COLLABORATIVE PROJECT: RESEARCH ON STRONGLY COUPLED PLASMAS

Final Technical Report

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The primary goal of the University of Vermont/Boston College joint research effort over the past four years was to develop methods for the analysis of strongly coupled plasmas and to apply these methods to the investigation of fundamental problems relating to static and dynamical properties of a variety of charged particle systems in the strongly correlated liquid phase.

The research reported here was carried out in accordance with the plan of the original Proposal. The following list of publications with abstracts summarizes the research supported by Grant DE-FG02-98ER54491 from 15 July 1998 to 14 July 2002.

Refereed journal publications (with abstracts)

[1] K. I. Golden, "Quadratic fluctuation-dissipation theorem for multilayer plasmas", *Physical Review E* **59**, 228-233 (1999). In this paper, the author formulates the static (zero frequency) and dynamical quadratic fluctuation-dissipation theorems (QFDTs) for multilayer classical one-component plasmas. The static QFDT is used to derive the lowest-order (in the coupling parameter) Mayer cluster expansion for the layer-space matrix elements of the equilibrium three-point correlation functions.

[2] G. Kalman, V. Valtchinov, and K. I. Golden, "Collective modes in strongly coupled electronic bilayer liquids", *Physical Review Letters* **82**, 3124-3127 (1999). The authors present the first reliable calculation of the collective mode structure of a strongly coupled electronic bilayer. The calculation is based on a classical model through the third-frequency-moment-sum rule preserving quasilocalized charge approximation, (QLCA) using recently calculated hypernetted-chain pair correlation functions. The out-of-phase spectrum exhibits a remarkable long-wavelength energy gap and the absence of a previously conjectured dynamical instability.

[3] De-xin Lu and K. I. Golden, "Third-frequency-moment sum rule for electronic multilayers", *Physical review E* **61**, 926-928 (2000). The authors establish the third-frequency-moment sum rules for the density-density response matrix of electronic multilayer structures modeled as an array of N parallel two-dimensional (2D) electron-plasma monolayers. As in [1] above, layer densities and spacings between adjacent layers need not be equal. The new sum rules hold for *arbitrary* degeneracy, that is, they are valid over the entire temperature domain down to zero temperature. Contact is made with previously established sum rules for the isolated electron layer and type-I infinite superlattice. The special case of the equal-density electronic bilayer is considered and its third-frequency-moment-sum rules for the in-phase and out-of-phase dielectric functions are formulated.

[4] K. I. Golden and G. Kalman, "The quasilocalized charge approximation in strongly coupled plasma physics", *Physics of Plasmas* **7**, 14-32 (2000). This paper is an in-depth review of the QLCA [G. Kalman and K. I. Golden, *Physical Review A* **41**, 5516 (1990)] as a formalism for the analysis of the dielectric response tensor and collective mode dispersion in strongly coupled Coulomb liquids. The approach is based on a microscopic model in which the charges are quasilocalized on a short time scale in

local potential fluctuations. The authors review the application of the QLC approach to a variety of systems which can exhibit strongly coupled plasma behavior: (i) the one-component plasma (OCP) model in three dimensions (e.g., laser-cooled trapped ions) and (ii) in two dimensions (e.g., classical 2D electron liquid trapped above the free surface of liquid helium), (iii) binary ionic mixture in a neutralizing uniform background (e.g., carbon-oxygen white dwarf interiors), (iv) charged particle bilayers (e.g., semiconductor electronic bilayers), and (v) charged particles in polarizable background (e.g., laboratory dusty plasmas).

This paper also presents new information about the longitudinal plasma and transverse shear mode eigenfrequencies in symmetric ionic mixtures where the charge to mass ratios are equal, i.e., $Z_2/m_2 = Z_1/m_1$ (e.g., $D^+ - He^{2+}$ plasma).

[5] M. P. Das, K. I. Golden, and F. Green, "Compressibility sum rule for the two-dimensional electron gas", *Physical Review E* 64, 012103-1 to 012103-4 (2001).

The authors establish formulas for the isothermal compressibility and long-wavelength static density-density response function of a weakly correlated two-dimensional electron gas in the $1 \ll \beta\epsilon_F < \infty$ and $0 \leq \beta\epsilon_F \ll 1$ degeneracy domains; $\beta\epsilon_F = \pi\hbar^2/(mk_B T)$. The calculation of the pressure in the former domain is based on the Ishihara-Toyoda formula [A. Ishihara and T. Toyoda, *Physical review B* 21, 3358 (1980)] for the exchange-correlation energy at finite temperature. The pressure calculated in the latter domain is based on the Totsuji classical cluster-expansion formula for the correlation energy [H. Totsuji, *Journal of the Physical Society, Japan* 40, 857 (1976); *Physical Review A* 19, 889 (1979)].

[6] M. P. Das, K. I. Golden, and F. Green, "Dynamical theory of strongly coupled two-dimensional Coulomb fluids in the weakly degenerate quantum domain", *Physical Review E* 64, 046125-1 to 046125-14 (2001). The authors study the problem of dynamical response and plasma mode dispersion in strongly coupled two-dimensional Coulomb fluids (2DCFs) in the weakly degenerate quantum domain. Adapting the nonlinear response approach of Golden and Kalman [*Physical Review A* 19, 2112 (1979)] to the 2DCF, the authors construct a self-consistent approximation scheme for the calculation of the density response functions and plasma mode dispersion at long wavelengths. The basic ingredients in the construction are (i) the first kinetic equation in the Bogoliubov-Born-Green-Kirkwood-Yvon kinetic equation hierarchy, (ii) the velocity-average-approximation (VAA) hypothesis, (iii) the quadratic fluctuation-dissipation theorem, and (iv) the dynamical superposition approximation (DSA) closure hypothesis. The reliability of the VAA-DSA theory is guaranteed by the fact that the principal coupling correction to the 2D temperature-dependent Lindhard function is identified as being precisely the part of the third-frequency-moment sum rule coefficient proportional to the potential energy.

[7] Z. Donko, G. Kalman, and K. I. Golden, "Caging of particles in one-component plasmas", *Physical Review Letters* 88, 225001-1 to 225001-4 (2002). Strongly coupled Coulomb systems are characterized by localization ("caging") of particles trapped and oscillating in slowly fluctuating local potential wells. This observation constitutes the

basic assumption underlying the QLCA. Using molecular dynamics simulation, the authors study the changes in the particles' surroundings (cages) in a three dimensional classical one-component plasma. The results of the analysis show that at high coupling values, the particle dynamics changes qualitatively: the particles are caged by their nearest neighbors and spend several oscillation cycles in local minima of the rough potential surface without experiencing substantial changes in their surroundings. The caging time is a rapidly increasing function of coupling strength. The caged particles exhibit a characteristic oscillation spectrum. Escape from the cage appears to be the dominating process for self-diffusion in the strong coupling regime. The conclusion is that the molecular dynamics simulation results support the physical basis of the QLCA.

