ENERGY LOSS AND PLASMON EXCITATION DURING ELECTRON EMISSION IN THE PROXIMITY OF A SOLID SURFACE

by

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ABSTRACT

We study the interaction with bulk and surface modes of electrons emitted in the proximity of a solid surface. We analyze the modifications in the energy loss, and in bulk and surface plasmon excitations, taking into account the effects due to the sudden creation of the electron and residual atomic hole, and the finite distance to the surface. The process is described using the dielectric function formulation and the specular reflection model. We derive expressions for the electrostatic potential in the medium and in vacuum, which include all the terms due to bulk and surface modes. The effect of each term in the energy loss rate and in the average number of plasmon excitations is discussed. The results illustrate in detail the different spatial dependences of the electron and ion interactions with the bulk and surface perturbations, through the relevant range of distances for studies of electron emission in the proximity of solid surfaces.

I. Introduction:

One of the main problems in the interaction of charged particles with solid surfaces is the excitation of bulk and surface plasmons. These excitations are of interest in studies of electron and ion interactions with surfaces or thin solid foils [1,2], and in studies of electron-energy-loss spectroscopy of solids [3].

The process of plasmon excitation in solids and surfaces is also an important aspect in electron emission induced by photons or ionizing particles, and the role of the hole created during the emission process is one of the interesting problems arising in these studies [4]. For instance, in XPS or Auger electron emission it becomes of interest to describe the interactions of the emitted electron and the residual atomic hole with bulk and surface plasmons, and the way in which they can affect the energy loss of the escaping electron or the probability of plasmon excitation.

The interaction of an emitted electron with an ion close to the surface is also of current interest to understand the effects of the dynamical electron-ion-surface interactions on the secondary-electron energy spectra obtained in ion-surface scattering experiments [5,6] or in ion-solid interactions [7,8]. A widely used assumption in secondary electron emission studies is the so-called three step model: electron production, transport inside the solid, and escape through the surface. It is clear that if the emission occurs close to the surface this separation in terms of independent processes is no longer applicable.

A useful approach to describe the interaction of charged particles with solid interfaces in terms of the dielectric properties of the bulk material, is provided by the so-called surface reflection model which was developed by previous authors [9]. The model has been quite useful for applications in studies of particle- surface interaction processes [10,11], and in calculations of the energy loss of particles reflected or moving in the proximity of a solid surface [1,12].

The purpose of this paper is to investigate in detail the effect of the interactions between a fast emitted electron and a stationary ion (or atomic hole) in the proximity of a solid surface. In particular, how the creation of a localized positive charge in the solid close to the surface, can influence the energy dissipation of the escaping electron, and the corresponding probability of bulk and surface plasmon excitation.

We provide here a detailed description of this process using a formulation based on the specular reflection model of particle-surface interactions. The approach permits to derive the expressions for the various interference terms that influence the energy dissipation, and to study the effects of the dynamical electron-hole-surface interactions on the probability of plasmon excitations.

II. The model

In the present work we study the cases where the emission process occurs inside or outside the solid. Therefore, we will derive the expressions for the fields and for the energy loss rate corresponding to each of these cases.

(a) **Internal emission process**

Let us consider the case where the electron and the atomic hole are created at time $t=-t_0$, and at a point $\vec{r}_0$ inside the solid. The electron is emitted with velocity $\vec{v}$, and at $t=0$ crosses the interface $z=0$, between the metal ($z<0$) and the vacuum ($z>0$), while the hole remains fixed at distance z_0 from the surface, as illustrated in Fig. 1.

According to the specular reflection model [9], the fields can be described in terms of the electron (*e*), the atomic-hole (*h*), their images (*e'*, *h'*), and a fictitious surface charge which is determined by the boundary conditions. The scheme is illustrated in Fig. 1, where we show the real system (part **a**), and the equivalent pseudo-media M (part *b*) and V (part *c*) introduced to evaluate the electrostatic fields in each case [9].

The charge densities of interest are the following:

$$\rho_e(\vec{r},t) = -e\ \delta(\vec{r}-\vec{x}_s-\vec{v}t)\ H_1(t) \tag{1a}$$

$$\rho_{e'}(\vec{r},t) = -e\ \delta(\vec{r}-\vec{x}_s-\vec{v}'t)\ H_1(t) \tag{1b}$$

$$\rho_h(\vec{r},t) = e\ \delta(\vec{r}-\vec{r}_0)\ H_1(t) \tag{1c}$$

$$\rho_{h'}(\vec{r},t) = e\ \delta(\vec{r}-\vec{r}_0')\ H_1(t) \tag{1d}$$

Here $\vec{r}_0=(0,0,-z_0)$ and $\vec{r}_0'=(0,0,+z_0)$ denote the hole and hole-image positions, $\vec{x}_s=(x_s,0,0)$ is the point on the surface where the electron emerges at time $t=0$, $\vec{v}=(\vec{w},u)$ and $\vec{v}'=(\vec{w},-u)$ are the electron and electron-image velocities in terms of its components, parallel ($\vec{w}$) and perpendicular ($\pm u$) to the surface, and $H_1(t)$ is a convenient switching function defined as

$$H_1(t)= \begin{cases} 0 & t < -t_0 \\ e^{\eta t} & -t_0 < t < 0 \\ e^{-\eta t} & t > 0, \end{cases} \qquad (2)$$

with $\eta \to 0^+$. The approximation of constant velocity holds for electron-kinetic energies much larger than the plasmon energy, i.e. $\frac{1}{2}mv^2 >> \hbar\omega_p$. Here we will consider values of $v \geq 4$ a.u. (and $\omega_p \cong 0.5$ a.u.).

To start the calculation one should first separate from Eqs.(1a-d) the Fourier components of the charge densities pertaining to each pseudo-medium. Thus, for the present problem the transformed charge densities acting on each medium are (note the different limits in the time integrals):

$$\rho^M_{ee'}(\vec{k},\omega)= \int_{-t_0}^{0} dt \int d^3r\ e^{-i\vec{k}.\vec{r}}\ e^{i\omega t}\ [\rho_e(\vec{r},t) + \rho_{e'}(\vec{r},t)] \qquad (3a)$$

$$\rho^M_{hh'}(\vec{k},\omega)= \int_{-t_0}^{\infty} dt \int d^3r\ e^{-i\vec{k}.\vec{r}}\ e^{i\omega t}\ [\rho_h(\vec{r},t) + \rho_{h'}(\vec{r},t)] \qquad (3b)$$

$$\rho^V_{ee'}(\vec{k},\omega)= \int_{0}^{\infty} dt \int d^3r\ e^{-i\vec{k}.\vec{r}}\ e^{i\omega t}\ [\rho_e(\vec{r},t) + \rho_{e'}(\vec{r},t)] \qquad (3c)$$

while $\rho^V_{hh'}(\vec{k},\omega)= 0$, since the hole never crosses the surface.

Hence, using Eqs.(1)-(3) we obtain:

$$\rho^M(\vec{k},\omega)= ie\ e^{-i\vec{k}.\vec{x}_s}\left[\frac{1-e^{-i(\omega-\vec{k}.\vec{v})t_0}}{\omega-\vec{k}.\vec{v}-i\eta} + \frac{1-e^{-i(\omega-\vec{k}.\vec{v}')t_0}}{\omega-\vec{k}.\vec{v}'-i\eta}\right] +$$

$$+ ie \frac{\left[e^{iqz_0} + e^{-iqz_0}\right] e^{-i\omega t_0}}{(\omega - i\eta)} \tag{4a}$$

$$\rho^V(\vec{k},\omega) = ie\, e^{-i\vec{k}.\vec{x}_s} \left[\frac{1}{\omega - \vec{k}.\vec{v} + i\eta} + \frac{1}{\omega - \vec{k}.\vec{v}' + i\eta}\right] \tag{4b}$$

Notice that the perturbation in the pseudo medium M contains terms from each source (*e*, *e'*, *h*, *h'*), while only the escaping electron and its image (*e*,*e'*) appear explicitly as external perturbations in the pseudo-vacuum V. Of course, due to the time dependence and matching conditions, the fields in the real vacuum will be influenced by all the charges, including the surface charge.

In terms of the bulk and surface charge densities, the fields in M and V can be written as follows,

$$\phi^M(\vec{k},\omega) = \frac{4\pi}{k^2\varepsilon(\vec{k},\omega)} \left[\rho^M(\vec{k},\omega) + \sigma^M(\vec{\kappa},\omega)\right] \tag{5a}$$

$$\phi^V(\vec{k},\omega) = \frac{4\pi}{k^2} \left[\rho^V(\vec{k},\omega) + \sigma^V(\vec{\kappa},\omega)\right] \tag{5b}$$

where $\sigma^{M,V}(\kappa,\omega)$ is a surface charge density and $\varepsilon(k,\omega)$ is the bulk dielectric function of the medium.

From the matching condition for the normal derivatives of the electrostatic potencial ϕ, we obtain $\sigma^M(\vec{\kappa},\omega) = - \sigma^V(\vec{\kappa},\omega) = \sigma(\vec{\kappa},\omega)$.

Expressing the wave vector $\vec{k}$ in terms of its components parallel and perpendicular to the surface, $\vec{k}=(\vec{\kappa},q)$, the surface charge density $\sigma(\vec{\kappa},\omega)$ can be obtained from the matching condition [9]:

$$\phi^M(\vec{\kappa},\omega;z)\Big|_{z=0^-} = \phi^V(\vec{\kappa},\omega;z)\Big|_{z=0^+} \tag{6}$$

where

$$\phi(\vec{\kappa},\omega;z)=\int_{-\infty}^{\infty}\frac{dq}{2\pi}\,e^{iqz}\,\phi(\vec{k},\omega) \tag{7}$$

Equation (6) then determines $\sigma(\vec{\kappa},\omega)$ as:

$$\sigma(\vec{\kappa},\omega)=\frac{\kappa}{\pi}\left[1+\frac{1}{\varepsilon_s(\vec{\kappa},\omega)}\right]^{-1}\cdot\int_{-\infty}^{\infty}\frac{dq}{k}\left[\frac{\rho^M(\vec{k},\omega)}{\varepsilon(\vec{k},\omega)}-\rho^V(\vec{k},\omega)\right] \tag{8}$$

Here $\varepsilon_s(\vec{\kappa},\omega)$ is the so-called surface dielectric function [9], defined in terms of the bulk function $\varepsilon(\vec{k},\omega)$ by

$$\frac{1}{\varepsilon_s(\vec{\kappa},\omega)}=\frac{\kappa}{\pi}\int_{-\infty}^{\infty}\frac{dq}{k^2\varepsilon(\vec{k},\omega)}\ , \tag{9}$$

where in Eqs. (7)-(9): $k^2=\kappa^2+q^2$.

According to this formulation, the results for the potential $\phi(\vec{r},t)$ and field $\vec{E}(\vec{r},t)$ can be obtained, through these expressions, from the corresponding quantities in the ω-$\vec{k}$ representation. The integrations can be treated analytically only for some model dielectric functions. In Appendix A we derive exact analytical solutions for a dielectric function that describes in a simple way both bulk and surface plasmon excitations.

