Higher harmonics of the magnetoplasmon in strongly coupled Coulomb and Yukawa systems

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The generation of higher harmonics of the magnetoplasmon frequency which has recently been reported in strongly coupled two-dimensional Yukawa systems is investigated in detail and, in addition, extended to two-dimensional Coulomb systems. We observe higher harmonics over a much larger frequency range than before and compare the theoretical prediction with the simulations. The influence of the coupling, structure, and thermal energy on the excitation of these modes is examined in detail. We also report on the effect of friction on the mode spectra to make predictions about the experimental observability of this new effect.

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I. INTRODUCTION

The behavior of two-dimensional (2D) systems is of continuing interest in many fields of physics as the reduced number of dimensions gives rise to a number of peculiar properties. In highly correlated systems, where the potential energy due to the interaction dominates over the thermal energy (for recent overviews see [1,2]), 2D many-particle systems exhibit a strongly collective behavior which manifests itself, e.g., in anomalous transport properties of 2D liquids [3–7]. Correlational effects are also responsible for additional shear mode excitations of 2D liquids [8,9] which do not occur in weakly coupled systems but have been experimentally observed in strongly coupled dusty plasmas [10,11].

Subjecting a 2D many-particle system to a perpendicular magnetic field gives rise to yet another line of research into the physics of low-dimensional systems [12]. The magnetic field effectively “mixes” longitudinal and transverse excitations, leading to two hybrid modes, the magnetoplasmon and the magnetoshear, which have, in recent times, been studied in Coulomb and Yukawa systems [13–15]. These modes are well understood from a theoretical perspective, including descriptions based on the quasilocalized charge approximation (QLCA) [16,17] or in harmonic lattice approximations [9,15].

However, besides these established modes, 2D Yukawa systems at strong coupling have recently been found to support additional high-frequency modes. These modes appear as higher harmonics of the magnetoplasmon in nondissipative 2D Yukawa systems [18] and are reminiscent of the classical Bernstein modes [19]. Unlike these, however, the observed higher harmonics are not a pure magnetic effect but are, additionally, fundamentally affected by the strong correlations between particles, as was demonstrated in Ref. [18].

In this work, we put the theoretical predictions of our earlier work [18] to the test by using more detailed simulations and observing considerably more high-frequency modes. In addition, we include the Coulomb case of vanishing screening in our analysis, and demonstrate that the higher harmonics are also generated under these circumstances, which are not only quantitatively but also qualitatively different from screened-interaction systems [2]. Finally, we assess the possibility of experimental verification by investigating the relative intensities of the modes and including dissipative effects in our simulations.

II. MODEL AND DETAILS OF THE NUMERICAL SIMULATION

Our model system consists of \( N \) point particles situated in a quadratic simulation box in the \( x, y \) plane with side-length \( L \). The particles are uniform in mass \( m \) and charge \( q \) and are subject to periodic boundary conditions to avoid surface effects. The particles propagate according to the coupled equations of motion,

\[
m \ddot{\mathbf{r}}_i = \mathbf{F}_i + q \mathbf{E}_i \times \mathbf{B} + \mathbf{S}_i, \tag{1}
\]

where the force \( \mathbf{F}_i \) follows from the Yukawa potential created by all other particles,

\[
\mathbf{F}_i = -\frac{q^2}{4\pi \varepsilon_0} \sum_{j=1}^{N} \left( \nabla \frac{e^{-r/j\lambda_D}}{r} \right) \bigg|_{r=r_i-r_j}.
\]

Here, \( \lambda_D \) denotes the Debye screening length and the primed sum indicates the omission of the term \( j = i \). For \( \lambda_D \to \infty \), we recover the well-known one-component plasma (OCP). The magnetic field is oriented perpendicular to the plane of the particles, \( \mathbf{B} = B_e \mathbf{z} \), and the Langevin term \( \mathbf{S}_i \) in Eq. (1) is defined as

\[
\mathbf{S}_i = -m_i \bar{\nu} \dot{\mathbf{r}}_i + \mathbf{R}_i.
\]

This Langevin term is only included in the simulations with friction \( \bar{\nu} \) and \( \mathbf{R}_i(t) \) is a Gaussian white noise [20] with zero mean and the standard deviation

\[
\langle R_{\alpha,i}(t_0) R_{\beta,j}(t_0 + t) \rangle = 2 k_B T \bar{\nu} \delta_{ij} \delta_{\alpha\beta} \delta(t),
\]

where \( \alpha, \beta \in \{x, y\} \) and \( T \) is the temperature.