[8] **K. I. Golden, G. Kalman, and S. Kyrkos, "Charged particle layers in the Debye limit", *Physical Review E* 66, 0311XX-1 to 0311XX-10 (to appear in the October, 2002 issue).** The authors develop an equivalent of the Debye-Huckel weakly coupled equilibrium theory for layered classical charged particle systems comprised of one single charged species. The two most important configurations are considered, namely, the charged particle bilayer and the infinite superlattice. The approach is based on the link provided by the classical fluctuation-dissipation theorem between the random-phase approximation response functions and the Debye equilibrium pair correlation function. Layer-layer pair correlation functions, screened and polarization potentials, static structure functions, and static response functions are calculated. The importance of the perfect screening and compressibility sum rules in determining the overall behavior of the system, especially in the $r \rightarrow \infty$ limit, is emphasized. The similarities and differences between the quasi-two- dimensional bilayer and quasi-three-dimensional superlattice are highlighted. An unexpected behavior that emerges from the analysis is that the screened potential, the correlations, and the screening charges carried by the individual layers exhibit a marked nonmonotonic dependence on the layer separation.

[9] **G. J. Kalman and K. I. Golden, "Sum rules, dynamical structure functions and collective mode spectrum for charged particle bilayers", submitted to *Physical Review Letters*.** The authors establish and use exact sum rules to analyze the behavior of the in-phase and out-of-phase dynamical structure functions for a charged particle bilayer over the entire classical to quantum domain. The frequencies and spectral weights of the collective modes and their strengths relative to the diffusive central peak are calculated. The results for the collective mode frequencies—including the prediction of the remarkable long-wavelength energy gap in the out-of-phase spectrum (see [2] above)—are valid over the entire temperature domain down to zero temperature. The prediction that the energy gap persists all the way down to zero temperature now opens up the possibility of actually observing it in Raman scattering experiments on high- r_s multiple quantum well structures in AlGaAs/GaAs.

[10] **Z. Donko, P. Hartmann, K. Kutasi, G. J. Kalman, and K. I. Golden, "Collective mode dispersion and energy gap in charged particle bilayers", submitted to *Physical Review Letters*.** The dynamical properties of strongly coupled charged particle bilayers are investigated by molecular dynamics (MD) simulation. The spectra of the current correlation functions show the existence of two (in-phase and out-of-phase) longitudinal

and two (in-phase and out-of-phase) transverse collective modes. The finite frequencies exhibited by the out-of-phase modes at long wavelengths confirm the existence of the predicted energy gap in the bilayer system (see [2] and [9] above). At small layer separation, the magnitude of the gap $\approx 1.4\omega_0$ (ω_0 being the nominal 2D plasma frequency); this magnitude decreases with increasing layer separation. The full MD-generated dispersion relation confirms the theoretical predictions and complements available experimental results.

Conference presentations

[11] K. I. Golden and G. J. Kalman, "Quasilocalized charge approximation in strongly coupled plasma physics", presented by K. I. Golden at Miniconference on Strongly Coupled Plasmas, American Physical Society Division of Plasma Physics 40, New Orleans LA, November 1998. (See Publication [4] above)

[12] G. J. Kalman, K. B. Blagoev, Z. Donko, K. I. Golden, G. McMullan, V. Valtchinov, and H. Zhao, "Charged particle bilayers: Equilibrium and dynamics", paper presented by G. Kalman at the 1999 International Conference on Strongly Coupled Coulomb Systems, Saint Malo, France (September 1999); *Journal de Physique IV, France 10, Pr 5-85 to 5-98 (2000)*. This review summarizes the results of analyses of the equilibrium structure, screening properties, and collective mode dynamics of electronic bilayers, based on the hypernetted chain calculation of the intralayer and interlayer correlation functions. A set of static sum rules for the response function are established which shed light on the origin of the anomalous screening properties of the system.

Summary

The following summarizes the main research accomplishments/findings of the project:

- ◆ Publication of an in-depth review article in *Physics of Plasmas* on the quasilocalized charge approximation (QLCA) in strongly coupled plasma physics and its application to a variety of Coulomb systems: the model one-component plasma in three and two dimensions, binary ionic mixtures, charged particle bilayers, and laboratory dusty plasmas.
- ◆ In the strongly coupled Coulomb liquid phase, the physical basis of the QLCA, namely, the caging of particles trapped in slowly fluctuating local potential minima, is supported by molecular dynamics simulation of the classical three-dimensional one-component plasma.
- ◆ The QLCA theory, when applied to the analysis of the collective modes in strongly coupled charged particle bilayers, predicts the existence of a remarkable long-wavelength energy gap in the out-of-phase excitation spectrum. Our more recent theoretical calculations based on the three principal frequency-moment sum rules reveal that the gap persists for arbitrary coupling strengths and over the entire classical to quantum domain all the way down to zero temperature. The existence of

the energy gap has now been confirmed in a molecular dynamics simulation of the charged particle bilayer.

- ◆ We formulated new compressibility and third-frequency-moment sum rules for multilayer plasmas, and we applied the sum rules to the analysis of the dynamical structure function of charged particle bilayers and superlattices.
- ◆ We formulated an equivalent of the Debye-Huckel weak coupling equilibrium theory for classical charged particle bilayer and superlattice plasmas.
- ◆ We formulated the quadratic fluctuation-dissipation theorem (QFDT) for layered classical plasmas.
- ◆ We applied the QFDT to a powerful kinetic theory-based description of the density-density response function and long-wavelength plasma mode behavior in strongly coupled two-dimensional Coulomb fluids in the weakly degenerate quantum domain.

There are no unexpended funds left at the end of the budget period.

SUM RULES, DYNAMICAL STRUCTURE FUNCTIONS AND COLLECTIVE MODE SPECTRUM FOR CHARGED PARTICLE BILAYERS

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We establish and use exact sum rules to analyze the behavior of the dynamical structure functions of a charged bilayer over the entire classical to quantum domain. The frequencies and spectral weights of the collective modes and their strengths relative to the diffusive central peak are calculated. We are lead to an inference concerning the effect of exchange on the intralayer and interlayer correlation functions.

