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Plasmons and diffraction for a circular aperture and a circular disk M. Apostol Department of Theoretical Physics, Institute of Atomic Physics, Magurele-Bucharest MG-6, POBox MG-35, Romania email: apoma@theory.nipne.ro

1 Introduction

In a previous paper[1] we reported on some negative, unphysical results concerning plasmons, polaritons and diffraction in structures with cylindrical geometries. In particular, we encountered ultraviolet divergencies for a circular aperture and a circular disk, and plasmons depending on the boundary conditions imposed at infinity for an infinite cylindrical hole and an infinite cylindrical rod. We show in this paper that a natural wavevector cutoff occurs in these structures, as given by $ka \ll 1$, where **k** is the in-plane wavevector of the motion and *a* is the radius of the hole (disk). We focus herein upon the circular aperture and the circular disk. We show that this wavevector cutoff allows an approximate method of computation for plasmons and for the diffracted field. We call this approximation the diffraction limit. The interest in plasmons and polaritons in structures with special, restricted geometries stems from the role played by these motion modes of the polarization in the diffraction problem. There were several attempts to approach this problem in the past for structures with cylindrical geometry.[2]-[9] In particular, we note the approximate treatment of the diffraction of a scalar field by a circular aperture and a circular disk, [10, 11] where, however, the polarization motion has been left aside.

The method employed here is based on the equation of motion of the electric polarizability and the radiation formulae of the Kirchhoff electromagnetic potentials. This method, which leads typically to coupled integral equations, was applied to a semi-infinite space,[12]-[14] a slab of finite thickness,[15] a sphere (where Mie's theory has been re-derived)[16] and to the electromagnetic eigenmodes of matter which led to the calculation of van der Waals-London and Casimir forces.[17] Usually, we are doing the calculations for an ideal model of jellium-like plasma, but the method is readily applicable to more realistic structures, like dielectrics, loss included. The method combines the elementary theory of dispersion[18] with the electromagnetic radiation formulae, and it was long sought in connection with the so-called Ewald-Osen extinction theorem.[19]

2 Plasmons in a circular aperture and a circular disk

We consider an infinite, two-dimensional, plane metallic screen (a sheet) with a cricular aperture of radius a. We assume a simple jellium-like model consisting of mobile charges -e, mass M and (superficial) density n_s moving in a rigid, neutralizing background of positive charges. For reasons of dimensionality we introduce a length d, much longer than the inter-atomic distances but much shorter than the relevant electromagnetic wavelengths, and write the charge density as $n_s = nd$,

183 (2009)

where *n* is the bulk density. We represent the density disturbances by $\delta n = -n \operatorname{div} \mathbf{u}$, where **u** is a displacement field in the positions of the charges. This representation is valid for $\mathbf{ku}(\mathbf{k}) \ll 1$, where **k** is the in-plane wavevector and $\mathbf{u}(\mathbf{k})$ is the Fourier transform of the displacement field. Under these circumstances, in the non-retarded (Coulomb) limit, the field **u** obeys the equation of motion

$$M\ddot{\mathbf{u}} = e^2 n_s grad \int d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} div \mathbf{u}(\mathbf{r}') - e\mathbf{E}_0 \quad , \tag{1}$$

where \mathbf{E}_0 is an external electric field.

For the circular aperture we write the displacement field as

$$\mathbf{u} \to \mathbf{u}\theta(r-a) \quad , \tag{2}$$

where $\theta(z) = 1$ for z > 1 and $\theta(z) = 0$ for z < 0 is the step function. We use the Fourier transform

$$\mathbf{u}(\mathbf{r},t) = \sum_{\mathbf{k}} \int d\omega \mathbf{u}(\mathbf{k}\omega) e^{i\mathbf{k}\mathbf{r}} e^{-i\omega t}$$
(3)

for the function **u** in the *rhs* of equation (1). Usually, we leave aside the argument ω in the Fourier transforms, for simplicity. Similarly, we use the well-known Fourier decomposition

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{\mathbf{k}} \frac{2\pi}{k} e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')} \tag{4}$$

for the Coulomb potential.

Making use of equation (2) the divergence entering equation (1) becomes

$$div\mathbf{u} \to div\mathbf{u} \cdot \theta(r-a) + \frac{\mathbf{ua}}{a}\delta(r-a)$$
, (5)

where **a** is the vector of magnitue a and the same orientation as the position vector **r**. We can see in equation (5) the occurrence of specific contribution arising from the rim of the aperture.

