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Relations between the longitudinal and transverse sound velocities in strongly coupled Yukawa fluids

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Two useful relations between the longitudinal and transverse sound velocities of the strongly coupled single component Yukawa fluids are derived. The first relates the sound velocities given by the quasilocalized charge approximation (QLCA) to the excess pressure of the system. This is shown to be a mathematical identity within QLCA, applicable to any soft isotropic interaction potential. The second relates the same quantities to the fluid sound velocity obtained via the thermodynamic route. Both three-dimensional and two-dimensional cases are considered. The accuracy of the relations is verified using the available results based on direct numerical simulations. [http://dx.doi.org/10.1063/1.4942171]

The quasilocalized charge approximation[1] (QLCA) is a powerful tool to describe collective mode dispersion in systems of strongly interacting particles. Developed originally for the Coulomb liquids,[2] in the last two decades, it has been successively applied to various strongly coupled systems, including in particular, the one-component-plasma (OCP) and Yukawa systems in both three (3D) and two (2D) dimensions.[1,3–6] Comparison with direct numerical simulations documented good performance of the approach, at least for weakly and moderately screened systems (OCP and Yukawa fluids with interparticle separation smaller than several screening lengths).[4,6–8]

In this Brief Communication, we focus on single component Yukawa systems and put forward two simple relations between the longitudinal and transverse sound velocities, resulting from the QLCA approach. Yukawa systems are characterized by the repulsive interaction potential of the form $V(r) = (Q^2/r)\exp(-r/\lambda)$, where Q is the particle charge, λ is the screening length, and r is the distance between a pair of particles. The phase state of the system is conventionally described by the two dimensionless parameters,[9] which are the coupling parameter $\Gamma = Q^2/aT$ and the screening parameter $\kappa = a/\lambda$. Here, T is the system temperature (in energy units), n is the particle density, and $a = (4\pi n/3)^{-1/3}$ (3D) or $a = (\pi n)^{-1/2}$ (2D) denote the mean interparticle separation. The Yukawa potential is a reasonable starting point to model interactions in complex (dusty) plasmas and colloidal dispersions,[10,11] although in many cases the actual interactions (in particular, their long-range asymptote) are much more complex.[12–19]

For a given interaction potential, the QLCA approach requires the equilibrium radial distribution function (RDF), $g(r)$, as an input, characterizing the spatial order in the system. Then, the dispersion relations of the longitudinal and transverse modes can be easily calculated. In the long-wavelength limit, Yukawa fluids exhibit acoustic dispersion for both longitudinal and transverse modes. The expressions for the corresponding sound velocities in the 3D case are[4,6]

$$C_L^2 = \frac{2}{15}\omega_{\rm p}^2 a^2 \int_0^\infty x g(x) e^{-\kappa x}\left(1+\kappa x+\frac{3}{4}\kappa^2x^2\right)dx,$$
$$C_T^2 = -\frac{1}{15}\omega_{\rm p}^2 a^2 \int_0^\infty x g(x) e^{-\kappa x}\left(1+\kappa x-\frac{1}{2}\kappa^2x^2\right)dx,$$

where $\omega_{\rm p} = \sqrt{4\pi Q^2 n/m}$ is the 3D particle-plasma frequency, m is the particle mass, and $x = r/a$ is the reduced distance. The main idea is to produce such a combination of C_L^2 and C_T^2 that the terms proportional to κ^2x^2 under the integrals cancel each other, and relate the rest to the reduced excess pressure, which, according to the virial expression,[20] is

$$p_{\rm ex} = \frac{\Gamma}{2}\int_0^\infty x g(x) e^{-\kappa x}(1+\kappa x)dx.$$

After some transparent algebra, we get

$$c_L^2 - 3c_T^2 = 2p_{\rm ex}, \tag{1}$$

where c_L and c_T are expressed in units of thermal velocity, $v_T = \sqrt{T/m}$. Note that since $p_{\rm ex}$ is always positive for a single component system of repulsive particles, Eq. (1) implies $c_L > \sqrt{3}c_T$, which is to be compared with the general inequality for elastic waves in an isotropic medium,[21] $c_L > \sqrt{2}c_T$.

