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Higher harmonic generation in strongly coupled plasmas

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Abstract
We present evidence for higher harmonic generation observed as additional peaks in the dynamical structure function and current–current fluctuation spectra in several types of strongly coupled plasmas. Results are presented on the dependence of the strength of the second and higher harmonic oscillations on the coupling parameter and the wave number.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Over the last decade we have performed extensive numerical studies on the wave dispersion properties of various kinds of strongly coupled ($\Gamma \gg 1$) many-particle systems with interparticle potentials of Coulomb ($\Phi(r) \propto 1/r$) and Yukawa ($\Phi(r) \propto \exp(-r/\lambda_D)/r$) types. Here $\Gamma = Q^2/ak_BT$, a is the Wigner–Seitz radius, T is the temperature and λ_D is the Debye length. The screening parameter of the Yukawa potential is defined as $\kappa = a/\lambda_D$. Collective modes are usually identified by the appearance of a strong peak in the density fluctuation power spectrum (the dynamical structure function) $S(k, \omega)$ (where k is the wavenumber and ω is the oscillation frequency). In many cases, one or more peaks in addition to the fundamental one can be identified in $S(k, \omega)$ at well-defined frequencies. The intensity of these higher harmonic excitations is usually three or more orders of magnitude weaker than the primary excitation. However, our molecular dynamics simulations are able to resolve these weak features in the density fluctuation spectra. During the course of our studies higher harmonics have been observed in single component systems:

- 3D Coulomb 'one component plasma' (OCP): harmonics of ω_p,
- 3D Yukawa OCP: harmonics of the plateau frequency,

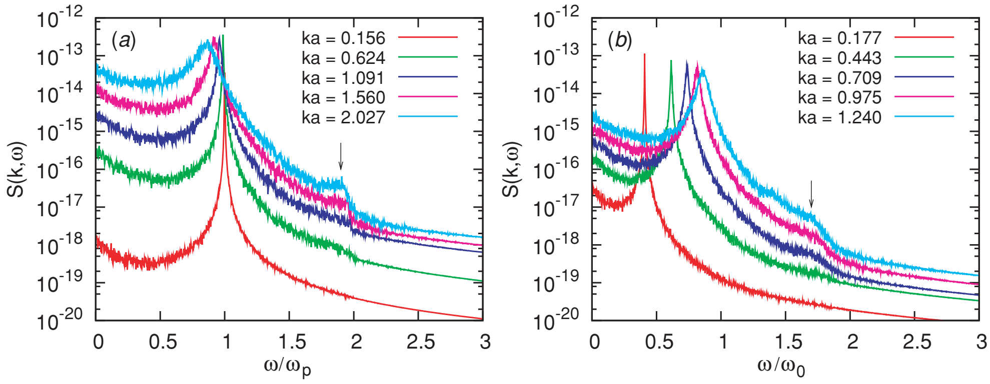

Figure 1. Dynamical structure function of (*a*) 3D Coulomb OCP at $\Gamma = 160$ and (*b*) 2D Coulomb OCP at $\Gamma = 120$. The wave numbers corresponding to the different curves are given in units of the inverse Wigner–Seitz radius. The arrows point at the second harmonic peaks.

- 2D Coulomb and Yukawa OCP: harmonics of the plateau frequency,

as well as in binary systems:

- electronic bilayer: harmonics of the out-of-phase gap and of the plateau frequency,
- electron–hole bilayer: harmonics of the out-of-phase gap frequency,

where ω_p is the 3D plasma frequency, the 'plateau frequency' is the frequency of the flat part of the primary wave dispersion (where $(\partial\omega/\partial k)|_{k_{\text{plateau}}} \approx 0$), the 'out-of-phase gap' is the $k \to 0$ limit frequency of the counter-oscillating modes in a bilayer system. Frequencies in 2D systems are presented in units of the nominal plasma frequency $\omega_0^2 = 2\pi n Q^2/ma$.

2. Single component systems

Dynamical structure functions of the 3D and 2D Coulomb OCPs, obtained from MD simulations [1] are shown in figure 1 for a series of wave numbers.

In these systems we have been able to identify the generation of second harmonics only. The harmonic frequency follows the plateau frequency. This frequency is nearly equal to the plasma frequency in 3D Coulomb systems. In (2D) Yukawa systems it depends on the screening parameter κ, as shown in figure 2(*a*).

