Effect of external screening on plasmons

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Abstract

To better understand the effect of external screening on the plasmon spectrum, the dynamic structure function of a system of charged bosonic particles on a neutralizing background is calculated beyond the RPA by systematically including three–excitation scattering processes. Attention is paid to the vanishing plasmon gap in the 3D spectrum and the emergence of an acoustic mode when screening is present, and anomalous dispersion at low densities.

Key words: plasmon, screening, electron gas

1. Introduction

Plasmons are collective excitations observed in systems consisting of charged particles. For the electron gas, a full calculation of the dynamic structure function $S(k,\omega)$, which provides a direct measure of the energy transfer from an experimental probe to the system, is a considerable task: besides the Coulomb interaction, one should incorporate the Fermi statistics and the periodic structure of the underlying ion lattice (band structure) into the calculation. (For an experimental point of view, see, *e.g.* Ref. [1].) However, the appearance of plasmons is not tied to statistics, so a model system consisting of bosons, for which the calculation is simpler, can also be used. Naturally, by doing so one misses the electron–hole excitations and plasmon damping. The ion background is commonly treated within the jellium model (uniform neutralizing background).

Besides the usual (Debye) screening inherent in charged systems, there can be impurities or other external sources, such as gates in mesoscopic systems, that can cause the Coulomb interaction to be screened. This work examines the effect of this external screening on the plasmon spectrum.

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2. Variational theory

We study a system driven out of its optimized ground state $|\Psi_0\rangle$ by a time–dependent infinitesimal external perturbation $U_{\rm ext}(k,\omega)$. This results in a change in the one–particle density, proportional to the perturbation within the linear response theory, $\delta\rho_1(k,\omega) = \rho_0\chi(k,\omega)U_{\rm ext}(k,\omega)$. Here $\chi(k,\omega)$ the density–density response function: the fluctuation–dissipation theorem states that $S(k,\omega) = -\frac{1}{\pi}\Im m\chi(k,\omega)$.

We see that to calculate $S(k,\omega)$ we need to establish a relation between $\delta\rho_1$ and $U_{\rm ext}$. We start by writing the trial state as

$$|\Psi(t)\rangle = \frac{1}{N}e^{-iE_0t/\hbar}e^{\frac{1}{2}\delta U}|\Psi_0\rangle\,, \qquad (1)$$

where N is a normalization factor, E_0 the ground–state energy, and $\delta U = \sum_i \delta u_1(\mathbf{r}_i;t) + \sum_{i<j}\delta u_2(\mathbf{r}_i,\mathbf{r}_j;t)$ is an excitation operator containing fluctuations in the one– and two–particle correlations u_1 and u_2 due to the perturbation, related to density fluctuations by the BGY equations. [2]

The time evolution of the correlations is governed by the least–action principle

$$\delta S = \delta\int_{t_0}^{t} dt' \left\langle \Psi(t') \left| H - i\hbar\frac{\partial}{\partial t'} \right| \Psi(t') \right\rangle = 0 \qquad (2)$$

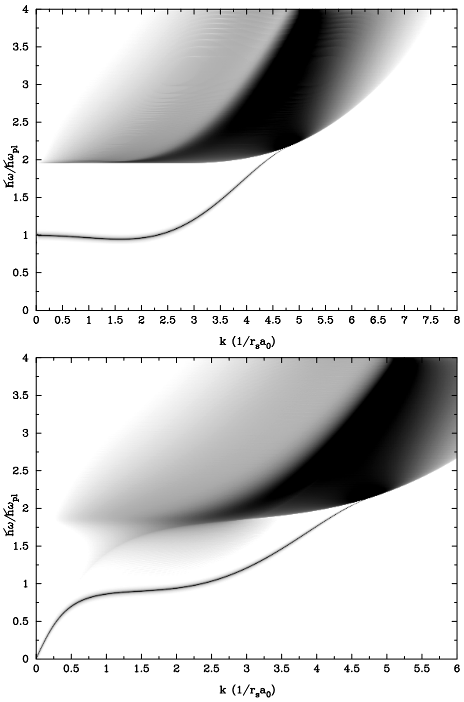

Fig. 1. $S(k,\omega)$ in 3D at $r_s = 5$ with $\sigma = \infty$ (Coulomb system) and $\sigma = 10$ Bohr radii. The strength of $S(k,\omega)$ is indicated by the gray scale: darker shade implies greater strength.

with the microscopic Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\left[\nabla_i^2 + U_{\rm ext}(\mathbf{r}_i;t)\right] + \sum_{i<j}\frac{e^{-|\mathbf{r}_i-\mathbf{r}_j|/\sigma}}{|\mathbf{r}_i-\mathbf{r}_j|} \quad (3)$$

leading to two coupled equations of motion for u_1 and u_2, from which $S(k,\omega)$ can eventually be solved. [3] In Eq. (3) σ is the screening length.

We recover the random–phase approximation (RPA) commonly used to interpret experimental data by including only $\delta u_1(\mathbf{r};t)$. Introducing δu_2 brings in three–excitation processes allowing high–energy excitations to decay, provided that energy and momentum are conserved. This is missing in the RPA.

We emphasize that the theory contains the correct summation of many–body diagrams so that Debye screening is built into it from the onset: the screening in the pair potential originates from an external source.

3. Results

Fig. 1 shows the calculated $S(k,\omega)$ at one representative density, $r_s = 5$, for two values of σ in 3D. In the figures, we see the plasmon mode (thin line) and the two–excitation continuum (large gray area). As expected, for unscreened Coulomb potential the plasmon

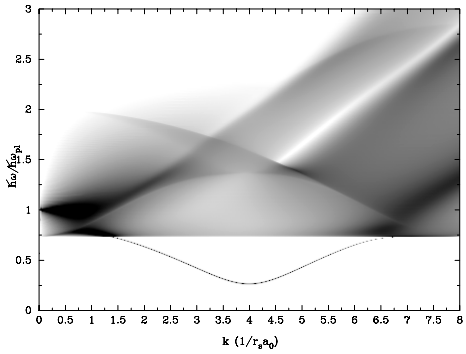

Fig. 2. $S(k,\omega)$ in 3D at $r_s = 100$ with $\sigma = \infty$ (Coulomb system) showing anomalous plasmon dispersion.

spectrum exhibits a gap in the long–wavelength (low momentum transfer k) limit: radiation with frequency below this plasma frequency cannot propagate in the medium. Additionally, we have shown [3] that the current theory leads to a negative plasmon dispersion coefficient for bosons (the single–excitation curve bends downwards) at all densities, in agreement with Monte Carlo calculations [4], whereas RPA predicts the coefficient to be zero with positive higher–order corrections.

If the potential is screened, the gap vanishes and the dispersion at low k becomes linear: the collective mode turns acoustic. The stronger the screening, the more the spectrum resembles that of a free particle.

Another important parameter considering the plasmon dispersion is the density of the system. At the usual metallic densities in 3D, the plasmon mode is well–defined (stays below the continuum) up to high k, but at lower densities it can happen that the dispersion becomes anomalous: the mode can decay into excitations of lower energy. The main strength is still concentrated around this decaying mode. This is seen in Fig. 2, along with growing multi–excitation resonances.

In 2D, there is no gap in the spectrum of an unscreened system, but the excitation energy vanishes as $\sqrt{k}$. [3] There is no anomalous dispersion and the collective mode is stable up to high k. Also here the screening turns the mode acoustic. For strong enough screening, the 3D and 2D spectra resemble each other.

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