Breathing Mode for Systems of Interacting Particles

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We study the breathing mode in systems of trapped interacting particles. Our approach, based on a dynamical ansatz in the first equation of the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy allows us to tackle at once a wide range of power-law interactions and interaction strengths, at linear and nonlinear levels. This both puts in a common framework various results scattered in the literature, and by widely generalizing these, emphasizes universal characters of this breathing mode. Our findings are supported by direct numerical simulations.

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Systems of trapped interacting particles are studied in many areas of physics: confined plasmas, trapped cold atoms, Bose-Einstein condensates, colloidal particles, trapped ions, astrophysical systems, the latter ones being self-confined by the interactions. The low-lying oscillatory modes of these systems are a natural object of study, as they are an important nondestructive tool to characterize the system and gain insight into the collective effects at work. As a consequence, there is abundant literature on the subject, corresponding to very diverse physical situations: (i) systems with short-range interactions, such as classical gases or shielded Coulomb interaction and (ii) systems with long-range interactions, such as non-neutral plasmas, Coulomb crystals, or astrophysical systems, in which the interactions may be weak (gases) or strong (liquids or crystals).

Diverse approaches and techniques are naturally used to investigate these phenomena. A trapped classical gas of interacting particles is studied using a Boltzmann-Vlasov equation in [1], where the nonlinear dynamics is approximated with a scaling ansatz, which captures the collective effects. Such an ansatz was used earlier for the Gross-Pitaevskii equation in [2,3]. In the confined plasma context, the problem is often studied through hydrodynamical equations, in the so-called "cold fluid approximation" [4], where the dispersion relation for fluid modes in a cold spheroidal plasma is derived. Following an idea of [5], Ref. [6] gives an approximate solution to the breathing mode of a 1D confined plasma beyond the cold fluid approximation, using an *ad hoc* closure of the hydrodynamical equations. Monopole modes of dusty plasmas interacting with a Yukawa potential are investigated in [7,8]. The breathing mode of trapped ions or colloids interacting via Coulomb or Yukawa interactions has been studied in 1D [9,10], 2D [11,12], and 3D [13] for crystallized systems, by a direct diagonalization of the linearized Newtonian equations of motion. Finally, breathing oscillations with attractive interactions have been studied in an astrophysical context using the virial theorem [14].

Each method applies to a specific situation: Newton equations are adapted to a crystallized state with negligible thermal fluctuations, linearization assumes a small amplitude, the Vlasov equation is limited to long-range interactions and weak correlations. Yet in all cases a similar equation for the breathing mode is obtained. In particular, it is intriguing that kinetic descriptions assuming small correlations between particles, fluid descriptions, and perturbative expansions around a crystallized state all yield similar predictions for the breathing mode, at linear and nonlinear levels. This stunning situation calls for a unified theory. In the limit of zero temperature, or equivalently infinitely strong interactions, such an endeavor has recently been undertaken in the linear regime [15]. A more general situation summarizing the different possible regimes for a binary isotropic power-law interparticle force $F(r) \sim 1/r^k$ in d space dimensions is shown in a diagram Fig. 1. We have organized the different cases along two axes. On the

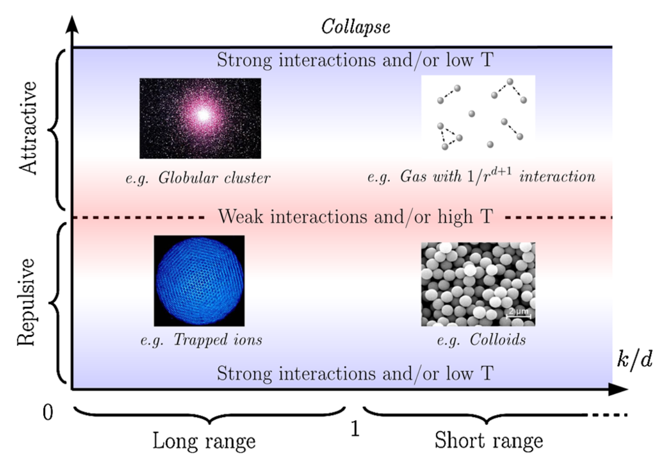

FIG. 1 (color online). Diagram of the different regimes for the breathing mode. On the horizontal axis, the interaction range, measured by k/d. The interaction strength is changing along the vertical axis. Pictures of some physical examples are inserted for illustration.

horizontal axis we represent the interaction range, which we will call long range if $k/d \leq 1$ and short range otherwise. The case $k/d \leq 1$ corresponds to nonintegrable forces at large distances [16]. The vertical axis represents the interaction strength with respect to the thermal energy.

