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Dispersion of two-dimensional plasmons in GaAs quantum well and Ag monolayer

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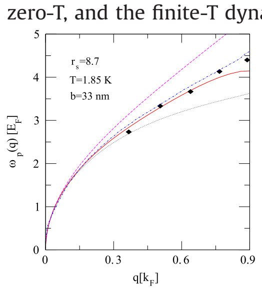
HIGHLIGHTS

- Corrections due to exchange-correlations and finite temperature are essential to explicate the measured 2D plasmon dispersion.
- Correlations are seen to introduce a noticeable red shift in plasmon frequency, while temperature has an opposite effect.
- At ultra low densities, the STLS theory seems to overestimate correlations which has the effect of over-suppressing plasmons into the single electron–hole pair continuum already at a relatively small q.
- The plasmon energy can be tuned to some extent by controlling the transverse confinement of 2D electrons.

GRAPHICAL ABSTRACT

Our study underlines that the exchange-correlation and finite-T corrections are crucial to explicate the measured 2D plasmon dispersion. Figure given below compares our results (solid curve) for 33 nm wide GaAs QW with experiment (symbols) for density $r_s = 8.7$ and $T = 1.85$ K. Other curves (from bottom) are zero-T, and the finite-T dynamical HA and RPA predictions.



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ABSTRACT

We study theoretically the role of finite temperature, exchange-correlations and finite layer width in explicating experimental findings on dispersion of two-dimensional plasmons in GaAs single quantum well and Ag monolayer. The plasmon energy is obtained from the poles of electron density response function determined by using the finite-temperature self-consistent mean-field theory of Singwi et al. Except for ultra low electron densities (as in GaAs system), our results exhibit a reasonably good agreement with the experimental data. While correlations are found to introduce a noticeable red shift in plasmon frequency, temperature has an opposite effect. Both of these effects become increasingly important with reduction in electron density. At ultra low densities, our predictions agree only for small wave vectors ($q < 0.6k_F$), with correlations over-suppressing plasmons into the single electron–hole pair continuum already at a relatively small q. This shortcoming may be arising due to the neglect of the dynamical nature of correlations in our study. Further, it is found that finite layer width gives rise to a red shift in plasmon dispersion, but its effect is significant when average electron-electron spacing is smaller than or comparable with layer width.

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1. Introduction

Experimental measurement [1,2] of plasmon dispersion of a two-dimensional electron gas (2DEG) for wave vectors q as large as the inverse average electron spacing r_0^{-1} has shown clear evidence of pronounced electron correlations in strong coupling regime; $r_0 = (\pi n)^{-1/2}$, with n as the areal electron number density. Among other things, this has provided an important means to test theories of short-range electron correlations directly against experiments. Hirjibehedin et al. [1] have probed plasmons in an ultra low density ($n \sim 10^9\,\mathrm{cm}^{-2}$) 2DEG produced in a narrow (33 nm) GaAs single quantum well (QW) for q of the order of Fermi wave vector k_F ($=\sqrt{2}/r_0$) by inelastic light scattering technique, including their dependence on n and temperature T. Here, the electron coupling parameter $r_s = r_0/a_0^*$ lies in the range 8.7–19.7, and electron correlation effects are expected to be significant; $a_0^* = \epsilon_0\hbar^2/(m^*e^2)$ is the effective Bohr radius, with ϵ_0 being the dielectric constant of substrate and m^* the effective mass of electron. It was in fact observed that correlations introduce a negative correction to the lowest-order dispersion relation $\omega_p \propto \sqrt{q}$, with temperature-induced positive correction determining the sign and magnitude of net correction. On the other extreme, Nagao et al. [2] have measured the dispersion of plasmons in a dense ($n \sim 10^{13}\,\mathrm{cm}^{-2}$) and atomically thin 2DEG realized in Ag monolayer (ML) grown on Si (111) surface by using the electron-energy-loss spectroscopy. Despite small r_s ($\sim$1) here, electron interaction effects may be pronounced due to exceptionally small width of the 2DEG. Also, such a 2DEG maps closely a perfect 2D system even at higher temperatures(90 K in Ref. [2]) as the energy spacing between the transverse electron energy levels is large due to strong transversal confinement. Again, electron correlations were found to show up clearly with increasing q in the plasmon dispersion.