Equation (1) is solved simultaneously for \( N = 4080 \) particles using standard molecular dynamics simulation with integrators adopted to the influence of the magnetic field [21]. When friction is included in the simulations, we apply an
additional Ornstein-Uhlenbeck process in momentum space [22,23]. For Coulomb systems, the appropriate Ewald summation techniques to calculate the forces are employed [24,25].

Starting from a random configuration of particles, the system is brought into equilibrium by a repeated rescaling of the particles’ momenta according to the desired temperature $T$. After equilibrium conditions are realized, the system is advanced only according to Eq. (1).

In the following, lengths are given in units of the Wigner-Seitz radius $a = [n\pi]^{-1/2}$, where $n$ is the areal number density of the particles. Time is given in multiples of the inverse of the nominal angular plasma frequency $\omega_p = [nq^2/(2\epsilon_0ma)]^{1/2}$. The system is characterized by four dimensionless parameters:

1. the temperature $T$ of the particles, given in terms of the system’s nominal (i.e., Coulomb) coupling parameter $\Gamma = q^2/(4\pi\epsilon_0ak_BT)$;
2. the inverse of the Debye screening length $\lambda_D$, normalized by the Wigner-Seitz radius, $\kappa = a/\lambda_D$;
3. the strength of the magnetic field, expressed as the ratio $\beta$ between the angular cyclotron frequency $\omega_c = qB/m$ and the nominal angular plasma frequency, $\beta = \omega_c/\omega_p$;
4. the strength of friction, given by $\nu = \nu/\omega_p$;

III. COLLECTIVE MODES

The collective excitations of the strongly coupled, interacting particles can be analyzed through the microscopic excitation spectra. The dispersion, i.e., the relation between the wavelength and the wave frequency of the collective excitations, can be obtained from the analysis of the autocorrelation (ACF) of the density and current fluctuations. For the Fourier components of the density fluctuations, we have [26]

$$\rho(k,t) = \sum_{j=1}^{N} e^{ikx_j(t)}. \quad (5)$$

The dynamical structure factor $S(k,\omega)$ follows as (assuming $k = ke_x$ and dropping the vector notation for $k$)

$$S(k,\omega) = \frac{1}{2\pi N} \lim_{T \to \infty} \frac{1}{T} |\mathcal{F}_t[\rho(k,t)]|^2, \quad (6)$$

where $\mathcal{F}_t$ denotes the temporal Fourier transform. The current operator is given by [26,27]

$$j(k,t) = \sum_{j=1}^{N} v_j(t) \exp[ikx_j(t)]. \quad (7)$$

Separating longitudinal $[\lambda(k,t)]$ and transverse $[\tau(k,t)]$ currents, one arrives at the microscopic quantities [28]

$$\lambda(k,t) = \sum_{j=1}^{N} v_{jx} \exp[ikx_j], \quad (8)$$

$$\tau(k,t) = \sum_{j=1}^{N} v_{jy} \exp[ikx_j]. \quad (9)$$

from which one can then obtain the fluctuation spectra $L(k,\omega)$ and $T(k,\omega)$ analogously to Eq. (6) [replacing $\rho(k,t)$ by $\lambda(k,t)$ and $\tau(k,t)$, respectively]:

$$L(k,\omega) = \frac{1}{2\pi N} \lim_{T \to \infty} \frac{1}{T} |\mathcal{F}_t[\lambda(k,t)]|^2, \quad (10)$$

$$T(k,\omega) = \frac{1}{2\pi N} \lim_{T \to \infty} \frac{1}{T} |\mathcal{F}_t[\tau(k,t)]|^2. \quad (11)$$

The dynamic structure factor $S(k,\omega)$ can be shown to be related to $L(k,\omega)$ as [29]

$$S(k,\omega) = \frac{k^2}{\omega^2} L(k,\omega). \quad (12)$$

$S(k,\omega)$, therefore, contains no additional information over $L(k,\omega)$, so we concentrate on $L(k,\omega)$ and $T(k,\omega)$ in the following [30].