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Sum rules dynamical and static structure functions are centrally important tools in many-body theory. In this Letter we address the formulation of sum rules and the character of structure functions in a charged particle bilayer system. Recently, bilayers have attracted attention from a number of directions. While most of the attention has been directed at semiconductor bilayers in a magnetic field, it has been realized at the same time that magnetic-field-free bilayers, both under classical conditions [1] and near zero temperature in semiconductor nanostructures [2, 3], are also endowed with a richness of unique physical effects. The effect of layering in double and multiple layered structures is also of importance in high- T_c cuprate superconductors [4]. The equilibrium structures of the correlation dominated strongly coupled solid [5] and liquid [6] phases are now well understood and the theoretical predictions have been experimentally corroborated [1]. Less understood is the strongly correlated ($r_s \gg 1$) quantum phase, where information on correlations is still lacking. The spectrum of collective excitations in the RPA limit has been known for a long time [7], but the analysis of the effect of correlations beyond the RPA, both in the weak coupling [8] and strong coupling [9] limits is more recent. The latter approaches are built upon a classical model, but it is not expected that quantum effects would substantially modify the nature of collective modes. The dynamical structure function $S(\mathbf{k}, \omega)$ contains, in principle, all the information on the collective mode spectrum and on exchange and correlations in the system for arbitrary degeneracy extending from the classical (high temperature) regime to the quantum (zero-temperature) regime. To date, no unified coupling independent representation of $S(\mathbf{k}, \omega)$ covering both regimes has been found for any many-body system. What makes the charged-particle bilayer unique in this respect is its quasi 2D character, combined with its isomorphism to a two-component system. The former makes it possible to apply the recently introduced [11] explicit representation for arbitrary degeneracy of 2D static response functions, while the latter renders this exercise highly non-trivial. In this Letter we exploit these features to obtain

structure functions in a manner valid for all temperatures and portraying the transition from the classical to the quantum regime. This is accomplished by the combination of exact sum rules, stated here the first time for bilayers, and an ansatz for the dynamical structure function, patterned as an extended Feynman-like structure.

We consider a bilayer model, consisting of two 2D layers of charged particles (with $Z=1$) of equal densities, separated by a distance d . The interaction matrix elements are $\phi_{11}(k) = \phi_{22}(k) = 2\pi e^2/k$, $\phi_{12}(k) = \phi_{21}(k) = (2\pi e^2/k)e^{-kd}$. With the aid of $\phi_{ij}(\mathbf{k})$ and $\bar{\chi}_{ij}(\mathbf{k})$, the screened (total) density response function, the dielectric matrix $\epsilon_{ij}(\mathbf{k})$, and its inverse $\eta_{ij}(\mathbf{k})$, and the full (external) density response $\chi_{\ell j}(\mathbf{k})$, can be constructed [6]):

$$\begin{aligned}\epsilon_{ij}(\mathbf{k}) &= \delta_{ij} - \phi_{i\ell}(\mathbf{k})\bar{\chi}_{\ell j}(\mathbf{k}), \\ \chi_{ij}(\mathbf{k}) &= \bar{\chi}_{i\ell}(\mathbf{k})\eta_{\ell j}(\mathbf{k}), \\ \eta_{ij}(\mathbf{k}) &= \delta_{ij} + \phi_{i\ell}(\mathbf{k})\chi_{\ell j}(\mathbf{k}).\end{aligned}\tag{1}$$

[Summation over repeated indices is understood; $\bar{k} = ka$, $\bar{d} = d/a$ (a being the Wigner-Seitz radius within a layer, $\pi a^2 n = 1$)].

Sum Rules. The perfect screening sum rule follows from the fact that a charged impurity placed in one of the layers (say layer 1) is screened by the combined effect of the two layers. The polarization charges, ρ_1 and ρ_2 surrounding the charge with $Z=+1$ in layer 1 are, respectively, $\rho_1(\mathbf{k}) = \eta_{11}(\mathbf{k}) - 1$ and $\rho_2(\mathbf{k}) = \eta_{12}(\mathbf{k})$. The total charges in the respective layers are $\rho_1(\mathbf{k}=0) + 1$ and $\rho_2(\mathbf{k}=0)$. Thus the perfect screening requirement is

$$\eta_{11}(\mathbf{k}=0) + \eta_{12}(\mathbf{k}=0) = 0.\tag{2}$$

$\eta_{11}(\mathbf{k}=0)$ and $\eta_{12}(\mathbf{k}=0)$ can assume any positive or negative value compatible with Eq. (2): $\eta_{ij}(\mathbf{k}=0) < 0$ (> 0) corresponds to overscreening (antiscreening) in the j -th layer. As it is discussed elsewhere [10], such situations may indeed occur in bilayers.

It is possible now, in view of Ref. [11], to provide an exact representation for the $\bar{\chi}_0$ screened (total) density response function $\bar{\chi}_{ij}$ in terms of L_{ij} , the inverse compressibility matrix and the density response of the 2D non-interacting electron gas :

$$\bar{\chi}_{ij}(\mathbf{k}=0) = \chi_0 L_{ij}^{-1}$$

$$L_{ij} = \left(\frac{\partial P_i}{\partial n_j} / \frac{\partial P_0}{\partial n} \right).$$

$$\chi_0 \square \bar{c}_0(\mathbf{k}=0) = - \frac{n}{e_0} [1 - \exp(-be_0)] \quad (3)$$

$[\beta=(kT)^{-1}, P_0$ and $\varepsilon_0 = \pi\hbar^2/m$ are, respectively, the pressure and the $T=0$ Fermi energy of the non-interacting 2D electron gas; $L = L_{11} = L_{22}$ (direct inverse compressibility) and $N = L_{12} = L_{21}$ (transverse inverse compressibility)].

The information available in Eq (3) is sufficient to generate a small- k expansion of the various response functions to $O(\bar{k})$, since $\bar{\chi}(\mathbf{k})$ is expected to be an analytic function of k . With this proviso one can obtain

$$\varepsilon_{11}(\mathbf{k} \rightarrow 0) = \frac{2\tilde{\Gamma}}{\bar{k}} \frac{1}{L+N} + 1 + 2\tilde{\Gamma}\bar{d} \frac{N}{L^2 - N^2} + O(\bar{k})$$

$$\varepsilon_{12}(\mathbf{k} \rightarrow 0) = \frac{2\tilde{\Gamma}}{\bar{k}} \frac{1}{L+N} - 2\tilde{\Gamma}\bar{d} \frac{L}{L^2 - N^2} + O(\bar{k}) \quad (4)$$

$$\|\varepsilon(\mathbf{k} \rightarrow 0)\| = \frac{4\Gamma}{\bar{k}} \frac{L - N + 2\Gamma\bar{d}}{L^2 - N^2} + O(1).$$