For the 2D case, the sound velocities can be expressed as[5,6]

$$C_L^2 = \frac{1}{16}\omega_{\rm p}^2 a^2 \int_0^\infty g(x) e^{-\kappa x}(5+5\kappa x+3\kappa^2x^2)dx,$$
$$C_T^2 = -\frac{1}{16}\omega_{\rm p}^2 a^2 \int_0^\infty g(x) e^{-\kappa x}(1+\kappa x-\kappa^2x^2)dx,$$

where $\omega_{\rm p} = \sqrt{2\pi Q^2 n/ma}$ is the 2D particle-plasma frequency. Following the procedure similar to the 3D case and using the 2D version of the pressure equation

$$p_{\rm ex}=\frac{\Gamma}{2}\int_0^\infty g(x)e^{-\kappa x}(1+\kappa x)dx,$$

we immediately recover Eq. (1). Thus, Eq. (1) is an exact result for Yukawa fluids within the QLCA theory, applicable in both 3D and 2D cases.

Moreover, it can be shown that Eq. (1) is a mathematical identity within the QLCA, which holds for any smooth (two first derivative of the potential with respect to distance are needed) isotropic interaction potential $V(r)$. This is a nice exercise; the derivation is fully analogous to the special case of Yukawa systems considered above. Only a brief sketch of the derivation is therefore given. The interaction potential is presented in the form $V(r)=\epsilon f(r/a)$, where ϵ is the energy scale. The generic expressions for the sound velocities within QLCA are then

$$C_{L/T}^2=\omega_0^2a^2\int_0^\infty dx x^{\mathcal{D}+1}g(x)\left[\mathcal{A}\frac{f'(x)}{x}+\mathcal{B}f''(x)\right], \quad (2)$$

where $\mathcal{D}(=2,3)$ is the dimensionality, $\omega_0^{\rm 3D}=\sqrt{4\pi n\epsilon a/m}$ and $\omega_0^{\rm 2D}=\sqrt{2\pi n\epsilon/m}$ are the nominal plasma frequencies in 3D and 2D, respectively. The coefficients $\mathcal{A}$ and $\mathcal{B}$ for the longitudinal and transverse modes in 3D and 2D are summarized in Table I. Combining this with the generic equation of state

$$p_{\rm ex}=-\frac{\omega_0^2a^2}{2\mathcal{D}v_T^2}\int_0^\infty dx x^{\mathcal{D}}g(x)f'(x), \quad (3)$$

Eq. (1) is immediately obtained.

Thus, the applicability of Eq. (1) is not limited to the strongly coupled Yukawa fluids. However, it can be particularly useful for Yukawa fluids, because accurate practical expressions for $p_{\rm ex}$ are available in this case.[22–25] Its consistency with the numerical results available in the literature will be verified below.

Now, we turn to the second relation between the longitudinal and transverse sound velocities. It originates from the observation that for an isotropic elastic medium, the longitudinal and transverse sound velocities can be expressed in terms of the bulk modulus, K, and shear modulus, G. For the 3D case, we have[21]

$$C_L=\sqrt{\frac{3K+4G}{3\rho}},\quad C_T=\sqrt{\frac{G}{\rho}},$$

where $\rho=mn$ is the mass density. Similarly, for the 2D case, we have

$$C_L=\sqrt{\frac{K+G}{\rho}},\quad C_T=\sqrt{\frac{G}{\rho}}.$$

TABLE I. The coefficients $\mathcal{A}_{L/T}$ and $\mathcal{B}_{L/T}$ appearing in Eq. (2) for the longitudinal (L) and transverse (T) sound velocities of simple strongly coupled systems with isotropic interactions in three (3D) and two (2D) dimensions.

$\mathcal{D}$	$\mathcal{A}_L$	$\mathcal{B}_L$	$\mathcal{A}_T$	$\mathcal{B}_T$
3D	$\frac{1}{15}$	$\frac{1}{10}$	$\frac{2}{15}$	$\frac{1}{30}$
2D	$\frac{1}{16}$	$\frac{3}{16}$	$\frac{3}{16}$	$\frac{1}{16}$

The thermodynamic sound velocity is defined as

$$C_{\rm Th}=\sqrt{\frac{K}{\rho}}.$$

Note that in the limit of strong coupling, the adiabatic index tends to unity for soft repulsive interactions, and the difference between the conventional adiabatic sound velocity and isothermal sound velocity becomes insignificant. We end up with the following relations between the longitudinal and transverse sound velocities

$$\begin{aligned} c_L^2-\frac{4}{3}c_T^2&=c_{\rm Th}^2, \quad (3D)\\ c_L^2-c_T^2&=c_{\rm Th}^2, \quad (2D)\end{aligned} \quad (4)$$

where the velocities are again expressed in units of the thermal velocity. The second of these relations has been discussed in the context of the acoustic velocities in the classical two-dimensional dipole lattice (point particles interacting via the repulsive $\propto 1/r^3$ potential).[26] Here, it is demonstrated that Eq. (4) is also relevant to the strongly coupled Yukawa fluids (at least in some vicinity of the fluid-solid phase transition), in both 3D and 2D cases, when c_L and c_T are evaluated using the QLCA approach.

