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THREE-PARAMETER APPROXIMATION OF THE SUM OF THE VIRIAL SERIES

K. I. LUDANOV

Faculty of Thermal Energy
NTTU "KPI" them. Sikorsky
No. 5, St. Polytechnic, 6; Kiev
Ukraine
e-mail: k.i.ludanov@ukr.net

Abstract

The article develops a three-parameter method of approximating the sum of the Maclaurin series by its first four terms of expansion, which allows obtaining analytical approximations for functions expanding into a power series. The expressions for the approximation parameters (a, b, c) of the exact sum $\sum(S)$ of the power series-basis of the geometric type are obtained in a general form and are determined by the coefficients in the second (A), third (B) and fourth (C) terms of the Maclaurin series. For rapidly converging series (their coefficients satisfy the inequalities $(a_n)^2 > a_{n-1} \times a_{n+1})$, the new method gives real values of the sum $\sum(S)$, and for slowly converging series (for them $(a_n)^2 < a_{n-1} \times a_{n+1})$, the method gives the complex-combined roots of

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the parameters of their sum $\sum(S)$. The paper gives examples of approximate determination of series sums by three-parameter and two-parameter methods based on the analysis of series coefficients. An assessment of the accuracy of two- and three-parameter approximation methods of $\sum(S)$ based on the determination of approximate sums of power series with an exact sum was carried out. On the basis of the new three-parameter method, the sum of the theoretically justified virial series was approximated and the closed expression of the virial equation was mathematically rigorously obtained.

1. Introduction

In the theoretical analysis of the fundamentally important regularities that make up our understanding of a new phenomenon, the role of analytical methods remains extremely high. Their role is also high in the qualitative determination of the parameters of physical phenomena, notes Cole [1]. Therefore, he points to the importance of various methods of perturbation theory, which are the main analytical tool for the study of nonlinear physical and technical problems. Realistically, only a few terms of the perturbed expansion can be calculated, usually no more than two or three. The resulting series often converge slowly or even diverge. Nevertheless, these few members contain significant information from which it is necessary to get the maximum possible, summarizes Van Dyke [2].

However, after the appearance of the works of Kantor et al. from set theory, mathematics was formed into a single whole, that is, into a complete science with its subject and method. And now “refined” mathematicians no longer consider the goal of mathematics to be the development of the “language” of natural science, that is, the apparatus for solving problems related to the exact sciences [3]. Modern mathematicians deal with the problems of the structure of mathematics itself and its individual aspects. The problems of “language” for the natural sciences are currently being dealt with only by specialists in applied mathematics. It is precisely this weakening of the interest of pure mathematicians in the problems of approximation of the sum of series that explains the fact that still in this field of higher mathematics one can find unexplained questions and some unsolved problems.

2. Review

Historically, the first method of accelerating the convergence of power series is the fractional-rational transformation of a variable in the form of the Euler transformation: $x = \varepsilon/(1+\varepsilon)$, [2, 3]. The purpose of the Euler transformation is to transfer the singularity $\varepsilon = -1$ to an infinitely distant point. At the same time, if there are no other features in the complex plane, then the radius of convergence becomes infinite.

The problem of approximate determination of the sum of an infinite series is generally solved by methods of approximating $\sum(S)$ by the first few coefficients of the expansion of the power series.

Among the low-parameter methods for approximating the sum of power series in mechanics, the Shanks method is well known [2]. It consists in approximating the sum of Maclaurin's series by its first three terms. Applying the non-linear Shanks transformation to the first three terms of the power series $S(\varepsilon) = 1 + a\varepsilon + b\varepsilon^2 + \ldots$ gives a simple rational fraction:

$$\sum S \cong \frac{a + (a^2 - b)\cdot\varepsilon}{a - b\cdot\varepsilon}, \tag{1}$$

which is often a more accurate approximation to the sum of the series than its fragment which is the sum of the first three terms. For example, this sum gives an exact value if the series is a geometric progression (both convergent and divergent). The sequence of members of a series is called a geometric progression because there is a relationship between adjacent members: $(a_n)^2 = a_{n-1} \times a_{n+1}$, i.e., each of its terms is the geometric mean between the term preceding it and the term following it. By the way, in the fundamental Handbook [4], in the Section of functional power series that have an analytical expression for an exact sum, the series S is written under No. 1, which is a geometric progression, the sum of which is equal to $\sum x^k = (1-x)^{-1}$ under the condition $x \neq 1$. Thus, we can say that power series of the form $\sum p(k) \cdot x^k$ generalize series of geometric type, which have an analytical expression for their exact sum. This sum $\sum(S)$ is finite under the condition $x \neq 1$ [4], and the series $S(x)$ diverges at the point $x \to 1$ $(\sum S(x) \to \infty)$.

