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Surface exciton modes for plane and spherical semiconductor-metal interfaces

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Abstract. An approximate method is developed for investigating the nature of interface exciton modes in a composite spatially dispersive medium. The method is general enough to be applicable to any composite system, in which each component is described by an arbitrary bulk dielectric function $\epsilon(q, \omega)$. It is based on the extension of the usual electrostatic-image method of solving the Poisson's equation, in the presence of an external point charge in the system. We have applied our general method to a composite system of a finite metal slab surrounded by a semiconductor on one side and the vacuum on the other side. Similarly, we have also considered the case of a metallic sphere of radius R, surrounded by a semiconductor, with a spherical interface between them. With assumed spatially dispersive model dielectric functions for the bulk metal and the bulk semiconductor, the nature of the electron-electron interaction and the interface exciton modes in the metallic region are obtained in both the cases. For the relevant size of the metal large compared to the atomic dimensions over which the bulk dielectric functions are non-local due to the spatial dispersion, it is shown that one can obtain the interface exciton modes by first defining new effective dielectric functions for each of the media making the particular interface, and then using the usual expression which determines the modes in the non-dispersive case.

Keywords. Interface exciton; semiconductor; metal.

1. Introduction

The study of interface exciton modes in a composite system of a semiconductor and a metal is of paramount importance in understanding the nature of effective electron-electron interaction near the junction. The exciton modes are in fact determined by the poles of the modified electron-electron interaction in the vicinity of the interface. Hence, they play a definite role in determining various physical properties of the systems, e.g., in determining the possible existence of the exciton-exchange mechanism of superconductivity (Ginzburg 1970; Ginzburg and Kirzhnits 1972) in composite systems or in explaining the details of Schottky effect (Inkson 1972). Though it is very difficult to obtain (Mills 1972; Ritchie and Marusak 1966; Fuchs and Kliewal 1971; Maradudin and Mills 1973; Agarwal 1972) the nature of these modes exactly, because of the complex nature of the interface, it is often possible to have an understanding about their approximate behaviour near the interface. In the first approximation, this may be enough to answer, for example, whether the exchange of these excitons leads to an attractive interaction between metal electrons, thereby enhancing the superconducting transition temperature, as envisaged by the exciton-exchange mechanism of superconductivity (Rangarajan and Jha 1976; Inkson 1974; Allender *et al* 1973).

In this paper, we obtain the effective electron-electron interaction between metal electrons in a semiconductor-metal system to obtain the surface exciton mode frequencies. The bulk regions of the metal and the semiconductor are described by model dielectric functions. The metal dielectric function represents a spatially dispersive medium with a single plasmon pole, which in the static limit leads to the usual screened static Coulomb interaction. We have considered the situations in which the semiconductor dielectric function is either spatially non-dispersive or spatially dispersive, but we have chosen only a single-oscillator model to describe the bulk semiconductor mode frequency. In the classical image approximation, the electrostatic potential in each region, due to a charge $-e$ at $\mathbf{r}'$ in the metal region, can be written in two parts. The first part is the frequency-dependent screened Coulomb potential due to the charges inside the bulk metal, while the second part arises due to the presence of the other medium. The latter is determined by matching the potentials and the normal components of the displacement vector at the interface. The interaction between electrons at $\mathbf{r}$ and $\mathbf{r}'$ inside the metal region is, then, nothing but the value of the above potential at $\mathbf{r}$ times the electronic charge $-e$.