Using the results of Appendix A, the potentials in M and V can be written as follows:

$$\phi^M(\vec{k},\omega)=\frac{4\pi ie}{k^2\varepsilon(\omega)}\left[F^M_{ee'}+F^M_{hh'}+F^M_{\sigma_1}\right] \tag{10a}$$

$$\phi^V(\vec{k},\omega)=\frac{4\pi ie}{k^2}\left[F^V_{ee'}+F^V_{\sigma_1}+F^V_{\sigma_2}\right] \tag{10b}$$

The expressions for the various terms that appear in ϕ^M and ϕ^V are given in Appendix A, Eqs.(A5 a-f), where we also discuss the physical origin of each term.

(b) **External emission process**

The case where the emission occurs outside the solid can be treated in a similar way than in the previous case of internal emission. The treatment here becomes simpler since the electron does not cross the surface.

The charge densities corresponding to this case are the following

$$\rho_e(\vec{r},t) = -e\ \delta(\vec{r}-\vec{r}_0-\vec{v}t)\ H_2(t) \qquad (11a)$$

$$\rho_h(\vec{r},t) = e\ \delta(\vec{r}-\vec{r}_0)\ H_2(t) \qquad (11b)$$

where $\vec{r}_0=(0,0,z_0)$ and $\vec{v}=(\vec{w},u)$, while the images $\rho_{e'}$ and $\rho_{h'}$ are obtained from ρ_e and ρ_h by substituting $\vec{r}_0$ by $\vec{r}'_0=(0,0,-z_0)$, and $\vec{v}$ by $\vec{v}'=(\vec{w},-u)$. We consider that the emission process occurs now at time t=0, and hence the switching function is defined by

$$H_2(t) = \begin{cases} 0 & t < 0 \\ e^{-\eta t} & t > 0\ , \end{cases} \qquad (12)$$

The charge densities in the vacuum V now become:

$$\rho^V_{ee'}(\vec{k},\omega) = \int_0^\infty dt \int d^3r\ e^{-i\vec{k}.\vec{r}}\ e^{i\omega t}\left[\rho_e(\vec{r},t)+\rho_{e'}(\vec{r},t)\right]$$

$$= -ie\left(\frac{e^{-iqz_o}}{\omega-\vec{k}.\vec{v}+i\eta}+\frac{e^{iqz_o}}{\omega-\vec{k}.\vec{v}'+i\eta}\right) \qquad (13a)$$

$$\rho^{V}_{hh'}(\vec{k},\omega) = \int_0^\infty dt \int d^3r\, e^{-i\vec{k}.\vec{r}}\, e^{i\omega t}\left[\rho_h(\vec{r},t) + \rho_{h'}(\vec{r},t)\right]$$

$$= \frac{ie}{\omega + i\eta}\left[e^{iqz_o} + e^{-iqz_o}\right] \qquad (13b)$$

and of course there are no charges inside the medium M.

The fields in M and V can now be readily obtained from

$$\phi^M(\vec{k},\omega) = -\frac{4\pi}{k^2}\frac{\sigma(\vec{\kappa},\omega)}{\varepsilon(k,\omega)} \qquad (14a)$$

$$\phi^V(\vec{k},\omega) = \frac{4\pi}{k^2}\left[\rho^V(\vec{k},\omega) + \sigma(\vec{\kappa},\omega)\right] \qquad (14b)$$

The surface charge density $\sigma(\vec{\kappa},\omega)$ is determined by Eq.(8), where now $\rho^M(\vec{k},\omega)=0$. The expression for $\sigma(\vec{\kappa},\omega)$ is given in Appendix A, Eq.(A6).

Finally, the potentials $\phi^M(\vec{k},\omega)$ and $\phi^V(\vec{k},\omega)$ can be determined from Eqs.(14 a,b), using (13 a,b) and the value of $\sigma(\vec{\kappa},\omega)$. Thus we get

$$\phi^V(\vec{k},\omega) = \frac{4\pi ie}{k^2}\left[\, G^V_{ee'}(\vec{k},\omega) + G^V_{hh'}(\vec{k},\omega) + G^V_{\sigma}(\vec{k},\omega)\right] \qquad (15a)$$

$$\phi^M(\vec{k},\omega) = \frac{4\pi ie}{k^2\varepsilon(\omega)}\; G^M_{\sigma}(\vec{k},\omega) \qquad (15b)$$

The expressions for the terms $G^{M,V}_{\nu}(\vec{k},\omega)$ appearing here are also given in Appendix A, Eqs.(A9 a-d).

III. Energy loss rates

The aim of this work is to calculate the energy loss due to plasmon excitation in the emission process. Therefore, in the following we will consider only the dissipative component of the induced field. Following the approach of previous authors [11], the energy- dissipation rate due to the fields acting on the emitted electron is given by

$$\dot{W}^{(e)}_{dis} = e \left. \frac{\partial \phi^{ind}(\vec{r},t)}{\partial t} \right|_{\vec{r}=\vec{r}_e(t)} \tag{16}$$

$$= ie \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \; \omega \; e^{i(\vec{k}.\vec{r}-\omega t)} \; \phi^{ind}(\vec{k},\omega) \Big|_{\vec{r}=\vec{r}_e(t)}$$

where $\vec{r}_e(t)$ is the electron trajectory, given in (1a) and (11a). To obtain the induced field ϕ^{ind} we subtract from Eqs.(10a) and (10b) the vacuum fields of the electron and hole (which correspond to the case $\varepsilon=1$).

The resulting expressions can be integrated analytically only for simple models of the dielectric function. Since we are interested in bulk and surface plasmon processes, we will use in this section the approximation:

$$\varepsilon(\omega) = 1 - \frac{\omega_P^2}{\omega(\omega+i\gamma)} \quad , \tag{17}$$

which describes the plasma resonance of simple metals, with plasma frequency ω_P and damping rate γ .

We separate the k integration as $d^3k=d^2\kappa\ dq$, and then we integrate in frequencies ω and wavevectors q, using complex-plane integration techniques. We apply this procedure to the fields previously obtained for the cases of internal and external emission. After some lengthy calculations we finally get the following expressions for the energy loss rate for normal incidence of the electron with respect to the surface.

Case a. Internal emission

As explained before, we consider that the electron is emitted at time $t=-t_0<0$, and at $t=0$ crosses the surface.

The results in this case are the following:

(i) $t<0$ (energy loss in the medium):

$$\dot{W}^{(e)}_{dis}=\dot{W}_{ee}+\dot{W}_{e-S_e[\omega_p]}+\dot{W}_{e-S_e[\omega_s]}+\dot{W}_{eh}+\dot{W}_{e-S_h[\omega_p]}+\dot{W}_{e-S_h[\omega_s]} \tag{18}$$

where we separate the terms corresponding to:electron self interaction (ee), interactions with the surface ($e-S_e$), with the hole (eh), and with the surface perturbation induced by the hole ($e-S_h$) (for a discussion of these results see Section V):

$$\dot{W}_{ee}=-e^2\omega_P^2\int_0^{k_c}d\kappa\left\{\frac{\kappa\ u}{\omega_P^2+\kappa^2u^2}+\frac{e^{-\kappa\ ut'}e^{-\gamma'/2}}{\omega_P^2+\kappa^2u^2}\left[\omega_P\ \sin(\omega_Pt')-\kappa u\cos\ (\omega_Pt')\right]\right\} \tag{18a}$$

$$\dot{W}_{e-S_e[\omega_P]}=e^2\omega_P^2\int_0^{k_c}d\kappa\left\{\frac{\kappa\ u\ e^{2\kappa ut}}{\omega_P^2+\kappa^2u^2}+\frac{e^{\kappa ut''}e^{-\gamma t'/2}}{\omega_P^2+\kappa^2u^2}\left[\omega_P\ \sin(\omega_Pt')-\right.\right.$$

$$\left.\left.-\kappa u\cos\ (\omega_Pt')\right]\right\} \tag{18b}$$

$$\dot{W}_{e-S_e[\omega_s]}=-e^2\omega_s^2\int_0^{k_c}d\kappa\left\{\frac{\kappa u e^{2\kappa ut}}{\omega_s^2+\kappa^2u^2}+\frac{e^{\kappa ut''}e^{-\gamma t'/2}}{\omega_s^2+\kappa^2u^2}\left[\omega_s\sin(\omega_s t')\right.\right.$$

$$\left.\left.-\kappa u\cos(\omega_s t')\right]\right\} \tag{18c}$$

$$\dot{W}_{eh} = e^2\omega_P\sin(\omega_P t')\,e^{-\gamma t'/2}\int_0^{k_c}d\kappa\; e^{-\kappa u(t+t_0)} \tag{18d}$$

$$\dot{W}_{e-S_h[\omega_P]} = -e^2\omega_P\sin(\omega_P t')\,e^{-\gamma t'/2}\int_0^{k_c}d\kappa\; e^{\kappa u(t-t_0)} \tag{18e}$$

$$\dot{W}_{e-S_h[\omega_s]} = e^2\omega_s\sin(\omega_s t')\,e^{-\gamma t'/2}\int_0^{k_c}d\kappa\; e^{\kappa u(t-t_0)} \tag{18f}$$

Here $t'=t+t_0$ and $t''=t-t_0$ (note that $t'>0$ and $t''<0$).

(ii) t>0 (energy loss in vacuum):

$$\dot{W}^{(e)}_{dis} = \dot{W}_{e-S_e} + \dot{W}_{e-S_h} \tag{19}$$

where

$$\dot{W}_{e-S_e} = e^2\omega_s^2 \int_0^{k_c} d\kappa \left\{ \frac{\kappa u e^{-2\kappa ut}}{\omega_s^2 + \kappa^2 u^2} - \frac{e^{-\kappa ut} e^{-\gamma t/2}}{\omega_s^2 + \kappa^2 u^2} \left[2\ \kappa u \cos\ (\omega_s t) \right] \right. \tag{19a'}$$

$$\left. + \frac{e^{-\kappa\ ut'} e^{-\gamma t'/2}}{\omega_s^2 + \kappa^2 u^2} \left[\kappa u \cos(\omega_s t') - \omega_s \sin\ (\omega_s t') \right] \right\}$$

$$\dot{W}_{e-S_h} = e^2\omega_s \int_0^{k_c} d\kappa\ e^{-\kappa ut'} e^{-\gamma t'/2} \sin\ (\omega_s t' \tag{19b'}$$

Case b. External emission

Since in this case the time where the electron is emitted is taken as t=0, we find non-zero results for t>0, as follows:

$$\dot{W}^{(e)}_{dis} = \dot{W}_{e-S_e} + \dot{W}_{e-S_h} \tag{20}$$

being

$$\dot{W}_{e-S_e} = \int_0^{k_c} d\kappa \frac{\omega_s^2\ e^{-2\kappa z_0}}{\omega_s^2 + \kappa^2 u^2} \left[\kappa u\ e^{-2\kappa ut} - e^{-\kappa ut}\ e^{-\gamma t/2} \right. .$$

$$\left. \cdot \left[\omega_s \sin\ (\omega_s t) + \kappa u \cos\ (\omega_s t) \right] \right] \tag{20a}$$

$$\dot{W}_{e-S_h} = \omega_s \int_0^{k_c} d\kappa\ e^{-2\kappa z_0}\ e^{-\kappa ut}\ e^{-\gamma t/2} \sin\ (\omega_s t) \tag{20b}$$

these results describe the interaction between the electron and the surface perturbations induced by the electron and by the hole.

In all these expressions k_c^{-1} is the usual cut off in the plasma response function [1-4].