Let us introduce the notation

$$\Phi(\mathbf{r}) = \int d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} div \mathbf{u}(\mathbf{r}') .$$
(6)

Making use of equation (5) and the Fourier transforms we can write

$$\Phi(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{k}'} \frac{2\pi}{k} \left[i\mathbf{k}'\mathbf{u}(\mathbf{k}') \right] e^{i\mathbf{k}\mathbf{r}} \int d\mathbf{r}' e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}'} \theta(r'-a) + \sum_{\mathbf{k}\mathbf{k}'} \frac{2\pi}{k} e^{i\mathbf{k}\mathbf{r}} \int d\mathbf{r}' \frac{\mathbf{u}(\mathbf{k}')\mathbf{a}'}{a} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}'} \delta(r'-a) \quad ,$$

$$(7)$$

where the vector \mathbf{a}' of magnitude *a* has the same orientation as the position vector \mathbf{r}' . The first integral in equation (7) can successively be transformed as

$$\int d\mathbf{r}' e^{i\mathbf{q}\mathbf{r}'}\theta(r'-a) = \int_a^\infty dr'r' \int d\varphi e^{iqr\cos\varphi} = 2\pi \int_a^\infty dr'r' J_0(qr') =$$

$$= 2\pi \int_0^\infty dr'r' J_0(qr') - \pi a^2 = \delta_{\mathbf{k}\mathbf{k}'} - \pi a^2 \quad , \tag{8}$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ and J_0 is the Bessel function of the first kind and zeroth order. In equation (8) we have used a series expansion in powers of a (actually aq) and restricted to the first non-vanishing

term (second-order), as a consequence of our general assumption $ak \ll 1$. A similar expansion is used for the exponential

$$e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}'} = 1 + i(\mathbf{k}'-\mathbf{k})\mathbf{r}' = \dots$$
(9)

in the second integral entering equation (7), and we can see easily that the first-order term (1) gives a vanishing contribution to the angular integration in equation (7). Consequently, we are left with

$$\Phi(\mathbf{r}) = \sum_{\mathbf{k}} \frac{2\pi}{k} [i\mathbf{k}\mathbf{u}(\mathbf{k})] e^{i\mathbf{k}\mathbf{r}} - \pi a^2 \sum_{\mathbf{k}\mathbf{k}'} \frac{2\pi}{k} [i\mathbf{k}'\mathbf{u}(\mathbf{k}')] e^{i\mathbf{k}\mathbf{r}} + \sum_{\mathbf{k}\mathbf{k}'} \frac{2\pi}{k} e^{i\mathbf{k}\mathbf{r}} \int d\varphi' [\mathbf{u}(\mathbf{k}')\mathbf{a}'] [i(\mathbf{k}'-\mathbf{k})\mathbf{a}'] .$$
(10)

Now, it is easy to see, by taking the gradient of $\Phi(\mathbf{r})$ and using the Fourier transform of the equation of motion (1), that $\mathbf{u}(\mathbf{k})$ is directed along the wavevector \mathbf{k} , as for longitudinal waves. We take therefore the projection of the equation of motion along the wavevector \mathbf{k} and denote this component of \mathbf{u} by u. The equation of motion becomes

$$\left(\frac{2\omega^2}{\omega_p^2 d} - k\right) u(\mathbf{k}) = -\pi a^2 \sum_{\mathbf{k}'} k' u(\mathbf{k}') + \sum_{\mathbf{k}'} \int d\varphi' u(\mathbf{k}') \frac{\mathbf{k}' \mathbf{a}'}{k'} \left[(\mathbf{k}' - \mathbf{k}) \mathbf{a}' \right] + \frac{1}{2\pi ned} E_0(\mathbf{k}) \quad ,$$
(11)

where $\omega_p = \sqrt{4\pi n e^2/M}$ is the (bulk) plasma frequency and $E_0(\mathbf{k})$ is the Fourier component of the external field directed along the wavevector \mathbf{k} . In equation (11) we may take φ' as the angle between \mathbf{a}' and \mathbf{k} . We introduce also the angle θ between \mathbf{k}' and \mathbf{k} , so that the angle between \mathbf{k}' and \mathbf{a}' is $\theta - \varphi'$. Under these circumstances, the angular integration over φ' can be performed in equation (11), so we get

$$\left(\frac{2\omega^2}{\omega_p^2 d} - k\right) u(\mathbf{k}) = -\pi a^2 k \sum_{\mathbf{k}'} \cos\theta u(\mathbf{k}') + \frac{1}{2\pi ned} E_0(\mathbf{k}) .$$
(12)

Here we perform a Fourier transform of the form

$$u(\mathbf{k}) = \sum_{m} e^{im\theta_1} u_m(k) \quad , \tag{13}$$

and a similar one for $u(\mathbf{k}')$ with the angle θ_2 . With these notations $\theta_2 = \theta_1 + \theta$. We use a similar Fourier transform for the external field $E_0(\mathbf{k})$, and get

$$\left(\frac{2\omega^2}{\omega_p^2 d} - k\right) u_{\pm 1}(k) = -\frac{\pi a^2 k}{2} \int dk' k' u_{\pm 1}(k') + \frac{1}{2\pi ned} E_{0\pm 1}(k) \tag{14}$$

and

$$\left(\frac{2\omega^2}{\omega_p^2 d} - k\right) u_m(k) = \frac{1}{2\pi ned} E_{0m}(k) , \ m \neq \pm 1 .$$
(15)

We can see that only the components $m = \pm 1$ are affected by the aperture within this approximation. For the other components, the plasma frequency

$$\omega = \omega_p \sqrt{\frac{dk}{2}} \quad , \tag{16}$$

as obtained from equation (15), is the same as for an infinite, continuous sheet without any aperture.

