Ion induced electronic excitations in a
spin-polarized electron gas

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Abstract

We calculate both the stopping power of a H atom and the number of electrons it excites, when it moves slowly in a spin-polarized electron gas. The potential induced by the projectile in which the medium electrons scatter off is obtained self-consistently within Density Functional Theory, in the Local Spin Density approximation. We show that both the stopping power and the number of excited electrons decrease slightly when increasing the polarization of the electron gas. Furthermore, the spin-polarization of the excited electrons increases with the projectile velocity and remains in all the cases lower than the polarization of the medium.

\textit{Key words:} Ions, spin-polarization, magnetic materials, Stopping power, Energy loss, electron emission

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1 Introduction

The study of the electronic excitations created by a charged particle moving inside a solid medium provides information on both the projectile and the target, as well as on the interaction between them. In the case of metal targets, the free electron gas model (FEG) has shown to be adequate to describe the valence band excitation spectrum. For high ion velocities one is faced to a weak-coupling problem, and linear response theory gives an accurate description of the medium response and of the projectile energy loss. However, for low projectile velocities ($v < v_F$, where $v_F$ is the Fermi velocity of electrons of the medium), the probe-target coupling is strong and non-perturbative approaches are required [1,2]. A slow ion loses energy mainly creating single particle excitations in the conduction band of the metal. If the energy of the excited electrons surpasses the work function of the metal, the electrons may be emitted giving rise to the so-called kinetic electron emission. Therefore, if one is interested in calculating the stopping power of the slow ion and/or the kinetic electron yield induced by it, one must go beyond linear response theory. A model that has proven to be successful in accounting for the inelastic processes that take place when an ion moves slowly through a free electron gas consists in performing an exact treatment of the scattering of the metal electrons at the potential induced by the projectile. The potential is approximated by the spherically symmetric static potential, calculated within density functional theory (DFT) for an impurity embedded in a free electron gas [3]. This approach has shown to constitute a substantial improvement over linear theory for the calculation of both the stopping power [1,2] and the kinetic electron emission [4] induced by slow ions in metals.
The above mentioned works were based on the spin-unpolarized electron gas. In a spin-polarized electron gas, the electrons of majority or minority spin respond differently to the projectile perturbation. Therefore, the screened potential becomes spin dependent. The natural question that arises and that we address here, is how the spin-polarization of the electron gas affects the stopping power of the ion and the number of electrons that it excites.

In addition to its fundamental interest, a motivation for this study can be found in the development of ion-based experimental techniques applied to the study of surface magnetism [5–7]. The experimental spectra of electrons discriminated in spin, and excited either by potential [8–12] or kinetic emission [9,12,13] provide surface-sensitive information on the magnetic properties of the material. In this respect, the work presented here is related to these experimental works in which the spin-polarization of the kinetic electron yield is measured [9,12,13]. Nevertheless, one should be careful when considering the applicability of our model results to a real situation. A ferromagnetic material presents a complex band structure that hardly can be approximated by the free electron gas model. In spite of that, provided that the Fermi velocity is adequately chosen, FEG has been successfullly applied to the calculation of the stopping power in transition metals like Au [14], and even in insulators like LiF [15] due to the strong perturbation that a slow ion represents. This leads us to believe that the results we obtain for an integrated quantity such as the stopping power are meaningful. In any case, the connection between our results for the number of excited electrons per unit time and the experimental spectra is by no means obvious. The electron emission is commonly considered as a three stage process: excitation, transport and crossing of the surface potential barrier [16]. We want to emphasize that here we only con-
sider the first stage of the process, i.e., the direct excitation of the electrons by the projectile. Therefore, in order to compare with the experimental data the two last steps of the process should also be taken into account. In this respect, the transport of electrons, which is spin dependent in a ferromagnetic material [17], constitutes also an intricate problem.

Finally, we stress that here we will only consider effects related to the spin-polarization of the target. Effects related to the spin polarization of the projectile will be presented elsewhere [18].

Atomic units (a.u.) will be used unless it is otherwise stated.