We have verified the consistency of Eqs. (1) and (4) with the available results from theory and simulations. The results are summarized in Tables II (3D case) and III (2D case). The values of c_L and c_T were obtained using the original QLCA, combined with MD simulations to produce the radial distribution functions, in Refs. 27 (3D case) and 6 (2D case). The excess pressure has been calculated using the practical expressions proposed in Refs. 22 (3D case) and 28 (2D case). The thermodynamic sound velocities have been obtained using the procedures detailed in Refs. 29 (3D case) and 30 (2D case). The pairs of (κ,Γ) values appearing in Tables II and III correspond to the isomorphs[31] $\Gamma/\Gamma_{\rm m}\simeq 0.8$ (3D) and $\Gamma/\Gamma_{\rm m}\simeq 0.9$ (2D), where $\Gamma_{\rm m}$ is the coupling parameter at the fluid-solid phase transition, i.e., in all cases, the system is in fluid state, but relatively close to the crystallization.

In the 3D case, Eq. (1) is satisfied to a very good accuracy. Equation (4) demonstrates excellent accuracy in the strongly coupled regime near the fluid-solid phase transition. For the 2D case, the agreement is also good, except for the state point with the largest screening strength, $\kappa=3.0$. This is not very surprising, because $p_{\rm ex}$ and $c_{\rm Th}$ have been estimated using the thermodynamic approach applicable for soft

TABLE II. The longitudinal (c_L) and transverse (c_T) sound velocities (in units of thermal velocity) of strongly coupled Yukawa fluids in 3D evaluated using the QLCA approach with the input of RDFs from direct MD simulations.[27] The excess pressure, $p_{\rm ex}$, and the thermodynamic sound velocity, $c_{\rm Th}$, are obtained using the expressions from Refs. 22 and 29, respectively.

κ	Γ	c_L	c_T	$c_L^2-3c_T^2$	$2p_{\rm ex}$	$\sqrt{c_L^2-\frac{4}{3}c_T^2}$	$c_{\rm Th}$
0.5	145	41.29	3.98	1657.34	1657.56	41.03	41.06
1.0	180	22.29	4.07	447.15	446.30	21.79	21.81
2.0	370	13.83	4.26	136.83	135.28	12.93	12.93
3.0	990	11.55	4.41	75.06	73.79	10.37	10.37

TABLE III. The longitudinal (c_L) and transverse (c_T) sound velocities (in units of thermal velocity) of strongly coupled Yukawa fluids in 2D evaluated using the QLCA approach with the input of RDFs from direct MD simulationsi.[6] The excess pressure, p_{ex}, and the thermodynamic sound velocity, c_{Th}, are calculated using the expressions from Refs. 28 and 30, respectively.

κ	Γ	c_L	c_T	$c_L^2 - 3c_T^2$	$2p_{ex}$	$\sqrt{c_L^2 - c_T^2}$	c_{Th}
1.0	163	14.62	4.12	162.82	162.70	14.03	14.10
2.0	362	11.25	4.28	71.61	69.78	10.40	10.38
3.0	1033	10.23	4.32	48.67	38.48	9.27	9.98

repulsive interactions near the OCP-limit.[28] It has been documented to deliver good accuracy for $\kappa \lesssim 2.0$, but apparently becomes much less relevant at $\kappa = 3.0$.

To conclude, two relations between the longitudinal and transverse sound velocities of strongly coupled Yukawa fluids in 3D and 2D have been discussed and verified. The first [Eq. (1)] is a mathematical identity within QLCA for arbitrary smooth isotropic interactions in both 3D and 2D. Strongly coupled Yukawa fluids represent just one example of its application. The second [Eq. (4)] demonstrates that in strongly coupled Yukawa fluids, the QLCA longitudinal and transverse sound velocities satisfy the general relationships for elastic waves in an isotropic medium. It is very likely that it applies also to other interaction potentials, but no rigorous proof has been presented, and hence, this has to be verified in each particular case. The discussed relationships are likely to be useful in the context of complex (dusty) plasmas, where the repulsive Yukawa potential can serve as a reasonable zero approximation of the actual interactions between highly charged microparticles, and the studies of waves and instabilities in the regime of strong coupling constitute a major research topic.

