EVALUATION OF NONLINEAR CONSTANTS FROM RESULTS OF ACOUSTIC MEASUREMENTS. REGULARIZATION OF PROBLEM

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The method of nonlinear constants B/A and C/A determination is discussed. It bases on comparison of experimental results of acoustic signal propagation with results of theoretical investigation of this problem. It is shown, that this problem, in general case, is ill-posed. So we use methods of ill-posed problem solution regularization. The values of the constants, which were extracted using this method, are in good accordance with estimations by other authors.

INTRODUCTION

A construction of solutions for problems of a continuous medium state perturbation is traditionally based on equations of hydrodynamics type. One of the important questions arising when one complete the equations of hydrodynamics set is a choice of the (caloric and thermic) equations of state [1]. More precisely a question is: how many and what equations of state correspond to the considered real medium? The equations of state of ideal gas form are frequently used. However, there is a serious contradiction. Viscosity and thermal streams for ideal gas are equal to zero, and the equations of hydrodynamics become inconsistent. The empirical equations of state for a real gas (for example, the equations of Van der Waals, Bertlo, Diterichi and others) also do not solve the problem. First, all of them contain a set of constants, which empirical definition or analytical calculation represents separate, rather uneasy problem. Second, all of them either works in narrow enough range of temperatures and pressure, or are too complicated. Especially, for liquids, even for most interesting of them - water up to now it was not possible to pick up the satisfactory equation of state.

The question on correctness of a choice of the equations of state becomes important when a state of a fluid goes up to a critical or phase transition points. It also relates the case of account of the physical effects connected with nonlinearity. It becomes clear, that nonlinear properties of fluids and their detail displays basically would be described, if exact equations of state of the medium under consideration were known. Unfortunately, in the majority of cases these equations till now are not established [2].

Accordingly, dependence of the pressure and the internal energy of a thermodynamic system on temperature and density, it is said the caloric and the thermic equations of state are independent despite a connection by a differential relation. If a system is simple, that is the system with a constant number of particles which equilibrium condition is defined only by the only external parameter (say, - density ρ) and the temperature T, the thermic and the caloric equations look correspondingly:

$$P = P(\rho, T), \quad U = U(\rho, T).$$

If the caloric and the thermic equations of state are known, it is possible to define all thermodynamic properties of systems. However, to deduce the equations of state in the thermodynamics frameworks is impossible. Originally they were established by experiment, the first, most simple and best known is the thermal equation - the equation of state for ideal gas - the Clapeyron - Mendeleev equation. However, the equation of ideal gas, describes satisfactory behavior of real gases in a narrow range of the external parameter values. It is because the equation for ideal gas does not take into account presence of forces of interaction between molecules and their internal structure.

With the purpose to bypass this lack, attempts to pick up the empirical equations were undertaken. Probably the most well-known one is the (thermic) empiric equation of Van der Waals. The further search has resulted in numerous attempts to pick up more exact equations. From the simple equations with two empirical parameters quite good results give equations of Diterichi and Bertlo. From the equations using five individual constants, the most successful seems to be the equation of Bitty - Bridgeman.

During some time it was applied to draw up of tables for real gases in wide range of pressure, volume and temperature. "Individual" constants in the empirical equations for different fluids have, generally speaking, individual values. Now the most exact tables of properties of real gases and for calculation of thermodynamic functions of gases use the equation Benedict - Webb - Roobin with eleven individual parameters.

For non-ideal gases to the present moment it is offered more than 150 empirical thermal equations of state.

Kammerling-Onnes and Kees, not aspiring to minimize number of individual parameters, were first who have offered the equation of state as series in powers of molecular volume V^{-1} or pressure P

$$PV = RT\left(1 + \frac{B_2(T)}{V} + \frac{B_3(T)}{V^2} + \ldots\right), \qquad (1)$$

Where $B_n(T)$ is a virial factor. The use of virial equations of state was also allowed to reach the good agreement with experiment. It is even more important, because the power expansion in V^{-1} has obtained a reliable theoretical explanation in the frameworks of more general, in comparison with thermodynamics, statistical physics. Mayer and Bogoliubov derived the expansion for real gases, in the assumptions, that intermolecular interactions are short-range. Factors B_n thus manage to be calculated theoretically, if a kind of potential of interaction between molecules is known.

