# Journal of Mathematics and System Science

Volume 7, Number 10, October 2017 (Serial Number 68)



David Publishing Company www.davidpublisher.com

#### **Publication Information:**

*Journal of Mathematics and System Science* is published monthly in hard copy and online (Print: ISSN 2159-5291; Online: ISSN 2159-5305) by David Publishing Company located at 1840 Industrial Drive, Suite 160, Libertyville, IL 60048, USA.

#### Aims and Scope:

*Journal of Mathematics and System Science*, a monthly professional academic and peer-reviewed journal, particularly emphasizes new research results in theory and methodology, in realm of pure mathematics, applied mathematics, computational mathematics, system theory, system control, system engineering, system biology, operations research and management, probability theory, statistics, information processing, etc.. Articles interpreting practical application of up-to-date technology are also welcome.

#### **Editorial Board Members:**

William P. Fox (USA) Wattanavadee Sriwattanapongse (Thailand) Zoubir Dahmani (Algeria) Claudio Cuevas (Brazil) Elisa Francomano (Italy) Baha ŞEN (Turkey) Assia Guezane-Lakoud (Algeria) Alexander Nikolaevich Raikov (Russia) Shelly SHEN (China)

Manuscripts and correspondence are invited for publication. You can submit your papers via web submission, or E-mail to mathematics@davidpublishing.org, jmss.mathematics@hotmail.com. Submission guidelines and web submission system are available at http://www.davidpublisher.com.

#### **Editorial Office:**

1840 Industrial Drive, Suite 160, Libertyville, IL 60048, USA Tel: 1-323-984-7526, 323-410-1082 Fax: 1-323-984-7374, 323-908-0457 E-mail: mathematics@davidpublishing.org, jmss.mathematics@hotmail.com

Copyright©2017 by David Publishing Company and individual contributors. All rights reserved. David Publishing Company holds the exclusive copyright of all the contents of this journal. In accordance with the international convention, no part of this journal may be reproduced or transmitted by any media or publishing organs (including various websites) without the written permission of the copyright holder. Otherwise, any conduct would be considered as the violation of the copyright. The contents of this journal are available for any citation. However, all the citations should be clearly indicated with the title of this journal, serial number and the name of the author.

#### Abstracted / Indexed in:

Database of EBSCO, Massachusetts, USA Index Copernicus, Poland CiteFactor, USA Google Scholar J-GATE database, India CSA Technology Research Database Ulrich's Periodicals Directory Electronic Journals Library (EZB) Public Affairs Information Service Universe Digital Library S/B, Proquest Norwegian Social Science Data Services (NSD), Database for Statistics on Higher Education (DBH), Norway Summon Serials Solutions Academic Keys Chinese Electronic Periodicals Service, Airiti Inc, Taiwan Online Computer Library Center, Inc., USA Chinese Scientific Journals Database, VIP Corporation, Chongqing, P. R. China

#### **Subscription Information:**

Price (per year): Print \$520; Online \$300; Print and Online \$560

David Publishing Company 1840 Industrial Drive, Suite 160, Libertyville, IL 60048, USA Tel: 1-323-984-7526, 323-410-1082; Fax: 1-323-984-7374, 323-908-0457 E-mail: order@davidpublishing.com Digital Cooperative Company: www.bookan.com.cn



David Publishing Company www.davidpublisher.com

# Journal of Mathematics and System Science

Volume 7, Number 10, October 2017 (Serial Number 68)

# Contents

269 The Conditional Heterocedasticity on the Argentine Inflation. An Analysis for the Period from 1943 to 2013

 Juan Carlos Abril and María De Las Mercedes Abril

 278 Quantization of Particle Energy in the Analysis of the Boltzmann Distribution and Entropy

 V.P. Malyshev, Yu.S. Zubrina, A.M. Makasheva

 289 New Results Subclasses of Analytic Functions Define by Opooladifferential Operator

 Fatunsin L. M. and Opoola T. O.



# The Conditional Heterocedasticity on the Argentine Inflation. An Analysis for the Period from 1943 to 2013

Juan Carlos Abril<sup>1</sup> and María De Las Mercedes Abril<sup>2</sup>

Universidad Nacional de Tucumán, Facultad de Ciencias Económicas and Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET). Tucumán. Argentina. <sup>1</sup>jabril@herrera.unt.edu.ar, mabrilblanco@hotmail.com<sup>2</sup>

Abstract. Numerous economic time series do not have a constant mean and in practical situations, we often see that the variance of observational error is subject to a substantial variability over time. This phenomenon is known as *volatility*. To take into account the presence of volatility in an economic series, it is necessary to resort to models known as *conditional heteroscedastic* models. In these models, the variance of a series at a given time point depends on past information and other data available up to that time point, so that a conditional variance must be defined, which is not constant and does not coincides with the overall variance of the observed series.

There is a very large variety of nonlinear models in the literature, which are useful for the analysis of any economic time series with volatility, but we will focus in analyzing our series of interest using *ARCH* type models introduced by Engle (1982) and their extensions. These models are non-linear in terms of variance.

Our objective will be the study of the monthly inflation data of Argentina for the period from January 1943 to December 2013. The data is officially published by the National Institute of Statistics and Censuses (or INDEC as it is known in Argentina). Although it is a very long period in which various changes and interventions took place, it can be seen that certain general patterns of behavior have persisted over time, which allows us to admit that the study can be appropriately based on available information. *Keywords:* Inflation, heterocedasticity, volatility, time series.

#### Introduction

Numerous economic time series do not have a constant mean and in practical situations, we often see that the variance of observational error is subject to substantial variability over time. This phenomenon is known as *volatility*.

To take into account the presence of volatility in an economic series, it is necessary to resort to models known as *conditional heteroscedastic models*. In these models, the variance of a series at a given time point depends on past information and other data available up to that time point, so a conditional variance can be defined, which is not constant and does not coincide with the overall variance of the observed series.

An important feature of any economic time series is that they are not generally serially

correlated but they are dependent. Thus linear models such as those belonging to the family of autoregressive moving average models or *ARMA* models may not be appropriate to describe these series.

The first inspection of series such as the one we will study suggests that they do not have a mean and a constant variance. A stochastic variable in which the variance is constant is said to be *homocedastic* as opposed to what would be a *heteroscedastic* variable. For those series where there is volatility, the unconditional variance can be constant even when the conditional variance in some periods is unusually large.

Our objective will be the study of the monthly inflation data of Argentina for the period from January 1943 to December 2013. The data is officially published by the National Institute of Statistics and Censuses (INDEC). Although it is a very long period in which basic changes, basket changes and interventions took place even in the INDEC itself, it can be seen that certain general patterns of behavior have persisted over time, which allows us to admit that the study is adequately based on the information available.

#### Method

#### **Research Model**

#### Modeling volatility

Linear models of the *ARMA* type, for example, admit that the disturbances have zero mean and constant variance, usually equal to one (this is equivalent to saying that these disturbances are white noise). Under these conditions, the conditional variance given over the past history, that is given  $F_{t-1}$ , is constant over time.

There is a very large variety of nonlinear models available in the literature to address these situations, but we will focus on *ARCH* models or *autoregressive conditional heteroscedastic models* introduced by R. Engle (1982) and their extensions. These models are nonlinear in terms of variance.

In the analysis of non-linear model, *errors* (also called *innovations*, because they represent the new part of the series that cannot be predicted from

the past) known as  $\varepsilon_t$ , are generally assumed IID

and the model has the form

$$y_{t} = g(\varepsilon_{t-1}, \varepsilon_{t-2}, ...) + \varepsilon_{t} h(\varepsilon_{t-1}, \varepsilon_{t-2}, ...)$$
  
=  $g_{t} + \varepsilon_{t} h_{t} = \mu_{t} + \varepsilon_{t} h_{t},$  (1)

where  $g(\bullet) = g_t = \mu_t$ , represents the conditional

mean and  $h^2(\bullet) = h_t^2$  is the conditional variance.

#### ARCH type models

The basic idea of this model is that a series  $y_t$  is not serially correlated but depends on past prices through a quadratic function.

An ARCH(q) model can be expressed as  

$$y_t = \mu_t + \varepsilon_t h_t$$
  
 $\varepsilon_t \sim i.i.d D(0,1)$  (2)  
 $\sigma^2 = h_t^2 = \omega + \sum_{i=1}^q \alpha z_{t-1}^2$ ,

where  $z_t = y_t - \mu_t$  and  $D(\bullet)$  is a probability density function with zero mean and variance equal to one.

An *ARCH* model such as the one just described adequately describes volatility clustering. The conditional variance of  $y_t$  is an increasing function of the square of the shock that occurs at time t-1. Consequently, if  $y_t$  is sufficiently large in absolute value,  $\sigma_t^2$  and thus  $y_t$  are expected to be also large in absolute value. It is necessary to take into account that even when the conditional variance in an *ARCH* type model varies with time, that is,  $\sigma_t^2 = E(z_t^2|F_{t-1})$ , the unconditional variance of  $z_t$  is constant and,

given that  $\omega > 0$  and  $\sum_{i=1}^{q} a_i < 1$ , we have

$$\sigma_t^2 = E\left\{ E\left(z_t^2 | F_{t-1}\right) \right\} = \frac{\omega}{1 - \sum_{i=1}^q a_i}.$$
(3)

In most practical applications, excess kurtosis in an *ARCH* model, along with a normal distribution, is not enough to be able to explain what a dataset like ours. Therefore, we can make use of other distributions. For example, we can suppose that  $\varepsilon_t$  follows a *t* Student distribution with mean 0, variance equal to 1 and  $\upsilon$  degrees of freedom, that is,  $\varepsilon_t$  is *ST* (0,1, v). In this case, the unconditional kurtosis for the *ARCH* (1) model is

$$\lambda (1 - \alpha_1^2)/(1 - \lambda \alpha_1^2)$$
 where  $\lambda = 3(\nu - 2)/(\nu - 4)$ .

Due to the additional coefficient v, the ARCH (1) model based on a *t* distribution will have heavier tails than one based on a normal distribution.

The calculation of  $\sigma_t^2$  in (2) depends on past

quadratic residues,  $z_t^2$ , that are not observed for t = 0, -1, ..., -q + 1. To initialize the process, unobserved quadratic residuals are set to a value equal to the sample mean.

#### GARCH type models

While Engle (1982) certainly made the greatest contribution to financial econometrics, *ARCH* type models are rarely used in practice because of their simplicity.

A good generalization of this model is found in the *GARCH* type models introduced by Bollerslev (1986). This model is also a weighted average of the past quadratic residuals. This model is more parsimonious than *ARCH* models, and even in its simplest form, has proven to be extremely successful in predicting conditional variances.

It should be noted that *GARCH* type models are not the only extension and there are at least twelve specifications related to them that will be the object of future research.

Generalized *ARCH* models (or *GARCH* models as they are also known) are based on an infinite *ARCH* specification and allow to reduce the number of parameters to be estimated by imposing nonlinear constraints on them. The *GARCH(p, q)* model is expressed as follows

$$\sigma_t^2 = \omega + \sum_{i=1}^q a_i z_{t-1}^2 + \sum_{j=1}^q \beta_j \sigma_{t-j}^2.$$
(4)

As in the case of *ARCH* models, it is necessary to impose some restrictions on  $\sigma_t^2$  to ensure that it is positive for all *t*. Bollerslev (1986) showed that ensuring that  $\omega > 0, a_i \ge 0$  (for  $i = 1, \dots, q$ ) and

 $\beta_j \ge 0$  (for i = 1, ..., p) is sufficient to guarantee

that the conditional variance is positive.

