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Closed-loop-based observer approach for tunneling current parameter estimation in an experimental STM^{*}

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Abstract

This paper is about parameter estimation in quantum effect of tunneling current, and is based on an experimental device of Scanning Tunneling Microscope (STM) type. Since this effect needs feedback control in order to be obtained and kept, a closed-loop stability analysis is first presented prior to any estimation. Then, in this context of closed-loop operation, an observer approach is proposed to estimate the couple of parameters which characterize the tunneling current (nonlinear) model. An extension of this observer technique to topography estimation is also discussed, and all the methodologies are illustrated with experimental data.

Keywords: Tunneling current, proportional integral control, nonlinear system, stability analysis, state observer, parameter identification.

1. Introduction

Tunneling effect is a quantum phenomenon which was first used by G. Gamow in 1928 to explain radioactivity [3]. It translates into what is called *tunneling current* when describing the electrical current that can be measured between a conductive tip and a surface subject to a voltage applied between them, and with a relative distance lower than 1 nm . This effect is typically at the heart of the so-called *Scanning Tunneling Microscope* (STM), invented in 1981 by G. Binnig and H. Rohrer [4], and allowing to obtain information about a surface, provided that some appropriate control is applied. This *intrinsic* need for feedback gave rise to advanced control studies *from the end of 1990's on, as in [5, 6] for instance, where inversion-based techniques were considered*, in [7], where a variable structure control was studied, in [8, 9], where methodologies of robust digital pole placement with sensitivity function shaping were proposed, in [10] with a multivariable Linear Quadratic Integral approach, up to more recent works as in [11, 12] presenting self-tuning PI control, [13] about MIMO H_∞ robust control, [14] with robust observer-based control, *or even in the very recent reference [15] proposing a MEMS-based STM system*.

In fact, tunneling current does admit a model, basically as an exponential law of the distance between tip and sample sur-

face, but with parameters depending on the operation conditions (such as materials and environment) [16]. The knowledge of such parameters is yet useful, for the control design on the one hand (see e.g. [17]), but also for topography applications of STM for instance, where the surface variations over a sample can be retrieved via this tunneling current model (e.g. as in [18]), *or even in other possible tunneling applications [19, 20]*. This motivates the study of estimation techniques for those parameters. In [17] for instance, a frequency-based closed-loop identification is proposed for an STM operation, providing in particular one of the two crucial coefficients of tunneling current model, and motivated by control improvement. In the present paper instead, a time-domain direct approach is studied, with observer techniques combining and extending our preliminary results of [1] for the case of one parameter to be estimated, and [2] for the case of two parameters, and rather focused on topography imaging improvement. The latter means that here the control is used for the estimation purpose, with a full stability analysis for the closed-loop system being provided, while the observer approach improves those of [1, 2], and includes an extension discussion towards surface variations estimation. *This observer approach thus provides a unifying framework for both tunneling current calibration and possible surface imaging, as an alternative to classical off-line current characterization (e.g. curve fitting) and control-based imaging [16]. In addition, it provides more information (two parameters) with less constraints (no dither for instance) than in so-called 'gap modulation methods' [11, 12], leading to some self-calibration tool, and possible quantitative analysis (see propositions 1 and 2 hereafter). Finally, all the proposed methodological developments are also illustrated with real data recorded on an experimental prototype of STM type developed in Gipsa-lab [21, 22], and can enrich the area of measurement and control at nanoscale that has been attracting an increasing attention in the*

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It combines and extends conference papers [1] and [2].

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last decade (as in [23, 24, 25, 26, 27, 28, 29] for instance, and references therein).

The paper is thus organized as follows: section 2 first states the tunneling current modeling problem under consideration (based on our STM prototype), and section 3 provides a full closed-loop stability analysis when considering a simple proportional integral control design. The proposed observer-based approach for estimation of tunneling current parameters is then presented in section 4, and extended to the estimation of surface variations. Section 5 is dedicated to illustrative results based on experimental data, while section 6 finally concludes the paper.

2. Modeling problem

The main problem we consider is that of estimating parameters of tunneling current (exponential) model. To that end, let us rely on a typical STM operation where tunneling current is measured. Such an operation means that a sharp conductive tip is approached close enough to a conductive sample, with a bias voltage being applied between both of them. The tip is driven by a piezo actuator fed via a voltage amplifier, while the tunneling current is measured via an appropriate sensor and used in a feedback loop to control the tip vertical position. This overall configuration is summarized by figure 1 hereafter, where u denotes the input driving voltage, u_a its amplified version, i_t the tunneling current which is established, and y_m its measurement (the feedback control loop is in grey dashed line).

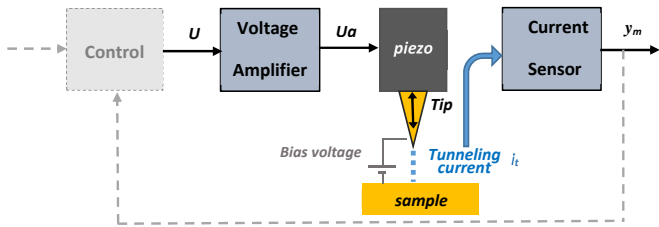


Figure 1: Tunneling current control.

For a formal dynamical description of this operation, we will refer to a corresponding prototype of Gipsa-lab [21], with a $120kHz$ PSt 150 actuator for the vertical motion, a $13kHz$ high gain sensor for current measurement, and a $4kHz$ voltage amplifier for piezo feeding, shown in figure 2.

