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# Mapping of the electron transmission through the wall of a quantum corral

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ABSTRACT

We report on a theoretical study of the escape of confined surface states electrons from quantum corrals made of Cu adatoms on a Cu(1 1 1) surface. This study maps electron transmission through the corral wall and provides an extension of our earlier work focused on confinement in Cu corrals [S. Díaz-Tendero, F.E. Olsson, A.G. Borisov, J.P. Gauyacq, Phys. Rev. B 77 (2008) 205403]. The existence of two decay modes for the confined surface state is stressed: (i) non-resonant tunnelling through the corral wall concentrated on the Cu adatoms and (ii) a resonant-induced decay involving the transient formation of a resonant state localized on top of the corral wall. The present mapping of the electron transmission reveals how the interference between the two decay modes works: there exist regions where the electron leaves the corral, balanced by regions where it enters the corral, though the global behaviour of the quasi-stationary states is electron escape from the corral.



## 1. Introduction

The possibility to build nanostructures at surfaces, in particular by atomic manipulation, opened a broad domain of research. Indeed, this leads to the hope of possibly tailoring the electronic properties of a given system, by carefully designing the atomic arrangement on the surface. One could thus control electron dynamics at surfaces and consequently the numerous processes in which electronic excitation plays a role. Among nanostructures, chains of atoms received a lot of attention both for electronic states located on the chain and for the confinement properties of an atomic line [1–9]. Indeed, certain surfaces, such as the (1 1 1) surface of noble metals, host a surface state and image states in which electrons are located in the surface region and are travelling quasi-freely parallel to it [10]. Surface state electrons are much perturbed by adsorbates on the surface. An individual adatom scatters efficiently surface state and image state electrons leading to decay and dephasing processes [11–16], as well as to patterns in scanning tunnelling microscopy (STM) imaging [17,18]. A line of adatoms on a surface also scatters surface state electrons and can be used to build so-called 'quantum corrals': these are formed by a closed chain of atoms adsorbed on a surface and defining an enclosure in which surface state electrons are confined. Confinement leads to the quantisation of the surface state continuum inside the corral. Quantum corrals have been the subject of many experimental and theoretical studies [19–28]. The circular chain of atoms forming the corral wall does not reflect perfectly the surface state electrons, and the quantised states resulting from the confinement of the surface state continuum are quasi-stationary states. A surface state electron hitting the corral wall has finite probabilities of being reflected, transmitted into the surface state continuum outside the corral or scattered into a 3D-propagating substrate state. The first phenomenon is at the origin of confinement and the two other contribute to the decay of the electronic states confined inside the corral. Electron reflection, transmission and scattering by a chain of atoms are thus key features for the properties of a quantum corral or, more generally, of confined systems at surfaces.

In the above context, the corral wall can be described by global properties, corresponding to a continuous wall acting as boundary conditions for the electronic states confined inside the corral. However, one can also wonder about the microscopic view of the confining action of a corral wall made of adsorbed atoms. In particular, one can wonder which part of the atomic chain reflects electrons, or equivalently how a transmitted electron goes through the wall. When escaping from the corral, is the electron sneaking underneath the wall, or between the atoms, is it going through the atom centre or is it jumping over the barrier? It is the aim of the present work to answer precisely to this question, i.e. to map the flux of outgoing electrons and the transparency of the corral wall. Expanding our earlier work on the confinement of the Cu(1 1 1) surface state electrons by a circular closed chain of Cu adatoms [28], we

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study how the confined electrons escape from the corral and how they travel or 'tunnel' through the corral wall. We can stress some link between the present study and STM imaging. In both cases, one looks for the spatial distribution of tunnelling electrons. However, in this work, (i) there is no bias and the electron current is generated by the quasi-stationary state decay, (ii) the directions of tunnelling with respect to the surface are different and (iii) the present flux mapping is very short range, the analysis being performed on the corral wall and not on an STM tip further away from the surface. The present flux analysis allows us to map the transmission of the wall as well as to illustrate the role of the states localized on the corral atoms in the decay of the confined states. Indeed, in our earlier work [28], we showed that the unoccupied sp-state that has been evidenced on individual Cu atoms and on finite and infinite straight Cu chains on Cu(1 1 1) [4,29–32] shows up as a circular sp-band located on the wall in the case of a circular Cu corral on Cu(1 1 1). This state mixes with the quasi-stationary states coming from the confinement of the surface state continuum, deeply affecting their energy and their lifetime [28]. Analyzing the electron escape from the corral allows us to further decipher the role of the sp-state as an intermediate in the decay of the confined states.

This paper is organized as follows. The next section briefly explains the theoretical methods employed. Results are shown and discussed in Section 3. We end the paper with conclusions in Section 4. Atomic units are used throughout, except otherwise stated.

## 2. Method

The system studied in the present work is schematized in Fig. 1. A circular closed chain of atoms is adsorbed on a Cu(1 1 1) surface and forms the corral wall. The Cu adatoms are adsorbed at the adsorption height obtained in DFT calculations on linear Cu chains on Cu(1 1 1) [31,32]. There are 70 atoms along the wall and the distance between two adjacent atoms is equal to $d_{Cu-Cu}$, the bulk Cu–Cu distance ($d_{Cu-Cu} = 4.8a_0$).