In section 2, we describe our model dielectric functions which can represent approximately the bulk metal and the bulk semiconductor. These are used here to study the exciton modes in plane as well as spherical interface systems. The exciton mode frequencies in the case of a plane interface are obtained in section 3. The metal is taken to be a slab of width L, with the semi-infinite semiconductor on one side and the vacuum on the other side. Here, $\mathbf{q}_t$, the tangential component of the wave vector of the exciton is still a good quantum number, though its component in the direction normal to the surface is no longer a constant of motion. Hence, we can plot the exciton mode frequencies as a function of q_t. The particular case of a spatially non-dispersive semiconductor in such a composite system has of course already been studied earlier (Rangarajan 1975; Rangarajan and Jha 1976). We consider a spherical interface system consisting of a metallic sphere of radius R inside an infinite semiconductor in section 4. Starting with a semiconductor which is spatially dispersive, we consider the limiting case when the semiconductor becomes spatially non-dispersive. This can be compared with the earlier results of Srinivasan and Jha (1977). In the case of a spherical interface, each of the exciton modes is labelled by its orbital l value, and the frequencies are obtained as a function of the radius of the metallic sphere. A discussion on the salient features of our calculations in the plane as well as the spherical interface systems is presented in section 5.

2. Model dielectric functions for the bulk metal and semiconductor

For many applications, the bulk metal may be represented by a wave vector and frequency dependent dielectric function

$$\epsilon_M(q,\omega)=\epsilon_{M\infty}+Q_s^2\Big/\left[q^2-\frac{\omega^2}{\omega_p^2}Q_s^2\right]=\epsilon_{M\infty}\left[1+q_s^2\Big/\left(q^2-\frac{\omega^2}{\Omega_p^2}q_s^2\right)\right] \tag{1}$$

where $q_s^2 = Q_s^2\,\epsilon_{M\infty}^{-1}$, $\Omega_p^2=\omega_p^2\,\epsilon_{M\infty}^{-1}$ and $\epsilon_{M\infty}$ is the contribution from completely full bands, and where the average screening wave vector Q_s due to

the conduction electrons is of the order of the Thomas-Fermi wave vector $q_{\mathrm{TF}} = (6\pi n e^2/E_F)^{\frac{1}{2}}$. Here, $\omega_p = (4\pi n e^2/m)^{\frac{1}{2}}$ is the free electron plasma frequency corresponding to the conduction electrons. In the spatially non-dispersive case, i.e. when $q \ll Q_s$, this function describes the collective plasma mode correctly in that limit, while in the static limit, we get the usual screened Coulomb interaction.

When we look for a representation of the dielectric function for the semiconductor, life is not so simple, if we want to take into account the spatial dispersion as well as the frequency dependence of its dielectric function. Under an isotropic version of the two band model (Penn 1962), this problem can, however, be simplified considerably. In this model, assumed to consist of an empty conduction band and a full valence band, the Bloch states of wave vector $\mathbf{k}$ is taken as the linear combination of two plane waves of wave vector $\mathbf{k}$ and $\mathbf{k}' \equiv (k-2k_F)\hat{k}$. In other words, the Bloch state of wave vector $\mathbf{k}$ in the band $b(=c$, the conduction band, or $=v$ the valence band) is

$$|\mathbf{k}, b\rangle = [\exp(i\mathbf{k}\cdot\mathbf{r}) + \alpha_k^b \exp(i\mathbf{k}'\cdot\mathbf{r})] / [1 + (\alpha_k^b)^2]^{1/2} \tag{2}$$

with the corresponding energy eigen values

$$E^c(\mathbf{k}) = \frac{1}{2}\left[E_k^0 + E_{k'}^0 + \left\{\left(E_k^0 - E_{k'}^0\right)^2 + E_g^2\right\}^{\frac{1}{2}}\right]$$

$$E^v(\mathbf{k}) = \frac{1}{2}\left[E_k^0 + E_{k'}^0 - \left\{\left(E_k^0 - E_{k'}^0\right)^2 + E_g^2\right\}^{\frac{1}{2}}\right] \tag{3}$$

Here,

$$\alpha_k^b = \frac{1}{2} E_g \Big/ \left(E^b(\mathbf{k}) - \frac{\hbar^2 k'^2}{2m}\right) \tag{4}$$