In this Letter, we present a theory of the breathing mode of systems of classical trapped interacting particles which classifies many cases studied in the references cited above in a common framework. The theory is valid both for short-range and long-range interactions, for any dimension, and for various interaction strengths. However, for short-range attractive interactions strong instabilities due to the unregularized short-range singularity are expected, and for strongly attractive long-range interacting systems, a gravitational-like collapse sets in. We did not verify to what extent our model may capture relevant features in these situations. Our theory describes both linear as well as nonlinear oscillations, and isolated systems as well as systems in contact with a thermal bath.

We consider a system of particles confined by a harmonic spherical trapping force $\mathbf{F}_{\rm trap}(\mathbf{r}) = -\omega_0^2\mathbf{r}$, with binary interaction forces $\mathbf{F}_{\rm int}$. In the canonical setting, particles are subjected to a positive constant friction k and diffusion D. In the microcanonical setting, $k = 0$, $D = 0$, and the dynamics is Hamiltonian. To overcome the limitations in the validity of the Vlasov equation, we describe the cloud of particles by its one-particle and two-particles distribution functions $f(\mathbf{r}_1, \mathbf{v}_1, t)$ and $g(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t)$. We start from the first equation of the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy, which we complement by a Fokker-Planck operator [18] to include the temperature in the canonical case:

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{r}}\cdot(\mathbf{v}f) + \mathbf{F}_{\rm trap}\cdot\nabla_{\mathbf{v}}f + C[g] = D\Delta_{\mathbf{v}}f + k\nabla_{\mathbf{v}}\cdot(\mathbf{v}f), \tag{1}$$

where $C[g]$ is the interaction term given by

$$C[g](\mathbf{r}_1, \mathbf{v}_1, t) = \int \mathbf{F}_{\rm int}(\mathbf{r}_1, \mathbf{r})\cdot\nabla_{\mathbf{v}_1} g(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}. \tag{2}$$

We stress that Eq. (1), in contrast with the Vlasov equation, can also describe strongly correlated systems. We assume in the following the existence of a stationary state f_0 and g_0, not necessarily the thermodynamic equilibrium [17]. We now drastically simplify the dynamics by using a scaling ansatz [1–3], which we extend here to the two-particles function g:

$$\begin{aligned} f(\mathbf{r}_1, \mathbf{v}_1, t) &= f_0(\varphi(\mathbf{r}_1, \mathbf{v}_1)) \\ g(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2, t) &= g_0(\psi(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2)), \end{aligned} \tag{3}$$

with $\varphi(\mathbf{r}_1, \mathbf{v}_1) = (\mathbf{R}_1 = \mathbf{r}_1/\lambda, \mathbf{V}_1 = \lambda\mathbf{v}_1 - \dot{\lambda}_{\mathbf{r}_1})$ and $\psi(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2) = (\varphi(\mathbf{r}_1, \mathbf{v}_1), \varphi(\mathbf{r}_2, \mathbf{v}_2))$. λ represents the dilatation of the cloud; the choice $\mathbf{R}_1 = \mathbf{r}_1/\lambda$ imposes the ansatz on velocities for consistency. All time dependence in the dynamics is now included in the positive parameter λ. Introducing Eq. (3) into Eq. (1) leads to

$$\sum_{i=1}^{d}\left\{\frac{V_i}{\lambda^2}\frac{\partial f_0}{\partial R_i} - R_i\lambda\frac{\partial f_0}{\partial V_i}(\ddot{\lambda} + \omega_0^2\lambda) - \kappa\frac{\partial(V_i f_0)}{\partial V_i} - \kappa\lambda\dot{\lambda}R_i\frac{\partial f_0}{\partial V_i} - D\lambda^2\frac{\partial^2 f_0}{\partial V_i^2}\right\} + C[g_0\circ\psi](\mathbf{r}_1, \mathbf{v}_1, t) = 0, \tag{4}$$

where the difficulty is to deal with the interaction term. We now assume that the two-body interaction satisfies