The radius of the corral, $R$, is thus:

$$R = \frac{70 d_{Cu-Cu}}{2\pi} \approx 53.5 a_0 \tag{1}$$

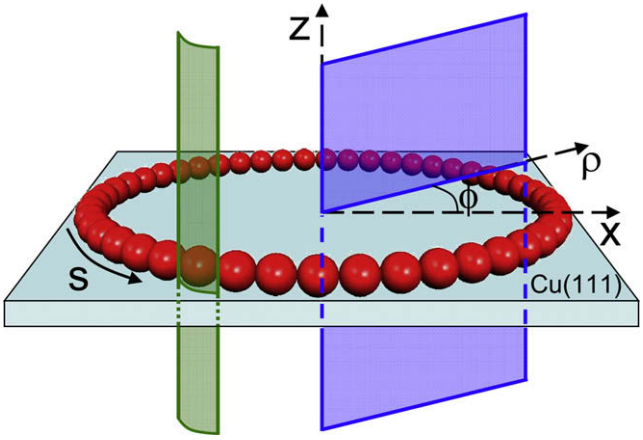


**Fig. 1.** Schematic view of the system studied. A circular chain of Cu atoms (red spheres) is adsorbed on a Cu(1 1 1) surface (blue plane). The cylindrical coordinate set used in the present calculation is shown in the figure: the $z$-axis is perpendicular to the surface plane and the origin of coordinates is at the centre of the corral in the plane defined by the adatom centres. The green and violet areas show the two surfaces ($z-\rho$ and $z-s$ surfaces) in which the outgoing electron flux is defined (see text). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The dynamics of excited electrons (electrons confined inside the corral) is studied using a one-electron wave-packet propagation (WPP) approach. The potential in which the excited electron evolves is obtained both from ab initio calculations and from modelling studies. Details about the WPP approach and about the potential construction can be found elsewhere [28,32,33] and only a general presentation together with the points specific to the present flux study are given below.

The dynamics of an excited electron is studied via the solution of the time-dependent Schrödinger equation:

$$\begin{aligned} i\frac{\partial \Psi(\vec{r},t)}{\partial t} &= H\Psi(\vec{r},t) = (T + V + V_{Abs})\Psi(\vec{r},t) \\ &= (T + V_{Substrate} + V_{Wall} + V_{Abs})\Psi(\vec{r},t) \end{aligned} \tag{2}$$

for the tri-dimensional electron wave function $\Psi(\vec{r},t)$. $T$ is the electron kinetic energy operator and $V$ is the interaction potential between the excited electron and the system (corral + substrate). $V$ is described as the sum of two terms describing the interaction with the clean Cu(1 1 1) substrate ($V_{Substrate}$) and with the corral wall ($V_{Wall}$). $V_{Substrate}$ is taken from Ref. [34], it accurately describes the electronic structure of the Cu(1 1 1) surface along the normal to the surface and assumes free-electron motion parallel to it. The wall potential, $V_{Wall}$, describes the potential induced by the presence of the Cu atom chain on the Cu(1 1 1) surface. It has been extracted from ab initio DFT calculations on the clean Cu(1 1 1) and on the Cu chain on Cu(1 1 1) systems (see [28,32] for details). $V_{Abs}$ is an absorbing potential put at the edges of the calculation box to impose a pure outgoing wave behaviour to the solution of Eq. (2).

Eq. (2) is solved by short time propagation on a grid of points in cylindrical coordinates [28,32,33]. The ($\rho$, $\phi$, $z$) coordinates are defined in Fig. 1. The ($\rho$, $\phi$, $z$) grid contains ($1100 \times 24 \times 768$) points. The system is periodic in $\phi$, so that Bloch boundary conditions are used and Eq. (2) is only solved in a small $\phi$ interval encompassing a single atom of the corral wall. Each Bloch function is associated to a given value of $m$, the projection of the electron angular momentum along the $z$-axis. Below, only $m = 0$ solutions are examined; considering a large set of $m = 0$ confined states should allow the illustration of the corral wall transparency over a broad energy range. We solve Eq. (2) with an appropriate initial condition ($\Psi(\vec{r}, t = 0) = \Phi_0$). From the survival amplitude, $A(t)$:

$$A(t) = \langle \Phi_0(\vec{r}) | \Psi(\vec{r},t) \rangle \tag{3}$$

the energy and lifetime of the quasi-stationary states in the system are extracted [33]. The success of the extraction procedure is directly linked to the choice of the initial state; the properties of the quasi-stationary states which have a large overlap with the initial wave packet, $\Phi_0$, are easily extracted from $A(t)$ (see a discussion specific to the corral case in Ref. [28]). In addition, the wave function associated with the quasi-stationary state at energy $E$ ($\Phi_E(\vec{r})$, pure outgoing wave at energy $E$) is obtained from the time dependent wave packet $\Psi(\vec{r},t)$:

$$\Phi_E(\vec{r}) = \int_0^{T'} e^{iEt} \Psi(\vec{r},t) dt \tag{4}$$

where $T'$ is a long enough propagation time.

It must be stressed that in such a one-electron WPP calculation, the quasi-stationary states decay by one electron energy-conserving transitions; many-electron decay terms, which possibly may contribute to the state decay, are absent (see a discussion in [28]). However, this should not influence the results of this work, which is devoted to the analysis of the spatial distribution of the one-electron decay.

In this study, we analyze the decay of the quasi-stationary states confined inside the corral. In practice, we run WPP calculations with $\Phi_E(\vec{r})$, the wave function of one of the confined states,