$E_k^0 = (\hbar^2 k^2/2m)$, and E_g is the energy gap parameter which is adjusted to yield the correct static dielectric constant. The dielectric response function for the semiconductor can then be written as

$$\epsilon_S(\mathbf{q}, \omega) = \epsilon_{S\infty} + (4\pi e^2/q^2\,\Omega_c) \sum_{\mathbf{k}} |\langle \mathbf{k}, c\,|\,\mathbf{k}+\mathbf{q}, v\rangle|^2 \times \left\{\frac{1}{E^c(\mathbf{k}) - E^v(\mathbf{k}+\mathbf{q}) - \hbar\omega} + \frac{1}{E^c(\mathbf{k}) - E^v(\mathbf{k}+\mathbf{q}) + \hbar\omega}\right\} \tag{5}$$

where Ω_c is the unit cell volume, and $\mathbf{k}$ runs over the entire first Brillouin zone. For completeness, we have also added the contribution $\epsilon_{S\infty}$ arising from other full bands in the semiconductor. In the zero frequency case, eq. (5) leads to the limiting values

$$\epsilon_S(\mathbf{q}, 0) \xrightarrow[q\to 0]{} \epsilon_{S\infty} + (\hbar\omega_{\mathrm{ps}}/E_g)^2 \tag{6}$$

$$\epsilon_S(\mathbf{q}, 0) \xrightarrow[q\to \infty]{} \epsilon_{S\infty} + (\hbar\omega_{\mathrm{ps}}/E_F)^2 \tag{7}$$

where, ω_{ps} is the plasma frequency corresponding to the free valence-electron density. We can interpolate between these two behaviours to choose, for all $\mathbf{q}$, the form

$$\epsilon_S(\mathbf{q},0) = \epsilon_{S\infty} + \frac{(\hbar\omega_{ps})^2}{E_g^2}\,\frac{1}{1+(E_F/E_g)^2\,(q^2/k_F^2)}$$

$$\equiv \epsilon_{S\infty} + (\epsilon_0 - \epsilon_{S\infty})/(1 + q^2/\gamma^2) \tag{8}$$

where

$$\epsilon_0 - \epsilon_{S\infty} = (\hbar\omega_{ps}/E_g)^2;\ \gamma^2 = (\hbar\omega_{ps})^2\,k_F^2\,(\epsilon_0 - \epsilon_{S\infty})/E_F^2 \tag{9}$$

Now, we must incorporate the frequency dependence also. But it can be shown that no simple interpolation procedure works well in all the regions of $\mathbf{q}$ and ω. However, since for $\mathbf{q} = 0$, eq. (5) gives

$$\epsilon_S(0,\omega) = \epsilon_{S\infty} + \hbar^2\omega^2{}_{ps}/(E_g^2 - \hbar^2\omega^2), \tag{10}$$

we can combine eqs (8) and (10) into a single expression of the form

$$\epsilon_S(\mathbf{q},\omega) = \epsilon_{S\infty}\left[1 + \frac{(\epsilon_0{}^* - 1)}{[1+(q^2/\gamma^2) - (\omega^2/\omega_0{}^2)]}\right],\quad \epsilon_0{}^* = \frac{\epsilon_0}{\epsilon_{S\infty}} \tag{11}$$

where

$$\omega_0 = \omega_{ps}\,(\epsilon_0 - \epsilon_{S\infty})^{1/2} \tag{12}$$

is the usual transverse bulk mode exciton frequency of the semiconductor. Although, expression (11) is very crude, it may be enough for many calculations of interest in physics. The bulk mode longitudinal frequency for the semiconductor is, of course,

$$\omega_L = \omega_0\,(\epsilon_0/\epsilon_{S\infty})^{1/2},\quad \gamma \to \infty \tag{13}$$

3. Plane interface exciton modes

We consider a composite system of a semiconductor and a metal with a plane interface taken to be the $z=0$ plane. The bulk semiconductor ($z<0$) is represented by the dielectric function $\epsilon_S(q,\omega)$ given by eq. (11). The metal is assumed to be of finite length L along the positive z-direction, beyond which is the vacuum. The model dielectric function given by eq. (1) represents the metal.