As an example, we can cite other series of geometric type, that is, those that have an analytical expression for their exact sum:

the series $S(x) = x + 2x^2 + 3x^3 + 4x^4 + \ldots$ has the sum

$$\sum S = \frac{x}{(1-x)^2}, \tag{2}$$

and the series $S(x) = 1 + 3x^2 + 5x^3 + 7x^4 + \ldots$ has the sum

$$\sum S = \frac{1+x}{(1-x)^2}. \tag{3}$$

The most powerful method of approximation is the Padé method [5], in which it is performed within the framework of approximating the sum of a series by rational functions. However, for many cases, the Padé approximation method is fundamentally unacceptable. For example, when only a few terms of the expansion are found in the solution by the small parameter method, the coefficients of which must receive a certain physical interpretation.

In this sense, the most promising method of approximating the sum of a static series by its first three terms turned out to be Ludanov’s method, the abstract of which (9B 832 DEP) was presented in the journal “Mathematics” about forty years ago (in No. 9 of 1984). In this article, a method of two-parameter approximation of Maclaurin’s power series by its first three terms was developed. As the comparison [6] showed, this method turned out to be much more accurate than the Padé method (other things being equal).

3. Formulation of the Problem

In cases where for a formula that approximately describes an exact expression or a fragment of a power series into which this expression decomposes, the coincidence of only the first two derivatives of this function is sufficient, the optimal solution to the problem is the method of two-parameter approximation of the sum of the Maclaurin series [6].

In this article, a method of two-parameter approximation of the Maclaurin power series by its first three terms in the form of the *N*th power of an arbitrary analytic function $y(x)$ was developed, in which the variable x is written as the product of the new variable ε by the parameter M $(x = M \cdot \varepsilon)$. Such a substitution makes it possible to "stretch" or "compress" the variable x and obtain one more parameter when constructing a multi-parameter approximation expression. The fact is that each additional parameter of the approximation gives a sharp increase in the accuracy of the approximation. For example, the error of the two-parameter approximation [6] is estimated as $R(x^3)$, while for the three-parameter approximation it is obvious that the error will be an order of magnitude lower than $R(x^4)$.

The most promising option for the development of a three-parameter approximation is the Maclaurin power series $S(x)$ of the geometric type, presented in Dwight's Handbook [7, No. 33.2]:

$$S(x) = 1 + a \cdot x + (a + b) \cdot x^2 + (a + 2b) \cdot x^3 + \ldots . \tag{4}$$

It also has an analytical expression for the exact sum:

$$\sum S = 1 + \frac{a \cdot x + (b - a) \cdot x^2}{(1 - x)^2} \text{ under the condition } x \neq 1. \tag{5}$$

This power series S and the generalized expression of its sum $\sum(S)$ already include two parameters (a and b) and if we try to include the third parameter c in the expression S and $\sum(S)$, then it is possible to obtain a generalized expression for the approximant of the sum of the Maclaurin series by to its four first members:

$$S(x) = 1 + A \cdot x + B \cdot x^2 + C \cdot x^3 + \ldots, \text{ where } \sum S(x) \cong f(x, A, B, C). \quad (6)$$

4. Research Results

4.1. Approximation of the sum of the Maclaurin series by the first four terms

Here we will use the technique that was used in the previous work of the author [6]. If the variable x is included with the factor c, then we get a “compressed” or “stretched” variable ε in the form of $x = \varepsilon/c$. By substituting a new variable ε/c instead of x (this is convenient for obtaining the same dimension), we obtain the expression for the three-parameter approximation:

$$S(x) \to S\left(\frac{\varepsilon}{c}\right) = 1 + a \cdot \left(\frac{\varepsilon}{c}\right) + (a + b) \cdot \left(\frac{\varepsilon}{c}\right)^2 + (a + 2b)\left(\frac{\varepsilon}{c}\right)^3 + \ldots . \quad (7)$$

Thus, a modified power series $S(\varepsilon)$ is obtained here, which has a different expression for its exact sum $\sum(S)$:

$$S(\varepsilon) = 1 + \frac{a}{c} \cdot \varepsilon + \frac{a + b}{c^2} \cdot \varepsilon^2 + \frac{a + 2b}{c^3} \cdot \varepsilon^3 + \ldots . \quad (8)$$

