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Dipole and quadrupole plasmon in confined quasi-one-dimensional electron gas systems

Reng-lai Wu, Yabin Yu *, Hong-jie Xue, Hui-fang Hu, Quan-hui Liu

School of Physics and Electronics, Hunan University, Changsha 410082, China

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ABSTRACT

An eigen-equation of plasmon excitation in confined quasi-one-dimensional systems is presented. Besides dipole plasmons, quadrupole plasmons are found in the systems by comparing the eigen-solutions with the dipole response. For both dipole and quadrupole plasmons, the plasmon frequencies decrease with the increase of the system's length, and their size dependence can be well fitted by the plasmon dispersion in the infinite systems calculated by the random phase approximation. Through extensively studies of eigen-charge density and induced charge density, we find that quadrupole plasmon corresponds to symmetric charge density distribution, and can only be excited by non-uniform electric field.

1. Introduction

The technology of precise manipulation of single atoms through a scanning tunneling microscope (STM) [1–3] makes it possible to experimentally investigate the electromagnetic response properties of the isolated nanostructure with few atoms. Collective excitations in low-dimensional nanostructures, such as nanowires and linear atomic chains, have been extensively studied [4–14]. In experimental studies, plasmon excitations have already been sensitively detected in nanorods and atomic wires in infrared spectroscopy; [4,5] in theoretical and simulation studies, plasmon excitations have been widely investigated in one-dimensional (1D) atomic systems based on the random-phase approximation (RPA) [7,8] and the time-dependent density functional theory (TDDFT) [9–14]. Recent investigations for the plasmon excitations in nanoscale clusters, plasmon modes are generally identified with the examination of either the dipole [7–14] and multipole [15,16] absorption spectrum, or other characters of plasmon resonances [17] induced by an external-field. However, the plasmon modes found by these ways are dependent on the applied external-field. This is implicated in Refs. [10,11], which show that a longitudinal field induces a longitudinal-mode plasmon resonance, and a transverse field induces a transverse resonance. On the other hand, the investigations of the collective excitations in one-dimensional atomic chain focused on dipole plasmons [7–14], and quadrupole plasmons have not yet been discussed. Different from the dipole plasmon, the quadrupole plasmon is a subradiative plasmon resonance mode which weakly couples to the incident light [18,19], so it is difficult to be excited by the incident light. The quadrupole plasmon may be excited via the near-field interaction [20–25] and retardation effects [26]. Quadrupole plasmons have been widely studied in a lot of nano-structure systems [15,16,27–40], however, in 1D atomic chain systems, they have not been reported.

In this paper, we use an eigen-equation approach to study the plasmon excitations in confined quasi-one-dimensional electron gas (Q1DEG) systems. The eigen-equation method has been used to calculate plasmon excitation in finite condensed-matter systems [41–45], and the plasmon modes found by this way are independent on the applied fields. We seek all plasmon modes in the Q1DEG systems by the eigen-equation, and then compare the eigen-plasmon with the dipole plasmon which obtained by the dipole response. Besides the dipole plasmons, the quadrupole plasmons are found in the systems. Unlike the dipole mode that corresponds to the anti-symmetric charge oscillation, the quadrupole mode corresponds to the symmetric charge oscillation. The dipole plasmon can be excited by both uniform and non-uniform electric fields and is shown as a consequence of the resonance of the dipole response. But the quadrupole plasmon can only be excited by non-uniform electric fields and is shown as a consequence of the quadrupole resonance. The dispersions of plasmons have been investigated. As demonstrated in Refs. [7–14], the plasmon is highly sensitive to the size of the system due to the local

* Corresponding author. Tel.: +86 13517312832.
E-mail address: apybyu@hnu.edu.cn (Y. Yu).

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confinement of atoms. Our results show that there are more plasmons in longer systems, and the plasmon frequencies decrease with the increase of the system's length. Furthermore, the dipole response and quadrupole response as functions of the system's length are discussed. With the increase of the system's length, the redshift of resonance frequency is found, and the intensities of dipole response and quadrupole response are increased.