Note that $\tilde{\Gamma} = [e^2/(a\epsilon_0)](1 - e^{-\beta\epsilon_0})$ is the coupling parameter for arbitrary degeneracy (for $T \rightarrow \infty$, $\tilde{\Gamma} = \Gamma = \beta e^2/a$, the classical coupling constant, and for $T=0$, $\tilde{\Gamma} = r_s$). Then

$$\eta_{11}(\mathbf{k}=0) = -\eta_{12}(\mathbf{k}=0) = \frac{1}{2} \frac{L-N}{L-N+2\tilde{\Gamma}\bar{d}} \quad (5)$$

in agreement with Eq. (2). With increasing layer separation N rapidly vanishes and L approaches a value, L_0 , appropriate for a single layer. One can track the evolution of the L, N compressibility coefficients through classical HNC calculations [12]. For $\Gamma \geq 3$, $L - N$ changes sign at a small ($\bar{d} \ll 1$) layer separation, but $L - N + 2\tilde{\Gamma}\bar{d}$ remains positive, since L_0 is bounded by $L_0 > -0.821\Gamma$ [13].

The Stillinger-Lovett (SL) condition that relates directly to the correlation function, rather than to the response functions, requires that $S_{11}(\mathbf{k}=0) + S_{12}(\mathbf{k}=0) = 0$. This requirement is statistics independent (i.e. valid for arbitrary degeneracy), although in the classical limit it is tantamount to the perfect screening sum rule.

Density response. Diagonalizing the commuting physical quantities in the space spanned by the $[+]$ (in-phase) and $[-]$ (out-of-phase) directions one finds

$$\begin{aligned} \chi_-(\mathbf{k} \rightarrow 0) &= \chi_0 X_-(\mathbf{k}), \\ X_-(\mathbf{k}) &= 2A + B \frac{\bar{k}}{4\tilde{\Gamma}} + O(\bar{k}^2) \\ A &= \frac{1}{2} \frac{1}{L-N+2\tilde{\Gamma}\bar{d}}, \quad B = \frac{4\tilde{\Gamma}^2 \bar{d}^2}{(L-N+2\tilde{\Gamma}\bar{d})^2} = 16\tilde{\Gamma}^2 \bar{d}^2 A^2 \end{aligned} \quad (6)$$

In $\chi_-(\mathbf{k})$, the $O(\bar{k}^2)$ terms cannot be found without the knowledge of the similar higher order terms in $\bar{\chi}_{ij}(\mathbf{k})$. In contrast, remarkably, the response function $\chi_+(\mathbf{k})$ can be obtained to $O(\bar{k}^2)$ without the

interference of these unknown terms;

$$\chi_+(\mathbf{k} \rightarrow 0) = \chi_0 X_+(\mathbf{k})$$

$$X_+(\mathbf{k}) = \frac{\bar{k}}{4\tilde{\Gamma}} - \left(\frac{\bar{k}}{4\tilde{\Gamma}} \right)^2 [L + N - 2\tilde{\Gamma}\bar{d}] + O(\bar{k}^3) \quad (7)$$

Eq. (6) and (7) are also valid for arbitrary degeneracy.

Structure functions. For the dynamical $S_{\pm}(\mathbf{k}, \omega)$ we invoke the Feynman type Ansatz

$$S_{\pm}(\mathbf{k}, \omega) = \pi [2p_{\pm}(\mathbf{k})\delta(\omega) + q_{\pm}(\mathbf{k})\{\delta(\omega - \omega_{\pm}(\mathbf{k})) + \delta(\omega + \omega_{\pm}(\mathbf{k}))\}] \quad (8)$$

The difference between Eq. (8) and the conventional Feynman-type Ansatz resides in the zero frequency term. The introduction of this term is motivated by the observation that in multicomponent systems the hydrodynamic diffusion dominates the low frequency behavior and its representation in $S(\mathbf{k}, \omega)$ is indispensable in view of the fact that $S(\mathbf{k}=0) \neq 0$. In contrast, in a single component plasma the central diffusion peak is suppressed for $k \rightarrow 0$ [14, 15]. The bilayer is more akin to a two-component system [6, 9] and thus the central peak is on a par with the peaks at the $\omega_{\pm}(\mathbf{k})$ resonances that represent the two, in-phase [+] and out-of-phase [-], longitudinal collective modes of a bilayer system. The representation of the central peak through a δ -function is not crucial since in the forthcoming analysis only the integral over the peak matters. A representation through a more realistic structure (a normalized Lorentzian, e.g.) would also be feasible: in this case, however, the width of the distribution could be determined by introducing additional considerations which are not constrained by exact sum-rule like constraints.

$S_{\pm}(\mathbf{k}, \omega)$ are required to satisfy low frequency and high frequency sum rules. The former follows from the combination of the general fluctuation-dissipation relation

$\text{Im } \chi_{\pm}(\mathbf{k}\omega) = -(n/\hbar)\tanh(z)S_{\pm}(\mathbf{k}\omega)$, ($z = \beta\hbar\omega/2$) and the compressibility sum rule Eq. (3). The high-frequency sum rules [16] are expressed via the $\langle\omega\rangle$ and $\langle\omega^3\rangle$ moments

$$\begin{aligned}\langle\omega^n\rangle_{\pm}(\mathbf{k}) &= (1/\pi)\int_{-\infty}^{\infty} d\omega\omega^n \text{Im } \chi_{\pm}(\mathbf{k},\omega) \\ \langle\omega\rangle_{\pm} &= -\frac{n}{m}k^2 \\ \langle\omega^3\rangle_{\pm} &= -\frac{n}{m}k^2\left\{\omega_{\pm 0}^2(\mathbf{k}) + [D_{11}(\mathbf{k}) \pm D_{12}(\mathbf{k})] + \frac{3}{ma^2}\langle E_{kin}\rangle\bar{k}^2 + \left(\frac{\hbar k^2}{2m}\right)^2\right\}\end{aligned}\quad (9)$$

Here $\omega_{\pm 0}(\mathbf{k}) = (n/m)k^2\varphi_{\pm}(\mathbf{k})$ are the mean field frequencies, $\langle E_{kin}\rangle$ is the average kinetic energy per particle for the interacting system. The $D_{\pm}(\mathbf{k})$ functions can be related to the pair correlations in the system; it should be noted that to lowest order in k , $D_{+}(\mathbf{k}) = -\omega_{+0}^2(\mathbf{k})\delta\bar{k}$, $D_{-}(\mathbf{k}) = g^2\omega_0^2$ where δ and g are system-dependent constants of order unity.