Thus it becomes clear, why the equations of state of real gas with two individual parameters are not enough for a good consistency with experiment. Statistical calculation shows, that presence of free parameters in the equation for energy interactions of molecules results in occurrence of individual constants in the equations of state.

The physical sense of virial factors B_n became clear also. The first one corresponds to ideal gas in which interaction between molecules is neglected. The second virial factor B_2 takes into account pair interaction between particles. The third B_3 is accordingly, threefold interaction and so on.

The difficulties connected to a choice of the equation of state, adequately describing a medium, have resulted in problems of nonlinear acoustics as the thermal equation of state, usually the equation of state in the form of virial expansion gets out, which for a perturbation of the pressure looks like:

$$P - P_0 = A(\frac{\rho - \rho_0}{\rho_0}) + \frac{B}{2}\left(\frac{\rho - \rho_0}{\rho_0}\right)^2 + \frac{C}{6}\left(\frac{\rho - \rho_0}{\rho_0}\right)^3 + \ldots, \qquad (2)$$

Here A, B, C - the coefficients of the expansion. The coefficient B/A after Beyer names the parameter of nonlinearity, it defines the relative contribution of the second order processes in investigated effects.

History of experimental evaluation of the nonlinear parameter B/A for various fluids totals more than 35 years. Size parameter in many respects defines many basic features of the behavior of a medium. In particular, parameter B/A defines characteristic lengths on which there is a formation shock wave. Knowledge of exact value of nonlinear parameter and its dependence on the temperature appears important in medical physics, for example, an influence on human bodies.

It is possible to tell, that now effective method of acoustic measurement of the first nonlinear parameter B/A are developed, giving satisfactory accuracy. Unfortunately, anything similar is impossible to tell concerning the second parameter nonlinearity C/A, included in (2). This parameter, obviously, defines the contribution of nonlinearity of the third order in a wave perturbation of a fluid. Cubic nonlinearity, according to theoretical researches is responsible such phenomena as self-focusing of an acoustic beam. It is obvious, that quantitative descriptions of specific effects in many respects are defined by value of constants of the virial expansion. On the other hand, it allows solving an inverse problem - under known quantitative characteristics of process to restore values of virial factors.

1. FORMULAS FOR SECOND AND THIRD HARMONICS FROM CIRCULAR PISTON EMITTER

In works [3, 4] formulas for the first, second and third harmonics of acoustic wave were obtained for perturbations with dimensionless amplitude of pressure Π on it and the given frequency ω. These formulas allow in principle to calculate nonlinear parameters B/A and C/A, by comparison amplitudes of harmonics behaviors with appropriate experimental measurements [6, 7].

Values of nonlinear parameter ε and, hence, the parameter B/A

$$\varepsilon = 1 + \frac{B}{2A}$$

may be easily found by comparison of theoretical and experimental curves for the second harmonics of the acoustic beam.

For simplification of comparison of analytical and experimental results we shall present the diffraction integrals, obtained in [3, 4]. For the first α and the second β harmonics it is possible to write down:

$$\alpha = \Pi I_1(\sigma, \xi), \qquad \beta = -2\Pi^2 \frac{(ka)^2}{A} \varepsilon I_2(\sigma, \xi), \tag{3}$$

where integrals I_1 и I_2 are equal accordingly

$$I_1 = \int_0^\infty J_1(\lambda) J_0(\lambda\xi) \exp\left(\frac{i\lambda^2}{4}\right) d\lambda \tag{4}$$

and

$$I_2 = -\int_0^\sigma \exp\left(-\frac{2i\xi}{\sigma - \sigma'} + 2\alpha_1 r_0 \sigma'\right) \frac{d\sigma'}{\sigma - \sigma'} \times$$
$$\times \int_0^\infty \alpha^2(\sigma', \xi') \exp\left(-\frac{2i\xi'^2}{\sigma - \sigma'}\right) J_0\left(\frac{4\xi\xi'}{\sigma - \sigma'}\right) \xi' d\xi'. \tag{5}$$

The diagrams the of integral I_2 is given for the second harmonic as a dimensionless function of the longitudinal coordinates σ on an axis of a beam $\xi = 0$ [4]. For more details about numerical scheme and plotting see [5].