In terms of the estimation process, we can say that many authors have proposed using a Student *t* distribution in combination with a *GARCH* model to adequately model heavy tails on economic or financial time series whose data are of high frequency, which will be seen below.

#### Sample

First, we proceed to plot the series. Within the study of a series, graphic methods are an excellent way to begin an investigation.

After plotting it, we can immerse ourselves in a detailed study of the subject under consideration. Among the functions that comply with the graphs that we will present are the following:

1. They make the data under study more visible, systematized and synthesized.

2. They reveal their variations and their historical or spatial evolution.

 They can show the relationships between the various elements of a system or a process and show indications of the future correlation between two or more variables.

In addition to this, the application of these methods suggests new research hypotheses and allows the subsequent implementation of statistical models ranging from the simplest to those that are much more refined, thus achieving a better analysis of the data and its fluctuations over time.

Section (a) of Figure 1 shows the monthly levels of the Consumer Price Index. In section (b) of the same figure we can see the first differences of the logarithm of the monthly IPC level. This is what is popularly known as *inflation* and will be the series object of our work.

#### The Conditional Heterocedasticity on the Argentine Inflation. An Analysis for the Period from 1943 to 2013

After a careful inspection of this last section, we can see that there are periods where the volatility is low and can be confused with the presence of seasonality especially within the period from January 1943 until the end of 1974. Then, there is a clear a period of very important volatility until late 1977, which is repeated with similar characteristics between 1983 and the end of 1985. Subsequently, between 1987 and the end of 1992 we have a period of high volatility. From late 2001, the volatility in the series under study is almost null, and it almost disappears from 2009.

Figure 1: (a) Monthly levels of the Consumer Price Index from January 1943 to December 2013. (b) First difference of the logarithm of the level of the Consumer Price Index from January 1943 to December 2013.

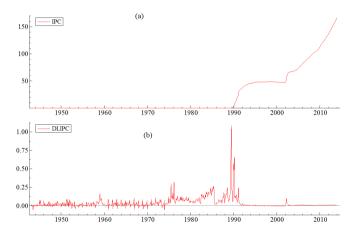
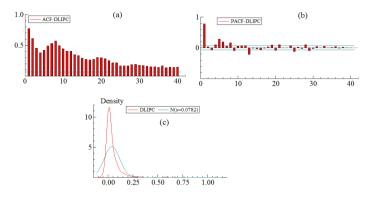


Figure 2 shows in section (a) the autocorrelation for the inflation series under study, also in section (b) we can see the partial autocorrelation function. Finally, in section (c), we have the estimated density function which is represented by a red line, compared to the normal density function which is represented by a green

line.

From the study of this figure we see that the series is not stationary, although it has some seasonal components and its distribution is different from that of a normal variable, so it is possible that we must make their corresponding estimates using a t Student distribution.

Figure 2: (a) Autocorrelation function of the inflation series for the period from January 1943 to December 2013. (b) Partial autocorrelation function of the same series under study. (c) Estimated density function compared to normal density (green line).



#### **Data Analysis and Discussion**

Different alternatives were tried with respect to the modeling of the inflation series in Argentina for the period between January of 1943 and December of 2013. After analyzing them and seeing the values of different goodness of fit statistics, like the Akaike Criterion, the Schwarz Criterion or the Hannan - Quinn Criterion, we are left with a model based on the equation (1), where

 $y_t$  is the series under study and its explicit specification is given by

$$y_t = \mu_t + \varepsilon_t h_t, \tag{5}$$

where  $\varepsilon_t$  has a t distribution with 2.21167

degrees of freedom. The conditional mean,  $\mu_t$  is equal to a general mean  $\mu$  a seasonal component and an *ARMA* (1, 1) process, which is explicitly

$$\mu_{t} = \mu + \gamma_{t} + \varphi \, y_{t-1} + \nu + \theta v_{t-1}, \tag{6}$$

where  $v_t = \varepsilon_t h_t$  and  $\gamma_t$  is a seasonal component that satisfies the following condition

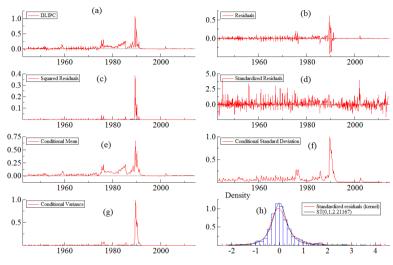
$$\gamma_t = -\gamma_{t-1} - \dots - \gamma_{t-11}, \tag{7}$$

that is, its sum is equal to zero over the previous year. This is achieved with the introduction of adequate dummy variables, Besides that, the conditional variance in (5) is given by

$$h_t^2 = \sigma_t^2 = \omega + \alpha (y_{t-1} - \mu_{t-1})^2 + \beta \sigma_{t-1}^2,$$
(8)

that is, a GARCH(1, 1) with a constant given by  $\omega$ . In the estimation process for our case, we could see that the constant was not significant different from zero, so we decided to remove it in the final formulation.

Figure 3: Characteristics of the inflation series for the period between 1943 and 2013. (a) Inflation series. (b) Residues from the inflation series. (c) Quadratic residues. (d) Standardized residuals. (e) Conditional mean from the application of the volatility. (f) Conditional standard deviation. (g) Conditional variance. (h) Standardized residuals compared to a t distribution with 0, 1 and 2.21167 degrees of freedom.

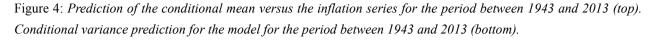


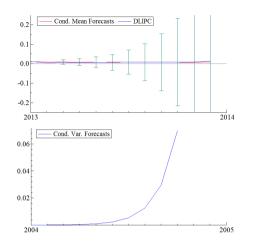
In the (a) the series of inflation again , in (b) we can see the residuals, in (c) we have the quadratic residuals while in (d) we have are the standardized residuals of the series. In section (e) of Figure 3 we show the estimated conditional mean for the proposed volatility model, in (f) we see the conditional standard deviation, while in (g) we observe the estimated conditional variance that arises from the application of the model to our series under study.

Looking closely at sections (a), (e), (f) and (g) of Figure 3, we can say that the model adequately

explains the inflation series of our country for the period between 1943 and 2013. This same characteristic arises again in section (h) when comparing the distribution of the standardized residuals with a Student t distribution with 2.21167 degrees of freedom.

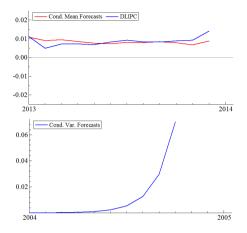
An interesting fact to note is that towards the end of the period under consideration, in particular from October or November 2004, the conditional variance or volatility of the series becomes practically insignificant.





At the top of Figure 4 we can see the last ten observations of the series under study, highlighted in blue, and the corresponding predictions of the conditional mean. The vertical bars correspond to the 95% confidence interval that serve to compare the predicted value with the one we observed. In the lower graphic we tried to predict the conditional variance corresponding to the last ten observations of our series under study, however, this was not possible. As we have already expressed, the conditional variance, or volatility, as of October 2004 is equal to zero. This situation corroborates the fact that from that date no volatility predictions can be made for this series, which is in line with the beginning of a period of lack of confidence in official statistics. Statistically, this involved the prediction of values different from those that may have been in reality, which gave rise to an extremely smooth series that does not coincide with the rest of it nor with the reality lived.

Figure 5 is similar to Figure 4, but in the latter the bars corresponding to the confidence intervals were removed and the vertical axis scale was changed in order to have a better observation of the original series and the predicted conditional mean. One can clearly see a great coincidence between both Figures and the analysis that we can do is exactly the same for both cases. Figure 5: Prediction of the conditional mean versus the inflation series for the period between 1943 and 2013 (top). Conditional variance prediction for the model for the period between 1943 and 2013 (bottom).



#### **Final Remarks**

In this initial stage of our investigation, we set out to analyze methods to treat a great variety of data with irregularities that happen in time series. Integrated autoregressive moving averages models (or *ARIMA* models) are often considered to provide the main basis for modeling in any time series. However, given the current state of research in time series research, there may be more attractive, and above all more efficient alternatives. Numerous economic time series do not have a constant mean and also in most cases phases are observed where relative calm reigns, followed by periods of important changes, that is, that the variability changes over time. Such behavior is what is called the *volatility*.

Among the models we have presented are the ones belonging to the *ARCH* family. The *ARCH* models or autoregressive models with conditional heteroscedasticity were first presented by Engle in 1982 with the aim of estimating the variance of inflation in Great Britain. The basic idea of this model is that  $y_t$  is not serially correlated but the conditional volatility or variance of the series depends on the past returns by means of a quadratic

function. However this kind of models are rarely used in practice because of their simplicity. A good generalization of this model is found in the *GARCH* type models introduced by Bollerslev (1986). This model is also a weighted average of the last quadratic residuals, but it is more parsimonious than the *ARCH* type models and even in its simplest form has proven to be extremely successful in predicting conditional variances, so we decided to make use of them when working with our data.

Before applying any statistical method to the data under study it is fundamental to observe them graphically in order to be able to become familiar with them. This can have numerous benefits, as we have explained at the beginning of our analysis, as this process will serve as an indicator of ideas for a more detailed later study. This was the first step of our work in which we could see the main features of the series and served us to make an appropriate adjustment of it. Again it is necessary to emphasize that although this is a very long period to analyze; where there were numerous changes such as the base, and interventions in the INDEC, it is possible to make a very interesting study where the main characteristics of the series are appreciated.

We decided to fit an appropriate GARCH type model that captures the main characteristics of the data. We saw that it takes adequately to the volatility of the series but however, it presents some difficulties when making predictions. It remains for later work to analyze if we can use another specification that takes into account this fact that captures even more the characteristics of the series that can do a GARCH model like the one we have seen. With this analysis we have been able to estimate that from October 2004, volatility is equal to zero. This situation corroborates the fact that from that date no volatility predictions can be made for this series, which is consonance with the beginning of a period of lack of confidence in the official statistics. Statistically, this gave rise to an extremely smooth series that does not match the rest nor with the reality lived.

#### References

- Abril, Juan Carlos. (1999), Análisis de Series de Tiempo Basado en Modelos de Espacio de Estado, EUDEBA: Buenos Aires.
- Abril, Juan Carlos (2004). *Modelos para el Análisis de las Series de Tiempo*. Ediciones Cooperativas: Buenos Aires.
- Abril, Maria de las Mercedes. (2014). El Enfoque de Espacio de Estado de las Series de Tiempo para el Estudio de los Problemas de Volatilidad. Tesis Doctoral. Universidad Nacional de Tucumán. Argentina.
- Baillie, R. T. y Bollerslev, T. (1989). The Message in Daily Exchange Rates: A Conditional-Variance Tale. *Journal of Business and Economic Statistics*, 7, 297-305.
- Bollerslev, T. (1986). Generalized autoregressive conditional heteroscedasticity. *Journal of Econometrics*, **31**, 307-27.
- Bollerslev, T. (1987). A Conditionally Heteroscedastic Time Series Model for Speculative Prices and Rates of Return. *Review*

of Economics and Statistics, 69, 542-547.