Our main interest lies in the mode spectra in the high-frequency range. We numerically evaluate the microscopic fluctuations (8) and (9) at multiples of the minimum wave vector $k_{\text{min}} = (2\pi/L)e_x$ as dictated by our use of periodic boundary conditions. The data are subsequently Fourier analyzed and the periodogram estimate of the power spectrum density is computed to obtain $L(k,\omega)$ and $T(k,\omega)$. Our simulations are typically thermalized for 20 000 plasma periods and data are collected during 400 000 or more plasma periods. The spectra are computed for different values and combinations of the coupling $\Gamma$, screening $\kappa$, magnetic field $\beta$ and friction $\nu$.

IV. RESULTS

In this section, we study the generation of the higher harmonics in detail. Using more accurate data, we confirm the theoretical formula of the mode spacing reported in Ref. [18] in Sec. IV A and then discuss the effect of the coupling, the structural properties and the thermal energy on the higher harmonics in frictionless systems in Sec. IV B. In Sec. IV C, we include dissipation and stochastic noise in our simulations to gauge the prospect of experimental verification.

A. Dependence of the spectrum on $\beta$

To obtain a first overview of the collective excitations, we depict in Fig. 1 several results for the longitudinal and transverse wave spectra at different strengths of the magnetic field for a Yukawa system with $\kappa = 2$ and $\Gamma = 200$. The density plots in Fig. 1 show the sum of transverse and longitudinal excitations. For the unmagnetized case (top row), the mode spectrum is well known and accurately described, e.g., within the QLCA [8]. The two branches associated with strongly coupled, unmagnetized Yukawa and Coulomb liquids (transverse and longitudinal branch) are not discernible on the scales of Fig. 1. At higher frequencies, the mode spectra appear structureless (cf. right columns of Fig. 1).

In the the magnetized case (lower three rows of Fig. 1), two features are immediately noticeable: i) The two modes from the unmagnetized case are now replaced by the upper- and lower-hybrid modes (UH and LH) with the $k \to 0$ limit $\omega_{0UH} = 0$ and $\omega_{0LH} = \omega_c$ [9]. ii) The qualitatively new feature reported in Ref. [18] is the emergence of multiple new branches at higher frequencies. These are higher harmonics reminiscent of the
Bernstein modes which have been observed half a century ago in strongly magnetized ideal plasmas [19]. Typical for these modes is that their frequencies are equally spaced, appearing at multiples of the cyclotron frequencies \( \omega_c \) and that they are undamped and exist in the entire wave number range.

The present modes show a number of fundamental differences which are caused by correlation effects: all modes are damped, and they appear only beyond a critical wave number which increases with the mode number. The most important difference is the mode frequency. Instead of being spaced by which increases with the mode number. The most important difference is the mode frequency. Instead of being spaced by the cyclotron frequency \( \omega_c \), here the modes appear at multiples of the magnetoplasmon frequency. The frequency of these “dressed Bernstein” modes, \( \omega_n \), \( n = 2, 3, \ldots \), were found to be well described by the relation [18]

\[
\omega_n^2(k) \approx n \omega_{E,\infty}^2, \quad \omega_n^2(\beta, \kappa) = \omega_0^2(\beta) + 2 n^2 \kappa_0(\kappa).
\] (13)

Here, the dominant single-particle oscillation frequency is denoted by \( \omega_E \), the Einstein frequency, which strongly varies with \( \kappa \) but also weakly depends on \( \Gamma \) [31]. Some values of \( \omega_E(\Gamma, \kappa) \) are collected in Table I.