We introduce the notation: $a/c = A$, $(a + b)/c^2 = B$ and $(a + 2b)/c^3 = C$, substitute them into the exact sum of the series $\sum(S)$, and then multiply the numerator and denominator of the fraction by c^2 and after reductions, we will get a modified series and an estimate of its sum:

$$S(\varepsilon) = 1 + A \cdot \varepsilon + B \cdot \varepsilon^2 + C \cdot \varepsilon^3 + \ldots, \tag{9}$$

$$\sum S(\varepsilon) \cong 1 + \frac{(a \cdot c) \cdot \varepsilon + (b - a) \cdot \varepsilon^2}{(c - \varepsilon)^2}. \tag{10}$$

And we will also get a system of three equations with three unknowns a, b and c:

$$\begin{cases} A = a/c, \\ B = (a + b)/c^2, \\ C = (a + 2b)/c^3. \end{cases} \tag{11}$$

Solving the obtained system of equations, it is possible to express the coefficients of the approximate series A, B and C through lowercase letters - the parameters of the sum of the series a, b and c. Expressions for a, b and c are determined as follows through the coefficients of A, B and C. Since the small b is included in only two equations of the system out of three, then by transforming the second and third equations of the system we find b from them, and by equating them - we exclude it from the system. Then, from the first notation of the coefficient A, we find c and, substituting the value of a/A in its place, we get a quadratic equation for a, solving which we find the roots:

$$a_{1,2} = \left(\frac{A}{C}\right) \cdot [B \pm \sqrt{(B^2 - A \cdot C)}], \text{ where } \mathrm{Det} = B^2 - A \cdot C. \tag{12}$$

Based on the found parameter a, others can be easily found from the above designations: $c = A/a$, and $b = B \cdot c^2 - a$. If in the expressions of the roots $a_{1,2}$ the root expression $(\mathrm{Det} = B^2 - A \cdot C)$ is negative $\mathrm{Det} < 0$, then there will be complex-conjugate roots, and accordingly the expression of the sum of the series $\sum(S)$ will also be complex - but these solutions are not considered in this paper.

4.2. Approximation of the sum of Maclaurin series of the form $\sum p(k) \cdot x^k$

Let us consider here the approximation of the sum of power series of the geometric type, which have an analytical expression for the sum $\sum (S)$.

Example 1.

Let us approximate the sum S of the rapidly converging Maclaurin series of the geometric type presented in the Handbook [4, §5.2.2, No. 4]:

$$S(x) = 1 + \sum k \cdot x^k = 1 + x + 2x^2 + 3x^3 + \ldots, \tag{13}$$

$$\text{where the sum } \sum k \cdot x^k = \frac{x}{(1-x)^2} \text{ provided } x \neq 1. \tag{14}$$

The expression of the sum of the two-parameter approximation is as follows:

$$\sum (S) \cong (1 + M \cdot x)^N.$$

By the coefficients $a = +1$, $b = +2$, we find the parameters: $M = -3$, $N = -1/3$. As a result of the substitution, we get $\sum S(x) \approx (1 - 3x)^{-1/3}$. The relative error δ of this formula is zero at $x = 0$, with increasing x, δ increases and at $x = 1/6$, reaches 1.6%, and at $x = 1/4$, reaches 8.5%, and with further growth of the variable ($x \to 1/3$) the series S diverges, and the value δ at $x \to 1/3$ increases indefinitely. Thus, the calculation of the approximate sum of the series according to MA No. 1 is very inaccurate here, and the range of approximation is extremely limited.

And now, in the case of $\text{Det} > 0$, we will approximate the sum of the same series, but within the framework of the three-parameter approximation of MA No. 2.

The coefficients of the corresponding Maclaurin series are obtained as follows: $A = +1$; $B = +2$; $C = +3$. We will calculate the parameters of the sum of the series-basis according to the formula: $a_{1,2} = (A/C) \cdot [B \pm \sqrt{(B^2 - A \cdot C)}]$. The substitution gives: $a_{1,2} = (1/3) \cdot (2 \pm \sqrt{1})$: $a_1 = +1$; $a_2 = +1/3$, for the second parameter c we get: $c_1 = +1$, $c_2 = +1/3$, for the third parameter we get: $b_1 = +1$; $b_2 = -1/9$.