In addition to these terms associated to the electron motion, the sudden creation of a hole in the medium is also a source for plasmon excitation. Using the same formulation, we can calculate the rate of energy dissipation due to the hole at $\vec{r}_h(t)=\vec{r}_0$, by the same simple formula, viz.

$$\dot{W}^{(h)}_{dis} = - e \left.\frac{\partial \phi^{ind}(\vec{r},t)}{\partial t}\right|_{\vec{r}=\vec{r}_0} \tag{21}$$

$$= - ie \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi}\, \omega\, e^{i(\vec{k}.\vec{r}-\omega t)}\, \phi^{ind}(\vec{k},\omega) \Big|_{\vec{r}=\vec{r}_0}$$

which leads to a set of integrals similar to the ones already presented.

IV. Energy loss and plasmon excitation

One of the main quantities in the process of electron emission is the total energy dissipated into bulk and surface modes, as well as the related probabilities for bulk and surface plasmon excitations.

The total (dissipated) energy loss can be obtained by a straightforward integration of the loss rate $\dot{W}$ derived in the previous sections. We will exploit here a useful relation between the energy loss and the probability of plasmon excitation, which is provided by a semiclassical description of the process. According to this description [4] the probability of exciting n plasmons of frequency ω_ν (with ν = P,S for bulk or surface plasmons), by a time- dependent perturbation like the one considered here, is given by a Poisson distribution

$$P_n(\omega_\nu) = \exp(-Q_\nu) \frac{Q_\nu^n}{n!} \tag{22}$$

where the coefficient Q_ν is the average number of plasmons excited.

In order to calculate the coefficient Q_ν from the present description, we note that the average energy absorbed by the plasmon field,

$$\langle \Delta W_\nu \rangle \equiv \sum_{n=1}^{\infty} n \hbar \omega_\nu P_n(\omega_\nu) = \hbar \omega_\nu Q_\nu , \tag{23}$$

should equal the dissipative loss calculated with our alternative approach.

To obtain the losses ΔW_ν associated to bulk and surface excitations we collect all the terms in $\dot{W}$ related to ω_P and ω_S, and integrate in time the resulting expressions. The results for each of the cases considered before will be discussed in the next section.

V. **Results and discussion**

In the previous sections we have derived analytical expressions for all the terms that contribute to the energy dissipation rate in emission processes that occur in the vicinity of a solid surface. We will now discuss the results of calculations of the energy loss rate, and of the total energy loss in the emission process.

(i) **Energy loss rates**

First we want to illustrate the behavior and physical origin of each of the terms that appear in the expressions for the energy loss. As before, we analyze the cases of internal and external emission. All the values are given in atomic units.

(i.a) **Internal emission:**

The results for $\dot{W}^{(e)}_{dis}$, Eqs.(18 a-f), consists of various terms representing the interaction of the electron with bulk and surface excitations. The notation indicates the electron interactions with surface perturbations induced by itself ($e-S_e$) or by the hole ($e-S_h$); the terms in ω_P and ω_S give the contributions from bulk and surface plasmons.

To illustrate the behavior of these terms we show in Figs.2 and 3 the results for the case of an electron emitted from a point inside a solid, at a distance z_0 for the surface. Here the rate $\dot{W}$ is plotted as a function of time $t=z/u$, where z is the instantaneous position of the emitted electron. Therefore, the results for $t<0$ describe the energy loss inside the medium, while those for $t>0$ correspond to the electron moving in vacuum. For simplicity, the curves representing each of the terms in Eqs.(18 a-f) are denoted by the corresponding letters, from a to f.

Let us first analyze the results of Fig.2, for velocity $u=4$ a.u. and time $t_0=30$ a.u. (hence, $z_0=120$ a.u.). In part (a) of this figure we show the electron-interaction terms of Eqs.(18 a-c). The first term in Eq.(18 a), independent of time, yields the normal stopping power associated to the *self energy* of an electron in a solid, namely

$$\dot{W}^{(e)}_{bulk} = - \frac{e^2\omega_P^2}{2u} \ln \left[1+ \frac{k_c^2 u^2}{\omega_P^2}\right] \tag{24}$$

In XPS studies this is usually called the "extrinsic" term [4,13]. The second term in (18a) provides the correction due to the "creation" of the electron at time $t=-t_0$. The sum of these two terms, curve *a* in Fig.2 (dotted line), shows how the electron self energy grows from zero and reaches asymptotically the bulk value of Eq.(24) (straight solid line). This effect determines a "self-energy formation distance" of the order of the wavelength $\Delta z=2\pi\omega_P/u$ of the oscillatory component (note that $\omega_P t' = \omega_P(t_0+z/u)$) in Eqs.(18 a-c)) as observed in this figure. We note incidentally that this coincides with the oscillation distance of the so-called *wake potential* [7]. In fact, this behavior illustrates how the wake potential develops after the electron motion starts.

Equations (18b,c) give modifications to the energy loss due to the electron interactions with bulk and surface plasmons in the vicinity of the surface. In particular, the first terms in each of these equations give rise to the following "begrenzung" effects: the *positive* term in ω_P , first term in (18b), reduces the intensity of the coupling to bulk plasmons in the vicinity of the surface, while the *negative* term in ω_S , first term in (18c), represents the energy loss in surface plasmon excitations.

Note that the positive first term in *b* exactly cancels the rate of bulk plasmon excitation when the particle crosses the surface (this is clearly illustrated by curve *ab* -the sum of *a* and *b*, in Fig.2(a)). Instead, the negative first term in *c* yields a maximum of surface plasmon excitation at the same crossing point.

The second terms in (18b, c), similar to the second term in (18a), yield the corrections to the electron-surface interaction due to the creation of the electron at time $-t_0$. These oscillatory components are very small for the case of Fig.2 (curves *b*, *c*), due to the relatively large value of t_0 (or z_0), but become more important if the emission process occurs closer to the surface (as in Fig.3, for t_0=10 a.u.). Finally, curve *abc* (solid line) gives the sum of the three curves.

On the other hand, the terms *d-f* correspond to the electron interactions with the hole-induced perturbations (Fig.2b). Thus, the term (18*d*) represents the interaction between the electron and the bulk-plasmon perturbation set up by the sudden creation of the atomic hole at time $-t_0$, while the terms *e* and *f* (corresponding to Eqs.18e anf 18f) account for the electron interactions with the bulk- and surface-plasmons perturbations induced by the appearance of the hole in the vicinity of the surface.

The term (18*d*) describes the electron-hole interaction inside the medium and it contains no surface effects; these effects are included in *e* and *f* , which are also very small in the case of

Fig.2, but become more important as the hole position approaches the surface (cf. Fig.3(b)).

Let us consider now the results for t>0. As already noted, they correspond to the energy loss of the electron moving in vacuum after escaping through the surface. The line **a'** in Figs.2(a), 3(a) shows the term (19*a*'), while the line ***b'*** in Figs.2(b), 3(b) corresponds to the term (19*b*').

The first two terms in (19a') join continuously with the begrenzung term in (18c), but the excitation of surface modes shows now an oscillatory component that dominates at larger distances (cf. also similar effects discussed in Ref.14). The remaining oscillatory terms in (19*a*'), depending on $t'=t+t_0$, are due to the sudden start of the electron motion at time $t=-t_0$, while the oscillatory term in (19*b*') is due to the interaction with the hole-induced surface-plasmon excitations. Again these terms are small in the case of Fig.2, but become more important the closer to the surface the emission process occurs (Fig.3).

In Fig.4 we summarize the results for the total dissipative energy loss rate. For comparison, we show the results for velocities, u=4, 10, 20 and 50 a.u., and for (a) t_0=30 a.u., and (b) t_0= 10 a.u.

(1.b) **External emission:**

Finally, we consider the case where the emission process occurs outside the solid (external emission). Since the coupling to surface plasmons decays exponentially with the distance z_0, we will consider here the interesting case of z_0=0 (emitting atom located at the surface). Note that this situation coincides also with the limit of the internal emission process, for $z_0 \to 0$.

This case is much simpler than the one described previously. The escaping electron interacts with the surface perturbations induced by the electron and hole created at time t=0, as given by (20 a) and (20 b) respectively. These results are shown in Fig.5, as a function of time t=z/u, where z is the instantaneous position of the electron. The solid line is the total (sum of *a* and *b*) dissipative energy loss rate. The oscillations here are rather out of phase and partially cancel each other.

(ii) **Integrated energy loss**

The results for the energy loss rates $\dot{W}$ already discussed have been integrated in time, from the expressions given in Sec.III, to obtain the total energy dissipated during the emission process ΔW. As noted in Sec.IV it is useful to separate the terms corresponding to bulk and surface plasmons (terms containing ω_P and ω_S in Eqs.(18)-(20)) and express the results in terms of the corresponding average numbers of bulk and surface plasmon excitations Q_ν , defined by $Q_P=-\Delta W[\omega_P]/\hbar\omega_P$ and $Q_S=-\Delta W[\omega_S]/\hbar\omega_S$.

The results for each of the cases considered in this section are given in Appendix B.

We show in Fig.6, parts (a) and (b), the results for Q_P and Q_S in the case of internal emission, as a function of the distance z_0 between the hole and the surface.

We see in Fig.6(a) how the bulk plasmon loss grows from zero when the emission occurs at the surface (z_0=0), almost independently of the value of the electron velocity u, but finally reaches a linear dependence on z_0, with a slope that decreases with u; this is due to the dominance of the extrinsic terms at large z_0 values. Therefore, the figure illustrates the existence of well defined intrinsic and extrinsic components in the probability of plasmon excitation. This point has been discussed in several works [4,13] and will not be discussed here; but we just note that this description provides a detailed account of the various terms that contribute to the interference between intrinsic and extrinsic components.

Fig.6(b) shows the energy loss due to surface plasmon excitation as a function of z_0. We also note that the behavior for small z_0 is rather independent of the velocity u, though in this case there is a maximum in surface plasmon excitation at z_0=0. For large z_0, the results approach constant Q values. This limit corresponds to the case of an electron crossing the surface of the metal after propagating a large distance through the bulk. The energy loss in this limiting case is given after Ritchie [15] by:

$$\Delta W_R \cong \frac{\pi}{2}\,\frac{\omega_S}{u}\ \text{arc tan}\,\left(\frac{k_c u}{\omega_s}\right) \qquad (25)$$

(the arctan(x) is a correction included here due to the finite upper limit k_c in the κ integral).

The corresponding asymptotic values of $Q_R = -\Delta W_R/\hbar\omega_s$ are indicated, for each velocity, on the right scale in this figure. The behavior in Fig.6(b) may be compared to the one resulting from intrinsic and extrinsic terms in Fig.6(a).

Finally, we show in Fig.7 the values of Q_S versus z_0, for the case of electron emission from points outside the metal (external emission). The results here show no structure. The maximum values occur again at z_0=0 and decrease nearly exponentially with z_0. The behavior for small z_0 coincides with that observed in Fig.6(b) (of course both results match at $z_0=0$).

VI. CONCLUSIONS

The dielectric formulation provides a useful approach to study the simultaneous interaction of electrons and ions (or atomic holes) with bulk and surface plasmons in the vicinity of a solid surface. The vicinage effect in the energy loss and induced surface excitations can be described in detail. The model provides a picture of how the interactions develop after the electron is emitted and moves through the solid, or escapes in vacuum after crossing the surface.

