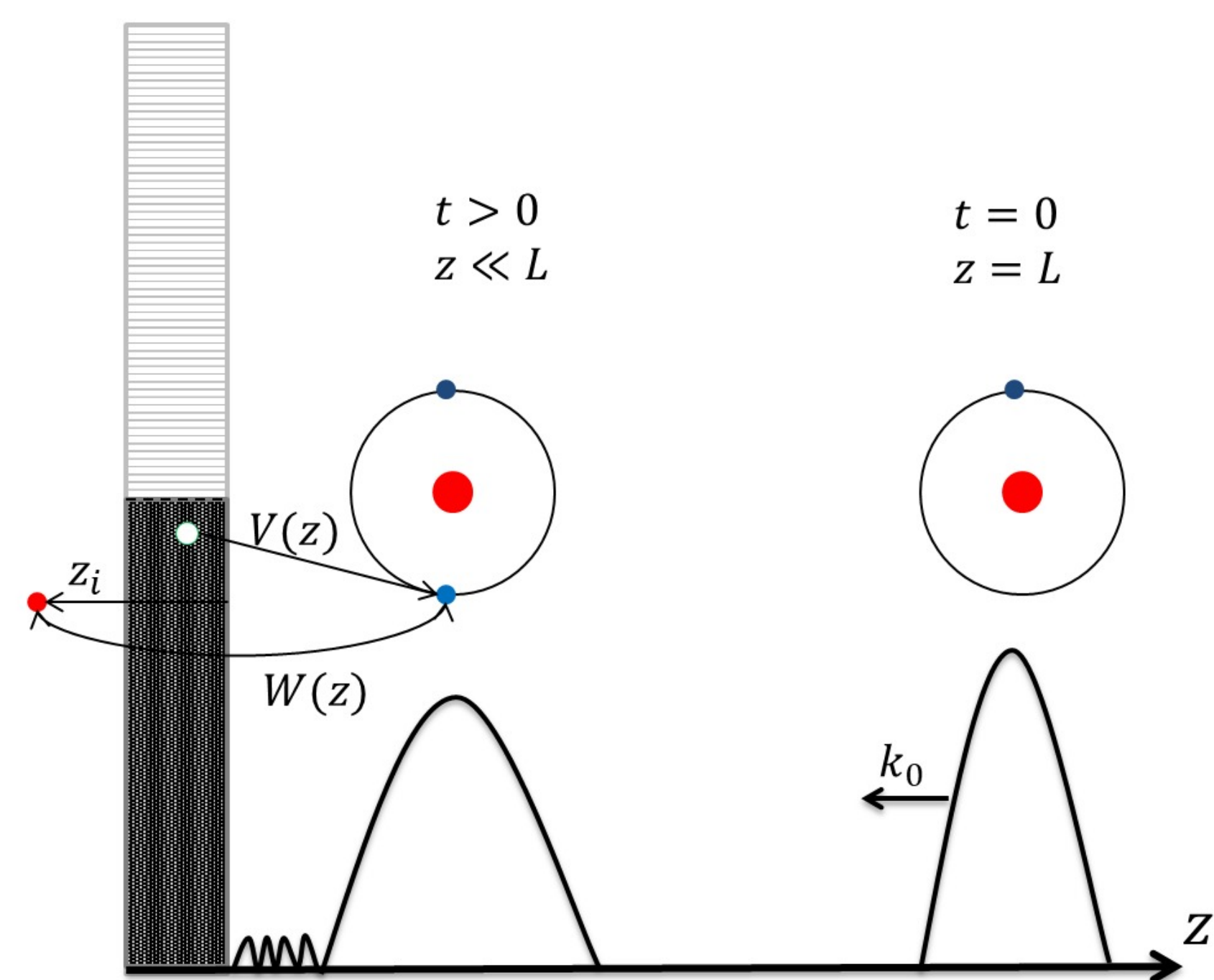


# Sticking coefficient for atoms impinging on metallic surfaces.

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## Introduction

The sticking coefficient is the probability that an initially neutral hydrogen atom with kinetic energy  $k_0$  incident upon a metallic surface be adsorbed. As the atom approaches the surface, the overlap  $V$  with the surface orbitals grows and allows electrons transfer. The atom becomes electrically charged, and the image charge potential  $W$  appears which accelerates the  $H^-$  ion. After the collision, the generation of phonons and electron-hole pairs in the metal steals energy from the particle, which could become trapped. Then the