$$\mathbf{F}_{\rm int}(\lambda\mathbf{r}_1, \lambda\mathbf{r}_2) = \frac{1}{\lambda^k}\mathbf{F}_{\rm int}(\mathbf{r}_1, \mathbf{r}_2), \tag{5}$$

as, for example, a pure power law. The important step is to replace the interaction term $C[g_0 \circ \psi](\mathbf{r}_1, \mathbf{v}_1, t)$ by a linear combination of f_0 and its derivatives. This is achieved using the condition (5) and the fact that f_0 and g_0 are stationary solutions of Eq. (1). Equation (4) becomes

$$\sum_{i=1}^{d}\left\{V_i\frac{\partial f_0}{\partial R_i}\left(\frac{1}{\lambda^2} - \lambda^{1-k}\right) + D\frac{\partial^2 f_0}{\partial V_i^2}(\lambda^{1-k} - \lambda^2) - R_i\frac{\partial f_0}{\partial V_i}[\lambda(\ddot{\lambda} + \omega_0^2\lambda) - \lambda^{1-k}\omega_0^2 + \kappa\lambda\dot{\lambda}] + \kappa\frac{\partial V_i f_0}{\partial V_i}(\lambda^{1-k} - 1)\right\} = 0. \tag{6}$$

Multiplying the previous equation by $R_j V_j/N$, and integrating over $d\mathbf{R}d\mathbf{V}$, we obtain a constraint on the parameter λ:

$$\ddot{\lambda} + \kappa\dot{\lambda} + \left(\lambda - \frac{1}{\lambda^k}\right)\omega_0^2 - \left(\frac{1}{\lambda^3} - \frac{1}{\lambda^k}\right)\frac{\langle V_j^2\rangle_{f_0}}{\langle R_j^2\rangle_{f_0}} = 0, \tag{7}$$

where j is a coordinate label, and we have set $\langle \mathcal{X}\rangle_f = \frac{1}{N}\times\int\mathcal{X}(\mathbf{r}, \mathbf{v})f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}$. In the dynamical equation for λ [Eq. (7)], all parameters are computed as averages over the stationary distribution f_0. For Eq. (7) to be a unique equation, it is necessary that the ratio $\langle V_j^2\rangle_{f_0}/\langle R_j^2\rangle_{f_0}$ does not depend on j, which is true if the trap and interactions are isotropic.

We introduce the dimensionless parameter $p = \langle V_j^2\rangle f_0/(\omega_0^2\langle R_j^2\rangle_{f_0}) \sim k_BT/E_{\rm trap}$, where k_BT is the thermal energy and $E_{\rm trap}$ the typical potential energy due to the trap. At the canonical equilibrium, $\langle V_j^2\rangle f_0 = \omega_0^2L^2$, where L is the typical size of the system without interaction. The parameter $p = L^2/\langle R_j^2\rangle_{f_0}$ thus describes change of the square of the size of the trap due to the interactions. The range $p < 1$ ($p > 1$) corresponds to a repulsive (attractive) interaction. A value of the parameter $p \sim 1$ means high temperature or negligible interactions. The limits $p \to 0$ and $p \to +\infty$ correspond to zero temperature or strong repulsive and attractive interaction. We can now rewrite Eq. (7) as $\ddot{\lambda} + \kappa\dot{\lambda} + \phi'(\lambda) = 0$, which corresponds to the equation of a damped anharmonic oscillator in the potential ϕ:

$$\phi(\lambda) = \begin{cases} \omega_0^2(\frac{1}{2}\lambda^2 + \frac{1}{2}\frac{p}{\lambda^2} + \frac{p-1}{1-k}\lambda^{1-k}) & \text{if } k \neq 1 \\ \omega_0^2(\frac{1}{2}\lambda^2 + \frac{1}{2}\frac{p}{\lambda^2} + (p-1)\log\lambda) & \text{if } k = 1. \end{cases} \quad (8)$$

The first term in Eq. (8) is the quadratic confining potential, the second one corresponds to a pressure term, and the last one is introduced by the two-body interaction. We stress that Eq. (8) does not explicitly depend on d. For repulsive interactions ($p < 1$), ϕ is strictly convex for all $k \geq 0$. It diverges as λ^{-2} when $\lambda \to 0$ and as $\omega_0^2\lambda^2/2$ when $\lambda \to +\infty$. Its unique minimum is $\lambda = 1$. The λ^{-2} divergence at small λ is due to pressure effects for very compressed clouds, and thus does not depend on the interaction. It yields a generic shape for the breathing oscillations in the nonlinear regime. For attractive interactions ($p > 1$), if $0 \leq k \leq 3$, ϕ has exactly the same qualitative properties as in the repulsive case. For $k > 3$, ϕ tends to $-\infty$ when λ goes to zero, indicating a possible collapse of the cloud. However, due to numerical difficulties, we have not tested this prediction.