- Bollerslev, T., Chou, R. Y. y Kroner, K. F. (1992). ARCH Modeling in Finance: A Review of the Theory and Empirical Evidence. Journal of Econometrics, 52, 5-59.
- Bollerslev, T. y Wooldridge, J. M. (1992). Quasi-maximum Likelihood Estimation and Inference in Dynamic Models with Time-varying Covariances. *Econometric Reviews*, **11**, 143-172.
- Box, G. E. P. y Jenkins, G. M. (1976). *Time Series Analysis: Forecasting and Control* (Revised edition), Holden-Day Inc.: San Francisco.
- Engle, R. F. (1982). Autoregressive Conditional Heteroscedasticity with Estimates of the Variance of the United Kingdom Inflation. *Econometrical*, **50**, 987-1007.
- Goldfarb, D. (1970). A Family of Variable Metric Updates Derived by Variational Means. *Mathematics of Computation*, 24 (109), 23-26.
- Harvey, A. C. (1989). Forecasting, Structural Time Series Models and the Kalman Filter. Cambridge University Press: Cambridge.
- Hsieh, D. A. (1989). Modeling Heteroskedasticity in Daily Foreign Exchange Rates. *Journal of Business and Economic Statistics*, 7, 307--317.
- Pagan, A. (1996). The Econometrics of Financial Markets. *Journal of Empirical Finance*, 3, 15-102.
- Palm, F. C. (1996). GARCH Models of Volatility. En Handbook of Statistics, edited by G. Maddala, y C. Rao, 209-240. Elsevier Science, Amsterdam.
- Palm, F. C. y Vlaar, P. J. G. (1997). Simple Diagnostics Procedures for Modeling Financial Time Series. *Allgemeines Statistisches Archiv*, 81, 85-101



# Quantization of Particle Energy in the Analysis of the Boltzmann Distribution and Entropy

V.P. Malyshev, Yu.S. Zubrina, A.M. Makasheva

Chemical and Metallurgical Institute named after Zh. Abishev, Karaganda, Kazakhstan

**Abstract.** The Boltzmann equilibrium distribution is an important rigorous tool for determining entropy, since this function cannot be measured, but only calculated in accordance with Boltzmann's law.

On the basis of the commensuration coefficient of discrete and continuous similarly-named distributions developed by the authors, the article analyses the statistical sum in the Boltzmann distribution to the commensuration with the improper integral of the similarly-named function in the full range of the term of series of the statistical sum at the different combination of the temperature and the step of variation (quantum) of the particle energy. The convergence of series based on the Cauchy, Maclaurin criteria and the equal commensuration of series and improper integral of the similarly-named function in each unit interval of variation of series and similarly-named function were established.

The obtained formulas for the commensuration coefficient and statistical sum were analyzed, and a general expression for the total and residual statistical sums, which can be calculated with any given accuracy, is found. Given a direct calculation formula for the Boltzmann distribution, taking into account the values of the improper integral and commensuration coefficient.

To determine the entropy from the new expression for the Boltzmann distribution in the form of a series, the convergence of the similarly-named improper integral is established. However, the commensuration coefficient of integral and series in each unit interval turns out to be dependent on the number of the term of series and therefore cannot be used to determine the sum of series through the improper integral. In this case, the entropy can be calculated with a given accuracy with a corresponding quantity of the term of series n at a fixed value of the statistical sum.

The given accuracy of the statistical sum turns out to be mathematically identical to the fraction of particles with an energy exceeding a given level of the energy barrier equal to the activation energy in the Arrhenius equation.

The prospect of development of the proposed method for expressing the Boltzmann distribution and entropy is to establish the relationship between the magnitude of the energy quantum  $\Delta \varepsilon$  and the properties of the system-forming particles.

Key words: distribution, entropy, sequence, commensuration, statistical sum, convergent series, analysis.

### Introduction

The Boltzmann equilibrium distribution is the most important, if not the only, rigorous tool for determining entropy, since this function cannot be measured, but only calculated in accordance with Boltzmann's law [1, 2]:

$$P_i = \frac{N_i}{N} = e^{-\frac{\varepsilon_i}{kT}} / \sum_{i=1}^m e^{-\frac{\varepsilon_i}{kT}} , \qquad (1)$$

where  $P_i$  is the fraction of particles with energy  $\varepsilon_i$ ;  $N_i$  is the number of particles possessing this energy; N is the total number of particles; m is the number of considered energy levels which can be infinite; k is the Boltzmann constant; T is the absolute temperature.

The fractional divisor in (1) is the sum of the states of particles or the statistical sum that is calculated for various objects in one way or another, including direct calculation by spectroscopic data, or as a continuous value with a transition from summation to integration [3]. However, the summation and integration are not identical procedures in either physical or mathematical terms, since in the first case it is necessary to take into account the actual quantization of energy, which is implied by the meaning of the Boltzmann constant, while in the second case the difference arises from inequality  $\Delta x \neq dx$  in discrete and continuous distributions, even when the number of levels of energy *m* tends to infinity.

Thus, the calculation of the statistical sum is more or less approximate. However, for all nonidentity of continuous and discrete distributions under certain conditions, their commensuration is ensured in the entire range of the function change, as we showed earlier [4], and this creates the possibility of a more rigorous direct calculation of the statistical sum and, together with it, entropy.

# The method for determining the commensuration of the statistical sum in discrete and continuous epressions

As is known, the basis of differential and integral calculations is the reducibility of discrete dependencies to continuous ones while the argument variability interval  $\Delta x$  tends to infinitely small quantity dx. But the relationship between discrete and continuous distributions can turn out to be definite and productive at fixed variability intervals  $\Delta x$ .

This is most evident in the establishment of the convergence of series; i.e. the sum of discrete quantities, using the Cauchy, Maclaurin integral convergence criterion [5], according to which the series  $\sum_{n=1}^{\infty} a_n$  converges if for a function f(x) that takes values of  $a_n$  at the points x = n, namely  $f(n) = a_n$ , and under the condition of a monotonic decrease of f(x) in the area  $x \ge n_0$  observing inequality  $f(x) \ge 0$ , providing the convergence of the improper integral  $\int_{n_0}^{\infty} f(x) dx$ .

Thus, this sign establishes a certain equivalence of the discrete and continuous distributions of the variable value. Our paper [4] justifies the possibility of calculating the sum of series through the improper integral of the similarly-named function if for any unit interval of variation of series,  $(n - 1) \div n$ , the ratio of the integral of similarlynamed function in this interval and hence of its mean value to the corresponding term of the series  $a_n$  is constant, independent of n:

$$K = \frac{\int_{n-1}^{n} f(x) dx}{a_n} = const \neq f(n). \quad (2)$$

In this case, all the improper integral also refers to the sum of series with the same coefficient of commensuration:

$$K = \frac{\int_0^\infty f(x)dx}{\sum_{n=1}^\infty a_n}.$$
(3)

From this the formula for calculating the sum of series follows

$$S = \sum_{n=1}^{\infty} a_n = \frac{1}{K} \int_0^{\infty} f(x) dx.$$
(4)

With respect to this expression, the statistical sum must be expressed through the general term of series, giving a certain energy variability interval (quantum)  $\Delta \varepsilon$  and providing the first energy level equal to zero in the following form

$$a_n = e^{-(n-1)\Delta\varepsilon/kT},\tag{5}$$

and the similarly-named function f(x) in the following form

$$f(x) = e^{-\frac{(x-1)\Delta\varepsilon}{kT}},$$
(6)

Here it should be borne in mind that the fraction  $\Delta \varepsilon/kT$  is a constant value for the undertaken analysis, i.e. as usual, the isothermal distribution of the function is considered at a some given value  $\Delta \varepsilon$ . This does not prevent to vary any further combinations of *T* and  $\Delta \varepsilon$ , including functionally related ones, for the solutions obtained. Therefore, in all calculations, this fraction can be designated as  $b = \Delta \varepsilon/kT$ .

But first we must verify the convergence of the statistical sum according to the Cauchy, Maclaurin criteria, taking the improper integral:

$$\int_{0}^{\infty} e^{-(x-1)\Delta\varepsilon/kT} dx = \int_{0}^{\infty} e^{-bx+b} dx$$
$$= -\frac{1}{b} |e^{-bx+b}|_{0}^{\infty} = \frac{e^{b}}{b}$$
$$= \frac{kT}{\Delta\varepsilon} e^{\frac{\Delta\varepsilon}{kT}}.$$
(7)

The integral converges for the constants Tand  $\Delta \varepsilon$ , therefore, the statistical sum also converges  $\sum_{n=1}^{\infty} e^{-(n-1)b} = \sum_{n=1}^{\infty} e^{-(n-1)\Delta \varepsilon/kT}$ .

The commensuration coefficient of continuous and discrete distributions (4) in this case is expressed as

$$K = \frac{\int_{n-1}^{n} e^{-bx+b} dx}{e^{-(n-1)b}} = \frac{-\frac{1}{b} \left| e^{-bx+b} \right|_{n-1}^{n}}{e^{-(n-1)b}} = \frac{e^{b} - 1}{b}$$
$$= \frac{kT}{\Delta \varepsilon} \left( e^{\frac{\Delta \varepsilon}{kT}} - 1 \right). \quad (8)$$

This coefficient does not depend on n; hence it is applicable to the whole multitude  $\sum_{n=1}^{\infty} a_n$ , that has a limit

$$\sum_{n=1}^{\infty} e^{-bn+b} = \frac{1}{K} \int_{0}^{\infty} e^{-bx+b} dx = \frac{b}{e^{b}-1} \cdot \frac{e^{b}}{b}$$
$$= \frac{e^{b}}{e^{b}-1}$$
$$= \frac{\frac{e^{b}}{e^{kT}}}{\frac{\Delta\varepsilon}{e^{kT}}-1}.$$
(9)

Thus, the statistical sum, and also the Boltzmann distribution, obtain a generalized mathematical certainty that in the familiar indexation of variables will take the following form Quantization of Particle Energy in the Analysis of the Boltzmann Distribution and Entropy

$$P_{i} = \frac{N_{i}}{N} = \frac{e^{-\frac{\varepsilon_{i}}{kT}}}{\sum_{i=1}^{\infty} e^{-\frac{\varepsilon_{i}}{kT}}} = \frac{e^{-\frac{(i-1)\Delta\varepsilon}{kT}}}{e^{\frac{\Delta\varepsilon}{kT}}} \left(e^{\frac{\Delta\varepsilon}{kT}} - 1\right)$$
$$= e^{-\frac{i\Delta\varepsilon}{kT}} \left(e^{\frac{\Delta\varepsilon}{kT}} - 1\right). \tag{10}$$

In the new form, this dependence, as well as the expressions for the commensuration coefficient (8) and statistical sum (9), and also for Boltzmann mathematical entropy,

$$H = -\sum_{i=1}^{\infty} P_i \ln P_i, \qquad (11)$$

are suitable not only for general, but also for numerical analysis, as well as for the direct calculation of all the characteristics discussed.