The frequency of the harmonics is largely independent of the wave number for $0 < k < k_{\text{max}}$, where $k_{\text{max}} \approx 2k_{\text{plateau}}$, as it can be seen in figure 2(*b*). In contrast to the frequency, the intensity of the harmonic, measured with respect to the thermal background, depends strongly both on the wave number and on the Γ coupling value. In general, it peaks at intermediate wave numbers and at Γ values that correspond to the strongly coupled liquid phase. Apparently, the generation of harmonics requires both strong coupling and disorder: the harmonic intensity markedly diminishes both in the weakly coupled liquid and in the highly ordered lattice-like phases (see figure 3).

3. Bilayer systems

In bilayer systems one could expect harmonics both of the out-of-phase mode gap frequency and of the in-phase plateau frequency to appear. In the electronic bilayer, however, the two

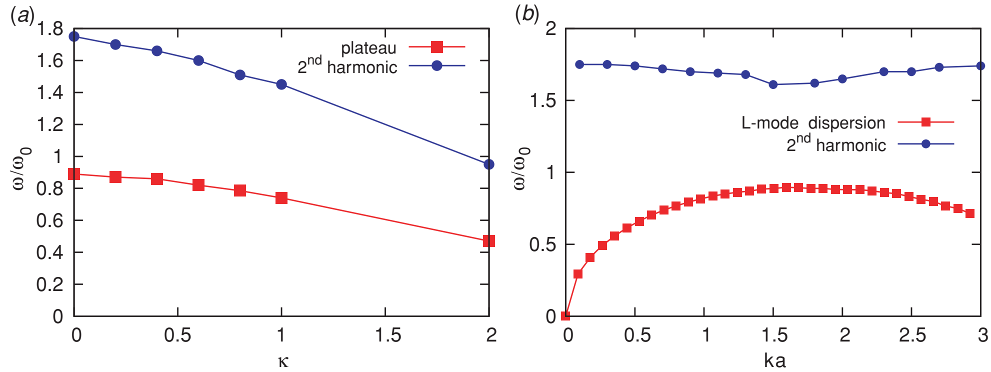

Figure 2. (*a*) 2D Yukawa OCP at $\Gamma = 120$, plateau and second harmonic frequencies versus Yukawa κ parameter. (*b*) 2D Coulomb OCP at $\Gamma = 100$: longitudinal mode dispersion and second harmonic frequency versus wavenumber.

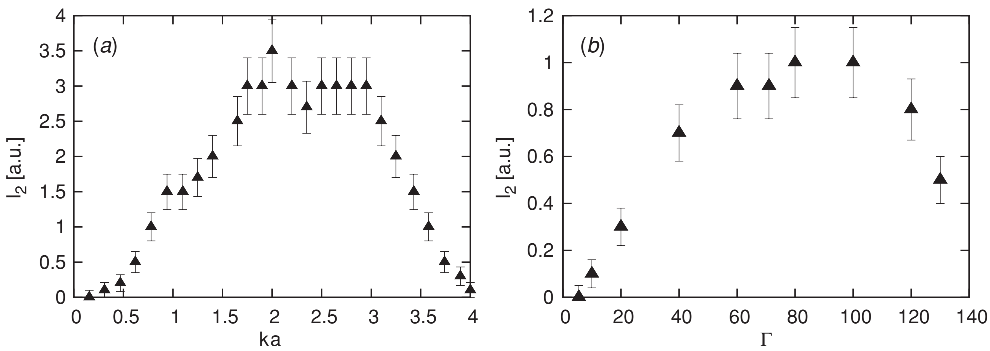

Figure 3. (*a*) 3D Coulomb OCP at $\Gamma = 160$, second harmonic peak relative intensity (I_2) versus wave number. (*b*) 2D Coulomb OCP at $\Gamma = 120$, second harmonic peak relative intensity (I_2) versus coupling parameter at wave number $ka = 0.62$.

frequencies (for layer separations of interest) are very close [2] and one cannot easily identify the primary frequency of a particular harmonic. In contrast, in the electron–hole bilayer the plateau frequency is too low for it to be of interest.

Electronic bilayers: The second and third harmonics of the out-of-phase (−) gap frequency (possibly intermingled with the plateau frequency) [2] appear both in the in-phase, and in the out-of-phase spectra, as shown for the longitudinal modes in figures 4(*a*) and (*b*).

