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Perturbative approach to the mode dispersion in charged particle bilayers

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Abstract
Earlier theoretical and computer studies on the dynamics of strongly coupled charged particle bilayers have revealed the existence of an *energy gap* ($\omega(k = 0) \neq 0$, optical behaviour) for the out-of-phase plasmon. This is in contrast to the correlationless RPA prediction of acoustic ($\omega \sim k$) behaviour. We have studied the question whether a classical perturbation calculation for weak coupling shows the onset of the energy gap, and whether there is a minimal coupling threshold for the formation of the gap. A formally exact lowest order expansion technique due to Zhang and Kalman (1992 *Phys. Rev.* A **45** 5935) has been used.

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1. Introduction

Bilayers of charged particles can be realized in various physical systems. In particular, advances in modern semiconductor nanotechnology have made it possible to routinely fabricate multiple quantum well structures of parallel electron layers in a strongly correlated liquid phase (for detailed references see [7]). We consider charged particle bilayers as described by a model with the following features:

(i) two equal-density ($n_1 = n_2 = n$) 2D classical electron liquids (each immersed in its own 2D uniform neutralizing background of positive charge) separated by distance d. The N electrons in each monolayer occupy the large but bounded area V_{2D} in the planes $z = 0$ and $z = d$ of a Cartesian coordinate system;

(ii) the interaction is described in species space by the symmetric interaction matrix

$$\phi(k) = \varphi(k) \begin{bmatrix} 1 & b \\ b & 1 \end{bmatrix} \qquad \text{where} \quad \varphi(k) = 2\pi e^2/k \quad b = \exp(-kd);$$

(iii) scattering on impurities, etc is neglected;
(iv) exchange and other quantum effects are ignored; there is no interlayer tunnelling.

These approximations are reasonable in the strong coupling regime where the particles are well localized. The interlayer coupling is characterized by the parameter $\Gamma \equiv \beta e^2 a^{-1} = \beta e^2 \sqrt{\pi n}$. While our treatment is classical, a qualitative correspondence between the classical model and a (partially) degenerate system can be established via the effective coupling constant $\tilde{\Gamma} = [e^2/(a\varepsilon_0)][1 - \exp(-\beta\varepsilon_0)]$, which turns out to be the measure of the coupling strength for arbitrary degeneracy; $\varepsilon_0 = \pi n\hbar^2/m$ is the zero-temperature Fermi energy of the non-interacting 2D electron gas, and $a = (\pi n)^{-1/2}$ is the 2D Wigner–Seitz radius [7], $\beta^{-1} = k_B T$ is the inverse temperature in energy units.

The scalar dielectric function of the system is defined as in [6]:

$$\epsilon(k, \omega) = 1 - \mathrm{tr}[\phi\chi] + \|\phi\| \cdot \|\chi\| \qquad (1)$$

$\chi = \chi(k, \omega)$ being the *screened (total) density response matrix*. (Note that the notation used here is different from the conventional one, where χ is reserved to designate the full (external) density response function.)

In the RPA [4, 5] the system is described by a diagonal response matrix $\chi^{(0)} = \mathrm{dg}\big(\chi_1^{(0)}, \chi_2^{(0)}\big)$. In the long-wavelength limit in a two-component system the *unperturbed* density response matrix is

$$\chi_A^{(0)}(k, \omega) = \chi_A^{(0)}(k \to 0, \omega) \simeq \frac{n}{m}\left(\frac{k}{\omega}\right)^2 \qquad A = 1, 2. \qquad (2)$$

The corresponding RPA mode structure consists of two longitudinal (in-phase [+] and out-of-phase [−]) modes, supported by the mean field, without any role played by particle correlations:

$$\omega_{\pm 0}^2(k) = \omega_{2\mathrm{D}}^2(k)[1 \pm \exp(-kd)].$$

We have introduced here the two-dimensional plasma frequency $\omega_{2\mathrm{D}} = \sqrt{2\pi n e^2 k/m}$. Thus the RPA predicts acoustic behaviour for the out-of-phase mode [4, 5].

For a strongly coupled bilayer the RPA is not appropriate. This situation was analysed via the quasilocalized charge approximation (QLCA) [1, 2]. The dispersion relation for the out-of-phase mode in this approximation is dramatically different from its RPA counterpart, exhibiting a remarkable *energy gap* at $k = 0$ induced by interlayer correlations:

$$\omega_{-}^2(k = 0) = -\frac{1}{2}\omega_0^2 \int_0^\infty \mathrm{d}(qa) \exp(-qd) n g_{12}(q) \qquad (3)$$

where $\omega_0 = (2e^2 m^{-1} a^{-3})^{1/2}$ and $g_{12}(q)$ is the off-diagonal element of the *correlation function matrix*.