Mathematically, the main characteristics of each element can be summarized as follows:

- The current sensor dynamics can be captured by a first order model of the form:

$$\begin{aligned} \dot{x}_1(t) &= -a_1 x_1(t) + i_t(t) \\ y_m(t) &= c x_1(t) + v_y(t) \end{aligned} \quad (1)$$

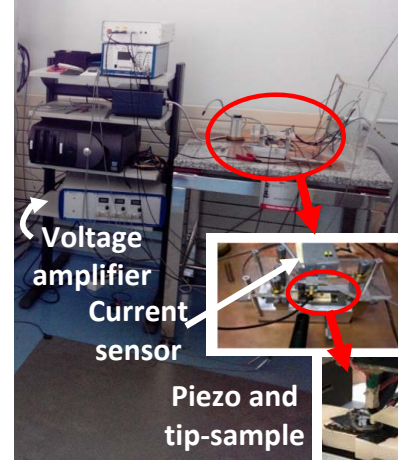


Figure 2: STM prototype (Gipsa-lab).

where x_1 denotes its state variable, a_1 represents its bandwidth, c adjusts its DC gain, and v_y represents some possible additive noise in its measurement y_m .

- The voltage amplifier can be also represented by a first order model as:

$$\begin{aligned} \dot{x}_2(t) &= -a_2 x_2(t) + u(t) \\ u_a(t) &= c_2 x_2(t) \end{aligned} \quad (2)$$

where x_2 is its state variable, and a_2 , c_2 gather bandwidth and gain parameters.

- The piezoactuator dynamics can be reduced to its DC gain only, denoted by G_p , since in our prototype it is much faster than the current sensor and the voltage amplifier.

Now the tunneling current can be obtained as a function of the distance between the tip and the sample surface [16], which can be expressed as:

$$d = z_s - z_t \quad (3)$$

where z_t refers to the vertical position of the tip, and z_s to that of the sample surface, both here considered downwards, with respect to a given reference (as in figure 3).

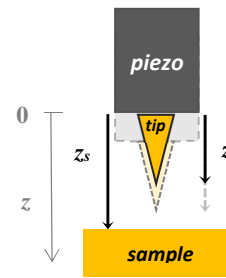


Figure 3: Tip and sample positions.

Formally, it is an exponential function of d , when d is small enough, as follows:

$$\begin{aligned} i_t(t) &= gV_b \exp(-kd(t)) \quad \text{if } d < d_i \\ &= 0 \quad \text{if } d \geq d_i \end{aligned} \quad (4)$$

where d_i is typically around 1 nm , k, g are positive constants depending on the materials (tip, sample), and V_b is the positive constant bias voltage which is applied (as shown in figure 1).

Now using model (2) and piezo gain G_p , we have:

$$z_t = G_p u_a = G_p c_2 x_2 \quad (5)$$

As for z_s , it is clear that when operating at a fixed horizontal position of the tip (only vertical motion along z axis), then it is a constant z_{s0} . Notice that in a scanning mode, where the tip is moved in the horizontal direction above the sample, then z_s will change according to surface variations, that is $z_s(t) = z_{s0} + \delta z_s(t)$. Finally, tunneling current model becomes:

$$i_t(t) = \alpha \exp(-\beta(\bar{\delta} z_s(t) - x_2(t))) \quad (6)$$

with $\alpha := gV_b \exp(-kz_{s0})$ (if d is kept below d_i), $\beta := kG_p c_2$ and $\bar{\delta} z_s := \frac{\delta z_s}{G_p c_2}$.

The main modeling issue we consider is that of getting estimates for α and β , which both contain parameters a priori unknown. To that end, we will consider a vertical motion operation only (that is with $\delta z_s = 0$), with an appropriate control so that distance d allows for tunneling current, giving rise to an overall dynamical model as:

$$\begin{aligned} \dot{x}_1(t) &= -a_1 x_1(t) + \alpha \exp(\beta x_2(t)) \\ \dot{x}_2(t) &= -a_2 x_2(t) + u(t) \\ y_m(t) &= c x_1(t) + v_y(t) \end{aligned} \quad (7)$$

where a_1, a_2, c are assumed to be known beforehand, and α, β are to be identified.

We will also show how estimates of the latter can then be used to further determine $\bar{\delta} z_s$ in case of scanning, and thus the sample surface variations by using the knowledge on piezo and voltage amplifier gains $G_p c_2$.

But the preliminary step is to ensure that the tunneling current can indeed be established, and kept under control, prior to any estimation. This is studied in next section.

3. Closed-loop operation with stability

The purpose in this section, is to show how a simple PI controller can ensure tunneling current regulation with stability. To that end, let us first omit the measurement noise, and use the fact that the sensor dynamics are here faster than the voltage amplifier dynamics. This means that the output can be expressed as: $y(t) := \frac{c}{a_1} \alpha \exp(\beta x_2(t))$, and model (7) can be reduced to the following one:

$$\begin{aligned} \dot{x}_2(t) &= -a_2 x_2(t) + u(t) \\ y(t) &= \alpha_1 \exp(\beta x_2(t)) \end{aligned} \quad (8)$$

with $\alpha_1 := \frac{c}{a_1} \alpha$, a_2, β , positive constants.

It is also clear that a regulation target i_t^* on i_t directly translates into a regulation target y^* on y .