Combination of (8) with the fluctuation-dissipation theorem, (3), and (9) yields the relationships determining the weight factors $p_{\pm}(\mathbf{k})$ and $q_{\pm}(\mathbf{k})$:

$$\begin{aligned}p_{\pm}(\mathbf{k}) &= -\frac{\chi_0}{\beta n}X_{\pm}(\mathbf{k}) - \frac{\bar{k}^2}{\beta ma^2\omega_{\pm}^2(\mathbf{k})} \\ q_{\pm}(\mathbf{k}) &= \frac{\hbar}{2ma^2\omega_{\pm}(\mathbf{k})} \frac{k^2}{\tanh(z_{\pm}(\mathbf{k}))}\end{aligned}\quad (10)$$

Thus the knowledge of the $S_{\pm}(\mathbf{k},\omega)$ enables one to obtain the static structure function for arbitrary degeneracy via the relation $S_{\pm}(\mathbf{k}\rightarrow 0) = p_{\pm}(\mathbf{k}) + q_{\pm}(\mathbf{k})$. Although it is not manifest from Eq. (10), the amplitude of the central peak $p_{\pm}(\mathbf{k})$ is always positive, as it should be (see Table I); this further corroborates the physical soundness of the present model.

Collective modes. The frequencies of the collective modes and their spectral weights now can be determined from evaluating the 3rd moment sum rule, Eq. (9) with the aid of Eq (10):

$$\omega_{\pm}^2(\mathbf{k} \rightarrow 0) = \omega_{\pm 0}^2(\mathbf{k}) + \left[D_{11}(\mathbf{k}) \pm D_{12}(\mathbf{k}) \right] + \frac{3}{m\alpha^2} \langle E_{kin} \rangle \bar{k}^2 \quad (11)$$

$$\frac{q_+(\mathbf{k})}{q_-(\mathbf{k})} = \frac{\omega_-(\mathbf{k}) \tanh[z_-(\mathbf{k})]}{\omega_+(\mathbf{k}) \tanh[z_+(\mathbf{k})]} \quad (12)$$

The frequencies are in agreement with earlier calculations, based on the Quasilocalized Charge Approximation (QLC) [9]: in particular, $\omega_-(\mathbf{k} \rightarrow 0)$ develops a finite energy gap and becomes an optic mode. While the QLC derivation is a strong coupling result, the present approach is formally coupling independent, and its result indicates that the gap is not supplanted by the RPA structure below some critical coupling value: it vanishes only with the vanishing of correlations. This result, however, has to be understood within the framework of the present approximation which ignores damping. More realistically, at low coupling the actual damping is expected to broaden the optic peak and merge it into the continuum.

Behavior of the structure functions. The results of the analysis of $S_{\pm}(\mathbf{k}, \omega)$ in the different temperature and frequency domains are summarized below in Table 1 and illustrated in Fig 1. The main features of the results displayed can be summarized as follows.

- (i) The fact that the central peak is related to thermal diffusion is clearly demonstrated by its strong temperature dependence; while for high temperatures the central peak saturates at a value dictated by the compressibility sum rule, for low temperatures it is proportional to T , both for S_+ and S_- and diminishes to zero as $T \rightarrow 0$. The vanishing of $S_{\pm}(\mathbf{k}, \omega=0)$ for $T=0$ has already been suggested by various approximate calculations [8]

- (ii) The out-of-phase ($S_{-}(\mathbf{k},0)$) diffusion peak, which is $O(1)$, always dominates over the $O(k^2)$ in-phase ($S_{+}(\mathbf{k},0)$) diffusion peak.
- (iii) The spectral weights of the collective modes are, qualitatively, in inverse proportion to their dispersion. Should the out-of-phase mode assume an acoustic behavior (as in the unphysical RPA limit) it would carry most of the strength, the in-phase mode being weaker. By contrast, the actual optic character of the out-of-phase mode, (for any finite coupling) transfers most of the strength to the in-phase mode. This tendency is more pronounced for high temperatures than for $T \rightarrow 0$. These results corroborate Ortnner's observation [18] concerning the weakness of the optic mode, but are at variance with his suggested behavior of the individual spectral weights.
- (iv) At low temperatures the static structure functions, both $S_{+}(\mathbf{k})$ and $S_{-}(\mathbf{k})$, are dominated by the contributions from the collective peaks. In contrast, at high temperatures the dominance of the collective peak prevails for $S_{+}(\mathbf{k})$ only, whereas for $S_{-}(\mathbf{k})$ the main contribution shifts from the collective to the central peak.

Pair correlation functions. The two pair correlation functions $g_{11}(\mathbf{r})$ and $g_{12}(\mathbf{r})$ are related to the static structure functions through their Fourier transforms by $S_{11}(\mathbf{k})=1+ng_{11}(\mathbf{k})$ and $S_{12}(\mathbf{k})=ng_{12}(\mathbf{k})$. In the $d=0$ limit, when the two layers collapse into a single 2D layer, classical considerations demand that $g_{11}(\mathbf{r}) = g_{12}(\mathbf{r})$. This, together with the SL condition fixes

$$ng_{11}(\mathbf{k}=0) = ng_{12}(\mathbf{k}=0) = -1/2 \quad (d=0, T \rightarrow \infty) \quad (20)$$

Once degeneracy sets in, the above equality is violated: in particular, at $T=0$

$$ng_{11}(\mathbf{k}=0) = -1, ng_{12}(\mathbf{k}=0) = 0 \quad (d=0, T \rightarrow 0). \quad (21)$$

The cause for this rather unexpected behavior is to be sought in the different roles exchange plays in the two correlation functions: exchange effects operate between particles within a layer, but not between particles in different layers. Thus g_{11} is enhanced by exchange interaction, and, as a consequence of the SL condition, g_{12} is simultaneously diminished. While for $d=0$ the effect is obviously spurious and results from the inadequacy of the model, it is real for distances greater than the tunneling distance (of the order of the effective Bohr radius), and it is expected that in the quantum domain, it will modify the classically predicted [5,6] structural phase transitions.

As to experimental results on bilayer collective spectra, a recent compilation [20] shows that at higher k values they do favor the QLCA prediction (and, consequently, that of the present paper) over the predictions of other theoretical approaches [21]. In the more crucial lower k domain, the existing low coupling results [22] do not provide conclusive evidence to distinguish between the QLCA and RPA behavior. At the same time, ongoing Molecular Dynamics studies [23] unambiguously show the existence of the $k=0$ frequency gap down to low coupling values.