We may observe that the out-of-phase plasmon in the strongly correlated liquid phase corresponds to the out-of-phase optical mode in the crystalline state, identified in [8]. Both of these are manifestations of a pure correlational effect. So is, of course, the gap which is isotropic in the liquid, but anisotropic in the solid phase. A more important difference is that in the Wigner crystal [8] the optical mode is not damped, while in the strongly correlated liquid phase the out-of-phase plasmon is damped, albeit with a damping rate that decreases as Γ grows.

The obvious discrepancy between the qualitative $k \to 0$ behaviour predicted by the RPA ($\omega = 0$) and the QLCA ($\omega \neq 0$) approaches raises the question of how *weak correlations* would modify the RPA result. In particular, one would like to know whether there is a critical minimal coupling value for the gap to appear, or whether even infinitesimally small correlations induce a gap-like behaviour. The purpose of this paper is to attempt to answer this question.

2. The perturbed system

In order to analyse the effect of a weak correlation introduced in the system we have carried out a perturbation study of the bilayer system in the long-wavelength limit. The calculations have been done on the basis of the Zhang–Kalman perturbation scheme for the dielectric response function of a multicomponent plasma [6], formally exact to the first order in the coupling parameter $\gamma = \kappa_{2D}^2/2\pi n$ ($\kappa_{2D} = 2\pi e^2 n\beta$ being the 2D Debye wavenumber), which, in 2D, is proportional to Γ^2.

The perturbation calculation for the first-order correction to the density response matrix in the $k \to 0$ limit provides

$$\chi_{AB}^{(1)}(k \to 0, \omega) = \frac{1}{m_A m_B \omega^4 \beta V_{2D}} \sum_{\mathbf{q}} (\mathbf{k}\cdot\mathbf{q})^2 \psi_{AC}(q) \times \int \delta_-(\nu)(\eta_{BA}\tilde{\eta}_{BC} - \tilde{\eta}_{BA}\eta_{BC})\big(\chi_B^{(0)} - \tilde{\chi}_B^{(0)}\big)\,\mathrm{d}\nu \tag{4}$$

where

$$\boldsymbol{\eta} = \boldsymbol{\eta}(k,\nu) = (\boldsymbol{\epsilon}^{(0)}(k,\nu))^{-1} = (\mathbf{I} - \phi(k)\boldsymbol{\chi}^{(0)}(k,\nu))^{-1}$$
$$\tilde{\boldsymbol{\eta}}(k,\nu) = \boldsymbol{\eta}(k,\omega-\nu),\ldots,$$
$$\delta_-(\nu) = \frac{1}{2\pi\mathrm{i}}\lim_{o\downarrow 0}\frac{1}{\nu - \mathrm{i}o} = \frac{P}{2\pi\mathrm{i}\nu} + \frac{\delta(\nu)}{2}.$$

One can easily see that if $m_A = m_B = m$, $\chi_{AB}^{(1)}(k \to 0,\omega) = -\chi_{AA}^{(1)}(k \to 0,\omega)$. Introducing the *static screening approximation (SSA)* [6, 9, 10], for the 2D-bilayer case we obtain

$$\chi_{AB}^{(1)}(k \to 0, \omega) = -\frac{(-1)^{A+B}}{m_A m_B \omega^4 \beta V_{2D}} \sum_{\mathbf{q}} (\mathbf{k}\cdot\mathbf{q})^2 \varphi^2(q)\exp(-2qd) \times \int \delta_-(\nu)\big(\chi_A^{(0)} - \tilde{\chi}_A^{(0)}\big)\big(\chi_B^{(0)} - \tilde{\chi}_B^{(0)}\big)(\epsilon_0)^{-2}\,\mathrm{d}\nu; \tag{5}$$

here $\epsilon_0 = \epsilon^{(0)}\,(k, \omega = 0) = 1 + \tilde{k}^2$, with $\tilde{k} = k/\kappa_{2D}$. Then, manipulations similar to those followed in [9] lead to

$$\boldsymbol{\chi}(k \to 0,\omega) = \boldsymbol{\chi}^{(0)}(k \to 0,\omega) + \boldsymbol{\chi}^{(1)}(k \to 0,\omega) = \frac{n}{m}\left(\frac{k}{\omega}\right)^2 \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} - \beta n(2\Gamma\tilde{k})^2 \begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\Lambda \tag{6}$$

$$\Lambda = \Lambda(z;\Gamma,\bar{d}) = \int_0^\infty \frac{Z(s)\,\mathrm{d}s}{s^2\big[s + \frac{z}{2\sqrt{\Gamma}}\exp\big(\frac{z\sqrt{\Gamma}\bar{d}}{s}\big)\big]^2} \tag{7}$$