In any medium, the electrostatic potential $\Phi(\mathbf{r},\omega)$ at $\mathbf{r}$ is determined from the solution of Poisson equation

$$\mathbf{D}(\mathbf{r},\omega) = 4\pi\,\rho_{ext}(\mathbf{r}) \tag{14a}$$

where the displacement vector **D** is given by

$$\mathbf{D}(\mathbf{r}, \omega) = \int d^3r' \; \tilde{\tilde{\epsilon}}\,(\mathbf{r}, \mathbf{r}', \omega) \cdot \mathbf{E}(r', \omega) \tag{14b}$$

in terms of the unknown dielectric tensor $\tilde{\tilde{\epsilon}}$ for the whole medium, and where the electric field is

$$\mathbf{E}(\mathbf{r}, \omega) = \vec{\nabla} \Phi(\mathbf{r}, \omega). \tag{14c}$$

Here, $\rho_{\text{ext}}(\mathbf{r})$ is the external charge density within the medium. The general solution of eqs (14) for an arbitrary unbounded composite medium is of course given by

$$\Phi(\mathbf{q}, \omega) = \int \frac{d^3q'}{(2\pi)^3} \frac{4\pi\rho\,(\mathbf{q}')}{qq'} \; \epsilon^{-1}\,(\mathbf{q}, \mathbf{q}', \omega) \tag{15a}$$

$$\Phi(\mathbf{r}, \omega) = \int d^3r' \; K(\mathbf{r}, \mathbf{r}', \omega)\, \rho(\mathbf{r}') \tag{15b}$$

where $\Phi(\mathbf{q}, \omega)$ is the spatial Fourier transform of the potential $\Phi(\mathbf{r}, \omega)$, and where in terms of the matrix elements of inverse dielectric matrix ϵ^{-1},

$$K(\mathbf{r}, \mathbf{r}', \omega) = \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3q'}{(2\pi)^3} \exp\,(i\mathbf{q}\cdot\mathbf{r}) \exp\,(-i\mathbf{q}'\cdot\mathbf{r}') \, \frac{4\pi\epsilon^{-1}\,(\mathbf{q}, \mathbf{q}')}{q\; q'} \tag{15c}$$

with

$$\epsilon\,(\mathbf{q}, \mathbf{q}') \equiv \mathbf{q} \cdot \tilde{\tilde{\epsilon}}\,(\mathbf{q}, \mathbf{q}', \omega) \cdot \mathbf{q}'/qq' \tag{15d}$$

$$\tilde{\tilde{\epsilon}}(\mathbf{r}, \mathbf{r}', \omega) = \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3q'}{(2\pi)^3} \exp\,(i\mathbf{q}\cdot\mathbf{r}) \exp\,(-i\mathbf{q}'\cdot\mathbf{r}') \; \tilde{\tilde{\epsilon}}(\mathbf{q}, \mathbf{q}', \omega). \tag{15e}$$

However, the formal solution given above is of not much value since we have no knowledge of $\tilde{\tilde{\epsilon}}(\mathbf{r}, \mathbf{r}', \omega)$ near the interface of a composite medium. We must, therefore, investigate the problem of composite systems in some other way, which may be only approximate. Of course, we may model the bulk metal and the bulk semiconductor fairly well by homogeneous dielectric functions depending only on the difference $\mathbf{r}-\mathbf{r}'$. In such a case, $\epsilon(\mathbf{q}, \mathbf{q}') = \epsilon(\mathbf{q}, \omega)\,(2\pi)^3\,\delta(\mathbf{q}-\mathbf{q}')$; $\epsilon^{-1}\,(\mathbf{q}, \mathbf{q}') = [1/\epsilon(\mathbf{q}, \omega)]\,(2\pi)^3\,\delta(\mathbf{q}-\mathbf{q}')$, and

$$\Phi\,(\mathbf{q}, \omega) = \frac{4\pi\,\rho\,(\mathbf{q})}{q^2\epsilon\,(\mathbf{q}, \omega)}. \tag{15f}$$

In other words, for the bulk homogeneous medium, we have

$$\epsilon(\mathbf{r}, \mathbf{r}', \omega) = \epsilon(\mathbf{r} - \mathbf{r}', \omega) \tag{16}$$