In Ref. [18], the data allowed to detect higher harmonics of the magnetoplasmon up to the third order \( \{n = 4 \text{ in Eq. (13)}\} \). The present data show higher harmonics up to \( n = 7 \) (cf. Fig. 1, third row). This provides us with the opportunity to verify the validity of Eq. (13) to a much higher precision. To this end, we depict in Fig. 2 the combined mode spectra for \( \beta = 1.0 \) in two different systems. The solid lines indicate the theoretical prediction of Eq. (13). A very good agreement between the theory and the simulations is evident. In addition, Fig. 2(a) illustrates that the generation of the dressed Bernstein modes also occurs in a Coulomb system in which the particle interaction is long ranged. This feature substantially expands the scope of the higher harmonics generation to other fields in plasma physics, including, e.g., ionic plasmas in traps [32,33] and electron-hole plasmas in semiconductors, e.g., [34].

<table>
<thead>
<tr>
<th>( \kappa )</th>
<th>( \Gamma )</th>
<th>( \omega_E/\omega_p )</th>
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<tr>
<td>0</td>
<td>100</td>
<td>0.62</td>
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<tr>
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<td>3</td>
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to observe the described effects. Figure 3b shows the relative
intensities at $ka = 2.0$ for the Yukawa and Coulomb spectra. Evidently, the data points are well described by a decay of the form $10^{-2.6(n-1)}$. The first of the higher harmonics (i.e., $n = 2$) appears with an intensity of about one hundredth of the magnetoplasmon. Such intensities are observable against the background noise in typical dusty plasma experiments [10].

FIG. 2. (Color) Combined mode spectrum $L(k, \omega) + T(k, \omega)$ for a) $\kappa = 0.0$, $\Gamma = 100$ and b) $\kappa = 2.0$, $\Gamma = 200$, and $\beta = 1.0$. Black lines are the theoretical prediction for higher harmonics according to Eq. (13).

We now quantify the higher harmonics in more detail. Figure 3 shows the frequency and oscillator strengths of the higher harmonics and the magnetoplasmon at $ka = 2.0$ and fixed $\Gamma$ and $\beta$. The agreement between relation (13) and the peak position from the simulations is again excellent (Fig. 3a), both for the OCP and a typical Yukawa system with $\kappa = 2$. Note that no free parameter enters the theoretical prediction and that the differences in the theoretical predictions are only mediated by $\omega_E$.

A quantity of central interest is the relative intensity of the generated higher harmonics. These values provide one with a first estimate of the required experimental sensitivity to observe the described effects. Figure 3b shows the relative intensities at $ka = 2.0$ for the Yukawa and Coulomb spectra. Evidently, the data points are well described by a decay of the form $10^{-2.6(n-1)}$. The first of the higher harmonics (i.e., $n = 2$) appears with an intensity of about one hundredth of the magnetoplasmon. Such intensities are observable against the background noise in typical dusty plasma experiments [10].

B. Dependence of the spectrum on the interaction, temperature, and structural order

The frictionless Yukawa system is (at fixed magnetization $\beta$) characterized by two parameters: The inverse temperature (Coulomb coupling parameter) $\Gamma$ and the interaction range (inverse Debye length) $\kappa$. The influence of the temperature is investigated by changing, at a fixed value of $\kappa$, the coupling parameter $\Gamma$.

In Fig. 4, different situations are depicted for a system with $\kappa = 2$, ranging from intermediate coupling ($\Gamma = 10; 40$) to strong ($\Gamma = 200$) and very strong coupling ($\Gamma = 1000$). Note that for $\Gamma = 1000$, the system is already far in the microcrystalline regime, $\Gamma_{\text{rel}} = \Gamma / \Gamma_{\text{melting}} \approx 2.4$. The decreased thermal background makes the fundamental and higher harmonics stand out very clearly at strong coupling, and the signal-to-noise ratio is higher in these cases. For example, harmonics with $n > 3$ are far easier to distinguish at $\Gamma = 1000$ than at $\Gamma = 40$. The intensity ratio $M = I_n/I_0$ between the intensity of the $n$th harmonic and the fundamental is, however, clearly decreased for stronger coupling [35]. This indicates that a certain degree of disorder is required for an effective generation of higher harmonics, which in turn might depend on anharmonic effects that are less important in highly ordered systems. Having established the influence of the temperature (inverse coupling), we now determine the influence of the interaction range. To this end, in Fig. 5, we show the combined mode spectra at a fixed $\Gamma = 100$ for different values of $\kappa$ and two
values of $ka$. The curves appear very similar, with comparable signal-to-noise ratios and similar relative intensities of the higher harmonics. This is despite the strong differences in structural order among the systems reflected in the different radial pair distribution functions (RPDF, inset of Fig. 5) defined as