Important effects here are the sudden creation of the electron-ion pair (including the sharp cut in the electron trajectory at the emission point), as well as the "vicinage" effects which appear when the emission occurs in the proximity of the surface.

It is of interest to note that the application of the surface reflection model to cases where one of the particles *crosses* the surface requires a careful separation of the Fourier charge-density components acting on each media, in the way explained in Sec. II; otherwise, spurious field terms will appear, and the continuity at the surface may also be broken.

The solutions given here show how the wake potential -due to bulk plasmon excitation- evolves into a stationary value, when the distance between the emitting point and the surface is much larger than the typical wavelength of the wake [7], $2\pi u/\omega_P$. If the distance to the surface is similar to the wake "formation distance" strong interference effects appear, and in particular, if the electron is emitted very close to the surface, bulk plasmons are not excited and the wake potential vanishes.

This effect gives a limit ($z_0 >> 2\pi u/\omega_P$) for the applicability of the electron-self-energy values, as normally calculated. For emission processes closer to the surface the self-energy values must be reconsidered taking into account the vicinage effects here discussed.

These conclusions may be also of interest for the analysis of the spectra, in angle and energies, of electrons emitted in the forward direction by ions emerging from solid foils [8]; a process where the wake potential and the dynamical electron-ion-surface interactions can influence the shape of the electron spectra [7,8]. Even though in our calculation the ion is at rest, it is straightforward to see that similar effects will appear if the ion moves in the proximity of the surface. Application of the present model to that case will be given elsewhere.

Another well-known excitation channel is provided by surface plasmons. These excitations are localized near the surface, in a range of distances given by k_c^{-1}. Therefore, hole-vicinage effects in the excitation of surface plasmons could be observed only if the electron is emitted from points closer than this value. On the contrary, electrons emitted from deeper points will show the normal surface plasmon losses [15], without any influence from the creation of the localized hole inside the bulk.

It is clear that this approach can be useful as well to study the spatial patterns of interactions with bulk and surface plasmon in photoelectron spectroscopy studies. The cases of ions implanted in the material [16], or atoms adsorbed at metal surfaces [17] are examples of the cases of internal and external emission considered here (besides the standard case of internal emission from pure metals [4,13]). Semiclassical models - based on quantum mechanical treatments of the plasmon field - have been previously used to describe some of these situations, but still some of the experimental results have not yet been explained satisfactorily [4,13,17].

Our results for the integrated energy loss and probabilities of excitations agree with existing results of previous authors if a simple plasmon-pole dielectric function is assumed. However, we note that the general formulation of the problem through the dielectric approach permits also to study the effects arising from different response functions.

Application of the present formalism to cases of interest in photoelectron spectroscopy [13,16,17] is currently under way.

Acknowledgments

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APPENDIX A

We derive in this appendix, from the general formulation given in the text for an electron emitted in oblique direction with respect to the surface, with velocity $\vec{v}=(\vec{w},u)$, the expressions for the surface charges and electrostatic potentials for a dielectric function of the form $\varepsilon(\omega)$. Note that this corresponds to the neglect of spatial dispersion, an approximation that holds in the limit of long-wavelength plasmon excitation.

We consider now the cases of *internal* and *external* emission.

(a) Internal emission

Using Eq.(8) and the expressions for $\rho^M(\vec{K},\omega)$ and $\rho^V(\vec{K},\omega)$, Eqs.(4a,b), we get the surface charge density as follows

$$\sigma(\vec{\kappa},\omega) = \sigma_1(\vec{\kappa},\omega) + \sigma_2(\vec{\kappa},\omega), \tag{A1}$$

with

$$\sigma_1(\vec{\kappa},\omega) = \frac{\kappa}{\pi}\frac{1}{(\varepsilon+1)}\int_{-\infty}^{\infty}\frac{dq}{(q^2+\kappa^2)}\,\rho^M(\vec{K},\omega) \tag{A2 a}$$

$$= \frac{2\,i\,e}{(\varepsilon+1)}\left[\frac{1-e^{-\kappa z_0}\,e^{-i\Omega t_0}}{\Omega - i\kappa u} + \frac{e^{-\kappa z_0}\,e^{-i\omega t_0}}{\omega - i\eta}\right]$$

$$\sigma_2(\vec{\kappa},\omega) = -\frac{\kappa}{\pi}\frac{\varepsilon}{(\varepsilon+1)}\int_{-\infty}^{\infty}\frac{dq}{(q^2+\kappa^2)}\,\rho^V(\vec{K},\omega) \tag{A2 b}$$

$$= \frac{2\,i\,e}{\Omega + i\kappa u}\,\frac{\varepsilon}{(\varepsilon+1)}$$

where $\Omega=\omega-\vec{\kappa}\cdot\vec{w}$, and $\varepsilon\equiv\varepsilon(\omega)$. The factors 2 in the final expressions are due to the equal contributions from e and e' to σ_1 (first term) and to σ_2 , and from h and h' to σ_1 (second term). This can be seen by integrating in (A2a) and (A2b), with the charge densities given in (4a) and (4b).

The potentials in M and V can be determined from Eqs.(5a) and (5b) using (4a,b) and the previous values if σ_1, σ_2. Thus we get

$$\phi^M(\vec{k},\omega) = \frac{4\pi\ i\ e}{k^2\varepsilon(\omega)}\left[F^M_{ee'} + F^M_{hh'} + F^M_{\sigma_1}\right] \tag{A3}$$

$$\phi^V(\vec{k},\omega) = \frac{4\pi\ i\ e}{k^2}\left[F^V_{ee'} + F^V_{\sigma_1} + F^V_{\sigma_2}\right] \tag{A4}$$

where:

$$F^M_{ee'}(\vec{k},\omega) = e^{-i\vec{k}.\vec{x}_s}\left\{\frac{\left[1-e^{-i(\Omega-qu)t_o}\right]}{\Omega-qu-i\eta} - \frac{\left[1-e^{-i(\Omega+qu)t_o}\right]}{\Omega+qu-i\eta}\right\} \tag{A5 a}$$

$$F^M_{hh'}(\vec{k},\omega) = \left(e^{iqz_o} + e^{-iqz_o}\right)\frac{e^{-i\omega t_o}}{\omega-i\eta} \tag{A5 b}$$

$$F^M_{\sigma 1}(\vec{k},\omega) = -\frac{2}{(\varepsilon+1)}\left\{\frac{\left[1-e^{-i\Omega t_o}e^{-\kappa z_o}\right]}{\Omega-i\kappa u} + \frac{e^{-\kappa z_o}\ e^{-i\omega t_o}}{\omega-i\eta}\right\} \tag{A5 c}$$

$$F^V_{ee'}(\vec{k},\omega) = -e^{-i\vec{k}.\vec{x}_s}\left[\frac{1}{\Omega-qu+i\eta} + \frac{1}{\Omega+qu+i\eta}\right] \tag{A5 d}$$

$$F^V_{\sigma 1}(\vec{k},\omega) = \frac{2}{(\varepsilon+1)}\left\{\frac{\left[1-e^{-i\Omega t_o}e^{-\kappa z_o}\right]}{\Omega-i\kappa u} + \frac{e^{-\kappa z_o}\ e^{-i\omega t_o}}{\omega-i\eta}\right\} \tag{A5 e}$$

$$F^V_{\sigma 2}(\vec{k},\omega) = \frac{2\varepsilon}{\varepsilon+1}\ \frac{1}{\Omega+i\kappa u} \tag{A5 f}$$

In order to analyze these expressions, we note that in the results for $\phi^M(\vec{K},\omega)$ and $\phi^V(\vec{K},\omega)$ we can distinguish: "surface" terms (depending on $(\varepsilon+1)^{-1}$), "bulk" terms (depending only on $1/\varepsilon(\omega)$), and "vacuum" terms (independent of $\varepsilon(\omega)$). In addition we shall consider the source of each of them. For instance, the term $F^M_{ee'}(\vec{K},\omega)$ in ϕ^M gives the potential in an infinite medium for an electron whose motion starts suddenly at time $t=-t_0$ (with velocity $v=(w,u)$), plus the analogous potential for the electron-image created at the same time (with velocity $v'=(w,-u)$). The term $F^M_{hh'}(\vec{K},\omega)$ gives the bulk potential due to the hole (h) and its image (h'), both created at $t=-t_0$ at distance z_0 on each side of the surface. The last term in ϕ^M, denoted $F^M_{\sigma 1}(\vec{K},\omega)$, includes the effect of the surface charges $\sigma_{ee'}$ and $\sigma_{hh'}$, induced respectively by e and e' (first term in (A2 *a*)), and by h and h' (second term in (A2 *a*)). The fact that e and e' (as well as h and h') contribute equally to the surface charge σ is the reason for the factor 2 in the expressions of σ_1 (Eq. A2 a) and F_{σ_1} (Eq. A5 c).

In analogous way, the term $F^V_{ee'}(\vec{K},\omega)$ is the vacuum potential for the semi-infinite trajectory of the outgoing electron e and image e', after the electron exits from the metal, while the last two terms are due to the surface perturbations induced by e, e', h and h' before leaving the metal ($F^V_{\sigma 1}(\vec{K},\omega)$) , and by e and e' after emergence in vacuum ($F^V_{\sigma 2}(\vec{K},\omega)$) (again, the factors 2 here have the same origin already mentioned).

Hence, the equations contain all the interference effects in bulk and surface plasmon excitation that originate from the time correlation between the hole creation and the electron emission.

(b) External emission

Proceeding as before, we now calculate σ using Eq.(8) and the charge densities for this case, Eqs.(13 a,b). Thus we get

$$\sigma(\vec{K},\omega)= \frac{ie\varepsilon}{(\varepsilon+1)}\,\frac{\kappa}{\pi}\int_{-\infty}^{\infty}\frac{dq}{k^2}\left[\frac{e^{-iqz_0}}{\Omega-qu+i\eta}+\frac{e^{iqz_0}}{\Omega+qu+i\eta}-\frac{\left(e^{iqz_0}+e^{-iqz_0}\right)}{\omega+i\eta}\right]$$

$$= \frac{2ie\varepsilon}{(\varepsilon+1)}\, e^{-\kappa z_0}\left[\frac{1}{\Omega+i\kappa u}-\frac{1}{\omega+i\eta}\right] \tag{A6}$$

and, from Eqs.(5a, b) the potentials in M and V become:

$$\phi^V(\vec{k},\omega)= \frac{4\pi ie}{k^2}\left[G^V_{ee'}(\vec{k},\omega)+G^V_{hh'}(\vec{k},\omega)+G^V_{\sigma}(\vec{k},\omega)\right] \tag{A7}$$

$$\phi^M(\vec{k},\omega)= \frac{4\pi ie}{k^2\varepsilon}\quad G^M_{\sigma}(\vec{k},\omega) \tag{A8}$$

with:

$$G^V_{ee'}(\vec{k},\omega)= -\left[\frac{e^{-iqz_0}}{\Omega-qu+i\eta}+\frac{e^{iqz_0}}{\Omega+qu+i\eta}\right] \tag{A9 a}$$

$$G^V_{hh'}(\vec{k},\omega)= \frac{1}{\omega+i\eta}\left(e^{iqz_0}+e^{-iqz_0}\right) \tag{A9 b}$$

$$G^V_{\sigma}(\vec{k},\omega)= \frac{2\varepsilon}{(\varepsilon+1)}\, e^{-\kappa z_0}\left[\frac{1}{\omega+i\kappa u}-\frac{1}{\omega+i\eta}\right] \tag{A9 c}$$

$$G^M_{\sigma}(\vec{k},\omega)= -\frac{2}{(\varepsilon+1)}\, e^{-\kappa z_0}\left[\frac{1}{\omega+i\kappa u}-\frac{1}{\omega+i\eta}\right] \tag{A9 d}$$

APPENDIX B

We give here the expressions for the average number of plasmons excited in the cases of internal and external emission, which are obtained from the corresponding expressions of ΔW, as discussed in the text. To obtain the terms related to bulk and surface plasmons, we separate the corresponding terms containing ω_P and ω_S, which we denote here by $\Delta W_{dis}[\omega_P]$ and $\Delta W_{dis}[\omega_S]$. In each case we give the contributions due to the electron (e) and hole (h).