Note Added in Proof: It came to the author's attention that S. Takeno and M. Goda [Prog. Theor. Phys. (1971) 45(2): 331–352; DOI: 10.1143/PTP.45.331S] previously derived a three-dimensional version of the elastic sound velocity, see Eqs. (4.19) and (4.20), which is comparable to Eq. (2).

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[1] K. I. Golden and G. J. Kalman, Phys. Plasmas **7**, 14 (2000).
[2] G. Kalman and K. I. Golden, Phys. Rev. A **41**, 5516 (1990).
[3] M. Rosenberg and G. Kalman, Phys. Rev. E **56**, 7166 (1997).
[4] G. Kalman, M. Rosenberg, and H. E. DeWitt, Phys. Rev. Lett. **84**, 6030 (2000).
[5] G. J. Kalman, P. Hartmann, Z. Donkó, and M. Rosenberg, Phys. Rev. Lett. **92**, 065001 (2004).
[6] Z. Donko, G. J. Kalman, and P. Hartmann, J. Phys.: Condens. Matter **20**, 413101 (2008).
[7] H. Ohta and S. Hamaguchi, Phys. Rev. Lett. **84**, 6026 (2000).
[8] S. Hamaguchi and H. Ohta, Phys. Scr. **T89**, 127 (2001).
[9] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, Phys. Rev. E **56**, 4671 (1997).
[10] V. E. Fortov, A. Ivlev, S. Khrapak, A. Khrapak, and G. Morfill, Phys. Rep. **421**, 1 (2005).
[11] A. Ivlev, H. Lowen, G. Morfill, and C. P. Royall, *Complex Plasmas and Colloidal Dispersions: Particle-Resolved Studies of Classical Liquids and Solids*, Series in Soft Condensed Matter (World Scientific Publishing Company, 2012).
[12] V. N. Tsytovich, Usp. Fiz. Nauk **40**, 53 (1997).
[13] V. E. Fortov, A. G. Khrapak, S. A. Khrapak, V. I. Molotkov, and O. F. Petrov, Usp. Fiz. Nauk **47**, 447 (2004).
[14] S. A. Khrapak, G. E. Morfill, V. E. Fortov, L. G. D'yachkov, A. G. Khrapak, and O. F. Petrov, Phys. Rev. Lett. **99**, 055003 (2007).
[15] A. V. Filippov, A. G. Zagorodny, A. I. Momot, A. F. Pal, and A. N. Starostin, JETP **104**, 147 (2007).
[16] S. A. Khrapak, B. A. Klumov, and G. E. Morfill, Phys. Rev. Lett. **100**, 225003 (2008).
[17] R. Kompaneets, G. E. Morfill, and A. V. Ivlev, Phys. Plasmas **16**, 043705 (2009).
[18] S. A. Khrapak, A. V. Ivlev, and G. E. Morfill, Phys. Plasmas **17**, 042107 (2010).
[19] I. L. Semenov, S. A. Khrapak, and H. M. Thomas, Phys. Plasmas **22**, 053704 (2015).
[20] J. P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Elsevier Academic Press, London, Burlington, MA, 2006).
[21] L. D. Landau, L. P. Pitaevskii, A. M. Kosevich, and E. Lifshitz, *Theory of Elasticity*, 3rd ed., Course of Theoretical Physics Vol. 7 (Butterworth-Heinemann, 1986).
[22] S. A. Khrapak and H. M. Thomas, Phys. Rev. E **91**, 023108 (2015).
[23] S. A. Khrapak, N. P. Kryuchkov, S. O. Yurchenko, and H. M. Thomas, J. Chem. Phys. **142**, 194903 (2015).
[24] P. Tolias, S. Ratynskaia, and U. de Angelis, Phys. Plasmas **22**, 083703 (2015).
[25] S. A. Khrapak, Plasma Phys. Controlled Fusion **58**, 014022 (2016).
[26] K. I. Golden, G. J. Kalman, P. Hartmann, and Z. Donkó, Phys. Rev. E **82**, 036402 (2010).
[27] S. A. Khrapak, B. Klumov, L. Couëdel, and H. M. Thomas, Phys. Plasmas **23**, 023702 (2016).
[28] S. A. Khrapak, I. L. Semenov, L. Couëdel, and H. M. Thomas, Phys. Plasmas **22**, 083706 (2015).
[29] S. A. Khrapak and H. M. Thomas, Phys. Rev. E **91**, 033110 (2015).
[30] I. L. Semenov, S. A. Khrapak, and H. M. Thomas, Phys. Plasmas **22**, 114504 (2015).
[31] A. A. Veldhorst, T. B. Schrøder, and J. C. Dyre, Phys. Plasmas **22**, 073705 (2015).