$$g(|r|) = \frac{L^2}{N^2} \left( \sum_{i,j} \delta(|r - r_{ij}|) \right).$$

The sole effect of an increase in $\kappa$ on the higher harmonics is a systematic shift toward smaller frequencies. This result is not unexpected and indeed predicted by Eq. (13): With increasing $\kappa$, the particle oscillations decrease in frequency as the interparticle potential becomes more lenient. The Einstein frequency, therefore, diminishes with increasing $\kappa$ (cf. Table I) and, consequently, so do the frequencies at which the higher harmonics appear.

So far we have investigated the influence of $\Gamma$ and $\kappa$ on the higher harmonics. A change of either of these parameters also affects the structural properties of the system. By changing $\Gamma$ and $\kappa$ simultaneously in such a way that the RPDF remains practically unchanged [31,36–38], we can compare systems with identical structural properties. We achieve this by fixing the ratio of the temperature to the point of (micro)crystallization, $\Gamma/\Gamma_{\text{melting}} \equiv \Gamma_{\text{rel}}$ [39,40]. Systems corresponding to the same $\Gamma_{\text{rel}}$ but different $\Gamma$ have thus the same structural order but different thermal energy.

The results are presented in Fig. 6, where a fixed value of $\Gamma_{\text{rel}}$ is maintained for systems with different values of $\kappa$. A combination of the two previously described effects is observed: The higher harmonics shift toward lower frequency with increasing $\kappa$, and decay more slowly albeit with a decreased signal-to-noise ratio with increasing temperature (inverse coupling).

In conclusion, we find that the generation of higher harmonics is nearly independent of the intricate details of the structure and the range of the interaction between the particles (except for a systematic frequency shift) but, instead, is dominated by the thermal energy available to the system.

C. Influence of dissipation on the higher harmonics. Prospects for experimental observation

Besides noise resulting from the measurement itself, many physical systems are also influenced by fluctuations due to the coupling to their surroundings. In many cases, these fluctuations and dissipation effects are well described by a
constant friction and stochastic noise, an approach which has been used extensively in the description of, e.g., dusty plasmas. We now introduce dissipation and stochastic noise in our MD simulations to estimate the effect of friction-induced noise on the fluctuation spectra. In other words, we now include the term (3) in Eq. (1).

In Fig. 7, we depict the longitudinal fluctuation spectrum $L(k, \omega)$ for fixed values of $k$, $\beta$ and $\Gamma$, while varying the magnitude of the friction $\nu$. As expected, the inclusion of friction has a twofold effect: a) The overall noise level in the spectrum is increased and begins to overlap the higher harmonics and b) the peaks in the spectra become increasingly broader with higher friction.

The noise resulting from the friction clearly dominates the intrinsic noise for the data depicted in Fig. 7. The high-$\omega$ limit of the spectra increases linearly with the friction coefficient. From the data presented in Fig. 7, we conclude that at a moderately coupled liquid state, $\Gamma = 200$ and $\kappa = 2$, the detection of the second harmonic is possible at $\beta = 0.5$ and a friction of $\nu \sim 0.01$ (note that $\nu$ is given here in units of the nominal plasma frequency).