We then have the following:

Theorem 1. Given a constant reference y^* for y in system (8), for any gains $\lambda_0, \lambda_1 > 0$, and any initial condition in (8), the PI control law:

$$u(t) = -\lambda_0 \int_0^t (y(\tau) - y^*) d\tau - \lambda_1 (y(t) - y^*) \quad (9)$$

ensures that $\lim_{t \rightarrow \infty} |y(t) - y^*| = 0$.

PROOF. The result can be established by using Lyapunov arguments: notice first that the closed-loop system (8)-(9) can written as follows

$$\begin{aligned} \dot{x}_0(t) &= \alpha_1 \exp(\beta x_2(t)) - y^* \\ \dot{x}_2(t) &= -a_2 x_2(t) - \lambda_0 x_0(t) - \lambda_1 [\alpha_1 \exp(\beta x_2(t)) - y^*] \end{aligned} \quad (10)$$

with $x_0 := \int_0^t (y(\tau) - y^*) d\tau$.

Now set $x_2^* := \frac{1}{\beta} \log\left(\frac{y^*}{\alpha_1}\right)$, and $x_0^* := -\frac{a_2 x_2^*}{\lambda_0}$. Then the closed-loop system can be restated in terms of errors $\tilde{x}_0 := x_0 - x_0^*$ and $\tilde{x}_2 := x_2 - x_2^*$ as:

$$\begin{aligned} \dot{\tilde{x}}_0(t) &= \alpha_1 \exp(\beta(\tilde{x}_2(t) + x_2^*)) - y^* \\ \dot{\tilde{x}}_2(t) &= -a_2 \tilde{x}_2(t) - \lambda_0 \tilde{x}_0(t) - \lambda_1 [\alpha_1 \exp(\beta(\tilde{x}_2(t) + x_2^*)) - y^*] \end{aligned} \quad (11)$$

For this system, let us consider a candidate Lyapunov function of the form:

$$V(\tilde{x}) := \frac{1}{\beta} [\alpha_1 \exp(\beta(\tilde{x}_2 + x_2^*)) - y^*] - y^* \tilde{x}_2 + \frac{\lambda_0}{2} \tilde{x}_0^2 \quad (12)$$

where \tilde{x} gathers \tilde{x}_0 and \tilde{x}_2 .

Clearly $V(0) = 0$ and V is positive definite w.r.t. \tilde{x}_0 . Let us now check that this also true for \tilde{x}_2 , that is $V_2(\tilde{x}_2) := \frac{1}{\beta} [\alpha_1 \exp(\beta(\tilde{x}_2 + x_2^*)) - y^*] - y^* \tilde{x}_2$ is always positive when $\tilde{x}_2 \neq 0$.

Noting that $y^* = \alpha_1 \exp(\beta x_2^*)$, by the mean value theorem, we have

$$\begin{aligned} V_2(\tilde{x}_2) &= \alpha_1 \exp(\beta(x_2^0)) \tilde{x}_2 - y^* \tilde{x}_2 \\ &= \alpha_1 [\exp(\beta(x_2^0)) - \exp(\beta x_2^*)] \tilde{x}_2 \end{aligned} \quad (13)$$

with x_2^0 lying between x_2^* and $\tilde{x}_2 + x_2^* = x_2$.

If $x_2 < x_2^*$, then $x_2^0 < x_2^*$ and consequently $\exp(\beta(x_2^0)) < \exp(\beta x_2^*)$, while $\tilde{x}_2 < 0$, meaning that $V_2(\tilde{x}_2) > 0$.

Similarly, if $x_2 > x_2^*$, then $x_2^0 > x_2^*$ and consequently $\exp(\beta(x_2^0)) > \exp(\beta x_2^*)$, with $\tilde{x}_2 > 0$, leading again to $V_2(\tilde{x}_2) > 0$. One can finally conclude that V_2 is indeed positive definite.

So V is a positive definite function, obviously globally defined and radially unbounded. It is also globally differentiable, and we can compute:

$$\begin{aligned} \dot{V} &= [\alpha_1 \exp(\beta(\tilde{x}_2 + x_2^*)) - y^*] \times [-a_2 \tilde{x}_2 - \lambda_0 \tilde{x}_0 \\ &\quad - \lambda_1 (\alpha_1 \exp(\beta(\tilde{x}_2 + x_2^*)) - y^*)] \\ &\quad + \lambda_0 \tilde{x}_0 (\alpha_1 \exp(\beta(\tilde{x}_2 + x_2^*)) - y^*) \end{aligned} \quad (14)$$

which gives

$$\dot{V} = -\lambda_1 \alpha_1^2 (\exp(\beta(\tilde{x}_2 + x_2^*)) - \exp(\beta x_2^*))^2 - a_2 \alpha_1 \tilde{x}_2 (\exp(\beta(\tilde{x}_2 + x_2^*)) - \exp(\beta x_2^*)) \quad (15)$$

From this, \dot{V} is negative definite in \tilde{x}_2 (it is clear that \tilde{x}_2 and $\exp(\beta(\tilde{x}_2 + x_2^*)) - \exp(\beta x_2^*)$ are of same signs).