The results are the following.

(a) *Internal emission:*

$$Q_P^{(e)} = \frac{\Delta W_{dis}^{(e)}[\omega_P]}{(-\hbar\omega_P)} = \frac{e^2}{\hbar}\int_0^{k_c} d\kappa \left[\frac{\omega_P\ \kappa u t_0}{(\omega_P^2+\kappa^2u^2)} - \frac{\omega_P}{2(\omega_P^2+\kappa^2u^2)} - \frac{2\omega_P\kappa^2u^2}{(\omega_P^2+\kappa^2u^2)^2} + \right.$$

$$+ \frac{\gamma\ \kappa\ u\ \omega_P}{2(\omega_P^2+\kappa^2u^2)^2} + \frac{\omega_P e^{-2\kappa u t_0}}{2(\omega_P^2+\kappa^2u^2)} - \frac{\gamma\ \kappa\ u\ \omega_P\ e^{-2\kappa u t_0}}{2(\omega_P^2+\kappa^2u^2)^2} +$$

$$\left. + \frac{2\ e^{-(\kappa u\gamma/2)t_0}}{(\omega_P^2+\kappa^2u^2)^2}\left[\omega_P\kappa^2u^2\cos(\omega_P t_0) + \kappa^3u^3\sin(\omega_P t_0)\right]\right] \qquad \text{(B1)}$$

$$Q_P^{(h)} = \frac{\Delta W_{dis}^{(h)}[\omega_P]}{(-\hbar\omega_P)} = \frac{e^2}{\hbar\omega_P}\int_0^{k_c} d\kappa \left[1-e^{-2\kappa z_0} - \frac{\gamma\kappa u}{2(\omega_P^2+\kappa^2u^2)}\left[1-2e^{-\kappa z_0} + e^{-2\kappa z_0}\right]\right]$$

(B2)

$$Q_S^{(e)} = \frac{\Delta W_{dis}^{(e)}[\omega_s]}{(-\hbar\omega_s)} = \frac{e^2}{\hbar}\int_0^{k_c} d\kappa \left[\frac{2\omega_s\ \kappa^2 u^2}{(\omega_s^2+\kappa^2u^2)} + \frac{\gamma\ \omega_s \kappa\ u}{(\omega_s^2+\kappa^2u^2)^2} - \right.$$

$$- \frac{\omega_s e^{-2\kappa u t_0}}{2(\omega_s^2+\kappa^2u^2)} - \frac{\gamma\ \omega_s\kappa\ u\ e^{-2\kappa u t_0}}{2(\omega_s^2+\kappa^2u^2)^2} - \frac{2e^{-(\kappa u\gamma/2)t_0}}{(\omega_s^2+\kappa^2u^2)^2}\Big[$$

$$\left.\Big[\omega_s\kappa^2u^2\cos(\omega_s t_0) + \kappa^3u^3\sin(\omega_p t_s)\Big]\right] \qquad \text{(B3)}$$

$$Q_S^{(h)} = \frac{\Delta W_{dis}^{(h)}[\omega_s]}{(-\hbar\omega_s)} = \frac{e^2}{\hbar\omega_s}\int_0^{k_c} d\kappa \left[e^{-2\kappa z_0} - \frac{\gamma\kappa u}{2(\omega_s^2+\kappa^2u^2)}\left[1+e^{-\kappa z_0} - e^{-2\kappa z_0}\right]\right]$$

(B4)

(b) External emission:

$$Q_e(\omega_s) = \frac{\Delta W_{dis}^{(e)}[\omega_s]}{(-\hbar\omega_s)} = \frac{e^2\omega_s}{2\hbar}\int_0^{k_c} dk\ \frac{e^{-2\kappa z_0}}{(\omega_s^2+k^2u^2)}\left[1- \frac{\gamma\kappa u}{2(\omega_s^2+k^2u^2+ \gamma\kappa u)}\right]$$

(B5)

$$Q_h(\omega_s) = \frac{\Delta W_{dis}^{(h)}[\omega_s]}{(-\hbar\omega_s)} = \frac{e^2}{\hbar\omega_s}\int_0^{k_c} dk\ e^{-2\kappa z_0}\left[1+ \frac{\gamma u\kappa}{2(\omega_s^2+\kappa^2u^2)}\right] \qquad \text{(B6)}$$

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FIGURE CAPTIONS

Fig. 1. Illustration of the problem:

Part (a): the electron is emitted at time $t=-t_0$ at a point $\vec{r}_0$ inside the solid, leaving a localized positive charge e (the hole) at that site. The electron moves through the solid and at time t=0 crosses the surface (at z=0) and escapes into vacuum.

Equivalent problem according to the specular reflection model [9]: Part (b): the extended pseudo-medium M ("metal") contains part of the electron (e), hole (h), and image (e',h') charge-density components, Eqs. (3a), (3b), and a fictitious surface charge σ^M.

Part (c): the pseudo-vacuum V contains the residual electron (e) and image (e') charge-density components, Eq. (3c), and a fictitious surface charge σ^V. (From the matching conditions one finds: $\sigma^M=-\sigma^V=\sigma$, as discussed in the text).

Fig. 2. Energy-loss rate for internal emission as a function of the time t and distance z of the electron to the surface (z=0), for an electron emitted with velocity u=4 a.u. at time $t=-t_0$, with $t_0=z_0/u=30$ a.u. Calculations correspond to $\omega_P=0.56$, $\gamma=0.034$ and $k_c=0.65$, as for aluminum [7]. Part(a) shows the terms of electron self-interaction with bulk and surface perturbations, Eqs. (18 a-c), while part (b) shows terms of electron interactions with the perturbations produced by the hole, Eqs (18 d-f). See the text for discussion.

Fig. 3. Same as in Fig. 2 for $t_0 = z_0/u = 10$ a.u.

Fig. 4. Total dissipative energy loss from Eqs. (18) and (19), for electron velocities u=4, 10, 20, and 50 a.u., and for (a) $t_0=30$, and (b) $t_0=10$ a.u.

Fig. 5. Electron energy loss terms for external emission, Eqs. (20 a) and (20 b) (lines *a* and *b*), as a function of time (t), or distance (z) of the electron to the surface, for u=10 a.u. and $t_0=z_0=0$ (emitting atom located at the surface). The solid line gives the sum of *a* and *b*.

Fig. 6. Average number of plasmons excited in an *internal* emission process from a depth z_0 in the medium, as a function of z_0, for electron velocities u = 3, 4, 5 and 10 a.u., for (a) bulk plasmons (Q_P) and (b) surface plasmons (Q_S). The marks on the right scale in part (b) show the limiting Q_R values given by Eq. (25).

Fig. 7. Average number of surface plasmons excited in an *external* emission process from a distance z_0 outside the medium, as a function of z_0 (in a.u.), for emission velocities u = 3, 4, 5 and 10 a.u.