Comparing our results and the data from [6, 7], we take the same values of constants which were used in the experiments for water: the radius a = 23 mm, ka = 97 ,external equilibrium pressure P_{00} = 258 kPa, equilibrium density of water $\rho_0 = 997 \frac{кг}{м^3}$, speed of a sound c_0 = 1492 m/s, temperature ,$T_0 = 25\,^0$C. Whence for the length of Rayleigh it is $r_0 = k\,\alpha^2/2 = 1{,}12$ m. Values of integral I_2 and experimental data for $<\rho_2>$ are given below:

X	$\lvert I_2 \rvert$	$< P_2 >$
0,2	0,034	13,0

The data from [6, 7] are given as the pressure of the Calculations of the factor ε are given with the second harmonic in percentage to peak pressure on the source. value ε = 3,6 ; while for nonlinear parameter B/A we obtain

$$\frac{B}{A} = 2(\varepsilon - 1) = 5{,}2,$$

that is in a good agreement with the data of other authors.

For the calculation of the second nonlinear parameter C/A we shall present the expression from [3, 4] for the third harmonic as, similar to (3)

$$< \gamma > = -i\Pi^3 \frac{3}{2} \frac{(ka)^2}{A^2} (2\varepsilon^2 (ka)^2 I_3 + \delta I_4). \tag{6}$$

Where

$$I_3(\sigma) = \int_0^\sigma \int_0^\infty I_1(\sigma', \xi) I_2(\sigma', \xi) \xi d\xi d\sigma',$$
$$I_4(\sigma) = \int_0^\sigma \int_0^\infty I_1^3(\sigma', \xi) \xi d\xi d\sigma'. \tag{7}$$

For evaluation of the numerical value of the second nonlinear parameter C/A we'll use the data from works [6, 7] for the second and third harmonics and calculations of integrals I_3 and I_4 by formulas (7) which comparison allows directly to establish the value of the parameter δ, describing the contribution of term with cubic nonlinearity. The parameter δ is linearly connected with the parameter C/A.

$$\delta = \frac{1}{6}\left(9\frac{B}{A} + \frac{9}{2}\frac{B^2}{A^2} - \frac{C}{A} + 6\right) \qquad (7)$$

It is necessary to take into account, that the functions determined by integrals (7), are complex and it is necessary to compare with experiment the absolute values of the sum of the integrals which are in brackets in the expression for $<\gamma>$ (6).

$$4(ka)^4 \varepsilon^4 |I_3|^2 + \delta^2 |I_4|^2 + 4(ka)^2 \varepsilon^2 \delta \left[\mathrm{Re}(I_3)\,\mathrm{Re}(I_4) + \mathrm{Im}(I_3)\,\mathrm{Im}(I_4)\right] =$$
$$= \frac{64}{9}\frac{A^4}{\Pi^4 (ka)^2}\left|< P_3 >^2\right|.$$

On fig. 1 the diagram of dependence of the third harmonic from axial coordinates σ is given.

2. THE C/A PARAMETER EVALUATION AS ILL-POSED PROBLEM AND REGULARIZATION

An evaluation of C/A from experiment, meet serious difficulties arise when trying to make exact numerical determination of the values of Π/A, which are connected to difficulties of experimental definition of values of peak pressure on a source and internal pressure in liquid. In calculations of the dimensionless parameter ε we have estimated the specified attitude as $8{,}6\cdot 10^4$. This gives values of parameter B/A, being in rather good agreements with experiment and it verifies formulas we use.