In summary, we have developed static sum rules for bilayer response functions and we have shown, for the first time, how these sum rules can be incorporated in the analysis of the bilayer dynamical structure function to obtain a representation over the entire temperature domain down to zero temperature. For finite temperatures, in $S_+(\mathbf{k}\omega)$ the central diffusive peak is suppressed, compared to the collective peak, whereas in $S_-(\mathbf{k}\omega)$ the central peak dominates; at zero temperature to lowest order in k only the two collective peaks survive, as usual [19], but with very different amplitudes ($k^{3/2}$ for ω_+ , and k^2 for ω_- , respectively). The result for the collective mode frequencies (including the prediction of an energy gap in the out-of-phase spectrum) is now free from the strong coupling approximation used earlier [9] (although encumbered by the limitations of the present approximation where damping is ignored). Examination of the information on the pair correlation

function gleaned from $S_{\pm}(\mathbf{k})$ shows how the classically prevailing g_{11} - g_{12} symmetry is broken in the general case, due to the in-layer exchange correlations.

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	Classical	Degenerate
S_+ , IN-PHASE		
$\omega_+(k \rightarrow 0),$	$\omega_0 \sqrt{\bar{k}} (1 - \frac{\bar{d}}{2} \bar{k} - \delta \bar{k} + \frac{3}{4\Gamma} \bar{k}), \quad \omega_0^2 = 4e^2 / ma^3$	
$S_+(\mathbf{k} \rightarrow 0),$	$\frac{1}{4\Gamma} \left[\bar{k} - \frac{1}{4\Gamma} (L + N - 2\Gamma \bar{d}) \bar{k}^2 \right] + \frac{1}{12} \beta \epsilon_0 \bar{k}$	$\frac{\bar{k}^{3/2}}{4r_s^{1/2}}$
$\frac{p_+(\mathbf{k} \rightarrow 0)}{q_+(\mathbf{k} \rightarrow 0)},$	$\frac{\bar{k}}{4\Gamma} (3 - (L + N) - 4\Gamma \delta)$	0
S_- , OUT-OF-PHASE RPA ACOUSTIC		
$\omega_-(\mathbf{k} \rightarrow 0),$	$s\bar{k}, \quad s = \sqrt{(\omega_0^2 \bar{d}/2) + [3/(ma^2)] E_{km}},$	
$S_-(\mathbf{k} \rightarrow 0),$	$\left[\frac{1}{L - N + 2\Gamma \bar{d}} + \frac{4\Gamma^2 \bar{d}^2}{(L - N + 2\Gamma \bar{d})^2} \left(\frac{\bar{k}}{4\Gamma} \right) \right]$	$\frac{\bar{k}}{2r_s \sqrt{\bar{d}}}$
$\frac{p_-(\mathbf{k} \rightarrow 0)}{q_-(\mathbf{k} \rightarrow 0)},$	$\frac{3 - (L - N)}{L - N + 2 + \bar{d}}$	0
S_- , OUT-OF-PHASE NON-RPA OPTICAL		
$\omega_-(\mathbf{k} \rightarrow 0),$	$g\omega_0$	
$S_-(\mathbf{k} \rightarrow 0),$	$\frac{1}{L - N + 2\Gamma \bar{d}} + \frac{4\Gamma^2 \bar{d}^2}{(L - N + 2\Gamma \bar{d})^2} \left(\frac{\bar{k}}{4\Gamma} \right)$	$\frac{\bar{k}^2}{r_s^{1/2}} \frac{1}{2^{3/2} g}$
$\frac{p_-(\mathbf{k} \rightarrow 0)}{q_-(\mathbf{k} \rightarrow 0)},$	$\frac{4g^2 \Gamma}{L - N + 2\Gamma \bar{d}} \frac{1}{\bar{k}^2}$	0
S_+/S_-		
$\frac{q_+(\mathbf{k} \rightarrow 0)}{q_-(\mathbf{k} \rightarrow 0)},$	$\frac{\omega_-^2}{\omega_+^2}$	$\frac{\omega_-}{\omega_+}$

Table I

CAPTIONS

Table 1.

The Table shows the leading terms for $k \rightarrow 0$ for the dynamical structure functions $S_{\pm}(\mathbf{k}, \omega)$ and the relative strengths of the central peak, $p_{\pm}(\mathbf{k})/q_{\pm}(\mathbf{k})$; the relative strength of the two modes ($q_{+}(\mathbf{k})/q_{-}(\mathbf{k})$) is also shown. Note that although it is not manifest from Eq. (10), the amplitudes both of the central and of the collective peaks are always positive, as they should be.

Fig. 1

Schematic representation of $S_{\pm}(\mathbf{k}, \omega)$ vs. ω . The heights of the central and collective peaks are shown for the classical ($T \rightarrow \infty$) and degenerate ($T \rightarrow 0$) limits in terms of the leading power of $\bar{k}$ and T . Note the vanishing of the central peak for $T \rightarrow 0$.

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Fig. 1

Collective mode dispersion and energy gap in charged-particle bilayers

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The dynamical properties of strongly coupled charged particle bilayers are investigated by molecular dynamics (MD) simulation. The spectra of the current correlation functions show the existence of two (in-phase and out-of-phase) longitudinal and two (in-phase and out-of-phase) transverse collective modes. The out-of-phase modes possess finite frequencies at wave numbers $k \rightarrow 0$, confirming the existence of the predicted long-wavelength energy gap in the bilayer system. The energy gap at low layer separation is $\approx 1.4 \omega_0$ at $\Gamma = 40$ (ω_0 being the nominal 2D plasma frequency) and it decreases with increasing layer separation. The full $\omega(k)$ dispersion relation confirms the theoretical predictions and complements available experimental results.

The dynamical properties of two-dimensional (2D) strongly-coupled classical Coulomb systems and complex plasmas have attracted considerable interest for many years [1]. The longitudinal and transverse waves existing in these systems have been thoroughly investigated both theoretically [2] and by molecular dynamics (MD) simulations [3]. Less understood is the more complex bilayer system consisting of two layers of identical charged particles separated by distance d . Such a model is relevant to supercooled ions in particle traps [4], semiconductor devices [5] and laboratory complex plasmas [6].