collision comprises two important regimes. With the H far from the surface, only low-energy electron-hole pairs are excited in the band. The ionization of the H orbital excites high-energy pairs and introduces non-adiabaticity.



**Figure 1:** Schematic representation of collision dynamics. The hydrogen atom is represented by a single level, and the metal is represented by its conduction band. Initially the H atom is neutral and the conduction band is half filled.

## Atomic-Surface Collision

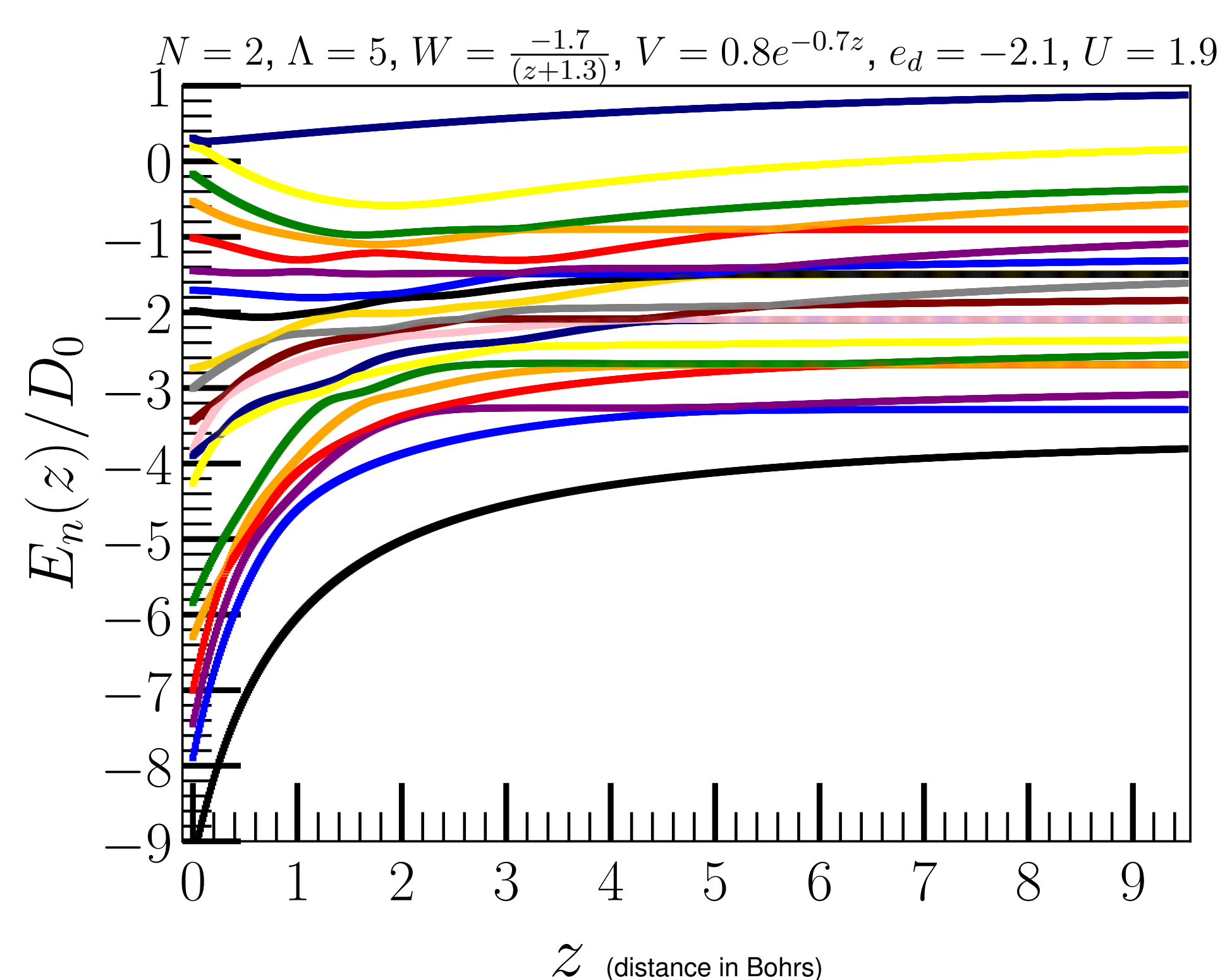
The dynamics of collision can be investigated using a Hamiltonian that includes the atomic kinetic energy  $\frac{P^2}{2M}$  and the electronic Hamiltonian  $H^e(z)$ . To follow the time evolution of the hydrogen  $\chi(z, t)$  we discretize the distance  $z$  and the time  $t$ . At fixed  $z$  the Numerical Renormalization Group <sup>[1]</sup> (NRG) approach allows for the diagonalization of the Anderson Hamiltonian. The Crank-Nicolson algorithm <sup>[2]</sup> then describes the time evolution between a given instant of time and the next. As mentioned we rely on the single-impurity Anderson model <sup>[3]</sup> with an additional scattering potential to the electronic dynamics. The NRG method discretizes the surface Hamiltonian  $H_b$  logarithmically on a basis defined by  $\Lambda > 1$  and converts it into a numerically tractable tight-bind with exponentially decaying couplings  $t_n \sim \Lambda^{-n/2}$ .