Equations (14) and (15) allow to compute the dielectric response to an external field E_0 . We limit ourselves here to give the eigenmodes corresponding to the dispersion equation

$$1 = -\frac{\pi a^2}{2} \int dk \frac{k^2}{\frac{2\omega^2}{\omega_p^2 d} - k} , \qquad (17)$$

where the integration is performed up to a certain cutoff k_0 . Since the plasmons should remain unchanged in the limit $k \to 0$ irrespective of the presence of the aperture, and their dispersion relation should be analytical in k, we look for a solution $\frac{2\omega^2}{\omega_p^2 d} - k = bk^2$ of equation (17). We get immediately $b = -\pi a^2 k_0/2$ and the dispersion relation given by

$$\omega^{2} = \omega_{p}^{2} \frac{dk}{2} \left(1 - \frac{\pi a^{2} k_{0}}{2} k \right) ; \qquad (18)$$

for $ak_0 = 1$ it reads

$$\omega^2 = \omega_p^2 \frac{dk}{2} \left(1 - \frac{\pi}{2} ak \right) . \tag{19}$$

Similar calculations for a circular disk leads to

$$\omega^2 = \omega_p^2 \frac{\pi dak^2}{4} . \tag{20}$$

3 Diffraction by a circular aperture and a circular disk

In the retarded regime the displacement field \mathbf{u} obeys the equation of motion

$$M\ddot{\mathbf{u}} = -e\left(\mathbf{E} + \mathbf{E}_0\right) \quad , \tag{21}$$

where **E** is the polarization field created by the moving charges. Equation (21) is restricted to the screen with the circular aperture, or to the circular disk. We assume an incident plane wave of the form $\mathbf{E}_0 e^{i\mathbf{k}\mathbf{r}} e^{i\kappa z} e^{-i\omega t}$, propagating with the wavevector $\mathbf{K} = (\mathbf{k}, \kappa)$ and frequency $\omega = cK$, where ω is the velocity of light. It is convenient to introduce the vector \mathbf{k}_{\perp} perpendicular to \mathbf{k} , $\mathbf{k}_{\perp}\mathbf{k} = 0$, and of the same magnitude k. We use notations $E_{01} = \mathbf{k}\mathbf{E}_0/k$ and $E_{02} = \mathbf{k}_{\perp}\mathbf{E}_0/k$ for the projections of the external field onto these vectors, and impose the transversality condition $KE_0 = kE_{01} + \kappa E_{03} = 0$, where E_{03} is the component of the external field along the z-axis. We use similar notations $u_1 = \mathbf{k}\mathbf{u}/k$ and $u_2 = \mathbf{k}_{\perp}\mathbf{u}/k$ for the displacement field \mathbf{u} and the polarization field \mathbf{E} .

The polarization field **E** is given by $E = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - grad\Phi$, where

$$\mathbf{A} = \frac{1}{c} \int d\mathbf{R}' \frac{\mathbf{j} \left(\mathbf{R}', t - |\mathbf{R} - \mathbf{R}'| / c\right)}{|\mathbf{R} - \mathbf{R}'|} , \ \Phi = \int d\mathbf{R}' \frac{\rho \left(\mathbf{R}', t - |\mathbf{R} - \mathbf{R}'| / c\right)}{|\mathbf{R} - \mathbf{R}'|}$$
(22)

are the retarded Kirchhoff potentials, $\mathbf{R} = (\mathbf{r}, z)$ and $\mathbf{R}' = (\mathbf{r}', 0)$. The curent and charge densities are given by $\mathbf{j} = -en\dot{\mathbf{u}}$ and, respectively, $\rho = endiv\mathbf{u}$, where the displacement field is given by equation (2). We use also the Fourier representation[20]

$$\frac{e^{i\frac{\omega}{c}\sqrt{r^2+z^2}}}{\sqrt{r^2+z^2}} = \sum_{\mathbf{k}} \frac{2\pi i}{\kappa} e^{i\mathbf{k}\mathbf{r}} e^{i\kappa|z|}$$
(23)

for the "retarded" Coulomb potential. We perform the Fourier transform given by equation (3) and apply the same approximation $ka \ll 1$ as described above for plasmons. After performing

the angular integral with respect to φ' as in equation (10) and rearanging the terms we get two coupled integral equations

$$\left(\omega^2 + \frac{1}{2}i\omega_p^2 d\kappa\right) u_1(\mathbf{k}) = \frac{1}{2}i\pi a^2 \omega_p^2 d\kappa \sum_{\mathbf{k}'} \left[\cos\theta u_1(\mathbf{k}') - \sin\theta u_2(\mathbf{k}')\right] + \frac{e}{M} E_{01} ,$$

$$\omega^2 \left(1 + \frac{i\omega_p^2 d}{2c^2\kappa}\right) u_2(\mathbf{k}) = \frac{i\pi a^2 \omega^2 \omega_p^2 d}{2c^2\kappa} \sum_{\mathbf{k}'} \left[\cos\theta u_2(\mathbf{k}') + \sin\theta u_1(\mathbf{k}')\right] + \frac{e}{M} E_{02} ,$$

$$(24)$$

where θ is the angle between **k** and **k'**.

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