The rest of this paper is organized as follows. In Section 2 we present the eigen-equation approach based on the quantum linear response and electromagnetic theory, and show in detail the application of this approach to the confined Q1DEG model systems. In Section 3 we present the results of numerical calculations and discussions about the excitation spectra of various Q1DEG systems. A brief summary is given in Section 4.

2. Theoretical approach and model

We will start with presenting the plasmon eigen-equation on the base of the quantum linear response and the electromagnetic theory. The quasi-one-dimensional (Q1D) system under investigation is formed by a virtual atomic chain with width $2a$ and length of $L = Na$, where $N = (N_a + 1)$, N_a is the numbers of virtual atoms, a is virtual lattice-constant. The ground electronic states of the Q1D system are modeled by the eigen-waves confined within an infinite wall in the x–y plane, where x and y is the direction parallel and perpendicular to the atomic chain respectively. The eigen-wave-function of the system can be written as

$$\Psi_m(x, y) = \sqrt{\frac{2}{Na}} \sin\frac{m\pi x}{Na} \sin\left(\frac{\pi y}{2a}\right), \tag{1}$$

where m is the wave number, $m = 1, 2, 3, \ldots, N_a$. According to the quantum linear response theory, when an external potential $V^{ex}(\mathbf{r}, \omega)$ is applied to the Q1D system, the induced charge density is

$$\rho^{in}(\mathbf{r}, \omega) = e^2 \int \Pi\left(\mathbf{r}, \mathbf{r}', \omega\right)\left(V^{ex}\left(\mathbf{r}', \omega\right) + V^{in}\left(\mathbf{r}', \omega\right)\right)d\mathbf{r}', \tag{2}$$

where e is the unit charge, $V^{in}(\mathbf{r}, \omega)$ is the induced inner potential. $\Pi(\mathbf{r}, \mathbf{r}', \omega)$ is Lindhard function

$$\Pi\left(\mathbf{r}, \mathbf{r}', \omega\right) = 2\sum_{mn} \frac{f(E_m) - f(E_n)}{E_m - E_n - \omega - i\gamma} \Psi_m(x, y)\Psi_n(x, y) \times \Psi_m\left(x', y'\right)\Psi_n\left(x', y'\right), \tag{3}$$

where E_m and E_n is the eigen-energy of the eigen-state $\Psi_m(\mathbf{r})$ and $\Psi_n(\mathbf{r})$, γ is the damping constant. $f(E_m)$ is the Fermi distribution function, for zero temperature, it is unity in the case of $m < N_m$, and zero in the case of $m > N_m$, where N_m is the occupation number of the energy state. We define

$$\rho_{mn}(\mathbf{r}) = \Psi_m^*(\mathbf{r})\Psi_n(\mathbf{r}), \tag{4}$$

and

$$V_{n,m}(\omega) = \int d\mathbf{r}' \rho_{nm}\left(\mathbf{r}'\right) V\left(\mathbf{r}', \omega\right). \tag{5}$$

Taking Eq. (4) and (5) into Eq. (2), we have

$$\rho^{in}(\mathbf{r}, \omega) = 2e^2 \sum_{mn} \frac{f(E_m) - f(E_n)}{E_m - E_n - \omega - i\gamma} \times \rho_{mn}(\mathbf{r})\left[V^{ex}_{n,m}(\omega) + V^{in}_{nm}(\omega)\right]. \tag{6}$$

On the other hand, based on the electromagnetic theory, the induced inner potential is given by

$$V^{in}(\mathbf{r}, \omega) = \int d\mathbf{r}' \frac{\rho^{in}(\mathbf{r}', \omega)}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|}. \tag{7}$$

