Plasmon excitations in cylindrical wires by charged particle beams: impact parameter dependence

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We study the interaction of external charged particles with electronic modes of cylindrical wires. The dielectric function approach is used to calculate the main induced effects and derive the average number of excited plasmons. The bulk plasmon fields are quantized and the corresponding processes of plasmon excitations are described in detail, as a function of the impact parameter of the particle.

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1 Introduction

The spectroscopy of small-size particles of various types is a very active field of research [1–3]. In previous studies we have considered with some detail the interrelations between the semiclassical dielectric models [4] and the quantum descriptions based on Hamiltonian models [5] for plasmon excitations [6]. More recently, we have done a comprehensive study of the quantization of bulk and surface modes for the case of small cylindrical structures in solids [7]. In this work we apply the formulation to study the probability and number of plasmon excitations, showing in particular the behaviour of the excitation of plasmons with respect to the impact parameter of the particle relative to the wire. This information is of great current interest for studies based on electron spectroscopy of nano-wire arrays.

The system we consider is illustrated in Fig. 1.

2 Electrostatic modes

In previous works [7], we studied the properties of electrostatic modes in cylindrical interfaces. We very briefly review this concept as it is important for the comprehension of the developments made in this work.

The electrostatic surface modes of a cylindrical wire of radius a are obtained from the Laplace equation, $\nabla^2 \phi = 0$, in terms of cylindrical Bessel functions $I_m(x)$ and $K_m(x)$, with $m = 0, \pm 1, \pm 2, \ldots$, subject to the boundary conditions at $\rho = a$. The solution to this equation provides the dispersion relation of the modes, $\omega = \omega_m(k)$, which becomes $\omega^2_{m,\text{wire}} = \omega^2_p x J'_m(x) K_m(x)$, with $x = ka$, and using the simple pole approximation for the dielectric function around the plasma resonance, given by $\epsilon(\omega) = 1 - \omega_p^2/\omega(\omega + i\gamma)$, where $\omega_p$ is the plasma frequency and $\gamma$ the damping constant.

On the other hand, the electrostatic bulk modes correspond to electron density oscillations within the volume of the sample with plasma frequency $\omega_p$ (such that $\epsilon(\omega_p) = 0$). These modes are characterized by electron density fluctuations $n_b(\rho, z, q)$ within the volume and should satisfy the Poisson
equation, \( \nabla^2 \phi_b(\rho, z, q) = -4\pi e n_b(\rho, z, q) \), as well as the boundary conditions for these modes: \( \phi_b|_{\rho=a} = 0 \), which yields: \( J_m(qa) = 0 \). Therefore, the values of \( q \) are given by \( q_{m,n} = x_{m,n}/a \), where \( x_{m,n} \) are the zeros of the Bessel function \( J_m(x_{m,n}) = 0 \) (with \( n = 1, 2, \ldots \)).

3 Interaction of the bulk plasmon field with external particles

The interaction of the bulk plasmon field with an external particle of charge \( Ze \) moving along a trajectory \( r(t) \) is given by \( H_{\text{int}} = Ze \phi_b|r(t)\rceil \), where \( \phi_b \) is the quantized plasmon field [7]:

\[
\phi_b(r, t) = -\sum_{k,m,n} \mu_{k,m,n} J_m(q_{m,n} \rho) \left( b_{k,m,n} e^{i(kz+mq)} + b_{k,m,n}^* e^{-i(kz+mq)} \right), \quad \rho < a
\]

where the coupling coefficients \( \mu_{k,m,n} \) are given by

\[
\mu_{k,m,n}^2 = \frac{2\hbar \omega_p}{L} \frac{1}{(q_{m,n} a)^2 + (ka)^2} \left[ J_{m+1}(q_{m,n} a) \right]^2 .
\]

Thus, from the previous equation, we obtain the expression for the interaction of the bulk plasmons with the particle moving inside the wire along a trajectory \( r(t) \)

\[
H_{\text{int}}^{(b)}(t) = -Ze \sum_{k,m,n} \left( b_{k,m,n}^{(b)} f_{k,m,n}(t) + b_{k,m,n}^{(b)} r_{k,m,n}(t) \right) ,
\]

where \( f_{k,m,n}(t) = \mu_{k,m,n} J_m(q_{m,n} \rho) e^{i(kz+mq)} \) for \( \rho < a \), and it vanishes for \( \rho > a \) (see details of the calculation in [7]).

The evolution of this system may be solved in an exact quantum mechanical way from the Schrödinger equation, \( i\hbar \partial |\Psi(t)\rangle /\partial t = H_{\text{int}} |\Psi(t)\rangle \), where \( |\Psi(t)\rangle \) denotes the quantum state of the plasmon field in the interaction picture and, expanding it in eigenstates \( |N_v\rangle \) of the plasmon field Hamiltonian (corresponding to the excitation of \( N_v \) bulk plasmons in mode \( \nu \) for simplicity we use the condensed notation \( \nu = (k, m, n) \) for bulk modes.

