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Virial Coefficients From Cubic KZK

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We start from the cubic KZK equation for ultrasonics beam that accounts first, second and third powers of density in pressure Taylor series expansion. In a condition of moderate amplitude and nearfield one can use approximate solutions provided by perturbation method including terms resonant to the multiple frequencies on a transducer. We consider three resonant harmonics within Rayleigh distance range. The second and third harmonics averaged over the beam cross-section are expressed in terms of some standard integrals and nonlinear constants. Fourier transforms of a signal on a receiver are equalized to the results of the evaluation that give equations for the non-linear constants determination. This in turn allows to compute constants B/A and C/A of the equation of state (virial expansion).

1. Introduction

The main goal of this paper is an attempt to construct a recipe for a calculation of non-linear constants and, via them, a virial coefficients in the framework of Khokhlov - Zabolotskaya (KZ) model for a weak nonlinear acoustic beam. The coefficients of the virial expansion we define as derivatives from Taylor series expansion of a dimensionless acoustic pressure as the function of a dimensionless density variations.

$$\frac{p-p_0}{p_0}=A\left(\frac{\rho-\rho_0}{\rho_0}\right)+\frac{B}{2}\left(\frac{\rho-\rho_0}{\rho_0}\right)^2+\frac{C}{6}\left(\frac{\rho-\rho_0}{\rho_0}\right)^3$$

Recently some direct extension of the classic model [1] was introduced [2]. We imply that the authors worked inside the original scheme of [1]. That resulted in the cubic KZK (cKZK) equation with additional cubic term under the second time derivative and coefficient combined from A,B,C similar to [3,4], but the expression for the coefficient is different. The discrepancy with the results is appeared due to a crucial assumption about the potential character of a medium motion (the introduction of the potential velocity function) of [4]. We do not forget about famous Thomson theorem but adopted a strightforward derivation because the following reasons.

1.The acoustic field pulsation produced by a transducer very close to an oscillating piston exibit a drastically nontrivial character. Some direct measurements by a point (about 0.5 mm) microphone discovered a fine structure with quite possible curly motion [6]. This phenomenon surely may be generated by a transverse medium movement that may launch vertical Tollmien - Schlichting waves at the piston boundary layer . A transverse nonzero modes of a membrane (piston) oscillations also influence the nearest layers of the medium.

2. The equation of state we use following the classic scheme (see [5] as well) is however non-standard from the general thermodynamics. It perhaps pose a constraint. Therefore the theory is a phenomenological model. Moreover the direct calculations we delivered do not give the zero rotV meaning [7].

So we exploit here approximate solutions of the equation for a weak non-linear sound beam nearfield in an homogeneous medium that generalize Khokhlov-Zabolotskaya one [1] .The solutions are obtained and evaluated by the perturbation scheme originated from [8] and applied and developed in [2,7,9]. The equations for the nonlinear parameters (see also [10]) realised to be non-linear as it is shown in the third section. The solutions of this cKZK equation are presented and an attempt to calculate the third virial coefficient (more exactly C/A) is done at the last section.

2. List of Symbols and Cubic KZK Equation

c_0	velocity of sound,
p	pressure,
ρ	mass density,
$\mathbf{V}$	hydrodynamic velocity with components $\{V_x, V_y, V_z\}$,
f	linear frequency
ω	angular frequency $\omega = 2\pi f$,
k	wave number $k = \omega / c_0$
J_n	Bessel function of the n-th order,
a	transducer radius,
r	radial variable;
r_0	Rayleigh distance, $r_0 = ka^2/2$;
x,y,z	Cartesian variables ;
ε	parameter of quadric nonlinearity,
δ	parameter of cubic nonlinearity,
σ	dimensionless coordinate along acoustic axis, $\sigma = x/r_0$.
ξ	dimensionless coordinate across acoustic axis, $\xi = r/a$,
τ	retarded time $\tau = t - x/c_0$,
b	dissipation coefficient
Π	dimensionless amplitude on transducer.

The cubic KZK equation for the acoustic pressure in the form we derived earlier [7] (for the cKZK in different contexts see also [2],[3],[11]) reads

$$p_{\tau x} - \frac{c_0}{2} \cdot \Delta_{\perp} p - b' \cdot p_{\tau\tau\tau} = \frac{\varepsilon}{2 A c_0} \cdot (p^2)_{\tau\tau} - \frac{\delta}{2 A^2 c_0} (p^3)_{\tau\tau} , \quad (1)$$

where the nonlinear constants are

$$\varepsilon = 1 + B/2A \quad (2)$$

$$\delta = 1 + 3B/2A + 3B^2/4A^2 - C/6A \quad (3)$$

The constant in the dissipative (Kuznetsov) term is

$$b' = b/2c_0^3\rho_0.$$

3. Fourier Harmonics From Perturbations

A solution of the equation (1) should be expanded into the Fourier series by introducing an amplitude parameter $\lambda = \max|p/p_0|$ as a small parameter for the perturbation theory (Taylor) series