$$H_d = \epsilon_d c_d^\dagger c_d + U n_{d\uparrow} n_{d\downarrow}, \quad H_b = \sum_{n=0}^{N-1} t_n (f_n^\dagger f_{n+1} + \text{H.c.}) \quad (1)$$

$$H^e(z) = H_d + H_b + \sqrt{2}V(z) (c_d^\dagger f_0 + f_0^\dagger c_d) + 2W(z)(n_d - 1)^2 f_0^\dagger f_0. \quad (2)$$

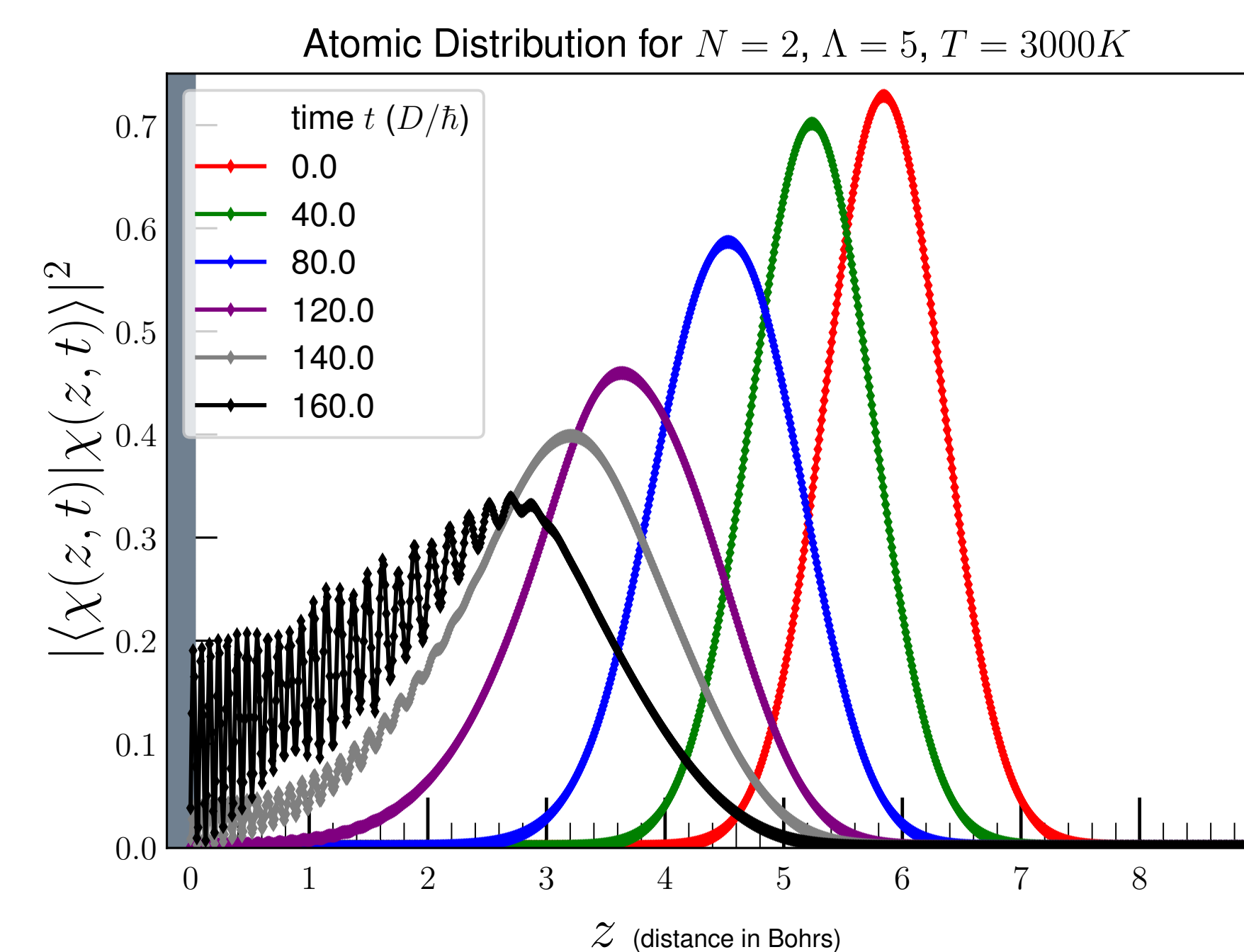
## Partial Results

Our work is in progress. We have computed the time evolution for the hydrogen atom initially neutral with initial distribution as a Gaussian centered in  $z = 6$  and kinetic energy of 0.3 eV. We are using for the electronic states  $N = 2$  and  $\Lambda = 5$ . For the atom close to the right side of the box  $W$  and  $V$  are almost zero so the atom and the band are decoupled and we know all the electronics configurations.