For the definition of the parameter C/A it is possible to compare the theoretical and experimental [6,7] diagrams for the third harmonic in two points. Thus the system of two algebraic equations of the second order for parameters ε and δ will be obtained. However there will appear above mentioned difficulties of comparison, and also a significant relative error in amplitudes definition. It makes such simple approach unstable to the specified error values. Hence because the second harmonic gives the much greater contribution, we arrive at the typical incorrect problem.

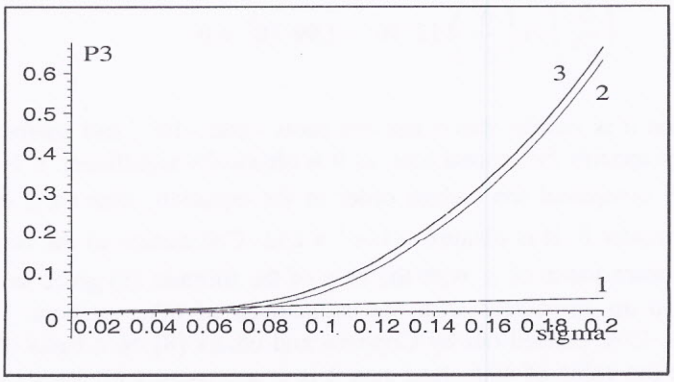

Fig. 1. ka = 97 . Dependence of the third harmonic $|< P_3 >|$ from axial coordinates σ; 1 - cubic nonlinearity, 2 - square-law nonlinearity, 3 - the sum.

However, this difficulty can be bypassed if to act in the following way. We shall compare the relation of amplitude of the third harmonic to the square of the second, then relation term in γ / β^2 disappears. Thus value of the parameter δ is defined at known ε from a expression

$$\frac{|<P_3>|^2}{|<P_2>|^4}\frac{16}{9}\varepsilon^4(ka)^4 10^4 =$$

$$= \frac{4(ka)^4\varepsilon^4|I_3|^2 + \delta^2|I_4|^2 + 4(ka)^2\varepsilon^2\delta\left[\mathrm{Re}(I_3)\mathrm{Re}(I_4) + \mathrm{Im}(I_3)\mathrm{Im}(I_4)\right]}{|I_2|^4}. \qquad (9)$$

The multiplier 10^4 in the left part of the equation has appeared because the experimental values $|<P_3>|$ and $|<P_2>|$ are given as the relation of absolute values of pressure of the appropriate harmonics to a peak pressure upon source, and are expressed in percentage.
Then evaluation the parameter C/A we shall use data, which are given below, for the values of I_2, I_3 and I_4 calculated by us and the values of amplitudes of the second and the third harmonics from [6, 7].

x	$\mathrm{Re}I_3$	$\mathrm{Im}I_4$	$\mathrm{Im}I_4$
0,4	$1{,}03\cdot10^{-3}$	$5{,}10\cdot10^{-2}$	$3{,}10\cdot10^{-2}$

$\lvert I_3\rvert$	$\lvert I_4\rvert$	$\lvert I_2\rvert$	$\lvert<P_3>\rvert$	$\lvert<P_2>\rvert$
$3{,}36\cdot10^{-3}$	$5{,}97\cdot10^{-2}$	$3{,}34\cdot10^{-1}$	10	23

Last columns represent the experimental of the pressure of the third and the second harmonics, accordingly. They are given, as it is told above, in percentage of peak pressure on the source Π.
Substituting the experimental data in (9), we obtain the quadratic equation for the parameter δ.

$$\left(\frac{\delta}{\varepsilon^2}\right)^2 + \left(\frac{\delta}{\varepsilon^2}\right)1{,}12\cdot10^7 - 1{,}99\cdot10^7 = 0.$$

From the equation it is visible, that it has two roots - one $\sim10^7$, and another about 1. Above given estimations specify the second root, as it is physically significant. It is easy to find it, if neglect by small composed the second order in the equation, then we'll obtain $\delta/\varepsilon^2 \approx 1{,}8$. Whence for parameter δ it is obtain $\delta = 1{,}8\varepsilon^2 \approx 23{,}1$. Calculation of the nonlinear parameter C/A using the known value of ε with the help of the formula (8) gives us the value C/A $\approx$ 36,1; which is in an agreement with the estimations of other authors. For example, the evaluation of the C/A, carried out by Coppens and others [8] on a basis of thermodynamic estimations give the value of 40,6. And also it is in a consent with results of estimations by Filipczynski and Grabowska [9] C/A=42 .