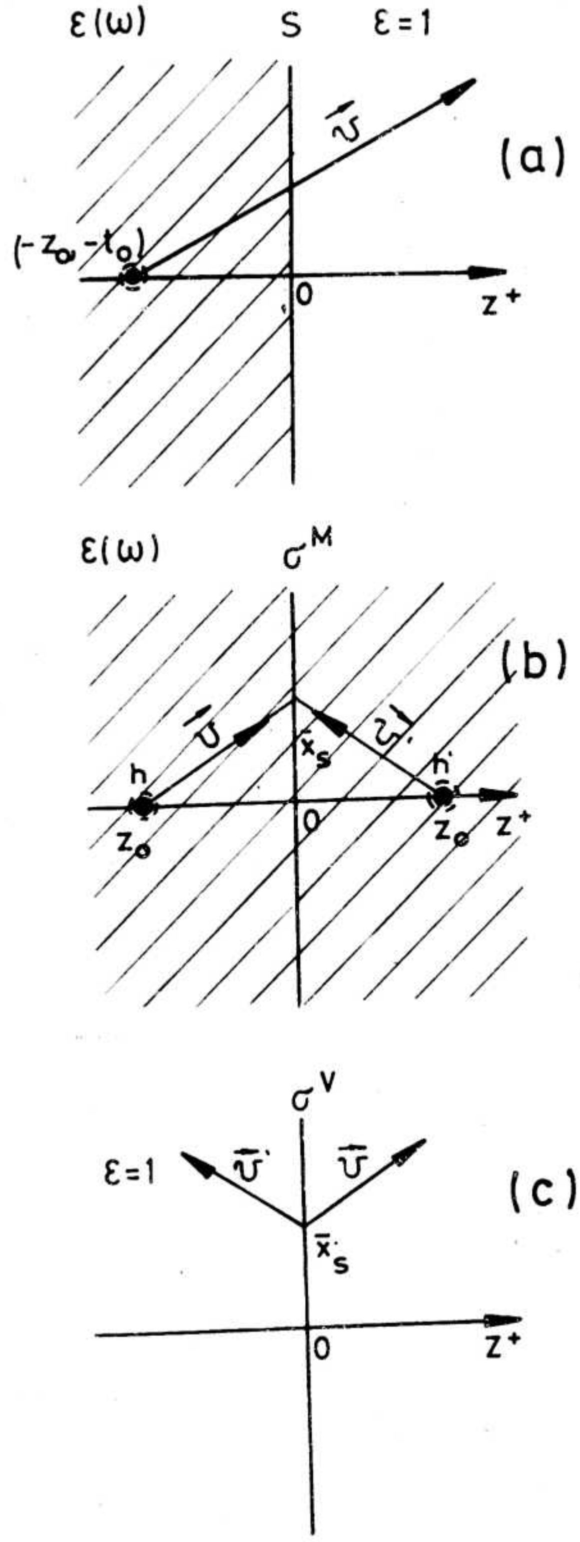


Fig. 1

Fig. 2a

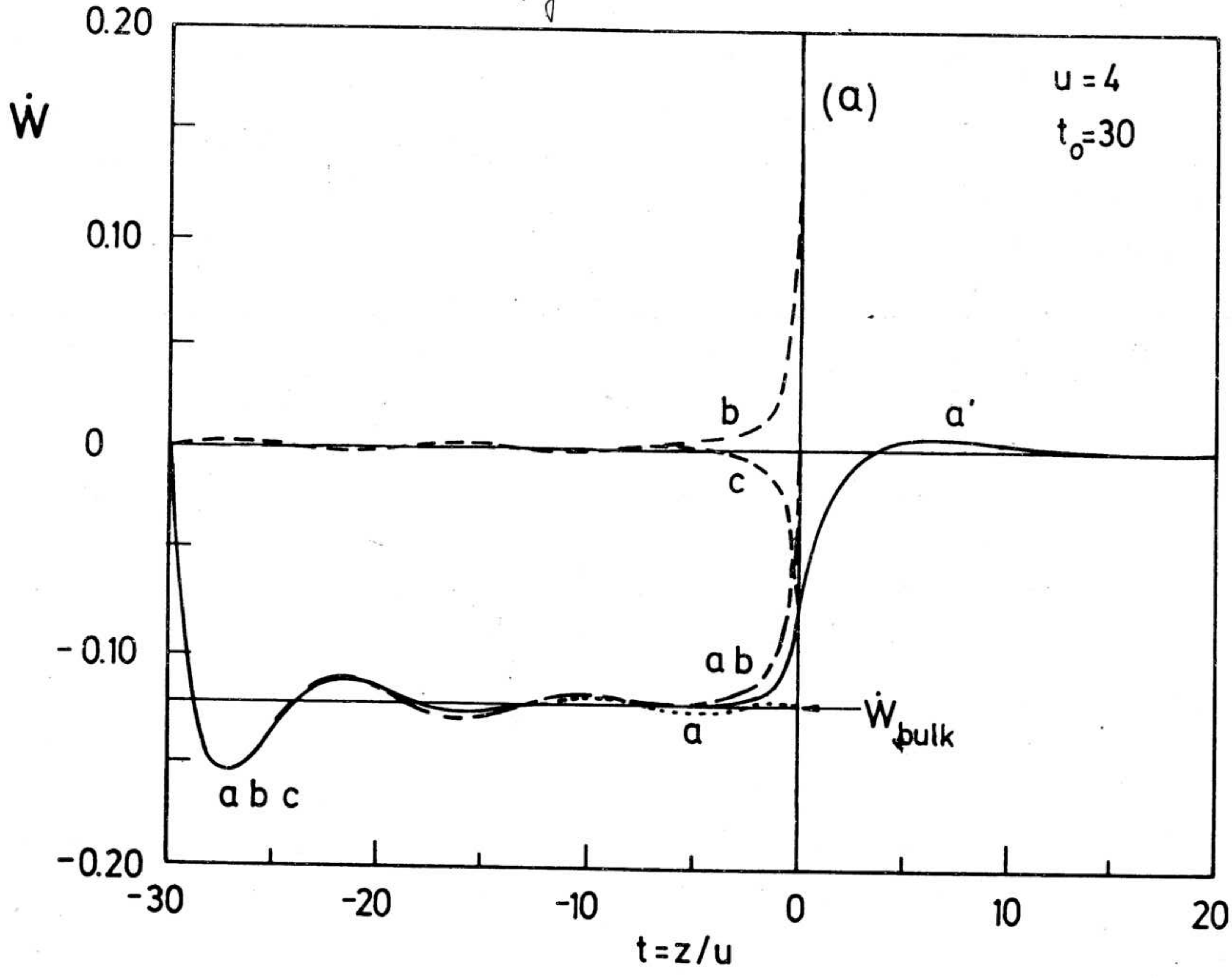


Fig. 2b

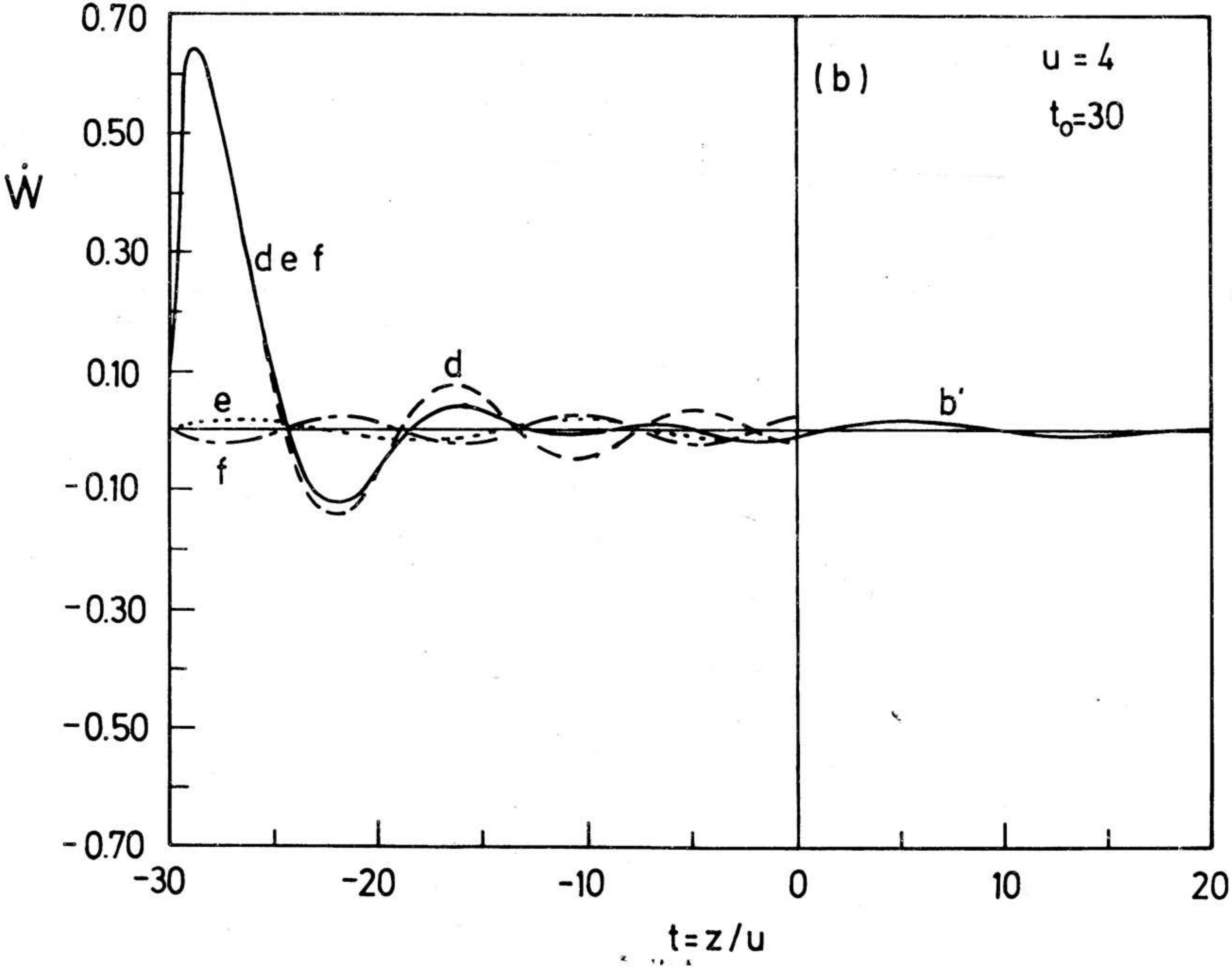
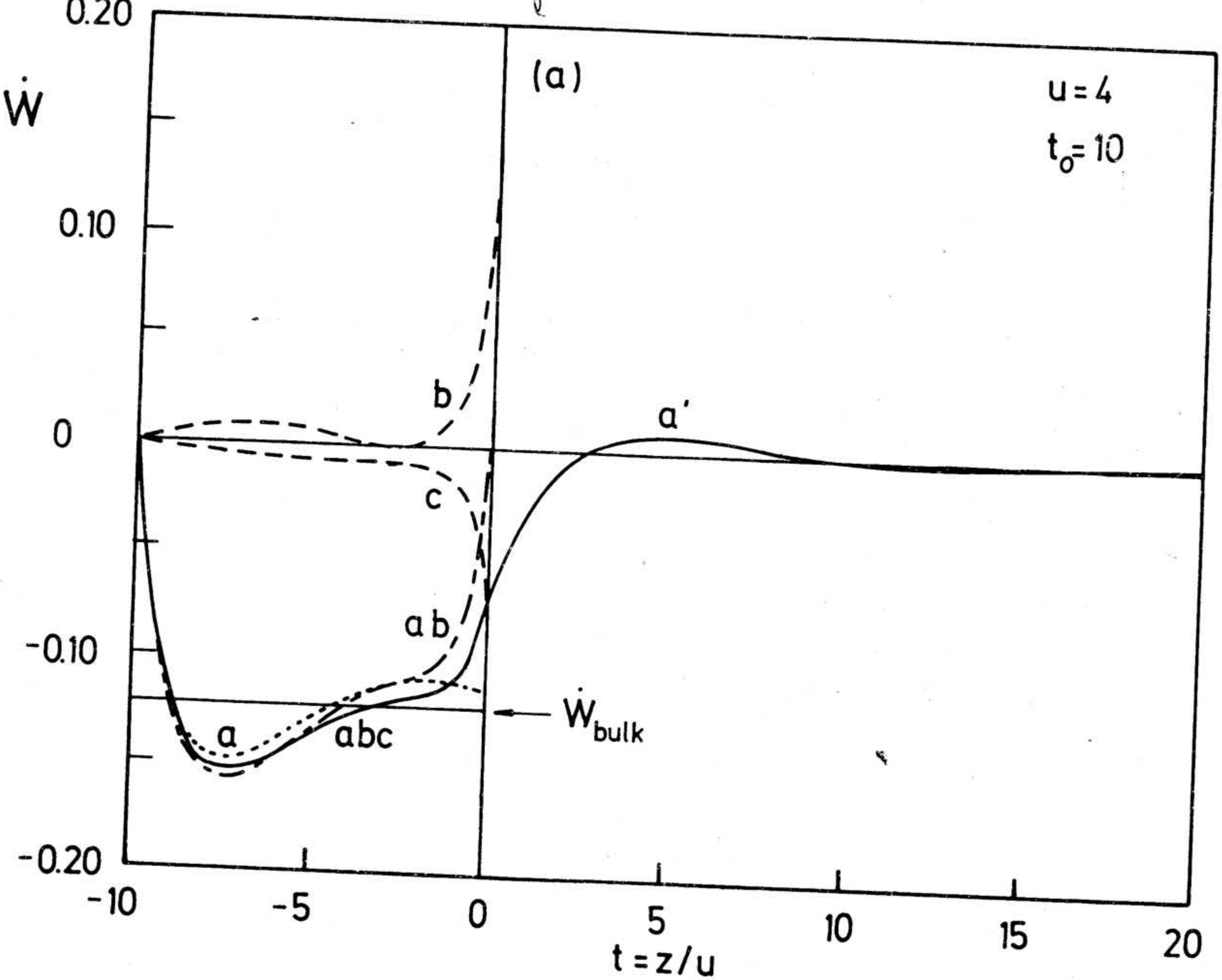

0.70
0.50
0.30
0.10
-0.10
-0.30
-0.50
-0.70
$\dot{W}$
-30
-20
-10
0
10
20
t = z / u
(b)
u = 4
t_0=30
d e f
d
e
f
b'

Fig. 3a



0.20
0.10
0
-0.10
-0.20
$\dot{W}$
(a)
$u = 4$
$t_o = 10$
b
a'
c
a b
a
abc
$\dot{W}_{bulk}$
-10
-5
0
5
10
15
20
$t = z/u$