Consequently, we get stability by Lyapunov's second method. We can finally conclude to (global) asymptotic stability by using La Salle's invariance principle (see e.g. [30]): $\dot{V} = 0$ indeed means $\dot{x}_2 = 0$, and this being constantly true in time means that $\dot{x}_0 = 0$ as well. Hence the set $\{\tilde{x} \in \mathbf{R} : \dot{V}(\tilde{x}) = 0\}$ contains no other solution than 0, and we can conclude that 0 is globally asymptotically stable. ▼

Notice that if the presence of measurement noise is taken into account, a local version of this stability result can be established as well (that is when the output which is used is y_m as in (7)). In that case indeed, closed-loop system (11) becomes:

$$\begin{aligned}\dot{\tilde{x}}_0(t) &= \alpha_1 \exp(\beta(\tilde{x}_2(t) + x_2^*)) - y^* + v_y(t) \\ \dot{\tilde{x}}_2(t) &= -a_2 \tilde{x}_2(t) - \lambda_0 \tilde{x}_0(t) \\ &\quad - \lambda_1 [\alpha_1 \exp(\beta(\tilde{x}_2(t) + x_2^*)) - y^*] - \lambda_1 v_y(t)\end{aligned}\quad (16)$$

where v_y can be assumed to be a zero-mean white noise. This gives rise to a possible local representation of variations $\delta\tilde{x}$ of \tilde{x} around 0 as:

$$\begin{aligned}\delta\dot{\tilde{x}}_0(t) &= \alpha_1 \beta \delta\tilde{x}_2(t) + v_y(t) \\ \delta\dot{\tilde{x}}_2(t) &= -a_2 \delta\tilde{x}_2(t) - \lambda_0 \delta\tilde{x}_0(t) - \lambda_1 \alpha_1 \beta \delta\tilde{x}_2(t) - \lambda_1 v_y(t)\end{aligned}\quad (17)$$

Hence, mean values of $\delta\tilde{x}_0$ and $\delta\tilde{x}_2$ satisfy a second order noise-free linear state equation, for which 0 is obviously asymptotically stable for any $\lambda_0, \lambda_1 > 0$.

It can also be noted that gain λ_1 can increase noise effects in the closed-loop system, meaning that low values should be preferred.

From the above stability analysis, one can finally conclude that no matter what are (positive) values of α, β , a proportional-integral control law stabilizes the operation at any desired value for the tunneling current, for any $\lambda_0, \lambda_1 > 0$.

In practice, they can be tuned experimentally, or based on features of model (17) for instance. But the important point is that this allows to settle experimental conditions for possible estimation of tunneling current model: use vertical motion to get the current, and use PI control to keep it under control. Next section is dedicated to the actual model estimation in such a context.

4. Tunneling current parameter estimation

4.1. Tunneling current model

Considering again model (7), and assuming some appropriate closed-loop operation for instance as in previous section, one can now focus on the estimation of parameters α, β in tunneling current model (6) (with $\delta z_s = 0$ in the vertical operation case).

To that end, the idea here is to proceed in two steps: first estimate the tunneling current itself, and then estimate its parameters α and β .

Tunneling current estimation. For this first step, let us only consider the sensor model (1), for which the problem translates into *unknown input estimation*, where i_t is the unknown input. There are various possible approaches to solve it, and one can for instance use the so-called *control-based observer* method of [31], in a similar fashion as it was applied in [18] for surface reconstruction: the idea in short is to drive an observer copying the dynamics of (1), by its input copying i_t , in such a way that its output tracks the measured output y_m .

A simple control strategy for this tracking problem can clearly take the form of a Proportional-Integral one, giving rise to the following observer for i_t :

$$\begin{aligned}\dot{\hat{x}}_0(t) &= c\hat{x}_1(t) - y_m(t) \\ \dot{\hat{x}}_1(t) &= -a_1\hat{x}_1 + v(t) \\ v(t) &= -k_0\hat{x}_0(t) - k_1(c\hat{x}_1(t) - y_m(t)) \\ \hat{i}_t &= v(t)\end{aligned}\quad (18)$$

for some $k_0, k_1 > 0$.

In the noise-free case, it has been shown in [31] that this system indeed provides an estimate \hat{i}_t for i_t as accurately as desired by appropriate tuning of k_0, k_1 .

In order to take noise into account, let us more precisely state the following:

Proposition 1. *System (18) for model (1) (with i_t bounded) ensures that for any $k_0 > 0, k_1 \geq 0$, and any initial conditions, \hat{x}_0, \hat{x}_1 remain bounded, and \hat{i}_t approaches i_t according to the following transfer functions:*

$$\begin{aligned}\hat{I}_t(s) &= F_i(s)I_t(s) + F_v(s)N(s) \\ \text{with } &: \\ F_i(s) &= \frac{k_1cs + k_0c}{s^2 + (a_1 + k_1c)s + k_0c} \\ F_v(s) &= \frac{k_1s^2 + (k_1a_1 + k_0)s + k_0a_1}{s^2 + (a_1 + k_1c)s + k_0c}\end{aligned}\quad (19)$$

where s stands for Laplace variable, and \hat{I}_t, I_t, N refer to Laplace transforms of \hat{i}_t, i_t, v respectively.

The proof is obtained by direct computations, and the remark that for any positive k_0, k_1 , all transfer functions only have poles with strictly negative real parts.

One can then notice that k_0, k_1 can be chosen according to desired tracking performances, with appropriate attenuation of noise effect. A simple tuning can for instance be as follows:

$$k_0 = \frac{a_1^2}{4c}, \quad k_1 = 0 \quad (20)$$

which yields a second order behaviour with characteristic polynomial

$$P(s) = s^2 + a_1s + \frac{a_1^2}{4}$$

that is a natural pulsation equal to $\frac{a_1}{2}$ and a damping coefficient equal to 1.