3. CONCLUSIONS AND DISCUSSION

Along Hadamard classification the problem of a medium parameter determination by a series of experiments belongs to ill-posed ones. In a strict mathematical sense the solution of such problem does not exist because the numbers of equations exceed the number of unknown values. In fact if we use some algorithm for evaluation of the parameter, using few experimental points, one arrives at overdetermined system even in the simplest algebraic case. Moreover in some case the problem looks unstable hence yields one of Hadamard ill-posed-problem conditions. In this case a small variation of the measurement results leads to a large deviation in the result of the parameter evaluation. In the first case the method of squares minimization is used [10]. In the second some regularization is necessary. In our case we consider linear equations (9) in which the left-hand side is taken from measurements while the coefficients in the right one are considered as exact, being calculated theoretically. It is the linear system for the $(k\ a)^2\ \varepsilon^2\delta$, δ^2 when $(k\ a)^2\ \varepsilon^2$ the coefficients are calculated theoretically but the right-hand-side are results of measurements. The value of ε is also considered as given, to b defined from the second harmonics measurements. So, consider such system for every set of l.h.s. values (more then two) as a source for the parameter determination. Our problem has both reasons to be ill-posed. We would use the method of regularization algorithm by Tikhonov [11]. Let us sketch the main features of the method briefly.

Let us consider the system·

$$A\,z = u\,, \tag{10}$$

for the vector z, when A is the matrix with elements a_{ij}, u is known vector. Let the r.h.s. of (10) is measured with the given error. Then instead of (10) we deal with an other system

$$\tilde{A}z = \tilde{u} \tag{11}$$

with the norms $\left\|\tilde{A} - A\right\| \le h$ and $\left\|\tilde{u} - u\right\| \le \delta$. As an approximate solution of (11) we shall take the vector z that minimize the functional

$$M^{\alpha}\left[z,\tilde{u},\tilde{A}\right] = \left\|\tilde{A}z - \tilde{u}\right\|^2 + \alpha\left\|z\right\|^2, \tag{12}$$

where the regularization parameter α is defined from the condition

$$\left\|\tilde{A}z^{\alpha} - u\right\| = 2(h\left\|z^{\alpha}\right\| + \delta) + \tilde{\mu}\,. \tag{13}$$

While the function $\varphi(\alpha) = \left\|\tilde{A}z - \tilde{u}\right\|^2$ increase and the $\psi(\alpha) = (h\left\|z^{\alpha}\right\| + \delta$ decrease. Therefore if the parameters h and δ are known, the α is determined uniquely. Here $\tilde{\mu} = \inf\left\|\tilde{A}z - \tilde{u}\right\|$.

He components of the vector z^{α} give solution of the linear algebraic system.

$$\alpha z_k^{\alpha} + \sum_{j=1}^{n} b_{kj} z_j^{\alpha} = d_k\,. \tag{14}$$

The notations are the following.

$$b_{kj} = \sum_{i=1}^{n} \tilde{a}_{ik}\tilde{a}_{ij} \qquad\qquad d_k = \sum_{i=1}^{n} a_{ik}\tilde{u}_i\,.$$

Starting from the seed value of the parameter of regularization α , we solve the system (14) ad find z^{α} .Having the vector z^{α} we plug it into (13) and find a new value of α . Hereafter we find the new value of z^{α} and so on.
In our case choosing the set of experimental points [4] one arrives at an over determined system. Using the method of minimal squares yields its normal form. Further by the regularization we obtain an optimal value of the parameter.
Accuracy of the method, under discussion unfortunately, is not too high. It is because, at first, not enough accuracy of experiments. So, mistakes in definition of values of parameters of nonlinearity are not consequence of the offered technique, and may be reduced by an increase of accuracy of measurements.

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