The dynamical properties of strongly-coupled charged bilayers have been studied theoretically with the aid of the Quasi-Localized Charge Approximation (QLCA) [7]. The QLCA analysis has shown the existence of four distinct collective excitations [8]: the longitudinal in-phase and out-of-phase (particles in the two layers oscillating in phase and 180 degrees out of phase, respectively) plasmon modes and the transverse in-phase and out-of-phase shear modes. The in-phase modes emulate a 2D behavior while the out-of-phase modes exhibit qualitatively new features. It has been predicted on the basis of the QLC theory that, in sharp contrast to the results of the RPA description where the long-wavelength out-of-phase plasmon is acoustic [9], this excitation exhibits a nonzero frequency at wave numbers $k \rightarrow 0$ [8]. At the same time, however questions have been raised about the actual existence of this so-called energy gap. The issue brought forward is the possible effect of damping [10] and the compatibility of the RPA and QLCA predictions [11]. Recent experiments on the dispersion of the out-of-phase plasmon have been carried out in the low-coupling, high

layer separation regime [5] (for a critical evaluation see also Ref. [12]). The possible relationship between these experimental findings, theoretical predictions, and the present MD simulations will be discussed below.

In order to provide a more definitive analysis of the dynamical behavior of charged particle bilayers, we have undertaken an MD calculation of the spectra of the longitudinal and transverse dynamical current correlation functions and of the corresponding dispersion relations for bilayers in their liquid state. The results of this classical simulation are also expected to provide a correct description of the qualitative features of the collective mode spectrum in the quantum domain. Our calculations are based on a P³M (particle-particle particle-mesh) [13] molecular dynamics code, used earlier to investigate the static properties of the system [14]. The number of particles is set to $N = 1600$ in both layers, and periodic boundary conditions are applied to the simulation squares having an edge length L . The bilayer is isomorphic to a binary liquid with interaction potentials $\phi_{11}(r) = \phi_{22}(r) = e^2/r$ and $\phi_{12}(r) = \phi_{21}(r) = e^2/\sqrt{r^2 + d^2}$ and is characterized by the coupling coefficient $\Gamma = e^2/(akT)$ and the layer separation d/a , where $a = 1/\sqrt{n\pi}$ is the Wigner-Seitz radius, and n is the areal density.

The central quantities in this study are the spectra of the correlations in the longitudinal and transverse current fluctuations and in the density fluctuations. Our goal is to deduce information on the collective modes and their dispersion from the analysis of these quantities. Using the phase space coordinates of particles situated in layers $m = 1$ and 2, data for

$$\lambda^{(m)}(k, t) = k \sum_i v_{ix}^{(m)} \exp(ikx_i^{(m)}), \quad (1)$$

are stored during the course of simulation for the calculation of the spectra of longitudinal modes, as well as

$$\tau^{(m)}(k, t) = k \sum_i v_{iy}^{(m)} \exp(ikx_i^{(m)}), \quad (2)$$

for the calculation of the transverse mode spectra and

$$\rho^{(m)}(k, t) = \sum_i \exp(ikx_i^{(m)}), \quad (3)$$

for the calculation of the density fluctuation spectra. (We assume that $\mathbf{k}$ is directed along the x axis (the system is isotropic) and accordingly omit the vector notation of the wave number.) The data are stored for a series of wave numbers, multiples of $k_{\min} = 2\pi/L$. The spectra of the modes are obtained through Fourier transforms of $\lambda(k, t)$, $\tau(k, t)$ and $\rho(k, t)$ [15,16]. For the bilayer system the intralayer and interlayer spectra are obtained as:

$$L_{11}(k, \omega) = \frac{|\mathcal{F}\{\lambda^{(1)}(k, t)\}|^2 + |\mathcal{F}\{\lambda^{(2)}(k, t)\}|^2}{2}, \quad (4)$$

and

$$L_{12}(k, \omega) = \frac{|\mathcal{F}\{\lambda^{(1)}(k, t) + \lambda^{(2)}(k, t)\}|^2}{2} - L_{11}(k, \omega). \quad (5)$$

It is useful to diagonalize L_{ij} by rotating it into a $\pm$ coordinate system: $L_+(k, \omega) = L_{11} + L_{12}$, $L_-(k, \omega) = L_{11} - L_{12}$. Similar relations are used for the transverse correlations and for the density correlation spectra, generating $T_{\pm}(k, \omega)$ and $S_{\pm}(k, \omega)$, respectively.

Most of our calculations have been carried out for $\Gamma = 40$, but we also illustrate the behavior of the fluctuation spectra at lower coupling, at $\Gamma = 5$. Layer separations have been chosen in the $0.1 \leq d/a \leq 5$ range.

Figure 1 shows a series of representative longitudinal (L_+ and L_-), and transverse (T_+ and T_-) current fluctuation spectra. The results are displayed as functions of the ratio of oscillation frequency to the nominal 2D plasma frequency $\omega_0 = (2\pi ne^2/ma)^{1/2}$. Collective modes show up as peaks at the collective mode frequencies in the correlation spectra. The longitudinal modes appear in $L_{\pm}$ or equivalently in $S_{\pm}$: we focus on $L_{\pm}$, where the noise is less prevalent. Transverse modes show up as peaks of $T_{\pm}$. In-phase modes appear in the (+) and out-of-phase modes appear in the (-) spectra.

The analysis of the correlation spectra unambiguously demonstrates the existence of all four predicted collective modes. While the peaks of $L_+(\omega)$ (see Fig. 1(a)) shift to $\omega = 0$ with decreasing k , both out-of-phase modes exhibit a finite frequency $\omega(0)$ at $k \rightarrow 0$, as it can be seen in Fig. 1(b) and (d). This behavior provides direct evidence for the presence of an energy gap in the out-of-phase mode spectrum of a strongly coupled bilayer.

The effect of layer separation on the L_- spectra (at fixed ka) and the energy gap as a function of layer separation d/a are shown in Fig. 2(a) and (b), respectively. One observes that the increasing layer separation results in a considerable change both in the position and in the width of the L_- spectra. The values of ω at $k \rightarrow 0$ for the L_- and T_- modes – as shown in Fig. 2(b) – are very close to each other and show a decreasing tendency with increasing layer separation. At layer separations $d \rightarrow 0$ the frequency tends to be saturated at $\omega(k=0)/\omega_0 \approx 1.43$. With increasing layer separation this value drops approximately to 0.35 at $d/a = 1$, reaching an extremely low (< 0.05) value by $d/a = 2$. In addition to the present results, data obtained from the QLCA gap formula [8]

$$\left(\frac{\omega}{\omega_0}\right)^2 = a \int_0^\infty dr \frac{r[1 + h_{12}(r)]}{(r^2 + d^2)^{3/2}} \left[\frac{3d^2}{r^2 + d^2} - 1 \right], \quad (6)$$

using pair correlation functions (h_{12}) obtained from hypernetted-chain [8] and MD [14] calculations are also plotted in Fig. 2(b). While the energy gap emerges as predicted by the QLC theory, one can observe that at small layer separations its magnitude is $\approx 30\%$ higher than the theoretical value. With increasing layer separation the energy gap value obtained from the simulations decreases faster than the QLC prediction, ultimately dropping below it around $d/a = 1$.