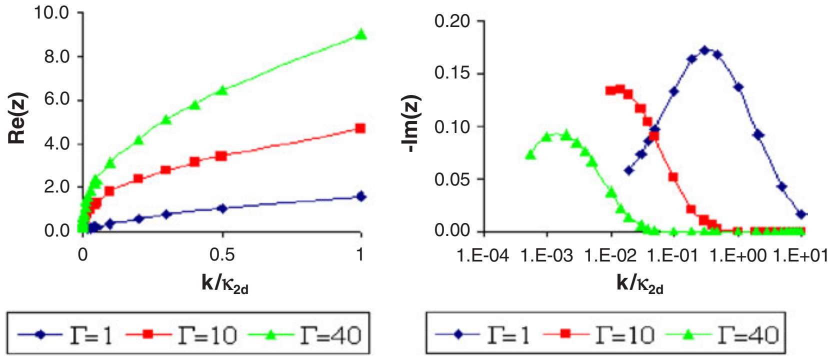
and

$$Z(s) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\exp(-t^2/2)\,\mathrm{d}t}{t - s} \qquad s \in \mathbb{C} \tag{8}$$

is the *plasma dispersion function* [10]. Moreover, in (7) we have introduced the dimensionless interlayer distance $\bar{d} = d/a$ and the dimensionless frequency $z = \omega/\omega_0$, $\omega_0 = (2e^2 m^{-1} a^{-3})^{1/2}$.

The dispersion equation, $\epsilon(k,\omega) = 0$, can be expressed as

$$\big[-m\omega^2\Lambda^{-1}\kappa_{2D}^2 - 8m\omega^2\kappa_{2D}k\Gamma^2(1-b) + m\omega_{2D}^2\Lambda^{-1}\kappa_{2D}^2(1-b)\big]\big[m\omega^2 - m\omega_{2D}^2(1+b)\big] = 0. \tag{9}$$



(*a*) (*b*)

Figure 1. RPA-like 2D-plasma branch for $\bar{d} = 1$.

The dispersion relation factorizes into two independent relationships, the first pertaining to the out-of-phase, the second to the in-phase mode. This latter, being a centre-of-mass mode, is unaffected to the order analysed here (as would be the plasmon mode in a 2D or 3D OCP, due to momentum conservation). We now focus on the out-of-phase mode whose dispersion relation becomes

$$\omega^2 = \frac{\omega_{2D}^2(k)(1-b)}{1 + 8\tilde{k}\Gamma^2(1-b)\Lambda}. \tag{10}$$

3. Asymptotic analysis

For small values of z the main contribution to the integral (7) originates from the region of the integration variable $s \to 0$; therefore we can write, see (8)

$$Z(s) = -\exp\left(-\frac{s^2}{2}\right)\int_0^s \exp\left(\frac{t^2}{2}\right)\mathrm{d}t + \mathrm{i}\sqrt{\frac{\pi}{2}}\exp\left(-\frac{s^2}{2}\right) \simeq -s + \mathrm{i}\sqrt{\pi/2}.$$

Then,

$$\Lambda(z \to 0; \Gamma, \bar{d}) \simeq -\frac{4\Gamma}{z^2}\int_0^\infty \frac{y}{[1 + y\exp(2\Gamma\bar{d}y)]^2}\,\mathrm{d}y + \mathrm{i}\frac{8\Gamma^{3/2}}{z^3}\sqrt{\frac{\pi}{2}}\int_0^\infty \frac{y^2}{[1 + y\exp(2\Gamma\bar{d}y)]^2}\,\mathrm{d}y. \tag{11}$$

For $\omega \to \infty$, $\Lambda \to 0$, which then leads to the asymptotic solution $z = \sqrt{ka} \to \infty$ as $k \to \infty$, for any value of Γ and $\bar{d}$. This is an *RPA-like 2D-plasma mode*: this feature, that for $k \to \infty$ the out-of-phase mode approaches the in-phase mode, is quite general and is already there in the RPA. This explains why there is only very little damping (see figure 1).

To determine the long-wavelength behaviour of (10), the asymptotic form (11) can be employed, with the new variable $\zeta = z(ka\sqrt{\bar{d}})^{-1}$. The dispersion relation can be written as

$$\frac{\zeta^2 - 1}{4\Gamma} = 4\Gamma\int_0^\infty \frac{y\,\mathrm{d}y}{[1 + y\,\exp(2\Gamma\bar{d}y)]^2} - \mathrm{i}\frac{8\sqrt{\frac{\pi}{2}\Gamma^3}}{\zeta ka\sqrt{\bar{d}}}\int_0^\infty \frac{y^2\,\mathrm{d}y}{[1 + y\,\exp(2\Gamma\bar{d}y)]^2}. \tag{12}$$

Should one ignore the imaginary term in (12), one would recover the RPA-like acoustic dispersion with a Γ-dependent increased phase velocity. It is clear, however, that for $k \to 0$ the imaginary term is dominant in (12).