Notice that various other tuning strategies could be used, including H_∞ optimal design as in [32] for instance.

170 From this, the measurement noise effect can be attenuated on
the tunneling current estimate (see also [33] for a subsequent
interest in surface imaging). However if the noise level is low
enough, then this first estimation step can be skipped, and an
estimate for tunneling current can simply result from approxi-
175 mation (8).

Tunneling parameter estimation. As soon as an estimate \hat{i}_t is
obtained for tunneling current i_t , a new output can be built from
its Logarithm $y_i := \log(\hat{i}_t)$.

From equation (6) indeed (with $\bar{\delta}z_s = 0$), we obviously have:

$$\log(i_t) = \log(\alpha) + \beta x_2 \quad (21)$$

and from dynamics of x_2 in equation (7), we get:

$$\frac{d\log(i_t)}{dt}(t) = -a_2 \log(i_t(t)) + a_2 \log(\alpha) + \beta u(t) \quad (22)$$

Setting $\xi := \begin{pmatrix} \log(i_t) \\ \log(\alpha) \\ \beta \end{pmatrix}$, we obtain a linear state equation of the

form

$$\dot{\xi}(t) = A(u(t))\xi(t) \quad (23)$$

with

$$A(u(t)) = \begin{pmatrix} -a_2 & a_2 & u(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Now considering $y_i = \log(\hat{i}_t)$ as the measurement for this sys-
tem, and the fact that \hat{i}_t approaches very well i_t after some tran-
sient (from equation (19)), a first order approximation allows to
consider:

$$y_i(t) = \log(i_t(t)) + \delta(t) = C\xi(t) + \delta(t) \quad (24)$$

where $C = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ and δ is a disturbance due to possible
mismatch between \hat{i}_t and i_t (formally indeed, if $\hat{i}_t = i_t + \bar{v}$ for
small disturbance \bar{v} , then $\log(\hat{i}_t) = \log(i_t) + \frac{1}{i_t}\bar{v} + \mathcal{O}(\bar{v}^2)$).

180 Since state-space representation (23)-(24) becomes linear time-
varying whenever u is chosen, a Kalman observer can be di-
rectly designed to get estimates for $\log(\alpha)$ and β , with the fol-
lowing result:

Proposition 2. *An observer for system (23)-(24) of the form:*

$$\begin{aligned} \dot{\hat{\xi}}(t) &= A(u(t))\hat{\xi}(t) - K(t)[C\hat{\xi}(t) - y_i(t)] \\ K(t) &= M(t)C^T/w \\ \dot{M}(t) &= \gamma M(t) + A(u(t))M(t) + M(t)A^T(u(t)) \\ &\quad - M(t)C^T C M(t)/w + V \end{aligned} \quad (25)$$

ensures that:

185 (i) if δ is a zero mean white noise of intensity Δ , then $(\hat{\xi}(t) - \xi(t))^2$ is minimized in mean value when $\gamma = 0$, $V = 0$, $w = \Delta$;

(ii) if δ vanishes, then $\|\hat{\xi}(t) - \xi(t)\|$ exponentially decays to zero for any $\gamma > 0$, $w > 0$, $V \geq 0$ whenever u is bounded and satisfies the regular persistency condition:

$$\exists T, \alpha > 0 \text{ and } t_0 \geq 0 \text{ s.t. } \forall t \geq t_0, \int_t^{t+T} \Phi_u(\tau, t)^T C^T C \Phi_u(\tau, t) d\tau \geq \alpha I \quad (26)$$

where $\Phi_u(t, \tau)$ is the transition matrix for (23).

(iii) if δ is bounded, then $\|\hat{\xi}(t) - \xi(t)\|$ remains bounded under same conditions as in item (ii) (ISS property of the error system w.r.t. input δ).

Item (i) is a direct consequence of Kalman result (see e.g. [34]), while items (ii) and (iii) result from the fact that under condition (26), M^{-1} can define a quadratic Lyapunov function for the error system (in $\hat{\xi} - \xi$) [35, 36].

Notice that one could even enhance the estimation, by taking into account filter model of (19) for noise δ . One can also implement a reduced order version of this observer (as in [37]) or a directly reduced design (as in [2]).

4.2. Surface variation estimation

Let us finally notice here that whenever α and β are estimated at a given horizontal position of the tip above the sample, then the tip can be moved in a scanning way, and the same observer approach allows to get an estimate for sample vertical variations δz_s with respect to the value of the original position. In that case indeed, the tunneling current will vary as in equation (6), which means that:

$$\log(i_t(t)) = -\beta \bar{\delta}z_s(t) + \beta x_2(t) + \log(\alpha)$$

Using again the dynamics of x_2 , and considering that time variations of $\bar{\delta}z_s$ can be neglected for the observer design, we get a state equation as:

$$\dot{\bar{\xi}}(t) = \begin{pmatrix} -a_2 & -a_2\beta \\ 0 & 0 \end{pmatrix} \bar{\xi}(t) + \begin{pmatrix} \beta u(t) + a_2 \log(\alpha) \\ 0 \end{pmatrix} \quad (27)$$

with $\bar{\xi} = \begin{pmatrix} \log(i_t) \\ \bar{\delta}z_s \end{pmatrix}$.

Using again output equation (24), we obtain a linear model for which a Kalman observer can be again designed, with similar properties as in proposition 2 regarding the effect of measurement disturbance.

