u_{C_m}(t,x)}{\sigma_{C_m}(t,x)} & if\ u \in V_{C_m}\ \&\ 2|m \\ \frac{1}{8}(m-1)(m-3)+n \sum\limits_{t \in V_{C_m}} \frac{\sigma^u_{C_m}(t,y)}{\sigma_{C_m}(t,x)} & if\ u \in V_{C_m}\ \&\ 2 \nmid m \end{cases}$$

4. OPEN PROBLEMS

In this section, we pose two open problems to develop the topic of betweenness centrality on other graph operations. The tensor product $G \otimes H$ of graphs G and H is the graph with vertex set $V_G \times V_H$ and (g_1, h_1) is adjacent with (g_2, h_2) whenever (g_1 is adjacent to g_2) and (h_1 is adjacent to h_2), see [10, 18] for details. The strong product $G \oplus H$ of graphs G and H is the graph with vertex set $V_G \times V_H$ and (g_1, h_1) is adjacent with (g_2, h_2) whenever (g_1 is adjacent to g_2 and $h_1 = h_2$) or (h_1 is adjacent to h_2 and $g_1 = g_2$) or (g_1 is adjacent to g_2 and h_1 is adjacent to h_2), see [10, 19].

We end this paper by the following two open questions:

1. Let G and H be two graphs and (g, h) be a vertex of $G \otimes H$. What is the value of $B_{G \otimes H}((g,h))$?

2. Let G and H be two graphs and (g, h) be a vertex of $G \oplus H$. What is the value of $B_{G\oplus H}((g,h))$?

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ABSTRACTS
IN
PERSIAN

An Algebraic Calculation Method for Describing Time–Dependent Processes in Electrochemistry– Expansion of Existing Procedures

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یک روش محاسباتی جبری برای توصیف فرایندهای وابسته به زمان در بسط- الکتروشیمی روش‌های موجود

ادیتور رابط : ایوان گوتمن

چکیده

در این مقاله، یک مدل جایگزین که امکان گسترش نظریهٔ دبای- هاکل (DHT) را با توجه به وابستگی به زمان به‌طور صریح فراهم می‌کند، ارائه می‌شود. از رویکرد الکترو- شبه ایستای (EQS) معرفی شده در مطالعات اخیر، پتانسیل های وابسته به زمان برای توصیف چندین پدیده بخصوص هدایت رسانه ها و نیز رفتار ذرات باردار (یونها) در الکترولیتها، مناسب هستند. این، منجر به اصلاح فرمولبندی مفهوم معادلهٔ غیرخطی پواسون- بولتسمن (PBE) می شود. اگر غلظت و یا گرادیان شار ذرات در نظر گرفته شود، ساختار اصلی PBE، به یک معادلهٔ دیفرانسیل جزئی غیرخطی (nPDE) از مرتبهٔ سوم تغییر داده خواهد شد. اینکه چگونه یک نفر می تواند کلاسهای جواب‌ها را برای تابع پتانسیل با استفاده از کاربرد گامهای جبری محض به صورت تحلیلی به دست آورد، نشان داده می‌شود. فایدهٔ ابزارهای ریاضی مورد استفاده در اینجا، این واقعیت است که شکل بسته جواب‌ها می توانند محاسبه شوند و بنابراین، روشهای عددی لازم نیست. نتیجهٔ مهم پژوهش حاضر، شامل دو قسمت معنادار است:

1. مدل معادله، اجازهٔ توصیف مسائل وابسته به زمان در نظریهٔ یونها را می‌دهد. 2. فرآیند ریاضی می‌تواند برای استنتاج کلاسهای جواب‌های nPDE های دلخواه، به خصوص برای مرتبهٔ بالاتر استفاده شود.

لغات کلیدی: nPDEها، nODEها، نظریهٔ دبای- هاکل (DHT)، معادلهٔ پواسون- بولتسمن (PBE)

The Irregularity and Total Irregularity of Eulerian Graphs

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بی‌نظمی و بی‌نظمی تام گراف‌های اویلری

ادیتور رابط : ایوان گوتمن

چکیده

برای یک گراف دلخواه G، بی‌نظمی و بی‌نظمی تام G به ترتیب به صورت

$$irr(G) = \sum_{uv \in E(G)} | d_G(u) - d_G(v) |$$

$$irr_t(G) = \frac{1}{2} \sum_{uv \in V(G)} | d_G(u) - d_G(v) |$$

تعریف می‌شوند که در آن، $d_G(u)$ درجهٔ رأس u است. در این مقاله، همه گراف‌های اویلری با دومین کمینهٔ بی‌نظمی و دومین و سومین کمینهٔ بی‌نظمی تام تعیین می‌شوند.

لغات کلیدی: گراف‌های اویلری، بی‌نظمی، بی‌نظمی تام، درجه رأس

Some Remarks on the Arithmetic-Geometric Index

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نکاتی دربارهٔ شاخص حسابی-هندسی

ادیتور رابط : تومیسلاو داسلیک

چکیده

با استفاده از یک اتحاد برای مقاومت‌های موثر، رابطه‌ای بین شاخص حسابی-هندسی و شاخص دورانی جهانی می‌یابیم. همچنین با کمک بیشینه‌سازی، کران های مقید بالایی و پایینی را برای شاخص حسابی-هندسی به‌دست می‌آوریم.