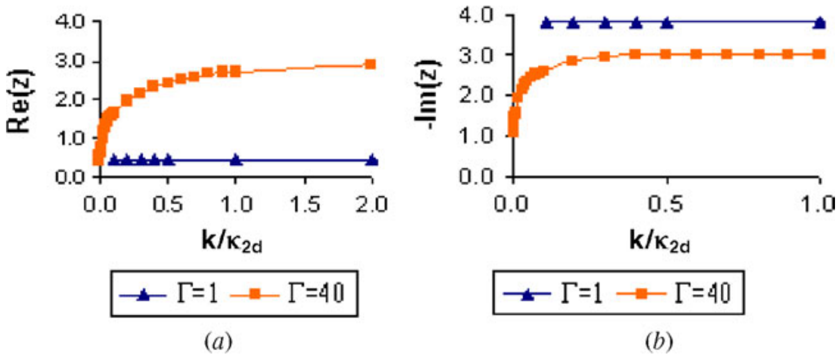


Figure 2. Gap-like branch for $\bar{d} = 1$.

Numerical analysis of the equation shows that as $k \to 0$, $\mathrm{Re}(\zeta)$ and the decay rate $\mathrm{Im}(\zeta)$ are of the same order of magnitude and grow as $k^{-1/3}$. This behaviour seems to indicate the breakdown of the perturbation expansion and a tendency to develop the non-perturbative optical mode predicted in earlier theoretical [5, 6] and computer [10] studies on the dynamics of strongly coupled charged particle bilayers.

For higher frequencies and k, the dispersion relation (10) now allows a solution such that $4\Gamma ka\Lambda \gg 1$. Then it seems reasonable to look for a solution of the full dispersion relation from the simplified expression

$$z_\infty^2 = \frac{1}{4\Gamma\Lambda(z_\infty; \Gamma, \bar{d})}. \tag{13}$$

The numerical solution of (13) leads to a finite (complex) frequency, whose value is almost independent of k. In this sense this is now a *gap-like mode*. The details of the numerical solution of (10) are discussed in the next section and are portrayed in the figures.

4. Numerical results and conclusions

The complex roots of equation (10) have been computed numerically. Some of the results are presented in figures 1 and 2 for various values of the interlayer distance $\bar{d}$ and the perturbation parameter Γ. As k grows we clearly distinguish two modes: the RPA-like one, with the real part of the frequency increasing as Γ, and the saturating one with the *gap* tendency.

In the immediate neighbourhood of $k = 0$ the acoustic behaviour is destroyed by the higher order correction. For somewhat higher k (but still for $k \ll k_{2\mathrm{D}}$) the slope and the decay rate of the acoustic mode values of the slope and of the decay rate of the acoustic mode grow as $k^{-1/3}$. For intermediate k values a bifurcation of the solutions seems to develop such that:

(i) the plasma mode assumes its RPA behaviour and approaches the in-phase mode with the dispersion relation $\omega = \omega_{2\mathrm{D}}(k)$ and with weak decay, and

(ii) a new mode develops which terminates in a frequency plateau, this latter has a value whose magnitude can be identified with that of the gap, this mode undergoes a strong collisional damping which decreases for higher values of the coupling parameter.

In conclusion, these results indicate that the RPA description is not robust, as it qualitatively breaks down even at arbitrary weak correlations. The emerging new behaviour exhibits the tendency to transform the acoustic mode into the predicted optical mode at any non-zero value of the coupling parameter. At the same time, one does not find the optical mode appearing as a direct outcome of the perturbation calculation. In retrospect, this may not be surprising, since the acoustic behaviour is caused by the mean field, whereas the energy gap is a pure correlational effect. Perturbation theory builds upon the mean field solution and thus, it is burdened with an inherent structural failure that prevents it from ever reproducing a mode whose main ingredient is not the mean field.

Acknowledgments

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References

[1] Golden K I and Kalman G J 2003 *J. Phys. A: Math. Gen.* **36** 5865–75
[2] Zhang H and Kalman G 1992 *Phys. Rev.* A **45** 5935
[3] Fetter A L 1974 *Ann. Phys., NY* **81** 367
[4] Das Sarma S and Madhukar A 1981 *Phys. Rev.* B **23** 805
[5] Kalman G *et al* 1999 *Phys. Rev. Lett.* **82** 3124
[6] Golden K I and Kalman G J 2000 *Phys. Plasmas* **7** 14
[7] Goldoni G and Peeters F M 1996 *Phys. Rev.* B **53** 4591
[8] Zhang H 1993 *PhD Thesis* Boston College, MA
[9] Carini P *et al* 1982 *Phys. Rev.* A **26** 1686
[10] Donko Z *et al* 2003 *J. Phys. A: Math. Gen.* **36** 5877–85