As shown in Ref. [8], from Eqs. (2) and (7), the excitation frequency can be solved self-consistently by iterating $V^{in}(\mathbf{r}', \omega)$ and $\rho^{in}(\mathbf{r}', \omega)$ with a given initial external potential $V^{ex}(\mathbf{r}', \omega)$. However, here we want to use an equivalent method to avoid large numerical and iterating calculations. Substituting Eq. (6) in Eq. (7), then multiplying $\rho_{n'm'}(\mathbf{r})$ at two sides of Eq. (7) and making an integral over the space as done in Eq. (5), we derive the oscillation equation for the induced potential

$$\sum_{mn}\left[\delta_{m'n',nm} - A_{m'n',mn}(\omega)\right]V^{in}_{nm}(\omega) = \sum_{mn} A_{m'n',mn}(\omega)V^{ex}_{n'm'}(\omega), \tag{8}$$

with

$$A_{m'n',mn}(\omega) = 2e^2 \frac{f(E_m) - f(E_n)}{E_m - E_n - \omega - i\gamma} \int d\mathbf{r}' \int d\mathbf{r} \frac{\rho_{n'm'}(\mathbf{r})\rho_{mn}(\mathbf{r}')}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}'|}. \tag{9}$$

To solve the oscillation equation of the system without the influence of external potential, we take $V^{ex}_{nm}(\omega) = 0$ in Eq. (8), and obtain the eigen-equation for the plasmon oscillation

$$\sum_{mn}\left[\delta_{m'n',nm} - A_{m'n',mn}(\omega)\right]V^{in}_{nm}(\omega) = 0. \tag{10}$$

According to the eigen-equation (10), the plasmon excitation frequency ω can be solved by

$$\det\left[\delta_{m'n',nm} - A_{m'n',mn}(\omega)\right] = 0. \tag{11}$$

However, due to the finite small imaginary part $i\gamma$, the practical calculation of plasmon excitation energy $\hbar\omega$ is carried out by the following equations,

$$\mathrm{Re}\left(\det\left[\delta_{m'n',nm} - A_{m'n',mn}(\omega)\right]\right) = 0, \tag{12}$$

with

$$\mathrm{Im}\left(\det\left[\delta_{m'n',nm} - A_{m'n',mn}(\omega)\right]\right) \sim 0. \tag{13}$$

Eqs. (12) and (13) imply that $A(N, N_m, \omega) = \mathrm{Im}(1/\det[\delta_{m'n',nm} - A_{m'n',mn}(\omega)])$ shows a peak at the plasmon frequency ω. Here we want to make clear that (13) should be exact zero for $i\gamma = i0^+$, and $A(N, N_m, \omega)$ will give an infinite peak at the plasmon frequency. However, for a realistic system the electrons always suffer some scattering, and γ can be understood as a scattering rate which makes the energy of plasmon a broadening. In this case, in general, Eq. (11) would have no real eigen-solutions for plasmon frequency ω, and ω would have a imaginary part corresponding to the decay time of plasmon. Equivalently, here we use Eq. (12) to give a real plasmon frequency which can be found at a finite peak of $A(N, N_m, \omega)$.

In the long wave length ($q \to 0$) limit, the plasmon dispersion calculated by the RPA in an infinite Q1D system is given by [46]

$$\omega_p \approx qa\omega_0\left|\ln(qa)\right|^{1/2} + O\left(q^2\right) \tag{14}$$

with $\omega_0 = \sqrt{2ne^2/m_e^*a^2}$ and n is the electron density. However, in our calculations for finite Q1D system, the wave length is discrete and scales as $q \propto \frac{1}{(N_a+1)a}$, the electron density scales as $n \propto \frac{1}{(N_a+1)a}$. So, keeping the numbers of electrons in the system fixed, the plasmon frequency is expected to scale as $(N_a+1)^{-3/2}|\ln(N_a+1)|^{1/2}$; while keeping the electron density fixed, the plasmon frequency is expected to scale as $(N_a+1)^{-1}|\ln(N_a+1)|^{1/2}$.