More precisely, the observer can be built for model (27) restated as:

$$\begin{aligned} \dot{\bar{\xi}}(t) &= \begin{pmatrix} -a_2 & -a_2\hat{\beta} \\ 0 & 0 \end{pmatrix} \bar{\xi}(t) + \begin{pmatrix} \hat{\beta}u(t) + a_2 \widehat{\log(\alpha)} \\ 0 \end{pmatrix} + \delta_z(t) \\ y(t) &= \begin{pmatrix} 1 & 0 \end{pmatrix} \bar{\xi}(t) + \delta(t) \end{aligned}$$

where $\hat{\beta}$ and $\widehat{\log(\alpha)}$ are the obtained parameter estimates, and δ_z gathers the effects of possible estimation errors $\delta_\beta, \delta_\alpha$ on those parameters: $\begin{pmatrix} (a_2 \bar{\delta}z_s - u)\delta_\beta - a_2 \delta_\alpha \\ 0 \end{pmatrix}$.

Here, clearly condition (26) is satisfied whenever $\hat{\beta}$ has converged (or is replaced by its steady state estimate), and all properties of proposition 2 (i) to (iii) hold w.r.t. disturbance vector $\begin{pmatrix} \delta_z \\ \delta \end{pmatrix}$. Finally, an estimate for δz_s can be obtained from the one $\hat{\delta}z_s$ of $\bar{\delta}z_s$ as $G_p c_2 \hat{\delta}z_s$.

The overall estimation methodology can be summarized by figure 4 hereafter.

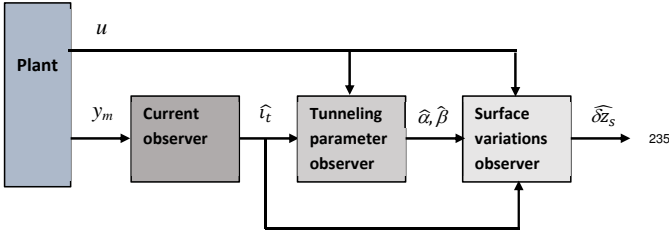


Figure 4: Overall observer structure.

5. Experimental results

Let us illustrate here the proposed methodology with experiments on our prototype of figure 2. In this prototype, the known parameters of current sensor and voltage amplifier models (1), (2) can be summarized as in Table 1 below.

a_1	$26\pi \times 1e3$	$[s^{-1}]$
a_2	$8\pi \times 1e3$	$[s^{-1}]$
c	$8.17 \times 1e13$	$[V.A^{-1}.s^{-1}]$

Table 1: STM known parameters.

The approach consists in operating the STM in closed-loop to obtain tunneling current as discussed in section 3, and in such a way that the corresponding control signal $u(t)$ satisfies condition (26) of proposition 2 in section 4, so that parameter estimation can indeed be achieved.

Let us first point that an operation under a simple square reference profile for the output is appropriate for this estimation purpose: in that case indeed, u chosen as in (9) will also clearly have a square profile, and it can be checked that condition (26) is in its turn satisfied for system (23) in that case.

Let us then consider a closed-loop operation for vertical tip motion, with a Proportional-Integral controller as in proposition 1, and with a square wave as a reference, of 1Hz, and varying between 0.25 and 2V.

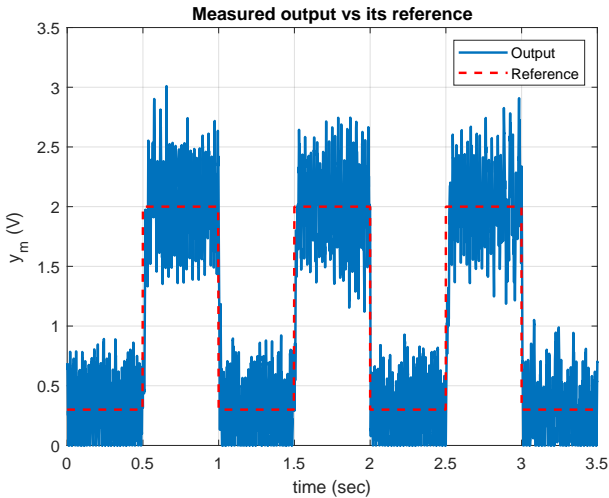


Figure 5: Measured output under PI control (solid line) vs square wave reference (dotted line).

The PI parameters are chosen empirically as $\lambda_0 = 1.5$, and $\lambda_1 = 0.007$ (much smaller than λ_0 , as commented before). The corresponding regulation performance is shown in figure 5, with reference in dashed (red) line and output in solid (blue) line. The corresponding control input u is presented in figure 6. Notice that in order to better emphasize the proposed estimation methodology, some drift effects which are quite common with such devices [38] have been removed beforehand in those signals.

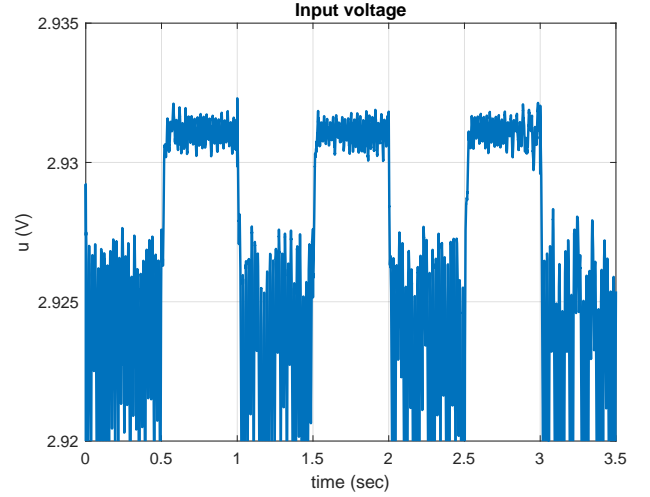


Figure 6: Control input under square reference variations.