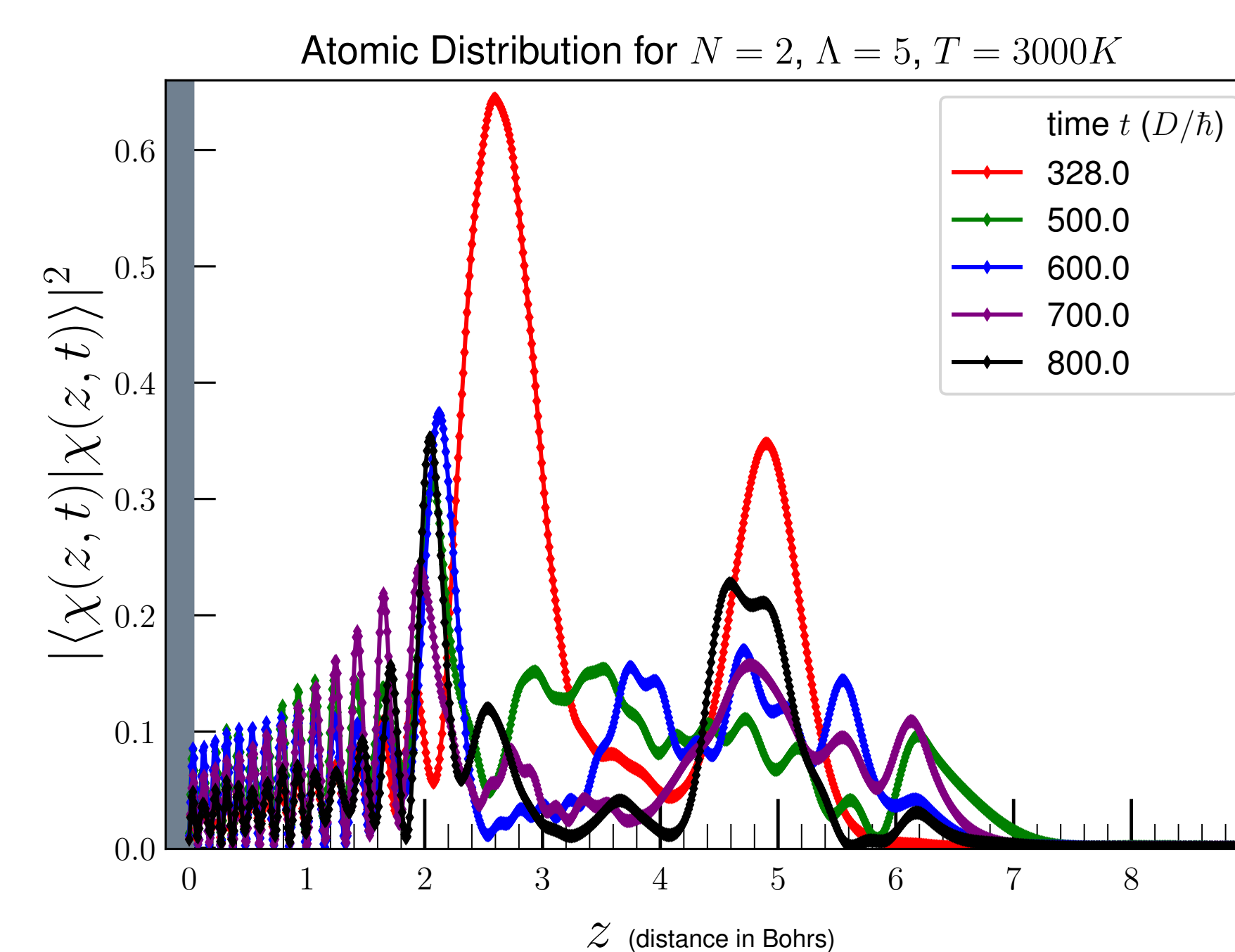


**Figure 2:** Energy levels for each electronic state along the distance  $z$ . The electronic states are mixing in the range  $z < 3$ .