Electron–hole bilayers: The generation of harmonics in the electron–hole bilayer is much more pronounced than in the simpler electronic bilayer. This may be related to the fact that the out-of-phase gap frequency here is strongly linked to the internal Kepler-type orbital frequency of the pair of oppositely charged particles in a dipole-like configuration. [3]. We observe the emergence of the third harmonic in the out-of-phase (−) spectra and the second and fourth harmonics in the in-phase (+) spectra, (see figures 4(*c*) and (*d*)).

As to the behavior of the intensity, the generation of harmonics is, similarly to what has been seen for the single component systems, the most pronounced around $\Gamma = 40$ in the

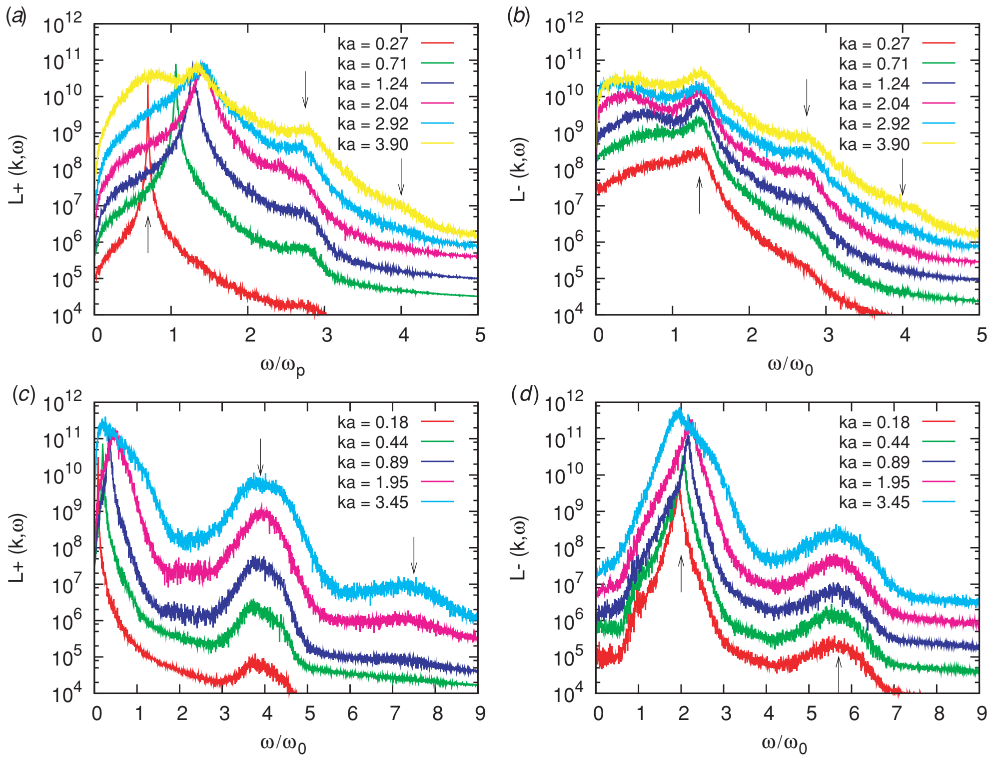

Figure 4. Longitudinal current fluctuation power spectra for (*a*) and (*b*) electronic bilayer at $\Gamma = 100$, $d/a = 0.3$ and (*c*) and (*d*) symmetric electron–hole bilayer at $\Gamma = 40$, $d/a = 0.6$. $L+$ (*a*) and (*c*) and $L-$ (*b*) and (*d*) denote in-phase and out-of-phase modes, respectively. Arrows point at (*a*) the peak of the in-phase mode, second and third harmonic; (*b*) the out-of-phase 'gap' frequency, the second and third harmonic; (*c*) the second and fourth harmonic; (*d*) out-of-phase 'gap' frequency and the third harmonic, respectively.