Substituting the first set of parameter roots into the expression of the sum of the series $\sum(S)$, we obtain:

$$S = 1 + 2x + 3x^2 + 4x^3 + \ldots, \text{ it has the exact sum:} \tag{15}$$

$$\sum(S) = 1 + \sum k \cdot x^k = \frac{x}{(1-x)^2} \text{ provided } x \neq 1. \tag{16}$$

The resulting expression also coincides with the exact sum of this series. That is, here the accuracy of the approximation of the sum of the series according to MA No. 2 is 100%. Therefore, it is obvious that when approximating the sum of series of a geometric type, which have an analytical expression for their exact sum, of the two methods MA No. 2 is more promising.

Example 2

Let us consider the approximation of the sum of the rapidly converging series of Maclaurin, given in Dwight's Handbook [5, No. 33.1].

$$S = 1 + 3x + 5x^2 + 7x^3 + \ldots, \text{ it has the exact sum:} \tag{17}$$

$$\sum(S) = \frac{1+x}{(1-x)^2} \text{ provided } x \neq 1. \tag{18}$$

The sum expression for the two-parameter approximation is as follows:

$$\sum(S) \approx (1 + M \cdot x)^N. \tag{19}$$

By the coefficients $a = +3$, $b = +5$, we find the parameters: $M = -1/3$, $N = -9$. As a result of the substitution, we get the formula: $\sum(S) \approx (1 - x/3)^{-9}$. The relative error δ of this formula is zero at $x = 0$, increases with an increase in x, and already at $x = 1/3$, reaches 3%, and further as $x \to 3$ increases, it grows indefinitely. Thus, the calculation of the approximate sum of the series according to MA No. 1 using the two-parameter formula is extremely inaccurate.

And now, in the case of $\mathrm{Det} > 0$, we will approximate the sum of the same series, but within the framework of the three-parameter approximation of MA No. 2.

We have the following coefficients of the corresponding Maclaurin series: $A = +3$; $B = +5$; $C = +7$. We will calculate the parameters of the sum of the series-basis according to the formula: $a_{1,2} = (A/C) \cdot [B \pm \sqrt{(B^2 - A \cdot C)}]$. Substitution gives: $a_{1,2} = (3/7) \cdot (5 \pm 2)$ ($a_1 = +3$; $a_2 = +9/7$), for the second parameter we get: $c_1 = +1$; $c_2 = +3/7$, for the third parameter we get: $b_1 = +2$; $b_2 = -18/49$.

Substituting the first set of roots-parameters ($a_1 = +3$; $c_1 = +1$; $b_1 = +2$) into the expression of the sum of the series-basis $\sum(S)$, we obtain:

$S = 1 + 3x + 5x + 7x + \ldots$, it has the exact sum:

$$\sum(S) = \frac{1 + x}{(1 - x)^2} \text{ provided } x \neq 1. \tag{20}$$

The resulting expression completely coincides with the exact sum of this series. And the accuracy of the approximation of the sum of the geometric type series according to MA No. 2 is 100%. Therefore, it is obvious that when approximating the sum of series having an analytical expression for the exact sum, of the two methods of MA, MA No. 2 is more promising.

1.3. Three-parameter approximation of the sum of the virial series

As a physical example of approximating the sum of the series $\sum(S)$, we use probably the most famous power series in physics - virial expansion. The virial equation of the state of a real gas is theoretically well-founded [9], as it is strictly obtained by the methods of statistical mechanics: the final form of the virial series was obtained in the works of Mayer-Bogolyubov [10]: In this expansion, the coefficients of the Maclaurin series thus correspond to the coefficients of the virial series: $A \equiv B_1$; $B \equiv B_2$; and $C = B_3$:

$$Z = 1 + B_1 \cdot \rho + B_2 \cdot \rho^2 + B_3 \cdot \rho^3 + \ldots \equiv 1 + \sum B_k \cdot \rho^k, \quad k \to \infty, \quad (21)$$

where Z is the compressibility coefficient of real gas; ρ is gas density; B_k are virial expansion coefficients, they depend only on the absolute temperature $B_k = f(T)$; B_1 is the first coefficient characterizing binary collisions of molecules; B_2 is the second coefficient characterizing triplet collisions; B_3 is the third coefficient characterizing quadruple collisions; k are natural numbers $(1, 2, 3, \ldots)$.