The estimation step can then be addressed: first obtaining an estimate for tunneling current, via system (18), with parameters as in (20), and then estimating its parameters as in (25), here choosing empirically $w = 0.04$, $V = Id_{3 \times 3}$, and $\gamma = 25$. The corresponding results are displayed in figures 7 and 8 respectively (where β/a_2 is shown instead of β , for scaling reasons).

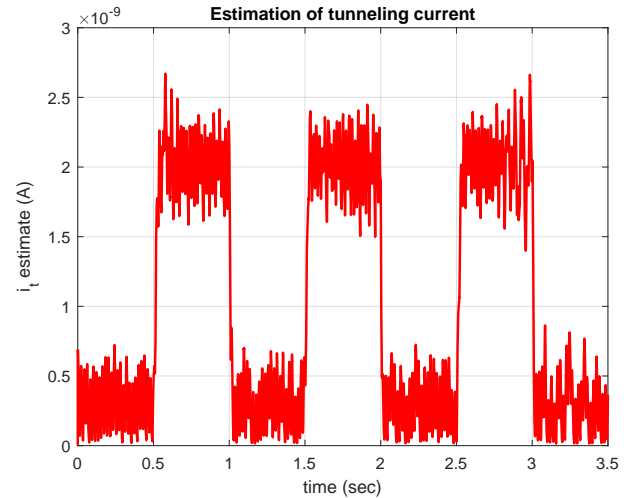


Figure 7: Estimation result for tunneling current i_t under square reference variations.

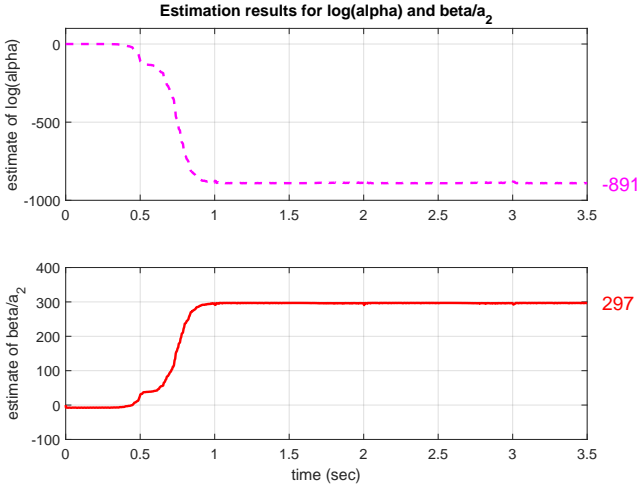


Figure 8: Estimate for parameter $\log(\alpha)$ (top dashed line) and β/a_2 (bottom solid line).

It can be seen that an estimate \hat{i}_t for tunneling current is indeed very rapidly obtained, and estimates for its parameters converge to some steady values in less than one second: the estimate for $\log(\alpha)$ reaches the value of about -891 , and that of β/a_2 the value of 297 .

In order to get some validation for those values, let us first underline that from the knowledge on piezo and voltage amplifier gains, we have $G_p c_2/a_2 = 18$, from which the tunneling exponential rate is identified as $\hat{k} = 16.5$, and this value is fully consistent with the one formerly obtained by some offline identification with the same prototype [22] (a theoretical value is about 20 [16]).

On the other hand, if we consider that g reduces to so-called *conductance quantum* equal to $77.5\mu S$ [16], we can get from $\widehat{\log(\alpha)}$ and \hat{k} (together with known bias voltage V_b , of about $1V$ here) an estimate for z_{s0} , and combine it with an estimate of z_t , which can be obtained from $\widehat{\log(\hat{i}_t)}$, $\widehat{\log(\alpha)}$ and $\hat{\beta}$, to get an estimate of the tip-sample distance: it is shown in figure 9, where it can be checked to be consistent with expected values (here varying between about 0.8 and 0.65 nm).

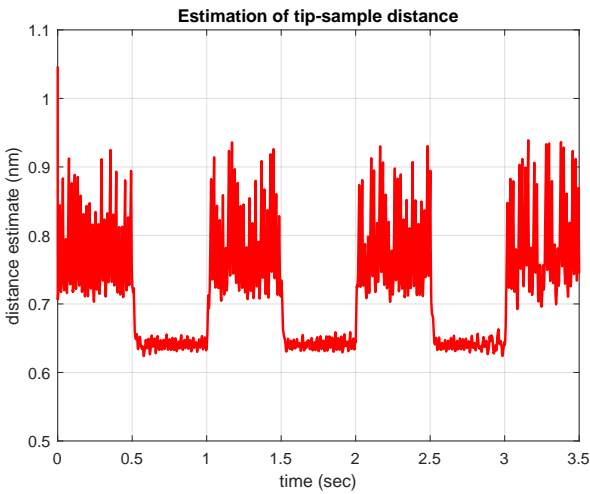


Figure 9: Estimated tip-sample distance under square reference variations.