From Eq. (8), we obtain the general expression of the breathing oscillation frequency in the small friction limit, as a function of the interaction range k and the interaction strength p:

$$\omega(k, p) = \omega_0[(3 - k)(p - 1) + 4]^{1/2}. \quad (9)$$

This expression recovers the well-known limits $\omega = 2\omega_0$ for a noninteracting gas ($p = 1$) and $\omega = \sqrt{3}\omega_0$ for a strongly interacting Coulomb plasma ($p = 0$, $k = 2$) [19]. It provides a generalization to the whole (k, p) plane shown in Fig. 2 and is independent of the dimension. We note that in 3D, the breathing frequency is a decreasing (increasing) function of the interaction strength for repulsive long- (short-)range interactions.

We can now compare the general Eq. (7) to the results found in the literature for various specific situations. Oscillations of crystallized systems [9,10,12,15] correspond to negligible pressure effects; i.e., $p = 0$ and the λ^{-3} term is absent. In [6], the authors consider a 1D plasma ($k = 0$) with p not too small, and introduce a pressure yielding the λ^{-3} term, which leads to the exact equivalent of Eq. (7). Note that Eq. (7) also contains the case of a classical gas with "mean field" interactions [1]. This work considers a Dirac δ potential, which corresponds to an interaction index $k = d + 1$. This result emphasizes that the present theory is not only valid for power-law forces.

In order to test the domain of validity of the ansatz solution, we have performed numerical simulations varying the force index k, parameter p, and amplitude of initial perturbation, in two and three dimensions, with (canonical ensemble) or without (microcanonical ensemble) a thermostat. We simulate the system using a molecular dynamics approach with $N = 4000$ particles. The integrator scheme is a Verlet-leapfrog algorithm [20]. The forces are exactly computed at each time step. As strong short-range singularities for parameters in the upper right corner of Fig. 1 create numerical difficulties, we have not tested the theory in this region. The computer simulations are performed as follows: we first equilibrate the system in a stationary state f_0. Then, at $t = 0$, we introduce a perturbation by rescaling the positions and velocities according to Eq. (3) and we let the system evolve. A similar simulation of a 1D Coulomb system in the microcanonical ensemble has been performed in [6]. The results of our extensive simulations may be summarized as follows. (i) Eq. (7) always picks up quite precisely the oscillation frequency, but not always the amplitude decay. (ii) For strongly repulsive interaction ($p \to 0$), Eq. (7) describes very precisely the whole dynamics. (iii) For a repulsive long-range or short-range interaction and intermediate p (i.e., $p \sim 0.5$) the agreement for the oscillation amplitude is not perfect (see Fig. 3). (iv) For attractive long-range interactions, the accuracy of the ansatz degrades as p increases (Fig. 4).

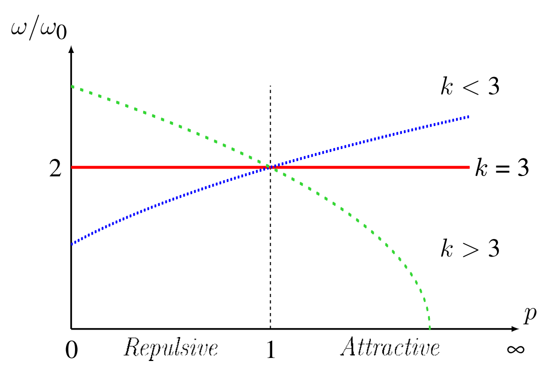

FIG. 2 (color online). Frequency of the linearized breathing mode as a function of the interaction strength p, for different values of interaction range k.