$$2p = \sum_{n=1}^{\infty} p_n \cdot \lambda^n \quad (4)$$

Here

$$p_n = p^{(n)}(x,y,z) \cdot \exp[i\omega\tau n] + \text{c.c.}$$

and c.c. means the complex conjugate

The substitution of (4) in (1) gives after transformations:

$$\frac{1}{2} \sum_{n=1}^{\infty} \lambda^n \cdot [(i\omega n p^{(n)}{}_x - c_0 \Delta_{\perp} p^{(n)} / 2 +$$
$$+ i n^3 \omega^3 b' p^{(n)}) e^{i\omega n\tau} + \text{c.c.}] =$$
$$-\frac{\omega^2 \varepsilon}{8 c_0 A} \sum_{l,m=1}^{\infty} \lambda^{l+m} (l+m)^2 \left[p^{(l)} p^{(m)} e^{i\omega\tau(l+m)} \right.$$
$$\left. + \text{c.c.} \right] +$$
$$+ \frac{\omega^2 \delta}{16 c_0 A^2} * \quad (5)$$
$$\sum_{l,m,k=1}^{\infty} \lambda^{l+m+k} [(l+m+k)^2 p^{(l)} p^{(m)} p^{(k)} \cdot$$
$$e^{i\omega\tau(l+m+k)} +$$
$$(l+m-k)^2 p^{(l)} p^{(m)} p^{(k)} \cdot$$
$$e^{i\omega\tau(l+m-k)} +$$
$$(l-m-k)^2 p^{(l)} p^{(m)} p^{(k)} \cdot$$
$$e^{i\omega\tau(l-m-k)} +$$
$$(l-m+k)^2 p^{(l)} p^{(m)} p^{(k)} \cdot$$
$$e^{i\omega\tau(l-m+k)} + \text{c.c.}]$$

The equation for the third harmonics is simplified if one introduce the new amplitudes

$$p^{(1)} = \alpha(r,x) \exp\left(-b' \omega^2 x\right),$$

$$p^{(2)} = \beta(r,x) \exp\left(-4 b' \omega^2 x\right),$$

$$p^{(3)} = \gamma(r,x) \exp\left(-9 b' \omega^2 x\right).$$

Here $r = \sqrt{y^2 + z^2}$ is the radial variable. Further we put $\lambda = 1$. The explicit solution of the linear problem for α with the cylindrical symmetry and boundary condition that follow from one for the acoustic pressure and a supposition that nonlinear generation of higher harmonics is negligible at the transducer surface.

$$\alpha(r,0) = \Pi, \qquad r < a,$$
$$\alpha(r,0) = 0, \qquad r > a.$$

where Π is the acoustic pressure amplitude on a circular piston transducer. The boundary conditions for β and γ are zeros. The resulting expressions for the functions β and γ may be taken from [8]. After transformations, one have

$$\alpha(\sigma,\xi) = \Pi \exp(-\alpha_1 \sigma r_0)\int_0^\infty J_1(\lambda) J_0(\lambda\xi) \exp\left(\frac{i\lambda^2\sigma}{4}\right) d\lambda \tag{6}$$

$$\beta(\sigma,\xi) = -\frac{\varepsilon (ka)^2}{A} e^{-4\alpha_1 \sigma r_0} \times \int_0^\sigma \exp\left(-\frac{2i\xi^2}{\sigma-\sigma'} + i4\alpha_1 r_0 \sigma'\right)\frac{d\sigma'}{\sigma-\sigma'} \times \times \int_0^\infty \alpha^2(\sigma',\xi') J_0\left(\frac{4\xi\xi'}{\sigma-\sigma'}\right) \exp\left(-\frac{2i\xi'^2}{\sigma-\sigma'}\right)\xi' d\xi' \tag{7}$$

where $\alpha_1 = b\omega^2/2\rho_0 c^3$ - linear absorbtion coefficient. Dimensionless coordinates $\xi = r/a$ and $\sigma = x/r_0$ are introduced.