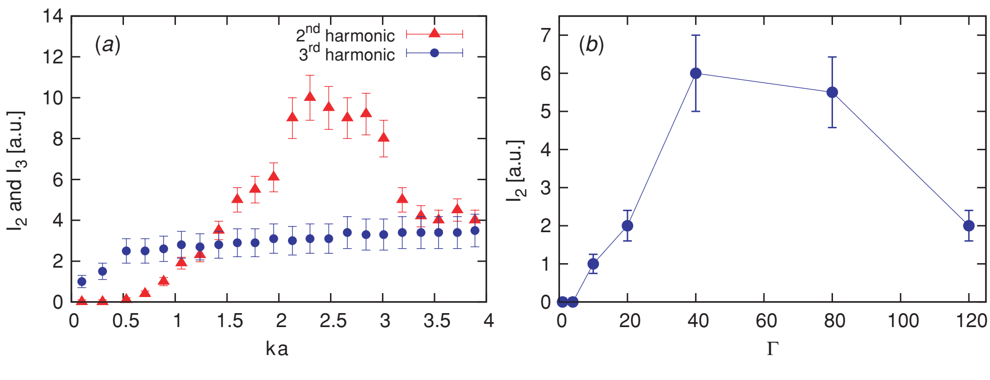

Figure 5. Relative intensities (I_2 and I_3) for a symmetric electron–hole bilayer with $\Gamma = 40$, $d/a = 0.6$ calculated from peak intensities in the $S_{\pm}(k, \omega)$ spectra. (*a*) wavenumber dependence; (*b*) Γ dependence of I_2 at $ka = 2.04$.

strongly coupled dipole–liquid phase [4], showing a diminishing trend both for lower and higher coupling values (see figure 5(*b*)). The intensity of the second harmonic is also similar to the previously observed non-monotonic dependence on the wave number; the different behavior of the third harmonic intensity is not explained, but may be due to the different phase space requirements relating to the 3-wave versus the 4-wave interaction. (see figure 5(*a*)).

3.1. Theoretical approach

The generation of harmonics can be described in terms of the nonlinear generalization of the QLCA equation of motion [5]

$$\ddot{\eta}_{\mathbf{k}}^{A} = D^{AB}(\mathbf{k})\eta_{\mathbf{k}}^{B} + \sum_{\mathbf{q}} D^{ABC}(\mathbf{k},\mathbf{q})\eta_{\mathbf{k}-\mathbf{q}}^{B}\eta_{\mathbf{q}}^{C} + \cdots, \qquad (1)$$

here $\eta_{\mathbf{k}}^{A}$ is the collective coordinate for density oscillations, $D^{AB}(\mathbf{k})$ is the dynamical matrix in AB layer space and $D^{ABC}(\mathbf{k},\mathbf{q})$ is its obvious generalization for 3-wave processes.

In the normal mode representation of (+) and (−) modes $D^{AB}(\mathbf{k})$ becomes diagonal and $D^{ABC}(\mathbf{k},\mathbf{q})$ assumes a particular structure [6]: $D^{+AB}(\mathbf{k},\mathbf{q})$ is completely diagonal, while $D^{-AB}(\mathbf{k},\mathbf{q})$ is completely off-diagonal, i.e. only $D^{+++}(\mathbf{k},\mathbf{q})$, $D^{+--}(\mathbf{k},\mathbf{q})$ and $D^{-+-}(\mathbf{k},\mathbf{q})$, $D^{--+}(\mathbf{k},\mathbf{q})$ are different from zero. This structure may be regarded as the manifestation of a 'parity' conserving symmetry.

By assigning a parity 'quantum number' ($P = +1$) to the in-phase and ($P = -1$) to the out-of-phase modes the conservation of parity will require that when the two or more modes interact, the resulting parity of the new mode be the product of the parities of the interacting modes. Thus, symbolically

$$[-+], [-++], [---] \Rightarrow [-]; \qquad \text{and} \qquad [++], [--], [+++], [+--] \Rightarrow [+].$$

However, the (−) mode frequency is the gap frequency, almost independent of k, while the frequency of the (+) mode at $k = 0$ is 0. Thus combining frequencies and wave vectors, for the first process

$$\begin{aligned} &k_- + k_+ = k, \qquad k_+ \simeq 0, \qquad k \simeq k_-, \\ &\omega_- + \omega_+ = \omega, \qquad \omega_+ \simeq 0, \qquad \omega_- \simeq \omega_{\mathrm{GAP}}, \qquad \omega \simeq \omega_{\mathrm{GAP},} \end{aligned} \qquad (2)$$

and similarly for all other processes. Therefore the frequencies (in units of the gap frequency) for the processes listed above become

$$\begin{aligned} &[1], [1], [3] \text{ for the } (-) \text{ mode;} \qquad \text{and} \\ &[0], [2], [0], [2] \text{ for the } (+) \text{ mode.} \end{aligned} \qquad (3)$$

This explains how the observed remarkable structure that restricts odd harmonics only to the (−) mode and even harmonics only to the (+) mode is brought about by the simple selection rule. The clear understanding of the physical origin of the parity assignment, however, still requires future work.

Acknowledgments

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