# Analysis of the limits of change in the commensuration coefficient, the statistical sum and the Boltzmann entropy

The commensuration coefficient (8) is convenient for analyzing the limits of variation in the following form

$$K = \frac{e^{\frac{\Delta\varepsilon}{kT}} - 1}{\frac{\Delta\varepsilon}{kT}}.$$
 (12)

In the methodological respect it is important to verify the desire for complete commensuration of the discrete and continuous expressions of the statistical sum as the variability interval of the energy of particles tends to zero. In fact, the initially arising uncertainty

$$\lim_{\Delta \varepsilon \to 0} \frac{e^{\frac{\Delta \varepsilon}{kT}} - 1}{\frac{\Delta \varepsilon}{kT}} = \frac{0}{0}$$

is further disclosed according to L'Hospital's rule with the result

$$\lim_{\Delta\varepsilon\to 0} \frac{d\left(e^{\frac{\Delta\varepsilon}{kT}}-1\right)}{d\left(\frac{\Delta\varepsilon}{kT}\right)} = e^{\frac{\Delta\varepsilon}{kT}} \Rightarrow 1,$$
(13)

that indicates the identification of the compared distributions for  $\Delta \varepsilon \rightarrow d\varepsilon$ .

But with a very rough specification of intervals of the energy of particles, the opposite result is obtained, and the distributions under consideration become incommensurate:

$$\lim_{\Delta\varepsilon\to\infty} \frac{e^{\frac{\Delta\varepsilon}{kT}} - 1}{\frac{\Delta\varepsilon}{kT}} = \frac{\infty}{\infty} \Rightarrow \frac{d\left(e^{\frac{\Delta\varepsilon}{kT}} - 1\right)}{d\left(\frac{\Delta\varepsilon}{kT}\right)} = e^{\frac{\Delta\varepsilon}{kT}}$$
$$= \infty. \tag{14}$$

This determines the inevitability of errors in the direct replacement of a discrete sum by a continuous one.

As to the effect of temperature on the commensuration of discrete and integral expressions of the statistical sum, the very formula of the commensuration coefficient implies the opposite character of this effect in comparison with  $\Delta \varepsilon$ : when  $T \rightarrow 0 \ K \rightarrow \infty$ , and when  $T \rightarrow \infty \ K \rightarrow 1$ . Such an effect is quite natural, since at an infinitely high temperature the relative role of any given energy variability intervals is reduced to zero, and at absolute zero temperature there is only a zero energy level, and any given energy variability interval with respect to the zero energy value becomes infinitely large, determining the impossibility of any distributions.

The effect of temperature on the statistical sum value (9) is expressed by the limits:

$$\lim_{T \to 0} \frac{\frac{\Delta \varepsilon}{kT}}{e^{\frac{\Delta \varepsilon}{kT}} - 1} = \frac{e^{\infty}}{e^{\infty} - 1} = 1, \quad (15)$$

$$\lim_{T \to \infty} \frac{\frac{\Delta \varepsilon}{kT}}{e^{\frac{\Delta \varepsilon}{kT}} - 1} = \frac{1}{1 - 1} = \infty.$$
(16)

Such limits are related to the fact that when T = 0 there exists only the first, zero energy level, which contribution to the statistical sum is always equal to one, which follows directly from the formula (5). At an infinitely high temperature, the improper integral (7) becomes divergent, and this according to the Cauchy, Maclaurin criterion determines the divergence of the similarly-named series. The physical picture of such a state is very conditional and reduces to a kind of uniform "smearing" of a finite number of particles over an infinite variety of energy levels [3] and even contradicts the information degeneration of the thermodynamic system at an infinitely high temperature, when the diversity of the system is determined only by the total number of particles and the corresponding limit of entropy [6-11]. However, this feature goes beyond the limits of the undertaken analysis of the statistical sum and is consistent with the existing formal approach to such an analvsis [1-3]. As for the effect  $\Delta \varepsilon$  on the statistical sum, it is also opposite to the effect of temperature: when  $\Delta \varepsilon \rightarrow 0$  this sum tends to infinity for a given temperature, and when  $\Delta \varepsilon \rightarrow \infty$  all the finite energy of the system formally refers to the first "interval" and also formally becomes zero with the first and only term of series equal to one.

It is theoretically and practically feasible to determine the sufficient number of terms of the statistical sum to calculate it with a certain accuracy. This is necessary to calculate the entropy by formula (11), which itself represents a new series requiring the determination of its sum, which includes the statistical sum (9). In the framework of the approach taken to consider such a sum as a convergent series, this problem has the following solution.

As shown in our paper [4], the commensuration coefficient of continuous and discrete distributions (2) can be used not only to express the total sum of the series (4), but also of any partial sum  $S_n$ through the improper integral of the similarlynamed function with the upper limit *n*:

$$S_n = \frac{1}{K} \int_0^n f(x) dx.$$
 (17)

This integral for the problem under consideration is defined as

$$S_n = \sum_{n=1}^n a_n = \frac{1}{K} \int_0^n e^{-(x-1)b} dx = -\frac{1}{Kb} \left| e^{-bx+b} \right|_0^n$$
$$= \frac{e^b}{Kb} (1 - e^{-bn}).$$
(18)

Substituting here the expressions for *K* (8) and  $b = \Delta \varepsilon / kT$ , we obtain a formula for calculating the partial sums

$$S_n = \sum_{n=1}^n a_n = \frac{e^{-\frac{n\Delta\varepsilon}{kT}} - 1}{e^{-\frac{\Delta\varepsilon}{kT}} - 1}.$$
 (19)

With its help you can determine the amount of the residual sum

$$R_n = S - S_n = \frac{e^{\frac{\Delta\varepsilon}{kT}}}{e^{\frac{\Delta\varepsilon}{kT}} - 1} - \frac{e^{-\frac{n\Delta\varepsilon}{kT}} - 1}{e^{-\frac{kT}{kT}} - 1}$$
$$= \frac{e^{\frac{(1-n)\Delta\varepsilon}{kT}}}{e^{\frac{\lambda\varepsilon}{kT}} - 1}.$$
(20)

The ratio of the residual sum to the total sum of the series can serve as a criterion for the accuracy of its calculation when the terms n are limited by the number. Using formulas (20) and (9), we find

$$\frac{R_n}{S} = e^{-\frac{n\Delta\varepsilon}{kT}}.$$
(21)

It is quite obvious that with an increase in the accounted terms of series, the contribution of the residual sum decreases and its fraction, as the calculation error, tends to zero. But the most important is that from here one can directly find the necessary number of terms of series to calculate the sum of series with a given accuracy equal to  $R_n/S$  in fractions of a unit:

$$n = -\frac{kT}{\Delta\varepsilon} \ln \frac{R_n}{S}.$$
 (22)

All the calculations of this section of the Article, which were previously described in detail in our paper [12], are subject to numerical verification for a certain idea of the possibilities of the discussed approach to the analysis of the Boltzmann distribution.

However, expression (21) is even more informative, since the product  $n\Delta\varepsilon$  has the meaning of an arbitrary value of energy  $\varepsilon_n$ , beginning from which all higher energy levels (i.e. residuals in the full range of the energy series) are related to the value of kT, which has a meaning of the store of thermal energy of the substance. This allows us to consider the value  $\varepsilon_n = n\Delta\varepsilon$  as some energy barrier, which overcoming corresponds to a fraction of the particles equal to  $R_n/S$ . In turn, this fraction acquires the meaning of exponential factor in the expression for the rate constant in the Arrhenius equation (in terms of molar quantities)

$$k = A_0 e^{-\frac{E_a}{kT}} = A_0 \frac{R_n}{S} = A_0 e^{-\frac{n\Delta\varepsilon}{kT}}.$$
 (23)

The same result is obtained by using integral expressions for the residual fraction of the statistical sum

$$\frac{\int_{x=n}^{\infty} e^{-(x-1)b} dx}{\int_{0}^{\infty} e^{-(x-1)b} dx} = \frac{-\frac{1}{b} |e^{-bx+b}|_{n}^{\infty}}{\frac{1}{b} e^{b}} = \frac{\frac{1}{b} e^{-bn} e^{b}}{\frac{1}{b} e^{b}}$$
$$= e^{-bn}$$
$$= e^{-\frac{n\Delta\varepsilon}{kT}}.$$
 (24)

Equality of expressions (23) and (24) is ensured by the commensuration of corresponding discrete and continuous distributions, so that the commensuration coefficients are reduced in their relative values.

The obtained independent treatment of statistical meaning of the exponential factor in the Arrhenius equation, in addition to confirming all the computations undertaken, makes it even more definite to emphasize the necessity of using equilibrium distributions in the mapping of kinetic processes, as well as probabilistic representations under the influence of chemical, physical and mechanical factors. Quantization of Particle Energy in the Analysis of the Boltzmann Distribution and Entropy

But first we must verify the convergence of the new entropy expression (11) in terms of the found statistical sum (9) for the particle distribution according to the energy  $P_i$  (10):

$$H = -\sum_{i=1}^{\infty} e^{\frac{-i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right) ln \left[ e^{\frac{-i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right) ln \left[ e^{\frac{-i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right) ln \left[ e^{\frac{-i\Delta\varepsilon}{kT}} \right] \right]$$

This sum is a functional series, general term of which can be expressed by taking into account the designation of constants for a given series of quantities  $b = \Delta \varepsilon / kT$  and  $A = e^{\frac{\Delta \varepsilon}{kT}} - 1$  as

$$a_n = Ae^{-bn} \ln(Ae^{-bn}). \tag{26}$$

A necessary condition for the convergence of series according to the Cauchy criterion is

$$\lim_{n \to \infty} a_n = 0.$$
Then
$$\lim_{n \to \infty} (Ae^{-bn}) \ln(Ae^{-bn}) = 0 \cdot \infty.$$

This uncertainty is revealed according to L'Hospital's rule by differentiating the fractional expression  $a_n$ :

$$\lim_{n \to \infty} \frac{Aln(Ae^{-bn})}{e^{bn}} = \frac{\infty}{\infty} \Rightarrow \frac{Adln(Ae^{-bn})}{de^{bn}}$$
$$= -\frac{A}{e^{2bn}} \Rightarrow 0.$$

The necessary condition is met, but sufficient can be established by the integral criterion of Cauchy, Maclaurin. Here the similarly-named function for the general term of series (26) will be

$$f(x) = Ae^{-bx} ln(Ae^{-bx}).$$
(27)

The improper integral of this function within the variation of  $a_n$  is expressed as

$$\int_{0}^{\infty} f(x)dx = \int_{0}^{\infty} Ae^{-bx} \ln(Ae^{-bx}) dx$$
$$= \int_{0}^{\infty} (A\ln A) e^{-bx} dx$$
$$- \int_{0}^{\infty} Ab x e^{-bx} dx.$$
(28)

This allows us to use table integrals of the following form

$$\int e^{ax} dx = \frac{1}{a} e^{-ax} \text{ and } \int x e^{ax} dx$$
$$= \frac{e^{ax}}{a^2} (ax - 1).$$