We now give estimates for the plasma parameters required to observe the generation of higher harmonics under experimental conditions. The main obstacle in attaining our simulation conditions in experiments are the required high magnetic fields. Combining the formulas for the cyclotron frequency $\omega_c$ and the plasma frequency $\omega_p$ and solving for the magnetic field, we obtain (in SI units)

$$B[T] \approx 2.7 \times 10^5 \beta \left( \frac{R}{a} \right)^2 \sqrt{\rho \left[ \frac{kg}{m^3} \right]}$$

where $\rho$ is the mass density. Typical 2D dusty plasma parameters are $R = 1$–10 $\mu$m, $\rho \approx 1g/cm^3$ and $a = 0.1$–1 mm, giving rise (for $\beta \approx 0.074$) to a required magnetic field of about 20T, which is at the edge of current experimental possibilities. That number can be reduced by using lighter particles or compressing the system to decrease the interparticle spacing (an increase of the average density by a factor of, e.g., 2 lowers the magnetic field requirements by 40%). Also note that the required magnetic field is independent of particle charge, which, however, enters into the coupling parameter $\Gamma$. 

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**FIG. 5.** (Color online) Combined mode spectra at $ka = 2.0$; $5.0$ for identical temperature ($\Gamma = 100$) and $\kappa = 1.0$; $2.0$; $3.0$ (highest to lowest curve), $\beta = 1.0$. The curves are shifted vertically for clarity. The inset shows the RPDF $g(r)$.

**FIG. 6.** (Color online) Combined mode spectra at $ka = 2.0$; $5.0$ for identical structural properties corresponding to $\Gamma_{rel} = 0.48$ but different $\kappa = 1.0$; $2.0$; $3.0$ (highest to lowest curve), $\beta = 1.0$. The inset shows the RPDF $g(r)$.

**FIG. 7.** (Color online) $\Gamma = 200$, $\kappa = 2.0$, $\beta = 0.5$: Combined mode spectra for different values of the friction strength, from $\nu = 10^{-4}$ (top curve) to $\nu = 10^{-3}$ (lowest curve).
The dissipation in 2D dusty plasma experiments can be quite low, a typical value is $\nu \approx 0.02$ [3]. Thus, according to our simulations, friction at this rate should not prevent the generation of the higher harmonics. It is, however, not uncommon to experience friction rates in excess of $\nu = 0.1$, at which the observation of the higher harmonics is not possible. In conclusion, the observation of higher harmonics appears as a possible experimental venue but poses several challenging restraints on the experimental setup.

V. SUMMARY

In this work, we have compared the previously derived theoretical description of the mode spacing of the higher harmonics with extended MD simulations and found excellent agreement over a wide range of coupling strengths and interaction range. We have also, for the first time, demonstrated that the generation of higher harmonics is present in strongly correlated systems with Coulomb interaction as well, which is especially interesting in the light of additional possibilities for experimental verification. The relative intensities of the higher harmonics have also been investigated and were found to decay, to a very good approximation, exponentially with the order of the harmonics. Finally, we have included dissipation in our simulations and estimated the maximum acceptable level of such friction for experiments. Combining estimates for the strength of the magnetic field and the maximum friction levels, we conclude that the experimental observation of higher harmonics is possible but challenging.

Finally, we expect that our results are also of direct relevance for strongly correlated quantum plasmas. In the case of magnetized ideal quantum plasmas the “traditional” Bernstein modes have been predicted theoretically long ago by Horing et al. [41] and were observed experimentally in electron-hole plasmas, e.g., [42]. In recent years strongly correlated quantum Coulomb systems, including liquid states and Wigner crystals of electrons [34], holes [43], and excitons, e.g., [44], moved into the focus of research. It is expected that these systems, if placed into a strong magnetic field, should exhibit a similar spectrum of “dressed Bernstein modes” as their classical counterpart studied in the present paper.

ACKNOWLEDGMENTS

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[28] Note that some authors insert a factor $k$ in front of the sums in Eqs. (8) and (9).
[30] Note that the displayed spectra are scaled for maximum visibility and are given in arbitrary units throughout this work.
[33] For Coulomb systems in a harmonic confinement the mean density is roughly constant as well, at sufficiently strong coupling, which justifies comparison with a homogeneous system, e.g.,


[35] We note that $M$ has been called “measurability” by some authors, e.g., A. Chatterjee and N. S. Vyas, J. Sound Vib. 268, 657 (2003).