Currently, in the calculations of the compressibility coefficient Z of a real gas, a “truncated” series of virial expansion is used, which includes only a few first terms, because until now only a few first virial terms have been calculated for realistic gas potentials [11] - usually 3-4 terms are tabulated in the reference books.

$$Z \cong 1 + \sum B_k \cdot \rho^k, \quad k = 3. \quad (22)$$

The calculation of terms of a series of higher powers is hampered by great difficulties of integration. On the other hand, many power potentials have already been proposed, and in order to choose the most suitable one, it is necessary to test them, i.e., first find out what they give the sum of the virial series. And as shown by the above calculations of sums, methods MA No. 1 and MA No. 2 (two- and three-parameter approximation methods) have quite sufficient accuracy, which is in no way lower than the accuracy of calculating theoretical potentials.

$$\sum S(\varepsilon) \cong 1 + \frac{(a \cdot c) \cdot \varepsilon + (b - a) \cdot \varepsilon^2}{(c - \varepsilon)^2} \text{ provided } \varepsilon \neq c. \tag{23}$$

If the coefficients of the virial series, which are included in the expressions $\sum(S)$, are replaced by parameters (a, b, c) and substituted instead of the parameters a, b and c in their expressions through the mediation of virial coefficients, then we get an exact analytical approximation for the expression of gas compressibility Z from gas density ρ:

$$Z \cong 1 + \frac{ac \cdot \rho + (b - a) \cdot \rho^2}{(c - \rho)^2}. \tag{24}$$

As part of the MA No.1, for the sum of the virial series using Newton's binomial, an expression is obtained that "works" only when $\rho > \rho c$, since it gives only one set of roots for the parameters M and N.

$$Z \approx (1 + M \cdot \rho)^N, \text{ where } M = B_1 - 2\,B_2/B_1,$$

$$N = B_1/(B_1 - 2B_2/B_1). \tag{25}$$

This presentation of the sum Z by "convolution" of the virial series is convenient in that it becomes possible to present the isotherms of the virial equation of state (within MA No.1) in double logarithmic coordinates:

$$\ln Z = N \times \ln(1 + M \cdot \rho), \tag{26}$$

where M and N are functions of virial coefficients that do not depend on ρ, but depend only on the absolute temperature.

And the approximation for $Z(\rho)$ according to MA No.2 can be used even under the condition $\rho < \rho c$, since the virial series accurately describes the state of a real gas up to the binodal (more precisely, to the saturated vapor line).

As part of the three-parameter approximation of MA No. 2 of the sum of the virial series, we obtain a closed expression for the virial equation of state:

$$Z(\rho) \cong 1 + \frac{ac \cdot \rho + (b - a) \cdot \rho^2}{(c - \rho)^2}, \tag{27}$$

where $a_{1,2} = (B_1/B_3) \cdot [B_2 \pm \sqrt{(B^2{}_2 - B_1 \cdot B_3)}]$; $c_{1,2} = a_{1,2}/B_1$; $b_{1,2} = B_2 \cdot (a_{1,2}/B_1)^2 - a_{1,2}$.

Since all the coefficients of the members of the virial series depend only on the temperature, then all the dependence parameters $Z(\rho)$ are also functions of T: $a_{1,2} = f_1(T)$, $c_{1,2} = f_2(T)$, $b_{1,2} = f_3(T)$.

The analysis of the parameters of the sum of the virial series shows that it also includes three sets of solutions: sets with real roots under the condition $\mathrm{Det} > 0$, sets with complex-combined roots when $\mathrm{Det} < 0$, and a set for $\mathrm{Det} = 0$. Here we can already assume that the expression $Z(\rho)$ with complex-combined roots describes the region of unstable and unstable states of a real gas located between the binodal and the O - Z axis. It is known that the region of unstable states of a real gas is limited by the spinodal. And the range between spinodal and binodal limits the region of metastable states. The expression $Z(\rho)$ with real root-parameters describes the region of the steady state of a real gas, located outside the region covered by the binodal and the O - Z axis. It can be assumed that one of the sets of roots-parameters of the virial equation at $\rho < \rho c$ describes a real gas in the “gas phase” state, and the other set describes a real gas in the “liquid phase” state.

It is obvious that the expression $Z(\rho)$ at $\mathrm{Det} = 0$ most likely represents, in fact, the saturation line, since it limits the region of the stable state of a real gas. And indeed, if we examine the expression for the binodal ($\mathrm{Det} = 0$) in more detail, it turns out that the condition $B^2{}_2 - B_1 \cdot B_3 = 0$ implies the presence of two branches of the binodal: $B_2 = \pm\sqrt{B_1 \cdot B_3}$. A similar dependence was obtained in [12]. It includes the aforementioned lines: saturated (dry) steam and saturated (boiling) liquid.