The first integral in (28) is equal to

$$= \frac{AlnA}{b}.$$

$$\int_{0}^{\infty} (AlnA) e^{-bx} dx = AlnA \left(-\frac{1}{b}\right) \left|e^{-bx}\right|_{0}^{\infty}$$
(29)

The second integral leads to the following uncertainty

$$\int_{0}^{\infty} Ab \, x e^{-bx} \, dx = \frac{A}{b} \left| -bx e^{-bx} - e^{-bx} \right|_{0}^{\infty}$$
$$= \frac{A}{b} (-\infty \cdot 0 + 1),$$

which is disclosed according to L'Hospital's rule

$$\lim_{x \to \infty} (bxe^{-bx}) = \lim_{x \to \infty} \frac{bx}{e^{bx}} = \frac{dbx}{de^{bx}} = \frac{1}{e^{bx}} = 0.$$
  
Then  
$$\int_{0}^{\infty} Ab xe^{-bx} dx = \frac{A}{b}.$$
 (30)

Both integrals converge, and so does their difference

$$\int_{0}^{\infty} Ae^{-bx} ln(Ae^{-bx}) dx = \frac{AlnA}{b} - \frac{A}{b}$$
$$= \frac{A}{b}(lnA - 1)$$
$$= \frac{kT}{\Delta\varepsilon} \left(e^{\frac{\Delta\varepsilon}{kT}} - 1\right) \left[ln\left(e^{\frac{\Delta\varepsilon}{kT}} - 1\right) - 1\right].$$
(31)

Therefore, the similarly-named series converges, and the Boltzmann entropy (25) does the same. However, the discrete expression of this entropy, as well as of other similarly-named series and functions, can lead to the same limit only under certain boundary conditions. In the general case, as shown above, it is required to establish the independence of the commensuration coefficient of discrete and continuous distributions from the number of terms of series,  $k \neq f(n)$ .

This coefficient can be determined by parts of the integral (28), correlating them with the corresponding general terms of series

$$k_{1} = \frac{\int_{n-1}^{n} (AlnA)e^{-bx} dx}{(AlnA)e^{-bn}} = \frac{\int_{n-1}^{n} e^{-bx} dx}{e^{-bn}}, (32)$$

$$k_2 = \frac{\int_{n-1}^{n} Abx e^{-bx} dx}{Abn e^{-bn}} = \frac{\int_{n-1}^{n} x e^{-bx} dx}{n e^{-bn}}.$$
 (33)

For  $k_1$  we find the solution

$$k_1 = \frac{-\frac{1}{b} \left| e^{-bx} \right|_{n-1}^n}{e^{-bn}} = \frac{e^b - 1}{b} \neq f(n).$$
(34)

This part of the continuous and discrete dependences is commensurate, and the corresponding sum of the series is expressed as

$$\sum_{n=1}^{\infty} (AlnA)e^{-bn}$$

$$= \frac{1}{k_1} \int_{0}^{\infty} (AlnA)e^{-bx} dx = \frac{b}{e^b - 1} \cdot \frac{AlnA}{b}$$

$$= \frac{AlnA}{e^b - 1}.$$
(35)

For  $k_2$  we obtain an expression depending on *n* 

$$k_{2} = \frac{\int_{n-1}^{n} xe^{-bx} dx}{ne^{-bn}} = \frac{\frac{1}{b^{2}} \left| e^{-bx} (-bx-1) \right|_{n-1}^{n}}{ne^{-bn}} = \frac{bn(e^{b}-1) + e^{b}(1-b) - 1}{b^{2}n} = f(n).$$
(36)

These parts of integral and the sum of series change their ratio in each unit interval, and therefore it is difficult to determine the ratio of the improper integral to the sum of series both in this part and in the whole according to (31). In any case, a direct computation of entropy according to (25) with a certain accuracy will be simpler, and besides, it will be possible to find the commensuration coefficient

$$K = \frac{\int_0^\infty Ae^{-bx} \ln(Ae^{-bx}) \, dx}{\sum_{n=1}^{n'} Ae^{-bn} \ln(Ae^{-bn})},\tag{37}$$

where n' - the number of terms in series that ensure the calculation of the sum of series with a given accuracy.

# Estimated part and examples of uing the obtained formulas

Table 1 shows the results of calculating the commensuration coefficient *K* and the statistical sum  $S = \sum_{n=1}^{\infty} a_n$  over a wide range of temperatures and the characteristic step of varying the energy of particles, rounded to four values of the figures. The first energy variability interval is given numerically equal to the Boltzmann constant,  $\Delta \varepsilon = 1.3806505 \cdot 10^{-23} \approx 1.381 \cdot 10^{-23}$  J. The calculations were performed with an accuracy of up to 7 digit order numbers in the range of  $10^{-99} \div 10^{99}$ .

From these tables it follows that at the smallest variation step  $\Delta \varepsilon = 1,381 \cdot 10^{-23}$  J, starting from 10 K, with accurate up to 5% and better the statistical sum is comparable according to the commensuration coefficient with the corresponding integral value. With a coarser variability interval  $\Delta \varepsilon$  such comparability shifts to higher temperatures: for  $\Delta \varepsilon = 10^{-22}$  J – starting from 100 K, for  $\Delta \varepsilon = 10^{-21}$  J – from 1000 K, for  $\Delta \varepsilon = 10^{-20}$  J – from 10<sup>4</sup> K,  $\Delta \varepsilon = 10^{-19}$  J – from 10<sup>5</sup>. At lower temperatures, the identification of discrete and continuous summation is unacceptable.

As for the very value of the statistical sum, it indirectly indicates the need to take into account the increasing number of terms of their sequence, of course, with some given accuracy in the calculation of each term of series. Proceeding from the fact that any statistical sum begins with one and continues with decreasing terms, it can be argued that in this sum it is necessary to take into account at least the number of terms n = S. This number increases with an increase in temperature and with a decrease in the variability interval  $\Delta \varepsilon$ . So  $\Delta \varepsilon =$ 1,381·10<sup>-23</sup> J and a temperature of 500 K will require accounting for more than 500 terms of the amount.

		S and K at $\Delta \varepsilon$ , J										
Т, К	1.381.10 <sup>-23</sup>		10 <sup>-22</sup>		10 <sup>-21</sup>	10 <sup>-21</sup>		10 <sup>-20</sup>		19		
	S	K	S	Κ	S	Κ	S	K	S	K		
0	1	8	1	8	1	8	1	8	1	x		
1	1.582	1.718	1.001	192.9	1.000	$3.94 \cdot 10^{29}$	1.000	>1099	1.000	>1099		
10	10.51	1.052	1.940	1.468	1.001	192.9	1.000	$3.94 \cdot 10^{29}$	1.000	>1099		
50	50.50	1.010	7.415	1.076	1.307	2.248	1.000	$1.35 \cdot 10^5$	1.000	$5.53 \cdot 10^{60}$		
100	100.5	1.005	14.31	1.037	1.940	1.468	1.000	192.9	1.000	$3.94 \cdot 10^{29}$		
200	200.5	1.002	28.12	1.018	3.291	1.205	1.028	10.05	1.000	$1.48 \cdot 10^{14}$		
300	300.5	1.002	41.92	1.012	4.662	1.131	1.098	4.217	1.000	$6.94 \cdot 10^8$		
400	400.5	1.001	55.73	1.009	6.038	1.096	1.196	2.825	1.000	$4.04 \cdot 10^{6}$		
500	500.5	1.001	69.53	1.007	7.415	1.076	1.307	2.248	1.000	$1.35 \cdot 10^5$		
1000	1000	1.000	138.6	1.004	14.31	1.037	1.940	1.468	1.000	192.9		
2000	2001	1.000	276.6	1.002	28.12	1.018	3.291	1.205	1.028	10.05		
3000	3000	1.000	414.7	1.001	41.92	1.012	4.662	1.131	1.098	4.217		
4000	4001	1.000	522.8	1.001	55.73	1.009	6.038	1.096	1.196	2.825		
5000	5001	1.000	690.8	1.001	69.53	1.007	7.415	1.076	1.307	2.249		
10 <sup>4</sup>	$10^{4}$	1.000	1381	1.000	138.6	1.004	14.31	1.037	1.940	1.468		
10 <sup>5</sup>	$10^{5}$	1.000	$1.38 \cdot 10^4$	1.000	1381	1.004	138.6	1.004	14.31	1.037		
$10^{6}$	$10^{6}$	1.000	1.39·10 <sup>5</sup>	1.000	$1.38 \cdot 10^4$	1.000	1381	1.000	138.6	1.004		

**Table 1** – Dependence of the statistical sum  $S = \sum_{n=1}^{\infty} a_n$  (9) and the commensuration coefficient *K* (8) on the temperature *T* and on the variability interval of the energy of particles  $\Delta \varepsilon$ 

In fact, at low temperatures and large energy variability intervals characterized by a steep decline in the distribution of the terms of sum, their necessary number for calculating this sum with a given accuracy is much greater *S*.

More directly and strictly it is revealed with the help of the derived formula (22) (Table 2) with rounding up to integers to the higher side.

**Table 2** – Dependence of the required number of terms *n* on the specified calculation accuracy  $R_n/S$  of the sum *S* with variation of the step  $\Delta \varepsilon$  and temperature *T* 

		S and <i>n</i> at $\Delta \varepsilon$	$= 10^{-22} \text{ J}$		S and n at $\Delta \varepsilon = 10^{-20}$ J			
<i>T</i> , K		i	<i>n</i> at $R_n/S$			<i>n</i> at $R_n/S$		
	S	10-3	10 <sup>-4</sup>	10-5	S	10-3	10-4	10-5
10	1.940	10	13	16	1.000	1	1	1
50	7.415	48	64	80	1.000	1	1	1
100	14.31	96	128	159	1.000	1	2	2
200	28.12	191	255	318	1.028	2	3	4
400	55.73	382	509	634	1.196	4	6	7
600	83.36	573	764	954	1.427	6	8	10
800	111.0	764	1018	1272	1.679	8	11	13
1000	138.6	954	1272	1590	1.940	10	13	16
2000	276.6	1908	2544	3180	3.291	20	26	32
3000	414.7	2862	3816	4770	4.662	29	39	48
4000	522.8	3816	5088	6360	6.038	39	51	64
5000	690.8	4770	6360	7950	7.415	48	64	80
$10^{4}$	1381	9540	12720	15900	14.31	96	128	159
10 <sup>5</sup>	$1.38 \cdot 10^4$	$9.54 \cdot 10^4$	$1.27 \cdot 10^5$	$1.59 \cdot 10^5$	138.6	954	1272	1590
10 <sup>6</sup>	$1.39 \cdot 10^5$	$9.54 \cdot 10^5$	$1.27 \cdot 10^{6}$	$1.59 \cdot 10^{6}$	1381	9540	12720	15900

Here, in addition to a more vivid expression of the increasing dependence of the required number of terms of sum on the given accuracy of calculating this sum and the apparent numerical superiority of *n* in comparison with the amount of the sum of *S* in all variations  $\Delta \varepsilon$  and *T* there are given numerical values of *n*, which are subject to direct verification.