لغات کلیدی: شاخص حسابی-هندسی، بیشینه‌سازی، شاخص دورانی جهانی

Novel Atom–Type–Based Topological Descriptors for Simultaneous Prediction of Gas Chromatographic Retention Indices of Saturated Alcohols on Different Stationary Phases

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توصیف‌کننده‌های جدید توپولوژیکی مبتنی بر نوع اتم برای پیش‌بینی همزمان شاخص‌های بازداری کروماتوگرافی گازی الکل‌های اشباع بر روی فازهای ساکن مختلف

ادیتور رابط : علیرضا اشرفی

چکیده

در این کار، شاخص‌های توپولوژیکی جدید مبتنی بر نوع اتم، به نام شاخص‌هایAT، به عنوان توصیف-کننده برای رمزگذاری اطلاعات ساختاری مولکول‌ها در سطح اتمی ارائه شدند.این توصیف‌کننده‌ها با موفقیت برای مدل‌سازی همزمان رابطه کمی ساختار-بازداری (QSRR) الکل‌های اشباع بر روی فازهای ساکن مختلف (SE-30، OV-3، OV-7،OV-11، OV-17 و OV-25) مورد استفاده قرار گرفتند. ابتدا مدل‌های رگرسیونی خطی چندگانه برای شاخص بازداری کوواتس (RI) الکل‌ها، با استفاده از شاخص‌هایAT و ارتباط مولکولی مرتبه اول راندیک ($^1\chi$) بر روی هر فاز ساکن به طور جداگانه توسعه داده شد. ضریب همبستگی تعدیل شده (R^2_{adj}) و خطای استاندارد (SE) برای مدل ها به ترتیب درگستره 0/999–0/994 و8/90 –4/40 قرار داشت. اعتبار آماری مدل‌ها، به وسیلهٔ اعتبارسنجی تقاطعی تأیید شد (R^2_{cv}>0/99). در مرحلهٔ بعد، کل مقادیر RI بر روی فازهای ساکن برای ایجاد یک سری داده-های جدید، ترکیب شدند و نتایج رضایت بخش بودند (SE=8/55 و R^2_{adj}=0/995). اعتبارسنجی خارجی مدل منجر به مقادیر میانگین 8/29 و 8/69 به ترتیب برای انحراف‌های استاندارد، درجه‌بندی و پیش‌بینی گردید. شاخص‌های توپولوژیکی، به خوبی ویژگی‌های مولکولی وابسته به شاخص بازداری ترکیبات مدل را پوشش دادند.

لغات کلیدی:رابطهٔ کمی ساختار-بازداری، شاخص‌های توپولوژیکی مبتنی بر نوع اتم، الکل‌های اشباع، مدل‌سازی

A Note on the Bounds of Laplacian–Energy–Like Invariant

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یادداشتی دربارهٔ کرانهای ثابت شبه- انرژی- لاپلاسی

ادیتور رابط : تومیسلاو داسلیک

چکیده

شبه- انرژی- لاپلاسی گراف همبند سادهٔ G به صورت $LEL = LEL(G) = \sum_{i=1}^{n} \sqrt{\mu i}$ تعریف می‌شود که $\mu_1(G) \geq \mu_2(G) \geq \ldots \geq \mu_n(G) = 0$ مقادیر ویژهٔ لاپلاسی گراف G هستند. در این مقاله، تعدادی از کران‌های بالایی و پایینی برای LEL و همچنین تعدادی از کران‌های پایینی برای شعاع طیفی گراف به دست می‌آوریم.

لغات کلیدی: طیف لاپلاسی، ثابت شبه- انرژی- لاپلاسی، نامساوی کوشی- شوارتز، اتحاد لاگرانژ، شعاع طیفی

On the Eigenvalues of some Matrices Based on Vertex Degree

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مقادیر ویژهٔ بعضی از ماتریسهای مبتنی بر درجهٔ رأس

ادیتور رابط : ایوان گوتمن

چکیده

هدف این مقاله، در ابتدا، محاسبهٔ تعدادی از کران‌های شاخص فراموش‌شده و سپس ارائهٔ خواص طیفی این شاخص توپولوژیکی است. در ادامه، نوع جدیدی از انرژی با نام انرژی ISI متناظر با شاخص ISI را تعریف می‌کنیم. سرانجام، تعدادی از کرانها را برای این گراف ثابت جدید تعیین می‌کنیم.

لغات کلیدی: شاخص زاگرب، شاخص فراموش‌شده، شاخص ISI، انرژی گراف

Further Results on Betweenness Centrality of Graphs

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نتایج بیشتری دربارهٔ مرز بین‌بودن گراف‌ها

ادیتور رابط : علیرضا اشرفی

چکیده

مرز بین‌بودن یکی از متغیرهای فاصله- مبنا از گراف‌ها است. در این مقاله، از ضرب‌های خط و لغت‌نامه‌ای برای محاسبهٔ مرز بین برخی از کلاس‌های مهم گراف‌ها استفاده می‌کنیم. در نهایت، تعدادی مسأله باز مرتبط با این عنوان مطرح می‌کنیم.

لغات کلیدی: مرز بین‌بودن، ضرب لغت‌نامه‌ای، خط، ضرب تنسور، ضرب قوی

این نشریه طبق مجوز شماره 89/3/11/104372 مورخه 89/11/27 دارای اعتبار **علمی -پژوهشی** از وزارت علوم ، تحقیقات و فناوری می باشد. همچنین این مجله در پایگاه اطلاعاتی ISC (Islamic World Science Citation Center) وابسته به وزارت علوم ، تحقیقات و فناوری نمایه می شود.

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