Let us analyze the equation of the saturation line (binodal).

If the determinant is zero, then the expression $B^2{}_2 - B_1 \cdot B_3 = 0$. And in this case, the sequence of coefficients B_1, B_2 and B_3 is a fragment of a geometric progression. In addition, only in this case the parameter $a_{1,2} \equiv a = (B_1 \cdot B_2)/B_3$; parameter $c = B_1/a = B_3/B_2$; and parameter $b = B_2 \cdot (a/B_1)^2 - a = B^3{}_2/B_3 - B_1 \cdot B_2/B_3 = (B_2/B^2{}_3) \cdot (B^2{}_2 - B_1 \cdot B_3)$. But $(B^2{}_2 - B_1 \cdot B_3) = 0$, i.e., in this case we get the value of the parameter $b = 0$ for the bimodal equation.

Thus, the sum of the series in the case $b = 0$ for $Z \cong \sum(S)$ is equal to:

$$Z \cong 1 + \left.\frac{ac \cdot \rho + (b - a) \cdot \rho^2}{(c - \rho)^2}\right|_{b=0} = 1 + a\rho/(c - \rho), \tag{28}$$

where parameter values $a = (B_1 \cdot B_2)/B_3$, $ac = B_3/B_2$.

We will rewrite the resulting equation binodally in the form:

$$Z_s \cong 1 + a\rho_s/(c - \rho_s), \tag{29}$$

where the subscript s means that this is the equation of the saturation line (binodal). The analysis of the binodal equation (29) shows that when

$\rho_s = c$ there is a discontinuity of the second kind, therefore the function $Z_s(\rho_s)$ is discontinuous (it means that $Z(\rho)$ is also discontinuous) and when $\rho_s \to c$ the derivative $|\partial Z_s/\partial\rho_s| \to \infty$, from which it follows that the point $\rho_s = c$ is the point binodal with the maximum - that is, with the critical density $\rho_s = \rho_c$. It can also be seen here that all the remaining points of the binodal are characterized by the inequality $\rho_s < \rho_c$. The same cannot be said about the density ρ in equation (29) - we can only assume that the isotherm $Z(\rho)$ consists of two parts: for one of them $\rho < \rho''$ (subcritical region), and for the other $\rho > \rho'$ (supercritical region). After all, the difference $(\rho_s - \rho_c)$ in the denominator (29) is represented in the square $(c - \rho)^2$ and the sign in parentheses does not affect the value of Z.

According to the existing formulas, it is possible to construct the isotherm of a real gas, which in the coordinates $Z \sim \rho$ undergoes a discontinuity of the second kind at $\rho_c = c$. From the reference book with tabulated virial coefficients - for the absolute temperature $T(\mathrm{K})$ we select the values B_1, B_2 and B_3, then using formula (27) we construct the curve $Z(T_J) = f(\rho)$ according to the first set of roots-parameters from $Z(0) = 1$ to the point Z'' on the saturated (dry) steam line, which is determined by the binodal equation from formula (29) by substituting the parameters $a = (B_1 \cdot B_2)/B_3$ and $c = B_3/B_2$ into it (they are defined above by $T(\mathrm{K})$. Based on the value of $Z''(\rho'')$ from the equation of the line of saturated steam (29), we find the value of ρ_s, then we look for the point of intersection of the curve (constructed on the second set of real roots) with the line of saturated (boiling) liquid (ρ', Z'). The coordinates of the point of intersection of the isotherm $Z(\rho)$ with the liquid saturation line $Z'(\rho')$ are determined by the solution of the system of equations of the binodal $Z_s(\rho_s)$ and the isotherm $Z(\rho)$ of a real gas built on the second set of roots - parameters (for the liquid). The liquid isotherm also undergoes a second-order discontinuity at $\rho = \rho_c$.