This can be illustrated by an example of calculating  $a_n$  by formula (5) at various temperatures, by setting an arbitrary value  $\Delta \varepsilon = 10^{-20}$  J (Table 3). Here are given the values of the sum of series (denoted as  $S_n$ ) calculated with rounding to the fourth decimal place, and hence with an accuracy of  $10^{-4}$ , and the total values of the sum calculated according to formula (9) (denoted as *S* and given with greater accuracy,  $10^{-5}$ ), as well as the fractional

values of the terms of sum calculated according to formula (10), with the aim of further determining the entropy by formula (11).

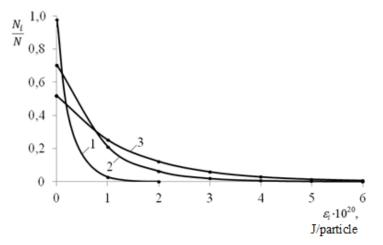
**Table 3** – Distribution of the terms of statistical sum  $a_n$  and their fractional values  $P_n$  depending on temperature

n	200 K		400 K		600 K		800 K		1000 K	
	$a_n$	$P_n$								
1	1	0.9732	1	0.8364	1	0.7009	1	0.5955	1	0.5152
2	0.0268	0.0260	0.1636	0.1368	0.2991	0.2096	0.4045	0.2409	0.4848	0.2498
3	0.0007	0.0007	0.0268	0.0224	0.0895	0.0627	0.1636	0.0974	0.2350	0.1211
4	0	0	0.0044	0.0037	0.0268	0.0188	0.0662	0.0394	0.1139	0.0587
5	0	0	0.0007	0.0006	0.0080	0.0056	0.0268	0.0159	0.0552	0.0284
6	0	0	0.0001	0.0001	0.0024	0.0017	0.0108	0.0064	0.0268	0.0138
7	0	0	0	0	0.0007	0.0005	0.0044	0.0026	0.0130	0.0067
8	0	0	0	0	0.0002	0.0002	0.0018	0.0011	0.0063	0.0032
9	0	0	0	0	0.0001	0	0.0007	0.0004	0.0030	0.0016
10	0	0	0	0	0	0	0.0003	0.0002	0.0015	0.0008
11	0	0	0	0	0	0	0.0001	0.0001	0.0007	0.0004
12	0	0	0	0	0	0	0	0	0.0004	0.0002
13	0	0	0	0	0	0	0	0	0.0002	0.0001
14	0	0	0	0	0	0	0	0	0.0001	0
15	0	0	0	0	0	0	0	0	0	0
$S_n$	1.0275	-	1.1956	-	1.4268	-	1.6792	-	1.9408	-
S	1.02750	-	1.19561	-	1.42681		1.67922	-	1.94082	-
$\Sigma P_n$	-	1.000	-	1.000	-	1.000	-	1.000	-	1.000

From this table it follows that with a given accuracy of calculation, taking into account seven significant digits and rounding up to 0.0001, the statistical sums coincide both at the term summing according to formula (5) and the direct calculation according to formula (9). Comparing with the data in Table 2 for  $\Delta \varepsilon = 10^{-20}$  J with a specified accuracy of  $10^{-4}$ , we make sure in practical coincidence of the necessary number of terms for calculating the partial sum in Table 3: at 200 K n = 3, at 400 K n = 6, at 600 K n = 8 and n = 9, at 800 K n = 11, at

1000 K n = 13 and n = 14. The same applies to the share distribution  $P_n$ .

The dependence of the absolute and fractional distributions of the terms of statistical sum on temperature becomes more smoothed as the temperature increases, and requires a larger number of terms. Fig. 1 shows a more graphic picture of the change in the fractional content of the terms of the statistical sum, and hence the fractional distribution of particles from the temperature and energy level of the particles. These data are directly needed to calculate the entropy of the system.



**Figure 1** – Dependence of the energy distribution of particles on temperature: 1 – at 200 K, 2 – 600 K, 3 – 1000 K. Points –  $a_n$  according to formula (5), lines – f(x) according to formula (6)

Correspondingly, the mathematical entropy of the system according to the data in Table 3 and in accordance with formulas (10) and (11) is cha-

<i>T</i> , K	200	400	600	800	1000
N	0.1266	0.5326	0.8703	1.1328	1.3441

Relatively low values of entropy completely correlate with sharp distributions of statistical sums in the chosen example of a rather rough variation of energy levels with step of  $\Delta \varepsilon = 10^{-20}$ J/particle. With a smaller value  $\Delta \varepsilon$ , as noted above, a much larger number of terms, hundreds and thousands, would have to be taken into account, and in this case an accurate knowledge of its limit according to the proposed formula (9) would make it possible to make informed decisions on limiting the number of terms in the sum according to formula (22) with the accuracy adopted for calculating the sum itself. In turn, this would determine the accuracy of calculating entropy.

In connection with the established possibility of direct calculation of the integral entropy of the Boltzmann distribution according to formula (31), it is expedient to compare it with formula (37) with the numerical definition of entropy as the sum of series, limited to the variation of temperature for  $\Delta \varepsilon = 10^{-20}$  J/particle and a sufficient number of terms of series according to formula (22), applicable for calculating the statistical sum. In this case, we can determine the accuracy of calculating the racterized by the following temperature dependence:

entropy in comparison with the given accuracy in accordance with (22) by calculating the last term of series

$$a' = Ae^{-bn'} \ln\left(Ae^{-bn'}\right) \tag{38}$$

with its ratio to the partial sum of series.

The corresponding expressions for the integral and total entropy have the following form

$$H_{int.} = -\int_{0}^{\infty} Ae^{-bx} \ln(Ae^{-bx}) dx$$
$$= \frac{A}{b} (\ln A - 1), \qquad (39)$$

$$H_{sum.} = -\sum_{n=1}^{n'} Ae^{-bn} \ln(Ae^{-bn}).$$
 (40)

Calculation results with determination accuracy n' up to 0,0001  $-a_{n'}$  are given in Table 4.

**Table 4** – Integral  $N_{\text{int.}}$  and partially summarized  $N_{\text{sum.}}$  Boltzmann entropy, their ratio  $K = N_{\text{int.}}/N_{\text{sum.}}$  at different temperatures

<i>Т</i> , К	N <sub>int.</sub>	n'	N <sub>sum.</sub>	K	$-a_{n'}$	$-a_{n'}$
						$H_{sum}$ .
400	1.1476	6	0.5324	2.1555	9.03·10 <sup>-4</sup>	$1.70 \cdot 10^{-3}$
600	0.5762	8	0.8696	1.8126	$1.32 \cdot 10^{-3}$	$1.52 \cdot 10^{-3}$
800	0.7885	11	1.1324	1.5794	6.67·10 <sup>-4</sup>	5.89·10 <sup>-4</sup>
1000	0.9415	13	1.3492	1.4454	8.10·10 <sup>-4</sup>	6.03·10 <sup>-4</sup>
5000	3.1550	64	2.9317	1.0762	1.63.10-4	5.57·10 <sup>-5</sup>
$10^{4}$	3.7596	128	3.6242	1.0374	8.37·10 <sup>-5</sup>	2.39.10-5
10 <sup>5</sup>	5.9493	1272	5.9262	1.0039	1.025.10-5	1.73.10-6
$10^{6}$	8.2334	12720	8.2289	1.0006	1.188.10-6	$1.44 \cdot 10^{-7}$

From these data it follows that the commensuration coefficient K decreases with the temperature increase, tending to a one. This corresponds to the ratio of decreasing similarly-named dependencies for continuous and discrete distributions over the sum of the corresponding areas, as shown in [4]. This confirms the correctness of the analytically found and calculated values of  $N_{int.}$  and  $N_{sum.}$ entropy. At the same time, the accuracy of calculations, determined on the basis of the accuracy of calculation of the statistical sum, is also generally preserved for calculation of the entropy, becoming even more strict for high temperatures. No violations of established regularities and at the variation  $\Delta \varepsilon$  - of value, most likely correlating with the properties of system-forming particles, are expected.

In any case, the possibility of freely combining the conditions affecting the calculation of the statistical sum, Boltzmann distribution and entropy, expands the limits of the use of these fundamental physical and chemical values and regularities.

## Conclusion

On the basis of the commensuration 1 coefficient of discrete and continuous similarlynamed distributions developed by the authors, we analyzed the statistical sum in the Boltzmann distribution to the commensuration with the improper integral of the similarly-named function in the full range of the term of series of the statistical sum at the arbitrary combination of the temperature and interval (step) of the energy variation of particles. The convergence of series based on the Cauchy, Maclaurin criteria and the equal commensuration of series and improper integral of the similarlynamed function in each unit interval of variation of series and similarly-named function were established.

2. Independence of the commensuration coefficient from the number of terms of series

$$K = \frac{\int_{x=n-1}^{x=n} e^{-(x-1)\Delta\varepsilon/kT} dx}{e^{-(n-1)\Delta\varepsilon/kT}} = \frac{kT}{\Delta\varepsilon} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right)$$

allows us to express the total statistical sum through this coefficient and certain value of the improper integral

$$\int_{0}^{\infty} e^{-(x-1)\Delta\varepsilon/kT} dx = \frac{kT}{\Delta\varepsilon} e^{\frac{\Delta\varepsilon}{kT}}$$

in the form of calculated formula

$$\sum_{n=1}^{\infty} e^{-(n-1)\Delta\varepsilon/kT} = \frac{1}{K} \int_{0}^{\infty} e^{-(x-1)\Delta\varepsilon/kT} dx$$
$$= \frac{e^{\frac{\Delta\varepsilon}{kT}}}{e^{\frac{\Delta\varepsilon}{kT}} - 1}.$$

Accordingly, the Boltzmann distribution, which is necessary for calculating entropy according to formula  $H = -\sum_{i=1}^{\infty} P_i \ln P_i$ , gets a more direct expression

$$P_i = e^{-\frac{i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right).$$

Within the framework of this same commensuration, we determined the possibility to calculate the necessary number of terms of sum to calculate it with a given accuracy equal to the ratio of the residual and total sum of the series  $R_n/S$  in the form of formula

$$n = -\frac{kT}{\Delta\varepsilon} \ln \frac{R_n}{S}.$$

3. An analysis of the expressions obtained for the commensuration coefficient and the statistical sum establishes its identity with the similarly-named improper integral only in the area of  $\Delta \varepsilon \rightarrow 0$  and  $T \rightarrow \infty$ . In other combinations  $\Delta \varepsilon$  and *T* a direct replacement of the statistical sum by an improper integral is accompanied by an error reaching  $K \rightarrow \infty$  at  $\Delta \varepsilon \rightarrow \infty$  and  $T \rightarrow 0$ . Therefore, the general expression for the total statistical sum is analytically correct and can be calculated with any given accuracy.

4. This amount for various combinations  $\Delta \varepsilon$  and *T* may vary from one (at  $T \rightarrow 0$  or  $\Delta \varepsilon \rightarrow \infty$ ) to infinity (at  $T \rightarrow \infty$  or  $\Delta \varepsilon \rightarrow 0$ ), respectively, determining either a steep decline or a complete uniformity in the distribution of the terms of sum, and thus close to zero or infinitely large entropy of the system. In any case, direct calculation of the statistical sum, as well as the particle's energy distribution in accordance with the Boltzmann law, makes it possible to apply this law more rigorously to various problems of statistical physics and physical chemistry.