There have been made attempts to explicate theoretically the above plasmon dispersion measurements. The authors of Ref. [1] have themselves shown that the random-phase approximation (RPA), which ignores completely the short-range correlations, overestimates plasmon energy and the extent of overestimation increases with q. Hwang and Das Sarma [3] went beyond the RPA by including correlations (through a static local-field correction (LFC) $G_{HA}(q;\,T)$ to the RPA interaction) within the T-dependent Hubbard approximation (HA). It was found that the correlation-induced softening of plasmon energy nearly cancels with the finite-T correction, thus explaining for the unexpected agreement between experiment [1] and the zero-T RPA. However, the HA results deviated increasingly from the experiment with increasing r_s. This is to be expected as the HA ignores the coulomb part of the correlation, which otherwise is known to grow with r_s. Yurtsever et al. [4] treated correlations within the so-called dynamical HA, which involved a frequency-dependent LFC factor $G_{HA}(q,\,\omega;\,T)$. More precisely, $G_{HA}(q,\,\omega;\,T)$ was constructed by approximating the *self-consistent* structure factor $S(q)$ in the LFC factor of the dynamical Singwi, Tosi, Land, and Sjölander (STLS) theory [5] with its finite-T Hartree–Fock estimate; the approximation was rather made to avoid heavy computation involved in the calculation of self-consistent $S(q)$. Although $\omega_p(q)$ thus obtained showed a good agreement with experiment, we argue that the HA may not be accurate at low densities probed experimentally [1]. On the other hand, Inaoka et al. [6] sought theoretical explanation of plasmon dispersion for the Ag ML [2] by treating exchange-correlations within the (static) self-consistent STLS theory [7]. However, these authors ignored both the finite temperature and the finite width of the Ag ML.

In this work, our aim is to determine the dispersion of plasmons for the above 2DEGs by taking into account the exchange-correlations as well as the experimental details (non-zero temperature and finite width) of the device hosting 2DEG. We shall treat exchange and coulomb correlations at the same footing within the self-consistent STLS theory [7]. Earlier, the STLS approach has been used [8,9] to study the finite temperature static correlations in an ideal (i.e., zero width) 2DEG. We present results both for GaAs and Ag systems, and make direct comparison with the respective experiments. The paper is organized as follows: In Section 2 we describe the 2DEG model and the finite-T STLS formalism. Results and discussion are given in Section 3, followed by concluding remarks in Section 4.

2. Theoretical formalism

2.1. 2DEG model

We model electrons in the GaAs QW or the Ag ML as a homogeneous 2DEG in the presence of a rigid charge neutralizing background. The transverse (z) motion of electrons is assumed to be confined by a strong potential $V_c(z)$ so that only the lowest energy subband is occupied. To be realistic with experiments, we take into account the finite extension of the transverse part $\phi(z)$ of the electron wave function. This results in an average electron interaction potential

$$V(q) = \frac{2\pi e^2}{\epsilon_0 q}F(q), \tag{1}$$

with the Form factor

$$F(q) = \int_{-\infty}^{\infty} \mathrm{d}z \int_{-\infty}^{\infty} \mathrm{d}z' |\phi(z)|^2 |\phi(z')|^2 \exp(-q|z-z'|), \tag{2}$$

representing the effect of finite width of the 2DEG. As a precise specification of $V_c(z)$ in actual samples is difficult, we consider different models for $V_c(z)$ to know its influence on plasmons. Infinite square QW has been the commonly used model for $V_c(z)$ in literature [10]. However, it should be more realistic to use a finite confinement potential, such as a finite square QW or a harmonic potential. For the finite QW, $\phi(z)$ (hence, $F(q)$) is to be obtained numerically, while $F(q)$ can be calculated analytically [11] for the harmonic potential as

$$F(q) = \exp\left(\frac{b^2q^2}{2}\right)\mathrm{erfc}\left(\frac{bq}{\sqrt{2}}\right), \tag{3}$$

where erfc(x) is the complementary error function and b is a measure of width of the 2DEG. Fig. 1 shows a comparison of $F(q)$ among the infinite square QW, finite square QW and harmonic confinement models for $b = 33$ nm. It may be noted that finite confinement results in a somewhat softer interaction potential, and softening is quite significant in the q region probed experimentally for plasmons. As expected, $F(q)$ for the finite QW approaches the result of infinite QW as the well depth is increased.

2.2. Finite temperature STLS formalism

The STLS approach has been used by Schweng and Böhm [8] to study the effect of temperature on exchange-correlations in an ideal 2DEG. Therefore, we give here only the essential STLS relations. The linear density response function $\chi(q,\,\omega;\,T,\,\mu)$, whose poles give the plasmon energy $\omega_p(q)$, is given by

$$\chi(q,\,\omega;\,T,\,\mu) = \frac{\chi_0(q,\,\omega;\,T,\,\mu)}{1 - V(q)[1 - G(q;\,T)]\chi_0(q,\,\omega;\,T,\,\mu)}, \tag{4}$$

where $\chi_0(q,\,\omega;\,T,\,\mu)$ is the finite-T non-interacting density response function,

$$G(q;\,T) = -\frac{1}{n}\int \frac{\mathrm{d}\mathbf{q}'}{(2\pi)^2}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\frac{V(q')}{V(q)}[S(|\mathbf{q}-\mathbf{q}'|;\,T) - 1], \tag{5}$$