The virial series can be transformed from the density expansion $Z(\rho)$ into the pressure expansion $Z(p) = 1 + \mathbf{B}_1 p + \mathbf{B}_2 p^2 + \mathbf{B}_3 p^3 + \ldots$. The formulas for such a transformation of the corresponding virial coefficients are also known:

$$\mathbf{B}_1 = B_1/RT\,; \;\; \mathbf{B}_2 = (B_2 - B^2{}_1)\,/\,(RT)^2;$$

$$\mathbf{B}_3 = (B_3 - 3B_1 \cdot B_2 + 2B^3{}_1)\big/\,(RT)^3. \tag{30}$$

Moreover, the dependence $Z(p)$ is usually used on the graphs, since it is much clearer and more convenient - because the node in the coordinates $Z \sim p$ is a vertical parallel to the O - Z axis.

As part of the three-parameter approximation of the sum of the virial series, it is possible to obtain a closed expression for this virial equation of state $Z(p)$:

$$Z(p) \cong 1 + \frac{ac \cdot p + (b - a) \cdot p^2}{(c - p)^2}\,, \tag{31}$$

where $a_{1,2} = (\,\mathbf{B}_1/\mathbf{B}_3) \cdot [\mathbf{B}_2 \pm \sqrt{\mathbf{B}^2{}_2 - \mathbf{B}_1 \cdot \mathbf{B}_3}\,]$; $c_{1,2} = a_{1,2}/\mathbf{B}_1$; $b_{1,2} = \mathbf{B}_2 \cdot (\,a_{1,2}/\mathbf{B}_1\,)^2 - a_{1,2}$.

Analysis of the obtained expression for the compressibility of a real gas as a function of pressure $Z(p)$ shows that it satisfies the a priori conditions. For example, for $p = 0$, we have $Z = 1$, i.e., at $p \to 0$, we get the equation of an ideal gas: see Figure 1.

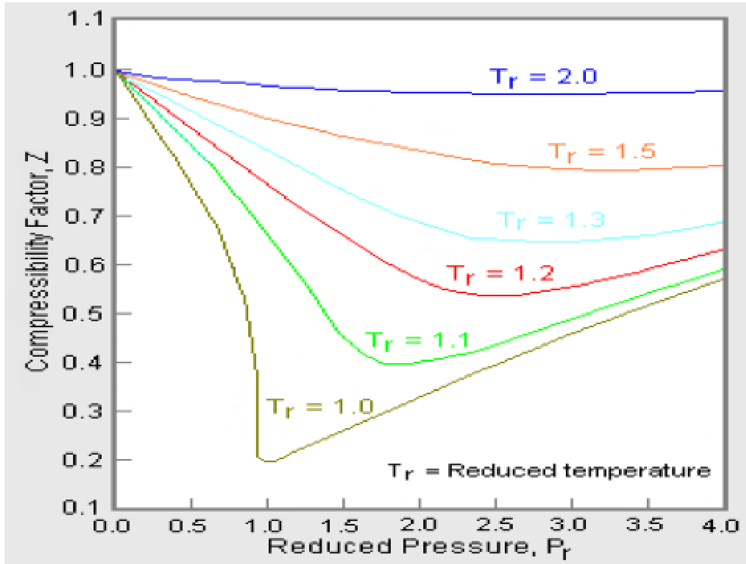

Figure 1. Real gas isotherms in coordinates $Z \sim P_r$ at $T \geq Tc$ ($P_r = p/Pc$).

5. Discussion

Based on the epigraph [3]: “The main goal of physical theories is to find a number, and what is more, with sufficient accuracy!” (R. Feynman) it can be said that this task in this article has been completed quite successfully. “Testing” of the methods proposed by the author for approximation of MA No. 1 and MA No. 2 of series sums on the given examples showed that the accuracy of the three-parameter approximation is almost 100%.

1. As shown by a comparative analysis of the two-parameter approximation of the author [3] based on the Newton binomial and the three-parameter approximation of the sum of the McLaren series developed in this article, its accuracy is significantly lower than the new one. However, the new method gives real roots for rapidly converging series, and complex conjugate roots for slowly converging series. This is due to the fact that it is built on the basis of the generalization of the sum

of a series of geometric type, in which adjacent terms are connected by a dependency: $a^2{}_n = a_{n-1} \times a_{n+1}$, unlike the well-known two-parameter approximation, where there is no such strict condition.

2. The developed approximation is unique in that it provides a new quality. The three-parameter approximation made it possible to substantiate a new interpretation of the phase transition line (binodal) of a real gas - not a physical one, but a mathematical one, as a line with $\mathrm{Det} = 0$. It should be noted here that, in fact, physical theories (including theories of phase transitions and critical phenomena) are relative truths, while mathematical truths are absolute.