5. To determine the entropy from the new expression for the Boltzmann distribution in the form of a series,

$$H = -\sum_{i=1}^{\infty} e^{-\frac{i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right) ln \left[ e^{-\frac{i\Delta\varepsilon}{kT}} \left( e^{\frac{\Delta\varepsilon}{kT}} - 1 \right) \right]$$

the convergence of the similarly-named improper integral is established.

$$\int_{0}^{\infty} e^{-\frac{\Delta \varepsilon x}{kT}} \left( e^{\frac{\Delta \varepsilon}{kT}} - 1 \right) ln \left[ e^{-\frac{\Delta \varepsilon x}{kT}} \left( e^{\frac{\Delta \varepsilon}{kT}} - 1 \right) \right] dx$$
$$= \frac{kT}{\Delta \varepsilon} \left( e^{\frac{\Delta \varepsilon}{kT}} - 1 \right) \left[ ln \left( e^{\frac{\Delta \varepsilon}{kT}} - 1 \right) - 1 \right].$$

However, the commensuration coefficient of integral and series in each unit interval turns out to be dependent on the number of the term of series and therefore cannot be used to determine the sum of series through the improper integral. In this case, the entropy can be calculated with a given accuracy with a corresponding quantity of the term of series n.

6. Given accuracy of the statistical sum of series  $R_n/S$  reveals the meaning of the exponential factor in the Arrhenius equation as the fraction of particles with energy above the energy level (the activation barrier)  $\varepsilon_n$ :

$$\frac{R_n}{S} = e^{-\frac{n\Delta\varepsilon}{kT}} = e^{-\frac{\varepsilon_n}{kT}} = e^{-\frac{E_a}{RT}}$$

7. The prospect of development of the proposed method for expressing the Boltzmann distribution and entropy is to establish the relationship between the magnitude of the energy quantum

 $\Delta \varepsilon$  and the properties of the system-forming particles.

## References

- Boltzmann L. Selected works. Molecular Kinetic Theory of Gases. Thermodynamics. Statistical Mechanics. Theory of Radiation. General Questions of Physics. – M.: Nauka, 1984. – 590 p.
- [2]. Cherchinyani K. Theory and Applications of the Boltzmann Equation. Trans. from Eng. – M .: Mir, 1978. – 496 p.
- [3]. Zhukhovitsky A.A., Shvartsman L.A. Physical Chemistry: Textbook for Universities – 4th ed., Rev. and add. – Moscow: Metallurgiya, 1987. – 688 p.
- [4]. Malyshev V.P., Makasheva A.M., Zubrina Yu.S. On the Interrelation and Commensuration of Discrete and Continuous Dependences // Reports of NAS RK. – 2016. - No.1. - p. 49-56.
- [5]. Bronstein M.N., Semendyaev K.A. Handbook on Mathematics for Engineers and Students of Technical Institutes. 13th ed., amended. – M.: Nauka, 1987. – 544 p.
- [6]. Malyshev V.P. Fundamentals of the Thermodynamics of Matter at an Infinitely High Temperature. – Alma-Ata: Nauka, 1986. – 64 p.

- [7]. Malyshev V.P., Bissenbayeva Sh.A., Muldahmetov Z.M. On the Information Degeneration of a Thermodynamic System under Isobaric Heating to an Infinitely High Temperature // Report. AS USSR. – T. 318. – No.2. – P. 368-371.
- [8]. Malyshev V.P. Probabilistic Deterministic Mapping.
   Almaty: Gylym, 1994. 376 p.
- [9]. Malyshev V.P., Kuspekova Sh.A., Nurmagambetova (Makasheva) A.M. Thermodynamics of matter at infinite high temperature // 5th World Congress of Theoretically Oriented Chemists "WATOC'99", London, 1999. P. 222.
- [10]. Turdukozhaeva (Makasheva) A.M. Application of the Boltzmann Distribution and Shannon Information Entropy to the Analysis of Solid, Liquid and Gaseous States of Matter (for example, metals): abstract of a thesis, Doctor of Engineering Science 05/16/08. – Karaganda. – 36 p.
- [11]. Malyshev V.P., Turdukozhaeva A.M. New physical and chemical constants and prospects of its use for the explicit expression of thermodynamic functions // Journal of Chemistry and Chemical Engineering, ISSN 1934-7375, USA, David Publishing Company. - 2013. - V. 7. - No. 5. - P. 468-482.
- [12]. Malyshev V.P., Zubrina Yu.S., Makasheva A.M. Boltzmann Distribution as an Infinite Sequence and a Convergent Series // Bulletin of NAS RK. – 2017. – No.1. – p. 49-58.



# New Results Subclasses of Analytic Functions Define by Opooladifferential Operator

Fatunsin L. M.<sup>1</sup> and Opoola T. O.<sup>2</sup>

1. Department of Mathematics Programme, National Mathematical Centre, Abuja, Nigeria.

Email: mfatunsin@gmail.com

2. Department of Mathematics, University of Ilorin. Ilorin, Nigeria.

Email:opoola\_stc@yahoo.com

Abstract: In this paper, using Opooladifferential operator, we introduce new subclasses of univalent functions and provide  $\delta$  –Neighbourhoods properties, Inclusion relations for the subclasses of univalent functions.

**Keywords:** Univalent functions, Normalised, Identity function,  $\delta$  – Neighbourhoods, Inclusion relations, Opoola differential operator.

# 1. Introduction

Let *A* denote the class of functions analytic in the unit disk  $\mathcal{U} = \{z: z \in \mathbb{C} ; |z| < 1\}$ . Denote by *S* a subclass of *A* consisting of functions univalent in *U* and have the form:

$$f(z) = z + \sum_{k=2}^{\infty} a_k z^k$$
(1)

For  $t \ge 0$ ,  $1 \le \mu \le \beta$ ,  $n \in \mathbb{N}_0$  and  $z \in \mathcal{U}$ , the Opoola Differential Operator  $D^n(\mu, \beta, t) f: A \to A$  is defined as follow:

$$D^{n}(\mu,\beta,t)f(z) = f(z)$$
$$D^{n}(\mu,\beta,t)f(z) = tzf^{\iota}(z) - z(\beta - \mu)t + (1 + (\beta - \mu - 1)t)f(z)$$
$$D^{n}(\mu,\beta,t)f(z) = \left(D\left(D_{t}^{n-1}f(z)\right)\right)$$

From the above, for f(z) given in (1)

$$D^{n}(\mu,\beta,t)f(z) = z + \sum_{k=2}^{\infty} [1 + (k+\beta-\mu-1)t]^{n} a_{k} z^{k}.$$
(2)

**Corresponding author:** Full name:Opoola, Timothy Oloyede, Academic tittle: Professor, Research field: Geometric Function Theory. Email:opoola\_stc@yahoo.com.

#### **Remarks:**

- 1). When  $t = 1, \mu = \beta$ ,  $D^n(\mu, \beta, t)f(z)$  becomes the Salagean Differential Operator [3].
- 2). When  $\mu = \beta_{\lambda} D^{n}(\mu, \beta, t) f(z)$  becomes the Al-Oboudi Differential Operator [2].

### 2. Definitions and Preliminaries

**Definition2.1:** For a function  $f \in A$  and  $\delta \ge 0$ ,  $\delta$  – neighbourhood of f is defined as

$$\mathcal{U}_{(\delta)}(f) = \{g(z) = z + \sum_{k=2}^{\infty} b_k z^k \epsilon A : \sum_{k=2}^{\infty} k |a_k - b_k| \le \delta\}$$
(3)

Notably, for the identity function e(z) = z,

$$\mathcal{U}_{(\delta)}(e) = \{g(z) = z + \sum_{k=2}^{\infty} b_k z^k \, \epsilon A \colon \sum_{k=2}^{\infty} k |b_k| \le \delta\}$$

The concept of neighbourhoods was first introduced by Goodman in [1] and then generalized byRuschewey in [6].

**Definition2.2:** Let f(z) and g(z) be analytic functions in the unit disk  $\mathcal{U}$ , then f(z) is said to be subordinate to g(z) in  $\mathcal{U}$  written as  $f(z) \prec g(z)$ . If there exist a Schwarz function  $\omega(z)$  which is analytic in  $\mathcal{U}$  with  $\omega(0) = 0$ ,  $|\omega(z)| < 1$  and  $f(z) = g(\omega(z))$ . If the function g is univalent in U, then  $f(z) \prec g(z), z \in \mathcal{U} \Leftrightarrow f(0) = g(0)$  and  $f(\mathcal{U}) \subset g(\mathcal{U})$ .

**Definition2.3:** A function  $f \in A$  belongs to the class  $L(n, m, A, B, t, \mu, \beta)$  if

$$\frac{D_t^{n+m}f(z)}{D_t^n f(z)} < \frac{1+Az}{1+Bz}, \quad z \in \mathcal{U}, \ t \ge 0, -1 \le B < A \le 1, \ n \in \mathbb{N}_0 \text{ and } m \in \mathbb{N}.$$

and  $D^n(\mu, \beta, t) f(z)$  is the Opoola Differential Operator.

If  $\beta = \mu$  in the differential operator  $D^n(\mu, \beta, t)f(z)$ , then we obtain the class  $\tau(j)$  studied by Hesam Mahzoonin [4].

**Definition2.4:** A function  $f \in A$  is said to be in the class  $K(n, A, B, t, \mu, \beta)$  if it satisfies the condition

$$(D^n(\mu,\beta,t)f(z))' < \frac{1+Az}{1+Bz}, \quad (z \in U), \ t \ge 0, \ n \in \mathbb{N}_0, and \ -1 \le B < A \le 1.$$

**Definition 2.5:** A function  $f \in A$  is said to be in the class  $R(n, m, C, D, t, \varphi, \mu, \beta)$  if there exist a function  $g \in L(n, m, C, D, t, \mu, \beta)$  such that the following inequality holds.

$$\left|\frac{f(z)}{g(z)} - 1\right| < 1 - \varphi, \qquad (z \in \mathcal{U}; 0 \le \varphi < 1), -1 \le D < C \le 1, t \ge 0.$$

If  $\mu = \beta$ , then the class  $R(n, m, C, D, t, \varphi, \mu, \beta)$  becomes the class  $K_j^{\lambda}(n, m, A, B, C, D)$  investigated by Hesam Mahzoon in [4].

In what follows, we discuss the main results in this paper.