3.1 Probability distributions

After some algebra, we can calculate the probability of excitation of \( N \) plasmons of a given state \( \nu \) as:

\[
P_N^{(\nu)} = |\langle N_v | \Psi(t) \rangle|^2 = \exp \left( -Q_v \left( \frac{Q_v}{N_v!} \right)^N \right),
\]

where \( Q_v = |X_v(t)|^2 \) and the term \( X_v^{(b)} \) is given by

\[
X_v(t) = \frac{Ze}{h} \int_{-\infty}^{t} f_v(t') \exp \left(-i\omega_v t' \right) dt',
\]

in terms of the coupling functions \( f_{k,m,n}^{(b)}(t) \) of Eq. (3).

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Alternatively, one may be interested in the excitation of a mode $m$, so that the appropriate $Q$-value for this would be

$$Q_m = \sum_k |X_{k,m}|^2 = \left( \frac{L}{2\pi} \right) \int_{-\infty}^{\infty} dk |X_{k,m}|^2,$$

(6)

The physical meaning of $Q_m$ is the average number of plasmons excited in mode $m$, i.e. $\langle N_m \rangle = Q_m$ [6].

4 Calculations: evaluation of $Q_m$ values

We study the case of a particle travelling across the wire with a trajectory perpendicular to the $z$-axis, with an impact parameter $b \neq 0$. Since the interaction with bulk modes is zero outside the wire we restrict the time integration in Eq. (5), in the case of bulk modes, to the range of particle positions $q_0 < a$.

Using Eqs. (5) and (6) and following a similar procedure to the one already indicated in [7], we obtain the following result for the average number of bulk plasmons in the mode $m$

$$Q_m(b) = \frac{4}{na} \left( \frac{ze}{v} \right)^2 c^2 \sum_{n=1}^{\infty} \frac{\alpha_n}{X_{n,m}} \left( \frac{g_{m,n}^\pm}{J_m(\alpha_n a)} \right)^2,$$

(7)

where

$$g_{m,n}^\pm(v) = \int_0^1 \frac{dx}{x} J_m \left( \frac{x_{m,n}}{a} \sqrt{b^2 + c^2 \frac{x^2}{v^2}} \right) \times$$

$$\begin{cases} 
\cos \left( m \arctg \left( b/(c\xi) \right) \right) - \frac{\alpha_n}{v} c\xi, & m \text{ even} \\
\sin \left( m \arctg \left( b/(c\xi) \right) \right) - \frac{\alpha_n}{v} c\xi, & m \text{ odd}
\end{cases}$$

(8)

with $c = \sqrt{a^2 - b^2}$ and using the integration variable $\xi$.

5 Analysis of results and concluding remarks

Results show that for parallel trajectories of the particle, the dependence with the impact parameter is in agreement with the results of [7] since in this case the radial coordinate $\rho$ plays the same role as $b$.

Let us consider now the case of transverse trajectories passing at a distance $b$ from the center of the wire. Figures 2a and b show calculations of the value of $Q_m(b)$ for $m = 0, 1$, from Eq. (7), as a function of the parameter $b$. We show here the contributions of the sub-modes with $n = 1, 2, 3 \ldots$, and the total $Q_m(b)$ value. We observe that in both cases, the principal contribution comes from the $n = 1$ term (i.e., the first root of the Bessel Function). Moreover, $Q_{m=0}$ has a maximum value for a null impact

**Fig. 2** Average number of bulk plasmon excitations, $Q_m(b)$, in modes $m = 0$ (left) and $m = 1$ (right) produced by a particle crossing the wire with a perpendicular trajectory with impact parameter $b$, calculated according to Eq. (7). We show here the results for the sub-modes with $n = 1, 2, \ldots$ (i.e., $(m,n) = (0,1), (m,n) = (1,1) \ldots$).
parameter, while that $Q_{m=1}^{(b)}$ has the maximum for $b = a/2$. These characteristics are due to the radial properties of bulk modes [7].

We finally consider the calculation of the probabilities of plasmon excitation for particles crossing the wire. Figure 3 shows the probabilities of bulk excitations for the modes $m = 0, 1$ of single ($N = 1$) and double ($N = 2$) bulk plasmon excitations as a function of the impact parameter $b$. We observe a similar behaviour as for the null impact parameter showed in [7]. In addition, the present study provides a complete characterization of the impact parameter dependence of the bulk plasmon excitation process. In particular, we obtain important interference effects in these excitations, which depend on the dwell time of the particles crossing the wire. A similar study of surface plasmon excitations is currently under way.

We finally note that the results obtained here will be of interest in experiments on electron energy loss spectroscopy of small nano-wire arrays.

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References