The full dispersion relations $\omega(k)$ for the four modes at $\Gamma = 40$ and layer separation $d/a = 0.3$, are plotted in Fig. 3(a). For low d/a values, the frequencies of the *out-of-phase modes* exhibit a weak dependence on wave number k over the whole domain shown in Fig. 3(a). Addressing the *longitudinal* (L_-) mode, for $d/a \geq 1.5$, the energy gap, which is now significantly lower (Fig. 2), is followed by a dispersion that bears a close resemblance to the well-known linear acoustic behavior predicted by the RPA. The slope of this quasi-linear portion is reduced by 66% (at $d/a = 1.5$) to 39% (at $d/a = 5$) from its RPA value due to the strong particle correlations. Fig. 3(b) also shows the results of the QLC theory calculation [8], which are in good agreement with the MD results.

For the *in-phase longitudinal mode* (L_+), the RPA predicts that for $k \rightarrow 0$, the dispersion is quasi-acoustic $\omega \sim \sqrt{k}(1 - kd/2 + 3ka/4\Gamma)$, while the QLCA predicts a further $O(k)$ correction due to correlations [8,9]. Our data reproduce this latter behavior. The dispersion of the mode is exhibited in Fig. 3(c), together with the RPA and QLCA predictions [8]. Agreement with the latter is very good. On the other hand, the RPA results increasingly deviate from the present data as ka increases.

The *in-phase transverse* (T_+) mode is also shown in Fig. 3(a): for this $\Gamma = 40$ value it is quite weak. This is similar to the behavior of the corresponding mode in the isolated 2D system where, however, the mode becomes stronger at higher values of Γ [3]. Here this mode is observable only at wave numbers $ka \geq 1$; for $ka \leq 1$, ω

$= 0$. The disappearance of the shear modes for $k \rightarrow 0$ is a well known feature of the liquid state [15,3,17] while the sharp cut-off $\omega \rightarrow 0$ for a finite k has also been observed in the case of Yukawa systems [18,19]. Comparison with the QLC theory shows an agreement as far as the linear acoustic dispersion is concerned, but the QLCA fails to predict the finite- k , $\omega = 0$ cutoff.

The widths of the peaks in the fluctuation spectra are indicative of the lifetimes of the corresponding modes. $L_+(\omega)$, which is maintained primarily by the mean field, is characterized by an extremely narrow peak and a long lifetime. In contrast, $T_+(\omega)$ and $T_-(\omega)$, which are supported by particle correlations, have broader peaks and shorter lifetimes. The peak for $L_-(\omega)$ is broad in the domain dominated by correlations, in particular in the gap region; it narrows dramatically, however, as it travels into the quasi-linear region which again is primarily maintained by the mean field, see Fig. 2(a). The difference in behavior between modes maintained by the mean field and those supported by particle correlations is reflected through the difference in their sensitivity to the change in coupling. The spectra of the longitudinal current fluctuations (L_+ and L_-) at $\Gamma = 5$ and $d/a = 0.3$ are shown in Fig. 4. Comparison of the $\Gamma = 40$ (see Fig. 1) and the $\Gamma = 5$ graphs shows that the longitudinal in-phase mode is extremely robust and is barely affected by the change in the coupling. In contrast, for all the other modes, their strengths substantially diminish at lower coupling values. It is clear, however, that the energy gap does survive even at the relatively low $\Gamma = 5$ value. Further lowering of the coupling results in the corresponding peak becoming swamped by the continuum noise.

In conclusion, we have presented MD simulation results for current fluctuation spectra for a charged particle bilayer liquid over a wide range of coupling and layer separation values. We have identified the four collective modes of the system and determined their dispersion characteristics: the existence of a frequency (energy) gap in the out-of-phase modes has been unambiguously established. Comparison with theoretical predictions shows that the qualitative conclusions of the QLCA for all four modes, in particular those concerning the emergence of the energy gap for the out-of-phase modes, are verified. Quantitatively, the agreement between the present MD and the QLCA results is excellent for the in-phase longitudinal mode; for the out-of-phase modes the value of the energy gap obtained in the present work is about 30 % higher than expected on the basis of the QLCA. The reason for this discrepancy is not understood at the present time. The MD results of the present work well complement the existing experimental findings [5,12] in laboratory experiments which were carried out for $r_s \approx 1.0 - 1.5$, equivalent to a much weaker coupling range than that investigated here. The high d/a , finite- k region accessed by the experiments can be identified with the quasi-linear portion of the lower dispersion curves in

Fig. 3(b).

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FIG. 1. Spectra of longitudinal $L_{\pm}(k, \omega)$ (a,b) and transverse current $T_{\pm}(k, \omega)$ (c,d) fluctuations at $\Gamma = 40$ and $d/a = 0.3$. The wave numbers are multiples of $(ka)_{\min} = 2\pi a/L = 0.0886$. The $\pm$ labels indicate in-phase and out-of-phase excitations. Note that very close to $\omega = 0$, the $L_{\pm}(k, \omega)$ curves descend steeply so that $L_{\pm}(k, 0) = 0$.

FIG. 2. (a) Longitudinal out-of-phase current fluctuation spectrum for fixed $ka = 0.353$ and layer separations $d/a = 0.3 - 5.0$. Note the sharpening of the collective peaks for high- d/a values. (b) Energy gap $\omega(k=0)/\omega_0$ as a function of layer separation d/a , obtained from the present simulations, and using the QLC formula (6). The inset portrays the high- d/a behavior.

FIG. 3. (a) Dispersion relations for the four modes, at $\Gamma = 40$ and layer separation $d/a = 0.3$. (b) Dispersion of the longitudinal out-of-phase mode (for $d/a = 0.8 - 5.0$) compared with the QLC theory calculations taken from Ref. [8]. (c) Dispersion of the in-phase longitudinal mode (for $d/a = 0.3$) compared with RPA calculations and with the QLC theory results taken from Ref. [8].

FIG. 4. Spectra of longitudinal current fluctuations $L_{\pm}(k, \omega)$ at $\Gamma = 5$ and $d/a = 0.3$. The wave numbers are multiples of $(ka)_{\min} = 2\pi a/L = 0.0886$. Note that very close to $\omega = 0$, the $L_{\pm}(k, \omega)$ curves descend steeply so that $L_{\pm}(k, 0) = 0$.

Donko et al. FIGURE 1.

Donko et al. FIGURE 2.

Donko et al. FIGURE 3.

Donko et al. FIGURE 4.