The results are obtained by the Green function method for the axial symmetry of equation and boundary condition for pressure and contain a minimal number of integrals (see e.g. [2, 3], ibid.). It is the case of the uniformly exited plain circular piston. The equation for the third harmonics is:

$$6 i\omega \gamma_x = c_0 \Delta_\perp \gamma - [9 \frac{\varepsilon}{c_0 A}\omega^2 \alpha\beta - \frac{9}{4}\omega^2 \frac{\delta}{c_0 A^2}\alpha^3 \cdot \exp\left(2b'\omega^2 x\right)] \exp\left(4b'\omega^2 x\right).$$

Now we restrict ourselves by the averaged signal at receiver. We use the infinite receiver as a good approximation for a receiver that is bigger than the beam cross-section. Integrating over the infinite receiver at the point x, one have:

$$\langle\gamma\rangle = \frac{1}{\pi a^2}\int_0^\infty 2\pi r\gamma\, dr = = i\frac{3\omega}{a^2 c_0 A}\varepsilon\int_0^x \exp\left(4b'w^2x\right)\int_0^\infty \alpha\beta\, r dr dx - - i\frac{3\omega}{4a^2 c_0 A^2}\delta\int_0^x \exp\left(6b'\omega^2 x\right)\int_0^\infty \alpha^3 r dr dx$$

The integrals of the term containing transverse Laplacian vanish as the beam field is spatially restricted. In fact, due to the cylindrical symmetry the integral by the radial variable gives

$$\int_0^\infty r\Delta_\perp \gamma\, dr = \int_0^\infty \frac{\partial}{\partial r} r \frac{\partial}{\partial r}\gamma\, dr = 0 \tag{8}$$

For $r\frac{\partial}{\partial r}\gamma$ is zero at $r = \infty$ and $r = 0$ due to the strong decay of the amplitude of the third harmonics and its derivatives at infinity. After simple scale transformations to the same spatial variables as for α, β: $\xi = r/a$, $\sigma = x/r_0$, one has

$$\langle\gamma(\sigma)\rangle = i\frac{3(ka)^2}{2A}\varepsilon\int_0^\sigma \exp\left(4b'\omega^2 r_0\sigma'\right)\int_0^\infty \alpha\beta\xi\, d\xi\, d\sigma' - - i\frac{3(ka)^2}{8A^2}\delta\int_0^\sigma \exp\left(6b'\omega^2 r_0 \sigma'\right)\int_0^\infty \alpha^3 \xi\, d\xi\, d\sigma' \tag{9}$$

4. Evaluation of the Virial Coefficient.

For the evaluation of the virial coefficients B/A and C/A we will use experimental data from the papers [6,9]. The meaning of the parameter ε and as a corollary the value of the parameter B/A one can easily find from the expression and data for the second harmonics. We do it as a test for the coefficient in cKZK by the quadratic term . It is evaluated from the times of [10]. Comparing the data from [9], for example

Table 1. *Second harmonics integrals.*

σ	Re(β)	Im(β)	$\lvert\beta\rvert$
0.362	-0.0162	-0.254	0.304

and the results of evaluation by (7) we extract the constant ε.

Now we define a dimensionless solution of the cKZK by (4) generated by the uniformly exited piston with the dimensionless amplitude pressure Π on it and definite frequency ω. Let us define the following diffraction integrals for α, β via:

$$\alpha = \Pi \cdot I_1(\sigma,\xi), \quad \beta = -\Pi^2 \frac{(ka)^2}{A}\varepsilon I_2(\sigma,\xi), \tag{10}$$

The forms of α and β (see the explicit expressions in the dimensionless variables (7)) are taken from [2] that is the transformed version from [8]. The averaged meanings of $<\gamma>$ (see (9)) is provided by

$$\langle\gamma\rangle = -i\frac{3\Pi^3}{8}\frac{(ka)^2}{A^2}\left(4\varepsilon^2(ka)^2 I_3 + \delta I_4\right) \quad (11)$$

The coefficient functions I_3, I_4 are proportional to integrals of $\alpha\beta$ and α^3 correspondingly. When $b=0$ (no dissipation) the expressions are more compact (9):

$$I_3(\sigma) = \int_0^\sigma\int_0^\infty I_1(\sigma',\xi)I_2(\sigma',\xi)\xi\,d\xi\,d\sigma' \quad (12)$$

$$I_4(\sigma) = \int_0^\sigma\int_0^\infty I_1(\sigma',\xi)^3\,\xi\,d\xi\,d\sigma' \quad (13)$$

For the evaluation of the virial coefficient *C/A* we use experimental data from the papers [6]. Especially we should note that in the work [6] the data about amplitude of perturbation is in form of percent of *Π*. Comparing the data which are derived by the formula for $|\beta|$ (that is the corollary of (7)) with experimental data we can see that $\varepsilon = 3.85$ that gives an estimation $B/A = 5.7$.