Finally, in order to illustrate the possible estimation of surface variations with the same approach, such variations are simulated in the control values. This simulation is made so as to emulate surface variations consistent with graphite atom organization (see e.g. [14]), and with a scanning speed of about 100 nm/s: referring to the distance of about 250 pm between two atoms seen as at 'highest positions' in such a case, and a height variation in between chosen as 0.2 nm in view of typical STM pictures, the control used in the observer is modified as if the tip had to follow a sine profile variation with peak-to-peak magnitude of 0.2 nm, and frequency of 400 Hz.

The observer is then designed as in subsection 4.2, based on estimates of tunneling current and its parameters, and under the Kalman form of (25), keeping $w = 0.04$, $V = Id_{3 \times 3}$ and increasing γ to 25×1000 so as to make the observer fast enough. The corresponding estimation results are shown in figures 10 and 11: the first one presents the surface estimation vs its 'simulated' sine reference (where a zoom on very first times emphasizes the estimation speed), and the second one focuses on the related error (which can be seen to be roughly lower than 10% of the sine magnitude, as highlighted by dashed lines).

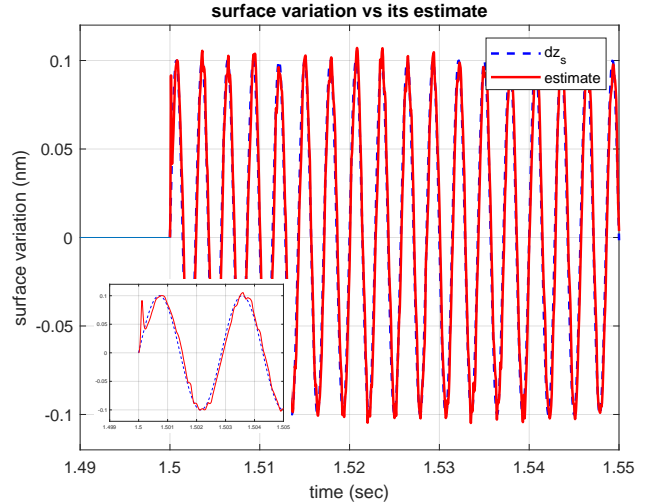


Figure 10: Estimated surface variations (solid line) vs its emulated sine wave (dashed line).

Remark. As an extension comment, let us notice that in the case when parameter k may vary during scanning, as emphasized for instance in [12], the methodology here proposed could be adapted, by considering some updates of tunneling current parameters from time to time over the fly. By adjusting observer tuning coefficients indeed, estimates can in fact be obtained here in less than $0.01s$ (picking γ larger than 25×100 for instance), as illustrated by figure 12 hereafter. As a consequence, with a scanning rate of about 100 nm/s, current parameters could be adjusted about every nanometer. Going up to video rate, as discussed in [39] for instance, can be part of future developments.

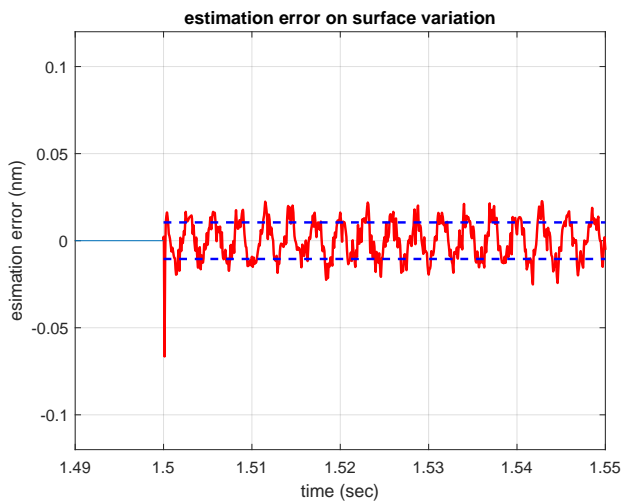


Figure 11: Estimation error on surface variation estimation.

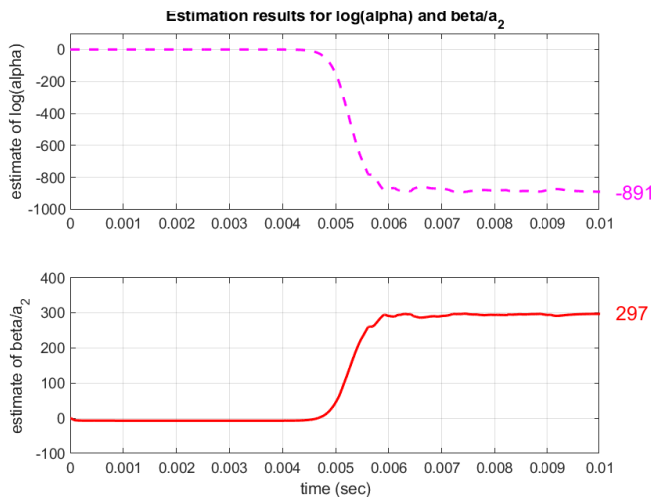


Figure 12: Parameter estimation results towards updating during scanning.

6. Conclusion

The problem of parameter estimation in tunneling current exponential model has been considered. Since obtaining tunneling current needs closed-loop operation prior to any possible identification, a stability analysis when using a simple Proportional-Integral controller has been first presented. On the basis of such an operation, an observer approach has then been proposed for the current model, further extended to surface variations estimation. All the methodology has been illustrated with experimental data, and the use of such a calibration approach will be next studied in various possible applications of such an STM operation.

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