ELECTRON TRANSFER IN SLOW ATOM–SURFACE COLLISIONS: A CLOSE–COUPLING APPROACH WITH CONTINUUM DISCRETIZATION

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Charge transfer during atom–metal surface collisions has received much interest in the last decade. In contrast to other close–coupling approaches[1], we discretize the active electron's motion inside the metal using Weyl wave packets[2]. These stationary wave packets have the advantage of being localized at the surface, where the electronic interactions occur. The use of discretized states to represent the conduction–band continuum allows for the convenient inclusion of (one electron) inelastic processes inside the substrate.

We solve the time–dependent Schrödinger equation as a system of coupled differential equations for the atomic and metallic population amplitudes, using a two–center expansion for the total wavefunction of the active electron[3]. The "metallic part" of the total wavefunction is discretized in momentum space in a finite triple sum (corresponding to the Ox, Oy and Oz directions) of Weyl wave packets. For the electron motion along the normal to the surface, wave packets are obtained by superimposing jellium wave functions within a small interval δ_z about the centroid momentum $\bar{k}_{z_i}$,

$$\phi_{\bar{k}_{z_i}}(z) \quad = \quad \sqrt{\frac{\delta_z}{2\pi}}\times$$

$$\left\{ \frac{2\sin(\frac{\delta_z z}{2})}{\delta_z z} \, [e^{i\bar{k}_{z_i} z} + \mathrm{R}e^{-i\bar{k}_{z_i} z}]\theta(-z) + \mathrm{T}e^{-\gamma z}\theta(z) \right\}$$

where the reflection and transmission coefficients, R and T, and the decay parameter γ are evaluated at the centroid momentum $\bar{k}_{z_i}$ and are assumed to be independent of k_z inside the interval $[\bar{k}_{z_i} - \delta_z/2, \bar{k}_{z_i} + \delta_z/2]$. For the electron motion in the surface plane, wave packets are obtained by superimposing plane waves within small intervals δ_x and δ_y about the centroid momenta $\bar{k}_{x_p}$ and $\bar{k}_{y_q}$, respectively.

The system of close–coupled equations is integrated numerically. We have studied the evolution of the atomic and metallic population amplitudes for a Hydrogen atom at perpendicular incidence on an Aluminum surface with speed v_z=0.02 a.u. Hybridization effects have been investigated, indicating that a significant part of the hybridization near a metal surface corresponds to the "Stark–like" mixing of spherical hydrogenic states in the non–uniform field of the surface.

Figure 1 shows the squared amplitudes in parabolic representation of the $n = 2, k = -1, +1$ states, of all $n = 3$ states, and of all 200 Weyl packets used to discretize the conduction band continuum, as a function of D-d_{min}. D is the atom–surface distance and d_{min}=0.5 a.u. the distance of closest approach.

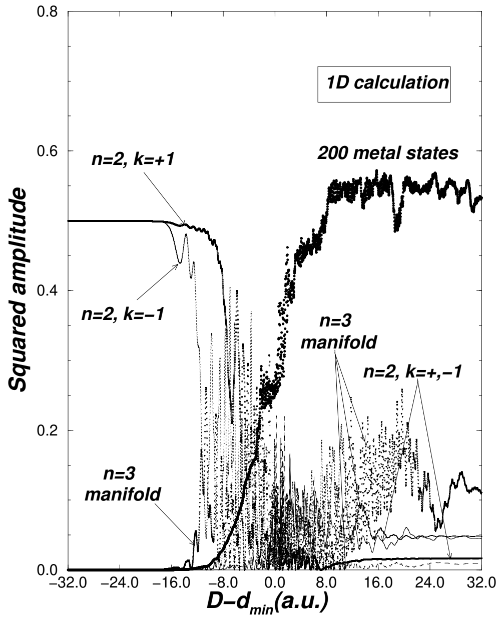

Figure 1. H/Al collision (see text)

We have also found that the atomic and metallic populations at the end of the collision are very sensitive to the screening of the interaction potential which couples the metal states.

References

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