3. Why is it important to approximate the sum of a virial series? The fact is that a mathematically rigorous conclusion of the closed equation of the state of a real gas is very necessary for practice. Although several hundreds of different empirical and semi-empirical equations are already known, a universal theoretical equation will allow predicting the parameters of the state of refractory substances at high and ultrahigh temperatures where there is no experimental data. And this is necessary for astrophysics, space technology, as well as high temperature technology.

4. Therefore, we can confidently say that a very useful tool for the analysis of mathematical solutions to complex nonlinear phenomena has been developed for the natural sciences, and the use of three-parameter approximation of series sums, the fragments of which physicists obtain in solving nonlinear problems using the small-parameter method, will allow finding on this basis not only quantitatively more accurate results, but will allow to reveal a different quality - a new physical interpretation of the phenomena under investigation.

Mathematical interpretation

The three-parameter approximation $\sum(S)$ is developed on the basis of a series-basis of the geometric type (with $\mathrm{Det} = 0$) and divides

Maclaurin series into two groups: those that converge faster $(\mathrm{Det} > 0)$ than series of the geometric type and those that converge slower than them $(\mathrm{Det} < 0)$, including those that diverge. In the case of $\mathrm{Det} = 0$, the sum of a series of geometric type is approximated, the expression having only one set of real roots. If $\mathrm{Det} > 0$ for the roots, then the series is approximated, which converges faster than the geometric series. In this case, two sets of common roots and two expressions for the sum of the series are obtained. If $\mathrm{Det} < 0$, then the series is approximated, converging more slowly than the geometric one, it has two sets of complex conjugate roots and complex expressions for the sum of the series.

Physical interpretation

The two-parameter approximation of the sum $\sum(S)$ of the virial series $Z(\rho)$ gives only one curve for any isotherm of a real gas, so it is suitable for representing only isotherms with a temperature above the critical $T > Tc$. The three-parameter approximation of $\sum(S)$ of the virial series immediately gives five sets of roots for expressing the compressibility of a real gas $Z(\rho)$: of them, two sets of real roots for the case $\mathrm{Det} > 0$. This is a case in the field of real gas steady state. It is obvious that the larger one is for the gas phase Z'', and the smaller one is for the liquid Z'. Two more sets of complex-combined roots are obtained for the case $\mathrm{Det} < 0$, it is obvious that they characterize the unstable and unstable region of a real gas in a two-phase state, which is covered by a binodal, the two branches of which are lines of saturated (dry) vapor and a line of saturated (boiling) liquid. The author previously showed [12] that the binodal equation is a parabola with two branches. And one real root in the case of $\mathrm{Det} = 0$ is obviously expressed by the point of intersection of the isotherm and the saturation line. From the expression for $\mathrm{Det} = 0$, the binodal line $B^2{}_2 = B_1 \cdot B_3$ can be determined, and it is also possible to calculate the values of the critical density ρ_c and the temperature T_c. At $\rho = \rho_c$, the $Z(\rho)$ curves undergo a break of the second kind, so the domain of the function $Z(\rho)$ is divided into two parts: subcritical and supercritical. The value of critical density and temperature are two very important parameters of the state of refractory substances, which determines the upper temperature limit of the existence of their liquid phase.

6. Conclusions

A new three-parameter method (MA No. 2) of approximation of the sum of power series, which is much more accurate than the two-parameter method (MA No. 1), has been developed on the basis of the generalized expression of the power series-basis of the geometric type.

A three-parameter approximation of the sum of the virial series was carried out and, for the first time, a closed expression $Z(\rho)$ for the virial equation of state of a real gas was mathematically rigorously obtained. This solution is the only theoretically justified equation of state of a real gas in a universal form.

A theoretically justified binodal equation was also found - the phase transition lines of a real gas $Z_s(\rho_s)$, including the line of saturated (dry) vapor and the line of saturated (boiling) liquid. It is contained precisely in the equation of state of a real gas under the condition $\text{Det} = 0$.

In addition, it is shown the possibility of creating another equation regarding the dependence of the compressibility of real gas on the density $Z(\rho)$ - also a closed analytical solution for Z, but this time in the form of its expression as a function of the pressure $Z(p)$.

It was established that the presence of two phases of a real gas is determined by a pair of solutions of the quadratic equation with respect to the parameters a, b, and c, its real solutions describe the region of the stable state of the real gas, and the imaginary solutions describe the region of the unstable state. The boundary between the regions of stable and unstable states, which is characterized by Det = 0, describes the phase transition line - binodal.

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