## 3. Results and Discussion

**Theorem 3.1:** A function  $f \in A$  belongs to the class  $L(n, m, A, B, t, \mu, \beta)$  if and only if

$$\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \{ (1 + B) [1 + (k + \beta - \mu - 1)t]^m - (1 + A) \} a_k \le A - B$$
(4)

 $t \ge 0, -1 \le B < A \le 1, n \in \mathbb{N}_0 and m \in \mathbb{N}.$ 

#### **Proof:**

Let  $f \in L(n, m, A, B, t, \mu, \beta)$ . Then

$$\frac{D^{n+m}(\mu,\beta,t)f(z)}{D^n(\mu,\beta,t)f(z)} < \frac{1+Az}{1+Bz}, \quad z \in \mathcal{U}$$

By the definition of subordination, there exists  $\omega(z) \in A$  such that

$$\frac{D^{n+m}(\mu,\beta,t)f(z)}{D^{n}(\mu,\beta,t)f(z)} = \frac{1+A\omega(z)}{1+B\omega(z)}, \quad \omega(0) = 0, \quad |\omega(z)| < 1$$
(5)

Which gives that

$$\omega(z) = \frac{D^{n+m}(\mu,\beta,t)f(z) - D^n(\mu,\beta,t)f(z)}{AD^n(\mu,\beta,t)f(z) - BD^{n+m}(\mu,\beta,t)f(z)}$$

It implies that

$$|\omega(z)| = \left| \frac{D^{n+m}(\mu,\beta,t)f(z) - D^{n}(\mu,\beta,t)f(z)}{AD^{n}(\mu,\beta,t)f(z) - BD^{n+m}(\mu,\beta,t)f(z)} \right| < 1$$
$$\left| \frac{z + \sum_{k=2}^{\infty} [1 + (k+\beta-\mu-1)t]^{n+m} a_{k}z^{k} - z - \sum_{k=2}^{\infty} [1 + (k+\beta-\mu-1)t]^{n} a_{k}z^{k}}{-B(z+\sum_{k=2}^{\infty} [1 + (k+\beta-\mu-1)t]^{n+m} a_{k}z^{k}) + A(z+\sum_{k=2}^{\infty} [1 + (k+\beta-\mu-1)t]^{n} a_{k}z^{k})} \right| < 1$$

i.e

$$\left|\frac{\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^n \left\{[1+(k+\beta-\mu-1)t]^m-1\right\}a_k z^k}{(A-B)z+\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^n \left\{A-B\left[1+(k+\beta-\mu-1)t\right]^m\right\}a_k z^k}\right| < 1$$

Since  $Rez \leq |z| < 1$ ,  $z \in \mathbb{C}$ . It implies that

$$Re\left\{\frac{\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^{n}\left\{[1+(k+\beta-\mu-1)t]^{m}-1\right\}a_{k}z^{k}}{(A-B)z+\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^{n}\left\{A-B\left\{[1+(k+\beta-\mu-1)t]^{m}\right\}a_{k}z^{k}\right\}}\le 1$$

Taking the values of z on the real axis as  $z \rightarrow 1$ , then we have

$$\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \{(1 + B)[1 + (k + \beta - \mu - 1)t]^m - (1 + A)\}a_k \le A - B$$

Conversely,

Suppose  $f(z) = z + \sum_{k=2}^{\infty} a_k z^k$ 

And

$$\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \{(1 + B)[1 + (k + \beta - \mu - 1)t]^m - (1 + A)\}a_k \le A - B$$

We show that

$$\frac{D^{n+m}(\mu,\beta,t)f(z)}{D^n(\mu,\beta,t)f(z)} < \frac{1+Az}{1+Bz}, \quad z \in \mathcal{U}$$

i. e we show that

$$\frac{D^{n+m}(\mu,\beta,t)f(z)}{D^{n}(\mu,\beta,t)f(z)} = \frac{1+A\omega(z)}{1+B\omega(z)}$$
(16)

Implies  $|\omega(z)| < 1$ 

$$\begin{aligned} |\omega(z)| \\ &= \left| \frac{\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \{ [1 + (k + \beta - \mu - 1)t]^m - 1\} a_k z^k}{(A - B)z + \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \{ A - B [1 + (k + \beta - \mu - 1)t]^m \} a_k z^k } \right| \end{aligned}$$
(17)

Taking z=1 and using (11) we have that

$$\begin{split} & \left| \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \left\{ [1 + (k + \beta - \mu - 1)t]^m - 1 \right\} a_k z^k \right| - |(A - B)z + \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \left\{ A - B \left[ 1 + (k + \beta - \mu - 1)t \right]^m \right\} a_k z^k | \le \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \left\{ (1 + B) [1 + (k + \beta - \mu - 1)t]^m - (1 + A) \right\} a_k z^k - (A - B)z \le 0 \end{split}$$

Hence,  $f \in L(n, m, A, B, t, \beta, \mu)$ .

We now provide a property of the neighbourhood of functions belonging to the class  $R(n, m, C, D, t, \varphi, \mu, \beta)$ .

**Theorem 3. 2:** If  $g \in R(n, m, C, D, t, \varphi, \mu, \beta)$  and

$$\varphi = 1 - \frac{\delta}{2} \cdot \frac{[1 + (\beta - \mu + 1)t]^n \{(1 + D)[1 + (\beta - \mu + 1)t]^m - (1 + C)\}}{[1 + (\beta - \mu + 1)t]^n \{(1 + D)[1 + (\beta - \mu + 1)t]^m - (1 + C)\} + (C - D)}$$

then

$$\mathcal{U}_{\delta}(g) \in R(n, m, C, D, t, \varphi, \mu, \beta).$$

**Proof:** 

Suppose  $f \in \mathcal{U}_{\delta}(g)$ . We then find from (3)that

$$\sum_{k=2}^{\infty} k|a_k - b_k| \le \delta$$

$$i.e\sum_{k=2}^{\infty}|a_k-b_k|\leq \frac{\delta}{2}$$

Since by definition of  $R(n, m, A, B, t, \varphi, \mu, \beta)$ ,  $g \in L(n, m, A, B, t, \varphi, \mu, \beta)$ , then we have from (4) that

$$\sum_{k=2}^{\infty} b_k \le \frac{C - D}{[1 + (\beta - \mu + 1)t]^n \{(1 + D)[1 + (\beta - \mu + 1)t]^m - (1 + C)\}}$$

so that

$$\begin{split} \left| \frac{f(z)}{g(z)} - 1 \right| &= \left| \frac{\sum_{k=2}^{\infty} (a_k - b_k) z^k}{z - \sum_{k=2}^{\infty} b_k z^k} \right| < \frac{\sum_{k=2}^{\infty} |a_k - b_k|}{1 - \sum_{k=2}^{\infty} b_k} \\ &\leq \frac{\delta}{2} \cdot \frac{1}{1 - \sum_{k=2}^{\infty} b_k} \\ &\leq \frac{\delta}{2} \cdot \frac{[1 + (\beta - \mu + 1)t]^n \{(1 + D)[1 + (\beta - \mu + 1)t]^m - (1 + C)\}}{[1 + (\beta - \mu + 1)t]^n \{(1 + D)[1 + (\beta - \mu + 1)t]^m - (1 + C)\} - (C - D)} \\ &= 1 - \varphi \end{split}$$

Hence,  $\left|\frac{f(z)}{g(z)} - 1\right| < 1 - \varphi$ 

Hence,  $f \in R(n, m, C, D, t, \varphi, \mu, \beta)$ 

**Theorem 3.3:** Let the function f in A defined by (1) be in  $K(n, A, B, t, \mu, \beta)$ , then

$$\sum_{k=2}^{\infty} (1+B)[1+(k+\beta-\mu-1)t]^n \, ka_k \le A-B \tag{6}$$

**Proof:** 

Let f(z) in A belongs to  $K(n, A, B, t, \mu, \beta)$ , then by the definition of the class  $K(n, A, B, t, \mu, \beta)$ 

$$(D^n(\mu,\beta,t)f(z))' \prec \frac{1+Az}{1+Bz}$$

By the definition of subordination, there exists  $\omega(z) \in A$  such that  $|\omega(z)| < 1$ ,  $\omega(0) = 0$  and

$$1 + \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n k a_k z^{k-1} = \frac{1 + A\omega(z)}{1 + B\omega(z)}$$
  
$$1 + A\omega(z) = (1 + B\omega(z)) \left( 1 + \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n k a_k z^{k-1} \right)$$
  
$$\Rightarrow |\omega(z)| = \left| \frac{\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n k a_k z^{k-1}}{(A - B) - B \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n k a_k z^{k-1}} \right| < 1$$

Since  $Re\vartheta \leq |\vartheta| < 1$ ,  $\vartheta \in \mathbb{C}$ . It implies that

$$Re\left\{\frac{\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^{n}ka_{k}z^{k-1}}{(A-B)-B\sum_{k=2}^{\infty}[1+(k+\beta-\mu-1)t]^{n}ka_{k}z^{k-1}}\right\} < 1$$

Using |z| = r, 0 < r < 1

$$\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \, ka_k r^{k-1} \le (A - B) - B \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \, ka_k r^{k-1}$$
$$\sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \, ka_k r^k \le (A - B)r - B \sum_{k=2}^{\infty} [1 + (k + \beta - \mu - 1)t]^n \, ka_k r^k$$

Choosing values of z on the real axis as  $z \rightarrow 1$ , then we have

$$(1+B)\sum_{k=2}^{\infty} [1+(k+\beta-\mu-1)t]^n \, ka_k \le A-B$$

Next, we provide the following inclusion property

#### Theorem 3.4: Let

$$\delta = \frac{A - B}{(1 + B)[1 + (\beta - \mu + 1)t]^n},\tag{7}$$

then

$$K(n, A, B, t, \mu, \beta) \subset \mathcal{U}_{\delta}(e)$$

#### **Proof:**

Let  $f \in K(n, A, B, t, \mu, \beta)$ , we have from (6) that

$$(1+B)\sum_{k=2}^{\infty} [1+(k+\beta-\mu-1)t]^n a_k \le A-B$$

And we have that

$$(1+B)[1+(\beta-\mu+1)t]^n\sum_{k=2}^\infty ka_k\leq A-B$$

Which implies that

$$\sum_{k=2}^{\infty} ka_k \le \frac{A - B}{(1 + B)[1 + (\beta - \mu + 1)t]^n} = \delta$$

Which implies that  $f \in \mathcal{U}_{\delta}(e)$ 

Thus,  $K(n, A, B, t, \mu, \beta) \subset \mathcal{U}_{\delta}(e)$ 

**Conclusions:** In this paper, using Opoola differential operator we defined new subclasses of univalent functions and established their properties. Results obtained provide new properties of certain subclasses of univalent functions.

## References

- A.W. Goodman, Univalent functions and non-Analytic Curves, Proceeding American Mathematical Society, 8 (1957) 598-601.
- [2]. F. M. Al-Oboudi, On Univalent functions Defined by a Generalised Salagean Operator, International Journal of Mathematics and Mathematical Sciences. No. 25-28 (2004) 1429-1436.
- [3]. G. S Salagean, Subclasses of Univalent Functions, Complex Analysis-Fifth Romanian Seminar, Part 1 (Bucharest, 1981) Lecture Notes in Mathematics. Vol. 1013, Springer, Berlin. 1983, pp 362-372.
- [4]. HesamMahzoon, On a Certain Subclasses of Analytic Functions Defined by Differential Subordination, International Journalof Mathematics and Mathematical Sciences, Vol. (2011).
- [5]. P. L. Duren, Univalent Functions, Springer, New York, NY, USA, 1983.
- [6]. S. Ruschewey, Neighbourhoods of univalent functions. Proceedings of the American Mathematical Society, vol. 81, no. 4, pp 521-527, 1981.
- [7]. S. S. Miller, P.T. Mocanu, Differential Subordination. Theory and Applications, Marcel-Dekker Inc., New York, 2000.
- [8]. T. O. Opoola. On a Subclass of Univalent Functions Defined by a Generalised Differential Operator. To appear in International Journal of Mathematical Analysis.