Fig. 3b

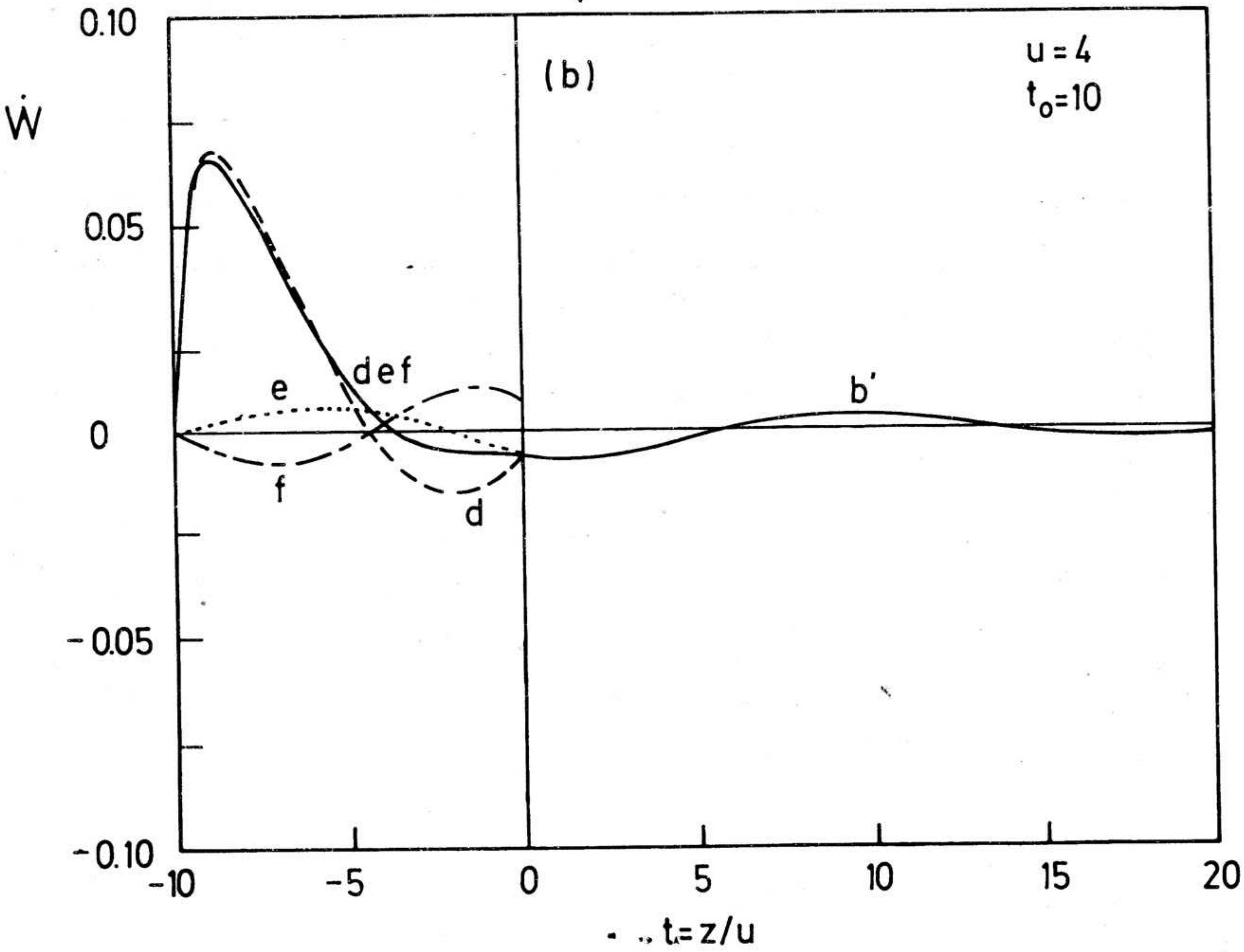


Fig. 4a

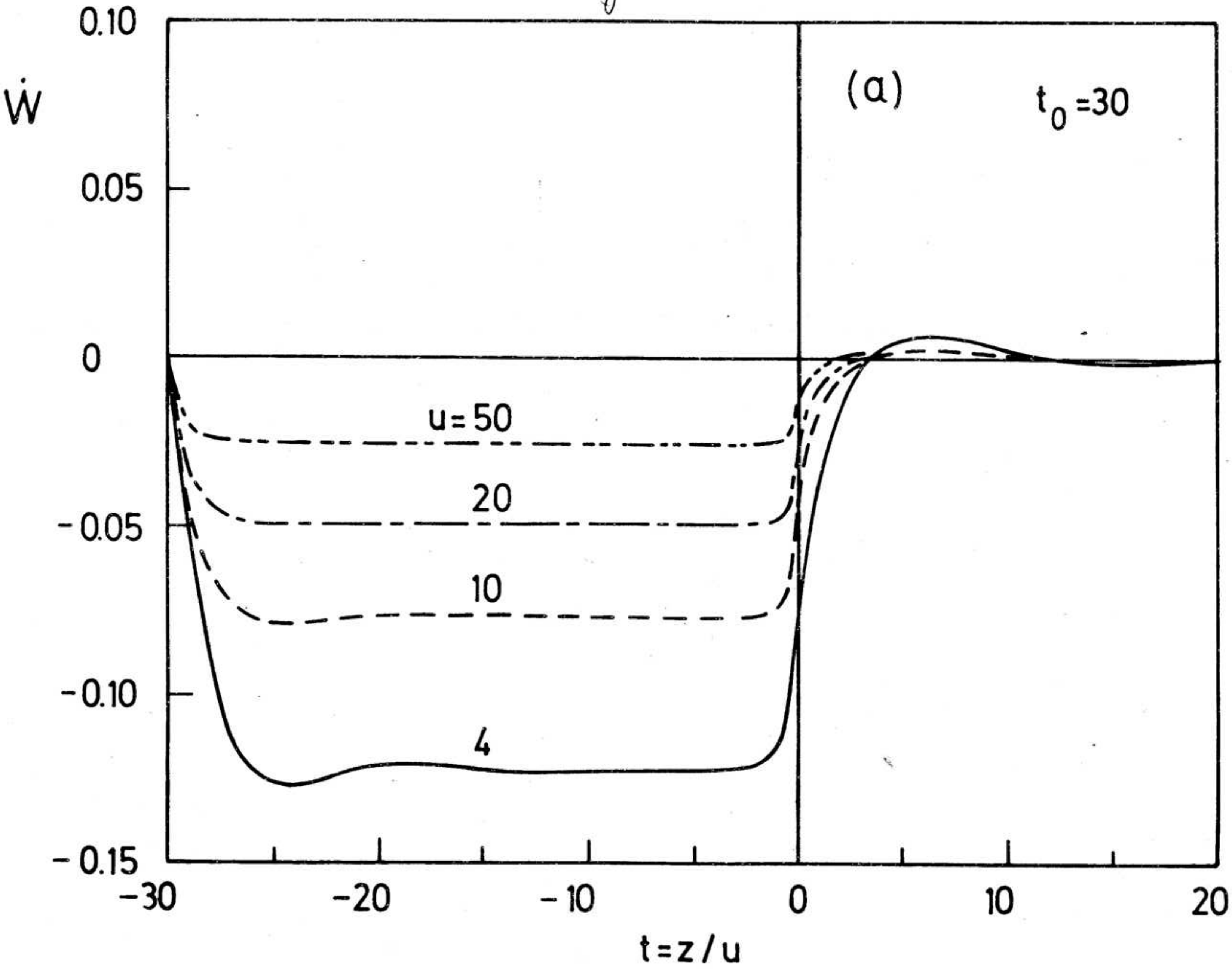


Fig. 4b

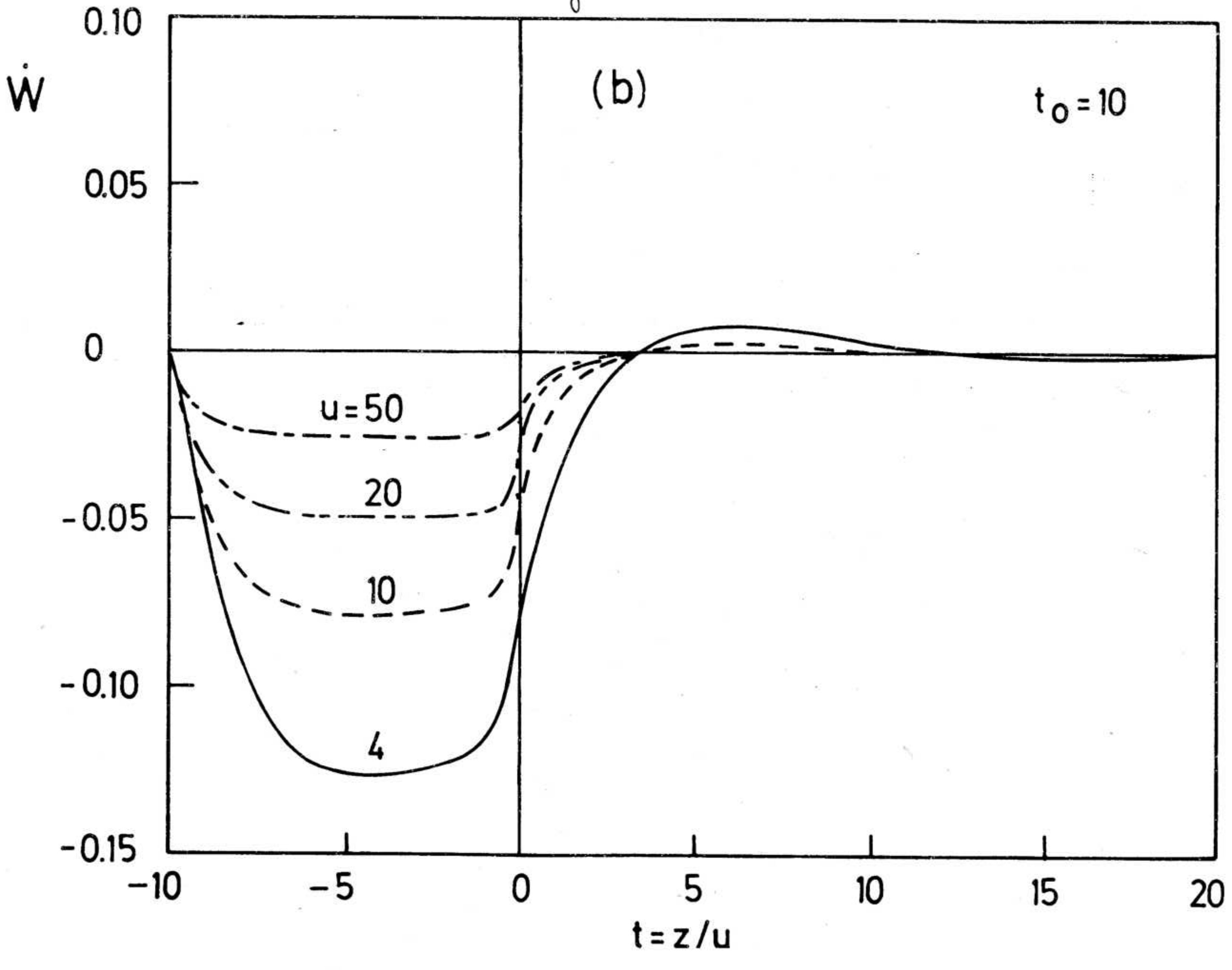