For definition of parameters δ and *C/A* we use data about the third harmonics of acoustic perturbation. The examples of the results of integrals calculations are given in the following table:

Table 2. *Modules of integrals for the third harmonics evaluation.*

σ	$\lvert I_3\rvert$	$\lvert I_4\rvert$
0.088	0.0000109	0.00173
0.137	0.0000373	0.00291
0.176	0.0000683	0.00400

Because of the experimental data in the paper [6] are given for $|\langle\beta'\rangle|$ and $|\langle\gamma'\rangle|$ let us transform the formula (11) to the following view:

$$16(ka)^4\varepsilon^4|I_3|^2 + \delta^2|I_4|^2 + 8(ka)^2\varepsilon^2\delta\left[\mathrm{Re}(I_3)\mathrm{Re}(I_4) + \mathrm{Im}(I_3)\mathrm{Im}(I_4)\right] = \frac{4}{9}\frac{A^4}{\Pi^4(ka)^2}|\langle\gamma'\rangle|^2 \quad (14)$$

We should remember that the harmonics amplitudes β', γ' are given also in percents of *Π*. The values of a real and imaginary parts of the integrals are given below for the same distances from the origin as in the previous table 2..

Table 3. *Real and imaginary parts of the third harmonics integrals.*

Re(I_3)	Im(I_3)	Re(I_4)	Im(I_4)
0.000009	0.00000	0.00173	-0.000041
0.000024	0.00002	0.00287	0.000440
0.000025	0.00006	0.00392	0.000758

There exist two ways to continue. First is by substitution into the equation the value of ε (we used the data for $x=0.2$), which was found above, and experimental data for γ from [5], and hence one arrive to a quadratic equation for δ. So we find that $\delta = 10^4$. Also we evaluate $C/A = 10^4$. We had divided the right-hand sides of the equation (14) at the different points and therefore excluded a mistake in the amplitude on the piston. The root of the quadric equation we choose by a physical reasons [12]. We should emphasize that the values we mention here may be considered only as an estimation of orders because the precision of experimental data seems to be low for such determination. Moreover the parameters of the experiment should be choosen specially. For example, it is better to take the parameter ka of less order to diminish the instability of the estimation.

For the estimations we used the following values of parameters:

$ka = 97$;

$A = 7.14$;

$\Pi = 4.5\ 10^{-4}$.

Second way is the use of experimental data for three points and derive this system of three linear equation for parameters ε^4, δ^2 and ε^2, δ of the form (14). After calculation we have, for example.

$\varepsilon^4 = 237$.

The result is close to the estimation given before and apparently leads to the close meanings for the parameter C/A.

As it was mentioned in the introduction during the calculation of integrals of a rapidly oscillating integrand of the expressions for $p^{(i)}$ we used the PASCAL program and the special algorithm for such case. The approximation of the integrands by this algorithm is more exact and converge more rapidly in comparison with one used in [2,7,9]. It gives a possibility for a rapid evaluation of constants in a technical applications of the theory.

For the averaged third harmonics the equation is obtained just analogously to [2,7] and to one mentioned in the previous section.

We see that the mean value of the third harmonics is the sum of two terms and both are proportional to Π^3. It means that the terms belong to the same order of nonlinearity. The dependence on parameters A,B,C is considerably different, moreover, the structure of the integrals and therefore the dependencies of the terms on distance σ is different as well. Hence one can estimate the constants from measurements of the third harmonics contribution as the function of distance in the nearfield. It is important however to determine the range of amplitudes and distances where the third harmonics is big enough and the results of the approximations are yet valid. For the purpose we estimate the result using the typical values of parameters from [2].

The comparison of the results of numerical calculation of the integrals are given at the Fig.3 at [7], where .the contributions of the terms proportional to $\alpha\beta$ and α^3 are evaluated separately .

Let us discuss now the results of the calculations. We would repeat that the curves for the terms in the expression (11) are essentially different that allow to divide the contributions and estimate the virial coefficients B and C. It is interesting that the sum of the curves at distances between 0 and 0.5 fit better the numerical calculations that the curve reproduced in [9] (originated from the usual KZK equation). It is understandable that in the range of big amplitudes the successive approximations that we develop here fails. But at "not very big" amplitude of the signal range we would hope that the difference between KZK (or generalized KZK (cKZK)) and our perturbation scheme is small. It is really supported by the comparison between our calculation and direct finite-difference integration approach [6,9].

When we substitute the expressions for α and β in the equation (6) and integrate it, we go to the formula for averaged third harmonics at a distance z. The resulting formula for the small distances (where $\exp(4b'\omega^2x) \cong 1+4b'\omega^2x$) may be expressed as a linear combination of ε'^2 , δ and $b'\varepsilon'^2$, etc. with diffraction integrals that depend only on x. It allows us to simplify calculations of nonlinear and absorption parameters by fitting of measurements to theoretical curves.

5.Conclusion

We see the physical applications of the higher terms account in the equation of state (virial coefficients) determination that are connected with the general theory of the condensed matter. The equation of state may help to calculate the coefficients of a model equation [11] or estimate models validity as in [12] where the choice of the model strongly influences the molecular dynamics simulations (a form of a potential of the intermolecular interaction). We also hope for such a development of the theory that may give rise to a environment physics aspects applications.

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