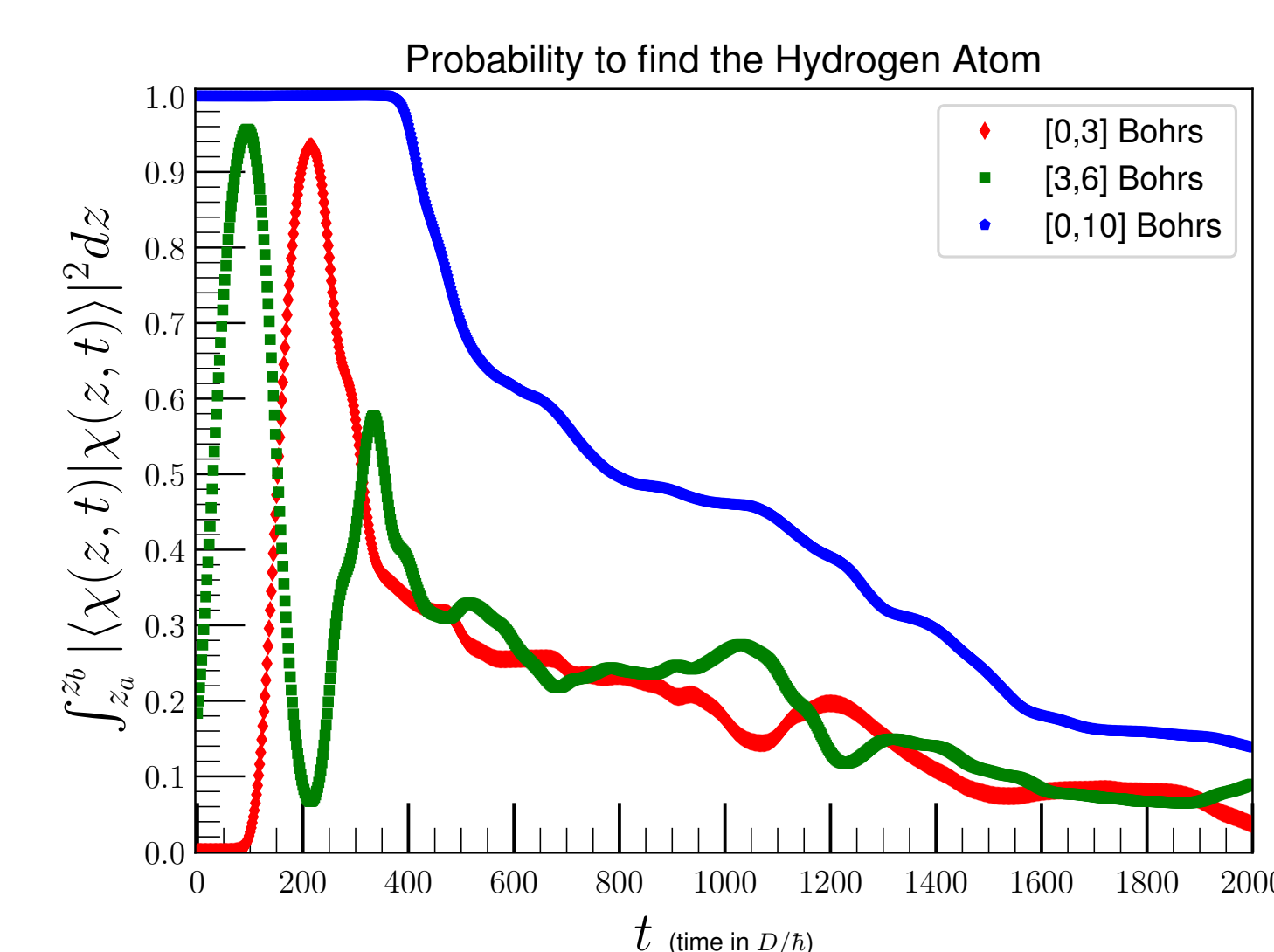
In this model there are 20 different electronic states, but in  $t = 0$  we know that the hydrogen is in the first excited state. As expected, for short times the hydrogen moves in the left direction until it collides with the surface. We can see from Fig. 2 that the energy levels become mixed near the surface  $z < 3$ . In this range the initial neutral electronic configuration is mixed with the ionized configuration which accelerates the atom. Then the atom experiences the non-adiabaticities and it has enough energy change to others electronic configurations. In this process the atom lose energy.



**Figure 3:** The hydrogen atom moves to the left direction until it collides with the surface.



**Figure 4:** The hydrogen distribution for larges times.



**Figure 5:** Probability to find the H atom inside a range of distances.

After the collision (at time around 328) the atomic distribution divides in two parts, one goes back to the surface direction and the other goes to the right side of the box. The remains atomic distributions are in ionized excited states with low kinetic energy close to the surface. It appears to form a bound state that stays almost the same for a long time. Therefore, around 20% of the distribution get stuck close to the surface. However, this bound state slowly evaporates. We suspect that the life-time of this state is associated with discretization.

## Conclusions

This simple model proves to be capable of explaining the phenomenon, but we need to do the calculations for larger  $N$  to approximate the continuum limit. However, the numerical cost of the simulation increases factorially with  $N$  so it is impractical to consider all the electrons in the conduction band, therefore, we need to select the most important electronic states. To do this, we are studding both the results obtained with only 20 electronic configurations and a similar but simpler problem: photoemission by a metal.

## Acknowledgment

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