2 Theory

We are interested in neutral Hydrogen atoms ($H^0$) moving with a velocity $v$ smaller than the Fermi velocity of the material $v_F$. As a first step, we perform a DFT calculation of the potential induced by a static $H^0$ atom embedded in a free electron gas, whose mean electronic density is $n_0 = 3/(4\pi r_F^3)$. The numerical procedure follows similar lines of previous work in the field [19]. However, we consider that the unperturbed electron gas is spin-polarized. The gas polarization is described by the fractional spin-polarization

$$\zeta_0 = \frac{n_0^\uparrow - n_0^\downarrow}{n_0^\uparrow + n_0^\downarrow},$$

(1)

where $n_0^\uparrow (n_0^\downarrow)$ is the background density of electrons with majority (minority) spin. Obviously, $n_0 = n_0^\uparrow + n_0^\downarrow$. We use the local spin density (LSD) approximation for the exchange-correlation potential, following the parametrization of Gunnarsson et al. [20].
For a value of $r_s > 2$ there are two bound Kohn-Sham (KS) states (one for each spin orientation) in the case of a Hydrogen atom[3]. Since we are not interested in effects related to the spin-polarization of the projectile we consider the impurity to be a neutral $H^0$ atom, where the bound electron wave function is calculated by using a linear combination (with identical weight) of the spin-up and spin-down KS orbitals.

The electronic stopping power $S$ is calculated in terms of the transport cross section at the Fermi level $\sigma_T(v_F)$ for scattering of electrons at the potential induced by the impurity:

$$S = n_0 v v_F \sigma_T(v_F) = v Q,$$

(2)

where $Q$ is the so-called friction coefficient. The transport cross section is obtained from the asymptotic behavior (phase shifts) of the KS continuum states, expanded in a spherical-harmonic basis set. In a spin-polarized system, the Fermi energy and the potential induced by the impurity are spin-dependent, and consequently $\sigma_T(v_F)$ is a spin-dependent quantity. The energy loss is thus obtained as the sum of two contributions, each of them related to the excitation of electrons with different spin:

$$S = S^+ + S^\perp = v (Q^+ + Q^\perp) = v (n_0 v_F^+ \sigma_T(v_F^+) + n_0 v_F^\perp \sigma_T(v_F^\perp)),$$

(3)

Notice that $S^+ (S^\perp)$ is the contribution to the stopping due to the excitation of majority (minority) electrons and $v_F^+ (v_F^\perp)$ is the Fermi velocity of the majority (minority) spin electrons.

The electron excitation mechanisms that give rise to kinetic electron emission constitute the stopping power of the incident ion. Using this, frequently applied
theoretical methods consider the total number of emitted kinetic electrons (the
total yield) to be proportional to the electronic stopping power [21,22]. In this
work, we go beyond this approximation and use the model developed in Ref. [4]
to calculate the number of excited electrons. In this model, the distribution of
excited electrons is directly obtained from the calculation of the scattering of
the conduction band electrons in the potential induced by the projectile. As in
the case of the stopping power, the scattering is calculated to all orders in the
projectile charge using phase shifts, and the potential is obtained within DFT
(see Ref. [4] for a detailed explanation of the expressions used). This approach
has shown to constitute a substantial improvement over linear theory [23] and
has been applied to a variety of situations [4,24]. Here, we use this model for
the case of the spin-polarized electron gas (with spin-dependent potentials),
and obtain the number of excited electrons of different spins.

3 Results

In the following, we present results for a neutral $H^0$ moving inside an elec-
tron gas of $r_s = 2.12$ (when the spin polarization is $\zeta_0 = 0.27$ this value of
$r_s$ represents a Fe target [25]). In Fig. 1 we plot the different contributions
to the friction coefficient $Q^\uparrow$ and $Q^\downarrow$ as a function of the spin polarization $\zeta_0$.
As $\zeta_0$ increases the energy loss associated to the excitation of majority (mi-
nority) spin electrons increases (decreases). Nevertheless, as a consequence of
the complex dependence of the transport cross section on the electron energy,
it is observed that the reduction that the medium $\zeta_0$ induces in $Q^\downarrow$ is more
important than the subsequent increase in $Q^\uparrow$. In order to see more clearly
this effect, the average value of the friction coefficient ($Q_{aver} = (Q^\uparrow + Q^\downarrow)/2$)
which decreases slightly with increasing the target spin-polarization, is plotted as well. This leads us to conclude that the ion projectile loses less energy in a spin-polarized medium (note that $Q = 2Q_{\text{aver}}$). In any case the correction is small (for $\zeta_0 = 0.5$ the reduction of the stopping is less than a 10%).