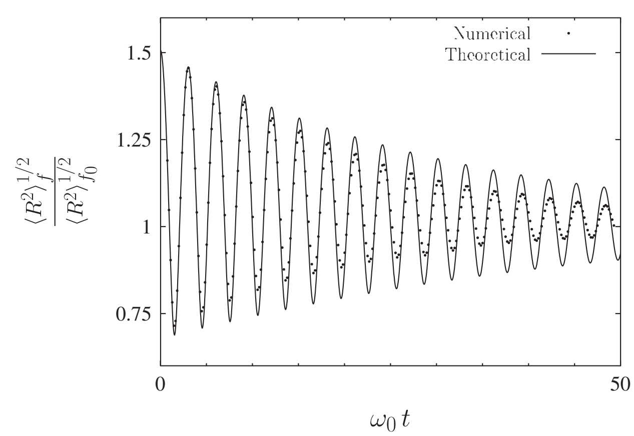

FIG. 3. Evolution of the typical size of the cloud. The space dimension is $d = 2$, and the interactions are repulsive. The parameters are $k = 4$ (short-range interaction), $\omega_0/\kappa = 17.8$ and $p = 0.63$.

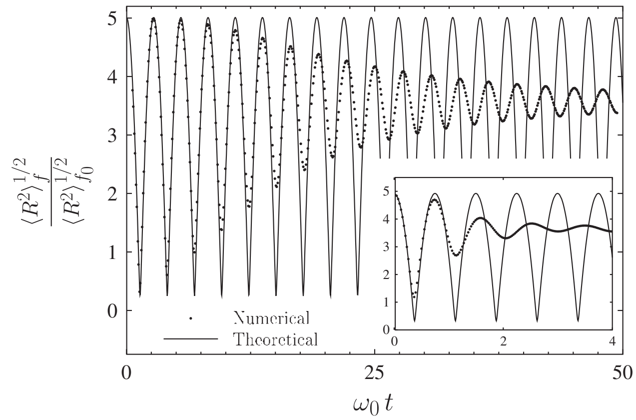

FIG. 4. Evolution of the typical size of the cloud in one of the few negative cases. The space dimension is $d = 3$, and the interactions are attractive. The parameters are $k = 0$ (long-range interaction), $\omega_0 = 17.8$, $\kappa = 0$ (microcanonical ensemble), and $p = 2.2$. Inset: Same parameters, except $p = 70$.

To explain these results, we first stress that in the limit $p \to 0$, Eq. (7) is *exact*. In this case, it may indeed be derived directly from Newton equations, as done in [15] in the linear approximation. The correct generalization for an arbitrary perturbation amplitude is given by Eq. (7). For intermediate p, we attribute the discrepancy between the predicted and simulated oscillation amplitudes to effects that are not taken into account in the simple dynamical ansatz (3), and thus limit the validity of Eq. (7). Indeed, for long-range interactions, one would expect collective effects (Landau damping, phase mixing, etc.) to play a role in the oscillation decay (beyond the friction κ), which are neglected in the ansatz. Similarly, for short-range interactions, two-body collisions should be important. This explanation is supported by the frictionless microcanonical simulations: when there is no amplitude decay in the microcanonical ensemble, which means that phase mixing and two-body collisions are negligible, Eq. (7) correctly predicts the breathing frequency and amplitude, with or without friction. Conversely, amplitude decay or modulation in the microcanonical ensemble is associated with discrepancies between theory and simulations.

In summary, starting from the first equation of the BBGKY hierarchy and a scaling ansatz for the dynamics, we have derived a nonlinear equation describing the breathing oscillations of trapped particles interacting via forces satisfying (5). The derivation and equation are valid independently of the temperature, interaction strength, interaction range, and dimensionality of the physical space, and it is successfully compared to direct numerical simulations. The main limitation is due to phase mixing phenomena for long-range interacting systems and two-body collisions in short-range interacting ones, especially for weak repulsive and attractive interactions, where they introduce damping and loss of coherence, unaccounted for in the scaling ansatz. We have concentrated on power-law interactions, but condition (5) for the force is more general. It includes, for instance, Dirac and dipolar potentials, and some nonpotential forces such as the attenuation force in magneto-optical traps [21]; the ansatz should be useful in such cases. Beyond the breathing mode, a generic study of quadrupolar modes would be very desirable, as harmonic traps are often anisotropic in experimental situations. This is not possible with the scaling ansatz, except in special cases. Even though no real breathing mode [15] exists when interactions are not power law, a generalization of this mode may exist. Following the lines of this Letter, and applying methods used in [8], a more general approach should be possible.

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