Fig. 5

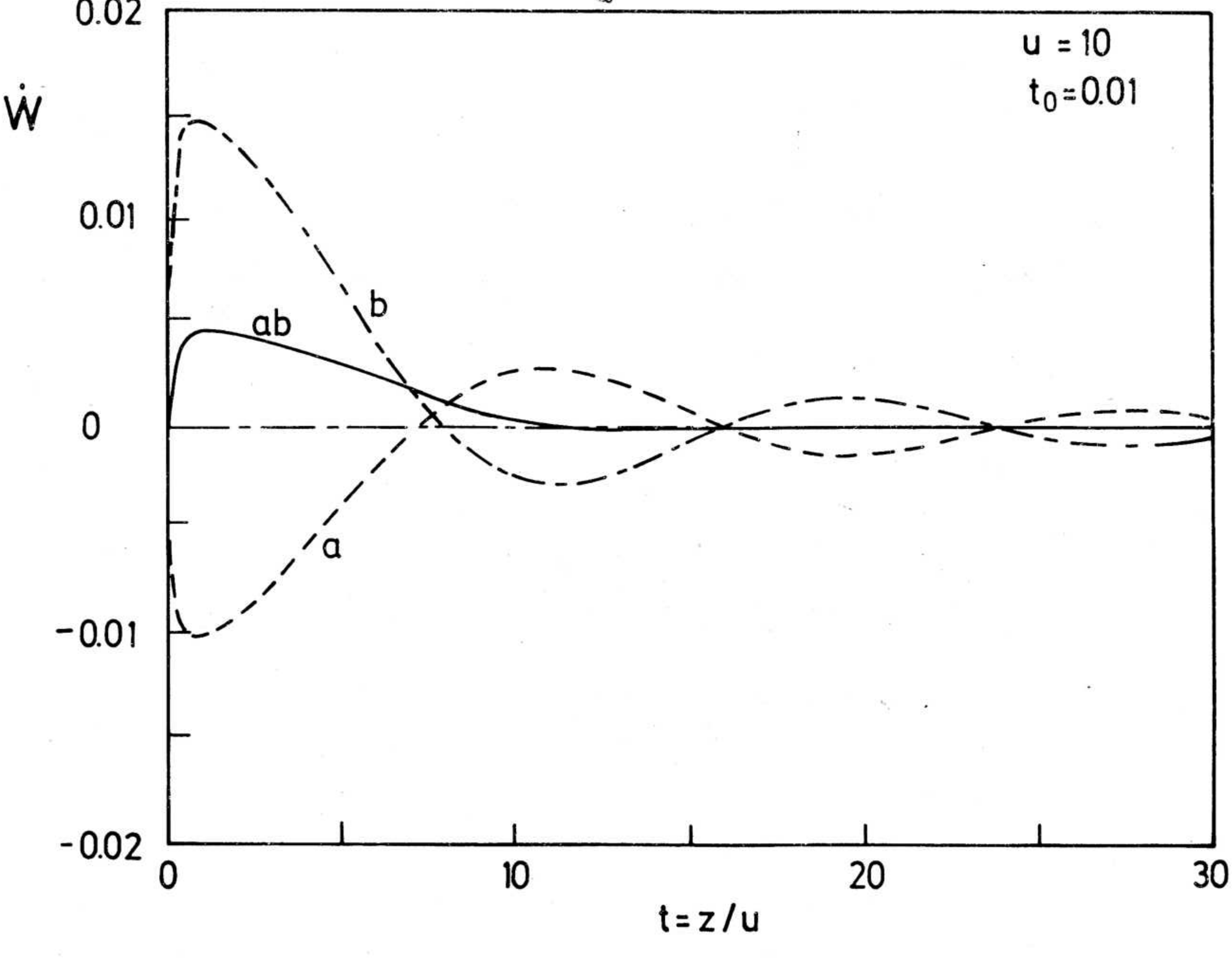


Fig 6a

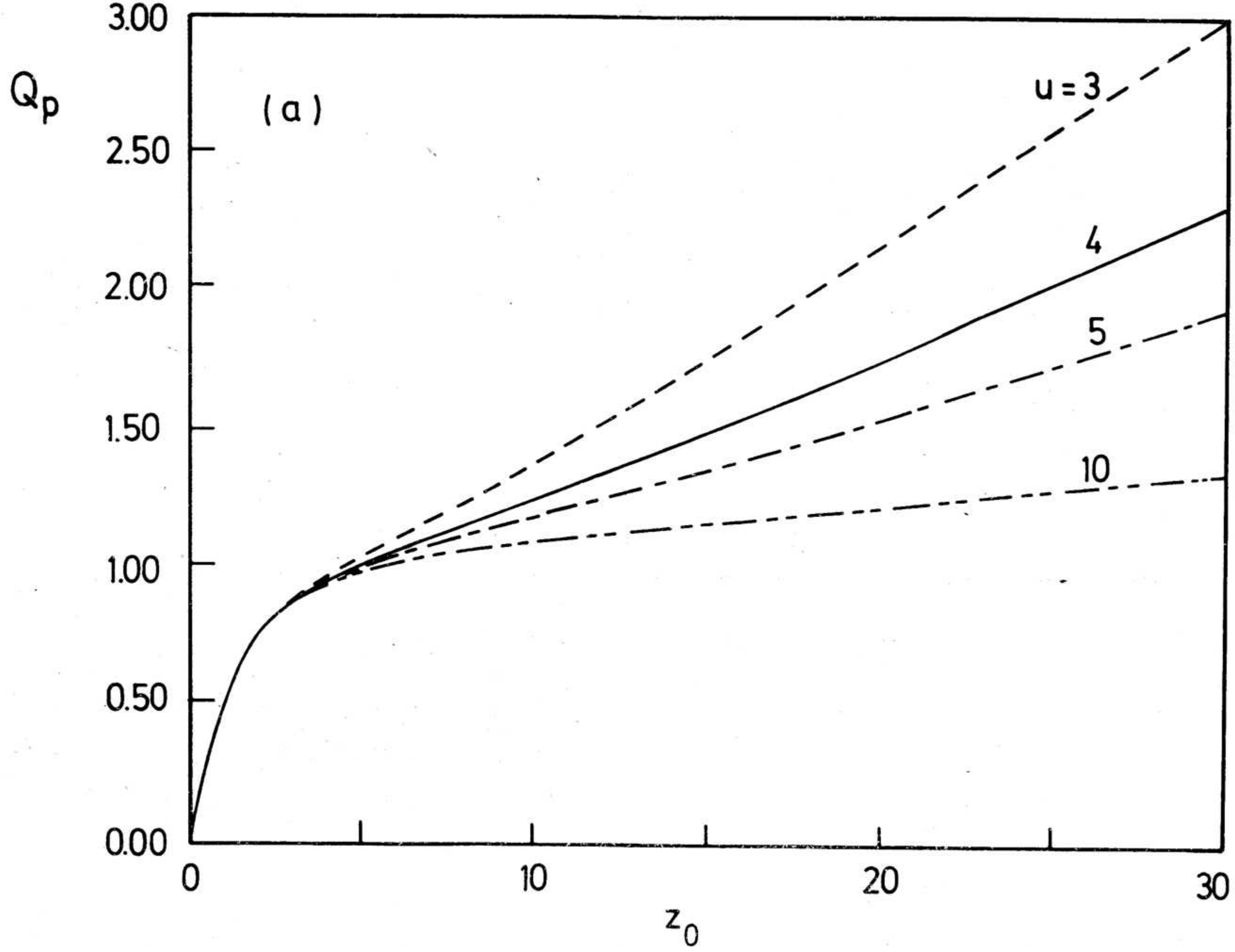


Fig. 6b

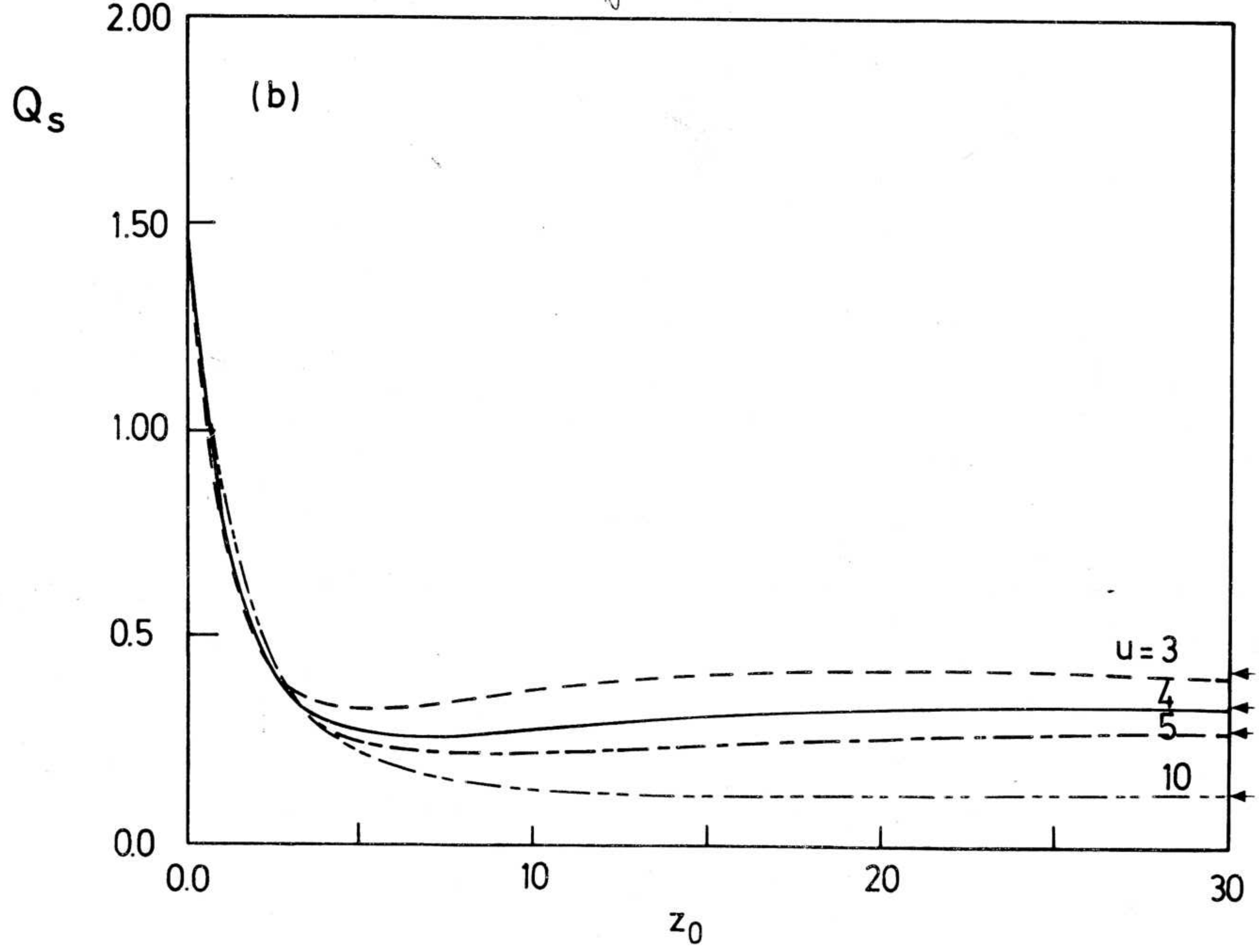


Fig 7