In Fig. 2 we show the number of majority and minority spin electrons excited per unit time by a $H^0$ atom with velocity $v = 0.5$ a.u. as a function of the spin polarization of the target. The polarization of the excitation increases with target polarization. The main reason for that is the reduction of minority spin excitation, which is stronger than the subsequent increase of the majority electron excitation. This implies a reduction of the total number of excited electrons. However, as in the case of the stopping power, this effect is small and even for the largest value $\zeta_0 = 0.5$ used in the calculation, it amounts to less than a 10% in the range of velocities studied ($v \leq 1$ a.u.).

Finally, the degree of the spin polarization of the excited electrons as a function of the velocity of the projectile is shown in Fig. 3, for different target polarizations. This quantity is defined as the difference between the number of excited majority and minority electrons relative to the total number of excited electrons. It is observed that the polarization increases with the projectile velocity, a behaviour that is consistent with experimental findings [9]. Note also that, in the range of velocities studied, the value of the polarization of the excitation is always below the target polarization. For instance for $\zeta_0 = 0.27$, that may represent a Fe target, the maximum value obtained for the polarization of the excited electrons is around 17% when $v = 1$ a.u.
4 Conclusions

In summary, we have studied the energy loss and the number of electrons excited by a slow $H^0$ atom travelling through a spin-polarized electron gas. Non-linear effects in both screening and scattering have been taken into account. It is found that both the number of excited electrons and the energy deposited in the medium decrease with target polarization. The excited electrons show a distinct spin polarization which is smaller in value than the target polarization, in all the cases. Moreover, it increases with projectile velocity, a behaviour that is consistent with the experiments. Nevertheless, we stress that one should be careful when comparing our theoretical results to the experimental kinetic electron yields. In order to perform a meaningful comparison with the experiments both the transport of the electrons and their transmission through the surface potential barrier should be taken into account. The transport of electrons is expected to enhance the spin polarization, due to the higher overall scattering probability of minority electrons [17]. The transmission through the surface potential barrier will also modify the spin polarization due to the discrimination in electron energies that it produces. In any case, the direct excitation of electrons by the ion that we investigate here, apart from being a process of fundamental nature, is a basic ingredient in any complete calculation of the total yield.

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References


Fig. 1. Friction coefficient $Q$ of $H^0$ travelling through a free electron gas ($r_s = 2.12$) as a function of the spin-polarization of the medium $\zeta_0$. The long-dashed line is the contribution of the excitation majority spin electrons $Q^\uparrow$, the short-dashed line is the contribution coming from minority electron excitation $Q^\downarrow$, and the solid line is the average $Q_{\text{aver}}$ of these two quantities. Note that the total friction coefficient is: $Q = 2 \ Q_{\text{aver}}$. 
Fig. 2. Number of electrons excited per unit time, by a $H^0$ moving with $v = 0.5$ a.u through a free electron gas ($r_s = 2.12$) as a function of the target spin polarization. Long-dashed line is the number of excited majority electrons, the short-dashed line is the number of excited minority electrons, and the solid line is the average, i.e., one half the total number of excited electrons.
Fig. 3. Polarization degree of the electrons excited by a $H^0$ travelling through a free electron gas ($r_s = 2.12$) as a function of the projectile velocity. In curve (a) the spin polarization of the target is $\zeta_0 = 0.1$, in curve (b) $\zeta_0 = 0.17$, in curve (c) $\zeta_0 = 0.27$ (this value corresponds to Fe), and in curve (d) $\zeta_0 = 0.5$. 